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AN A_∞ VERSION OF THE POINCARÉ LEMMA

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We prove a categorified version of the Poincaré lemma. The natural setting for our result is that of ∞-local systems. More precisely, we show that any smooth homotopy between maps f and g induces an A_∞-natural transformation between the corresponding pullback functors. This transformation is explicitly defined in terms of Chen's iterated integrals. In particular, we show that a homotopy equivalence induces a quasiequivalence on the DG categories of ∞-local system.

1. Introduction

Higher versions of local systems on a smooth manifold has been considered in several recent works. Some of the references include [Block and Smith 2014; Arias Abad and Schätz 2018; 2013; Holstein 2015; Malm 2011; Ben-Zvi and Nadler 2012; Brav and Dyckerhoff 2019; Rivera and Zeinalian 2018]. These references contain different points of view on such ∞-local systems, as they are now called. Crucially, each of the points of view can be used to define a DG category of ∞-local systems, and it has been shown that all resulting DG categories are A_∞-quasiequivalent [Holstein 2015; Arias Abad and Schätz 2013; Block and Smith 2014].

In this paper, we take the de Rham point of view that an ∞-local system on a manifold M is a $\mathbb{Z}$-graded vector bundle equipped with a flat $\mathbb{Z}$-graded superconnection. We denote the corresponding DG category by $\mathbf{Loc}_\infty(M)$ and study its behavior with respect to homotopies. It has been proved by Holstein [2015], using a different but equivalent version of ∞-local systems, that the pullback by a homotopy equivalence induces a quasiequivalence on local systems. We use the de Rham point of view on ∞-local systems to provide a more explicit version of this homotopy invariance property. The precise result is as follows:

Theorem 4.5. *Let M, N be smooth manifolds, and let h be a smooth homotopy between maps $f, g : M \to N$. Then there exists an A_∞-natural isomorphism* $\mathrm{hol} : f^* \Rightarrow g^*$ *between the pullback functors* $f^*, g^* : \mathbf{Loc}_\infty(N) \to \mathbf{Loc}_\infty(M)$. *Such*

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an A_∞-natural isomorphism depends only on h and is given explicitly by Chen's iterated integrals.

This result should be contrasted with the A_∞ version of de Rham's theorem due to Gugenheim [1977], which plays a key role in the construction of the higher Riemann–Hilbert correspondence given in [Block and Smith 2014; Arias Abad and Schätz 2018]. There are also some important corollaries that follow directly from it, including the following:

Corollary 5.1. *If $f : M \to N$ is a smooth homotopy equivalence, then the pullback functor $f^* : \mathbf{Loc}_\infty(N) \to \mathbf{Loc}_\infty(M)$ is a quasiequivalence.*

Corollary 5.2. *If M is contractible, then $\mathbf{Loc}_\infty(M)$ is quasiequivalent to $\mathbf{DGVect}_\mathbb{R}$.*

The latter should be thought of as a categorified version of the Poincaré lemma. It provides a local normal form for flat superconnections, which we believe is of independent interest.

Corollary 5.4. *For an arbitrary manifold M, any ∞-local system (E, D) is locally isomorphic to a constant ∞-local system, that is, every point has an open neighborhood U in which $(E|_U, D|_U)$ is isomorphic to a constant ∞-local system.*

We remark that an analogous result in the complex-analytic context has been established by Bondal and Rosly [2011]. Some other related results are also considered in [Demessie and Sämann 2015].

The paper is organized as follows. Some preliminaries on DG categories, DG functors, A_∞-natural transformations, and ∞-local systems are presented in Section 2. In Section 3, we describe some properties of Chen's iterated integrals that are used in our construction. The main section of the paper is Section 4, which contains the proof of the homotopy invariance of the DG category of ∞-local systems. In Section 5, we derive some corollaries of our main result, including the categorified version of the Poincaré lemma. Finally, Appendix A contains some technical computations which are essential for the proof of the main result and Appendix B a short compilation of the basic definitions of A_∞-categories.

Note added. While we were writing this paper, the work [Chuang et al. 2018] appeared. Among other results, this paper discusses a higher version of the Riemann–Hilbert correspondence which generalizes and extends the results of [Block and Smith 2014]. In this reference the notion of ∞-local system is replaced by that of cohomologically locally constant DG sheaf with cohomology sheaves of finite rank, and their results are therefore closely related to ours.

Notation and conventions. If K is a field and $V = \bigoplus_{k\in\mathbb{Z}} V^k$ is a $\mathbb{Z}$-graded K-vector space, we denote by sV its suspension, that is, the $\mathbb{Z}$-graded K-vector space

with grading defined by
$$(sV)^k = V^{k+1}.$$
Vector spaces and tensor products are defined over the real numbers unless otherwise stated.

If $E = \bigoplus_{k\in\mathbb{Z}} E^k$ is a $\mathbb{Z}$-graded vector bundle over a smooth manifold M, we define
$$\Omega^\bullet(M, E) = \Gamma(\Lambda^\bullet T^*M \otimes E).$$
This space is graded by the total degree
$$\Omega^\bullet(M, E)^n = \bigoplus_{p+q=n} \Omega^p(M, E^q).$$
Given an element $\omega \in \Omega^p(M, E^q)$ we will say that ω is of partial degree p.

2. Preliminaries

In this section we review some facts regarding DG categories and higher local systems that will be used throughout the paper. For a more thorough discussion on the topics treated here, see for example [Keller 2006; Positselski 2011; Block 2010; Block and Smith 2014; Arias Abad and Crainic 2012; Arias Abad and Schätz 2013].

2A. ***DG categories, DG functors, and A_∞-natural transformations.*** A *DG category* (where DG stands for "differential graded") over a field K is a K-linear category $\mathscr{C}$ such that for every two objects X and Y the space of arrows $\mathrm{Hom}_{\mathscr{C}}(X, Y)$ is equipped with a structure of a cochain complex of K-vector spaces, and for every three objects X, Y, and Z the composition map
$$\mathrm{Hom}_{\mathscr{C}}(Y, Z) \otimes_K \mathrm{Hom}_{\mathscr{C}}(X, Y) \to \mathrm{Hom}_{\mathscr{C}}(X, Z)$$
is a morphism of cochain complexes. Thus, by definition,
$$\mathrm{Hom}_{\mathscr{C}}(X, Y) = \bigoplus_{n\in\mathbb{Z}} \mathrm{Hom}^n_{\mathscr{C}}(X, Y)$$
is a $\mathbb{Z}$-graded K-vector space with a differential $d : \mathrm{Hom}^n_{\mathscr{C}}(X, Y) \to \mathrm{Hom}^{n+1}_{\mathscr{C}}(X, Y)$. The elements $f \in \mathrm{Hom}^n_{\mathscr{C}}(X, Y)$ are called *homogeneous of degree n*, and we write $|f| = n$. We shall denote the set of objects of $\mathscr{C}$ by $\mathrm{Ob}\,\mathscr{C}$.

The prototypical example of a DG category is the category of cochain complexes of K-vector spaces, which we denote by $\mathbf{DGVect}_K$. Its objects are cochain complexes of K-vector spaces and the morphism spaces $\mathrm{Hom}_{\mathbf{DGVect}_K}(X, Y)$ are endowed with the differential defined as
$$d(f) = d_Y \circ f - (-1)^n f \circ d_X,$$
for any homogeneous element f of degree n.

Let $\mathscr{C}$ be a DG category, and let $X \in \operatorname{Ob}\mathscr{C}$. Given a closed morphism $f \in \operatorname{Hom}^0_{\mathscr{C}}(Y, Z)$ we define $f_* : \operatorname{Hom}_{\mathscr{C}}(X, Y) \to \operatorname{Hom}_{\mathscr{C}}(X, Z)$ by $f_*(g) = f \circ g$ for $g \in \operatorname{Hom}_{\mathscr{C}}(X, Y)$. It is not difficult to see that f_* is a morphism of cochain complexes. Similarly, if we define $f^* : \operatorname{Hom}_{\mathscr{C}}(Z, X) \to \operatorname{Hom}_{\mathscr{C}}(Y, X)$ by $f^*(h) = h \circ f$ for $h \in \operatorname{Hom}_{\mathscr{C}}(Z, X)$, then f^* is a morphism of cochain complexes.

Given a DG category $\mathscr{C}$ one can define an ordinary category $\mathbf{Ho}(\mathscr{C})$ by keeping the same set of objects and replacing each Hom complex by its 0-th cohomology. We call $\mathbf{Ho}(\mathscr{C})$ the *homotopy category* of $\mathscr{C}$.

If $\mathscr{C}$ and $\mathscr{D}$ are DG categories, a *DG functor* $F : \mathscr{C} \to \mathscr{D}$ is an K-linear functor whose associated map for $X, Y \in \operatorname{Ob}\mathscr{C}$,

$$F_{X,Y} : \operatorname{Hom}_{\mathscr{C}}(X, Y) \to \operatorname{Hom}_{\mathscr{D}}(F(X), F(Y)),$$

is a morphism of cochain complexes. Notice that any DG functor $F : \mathscr{C} \to \mathscr{D}$ induces an ordinary functor

$$\mathbf{Ho}(F) : \mathbf{Ho}(\mathscr{C}) \to \mathbf{Ho}(\mathscr{D})$$

between the corresponding homotopy categories. A DG functor $F : \mathscr{C} \to \mathscr{D}$ is said to be *quasi fully faithful* if for every pair of objects $X, Y \in \operatorname{Ob}\mathscr{C}$ the morphism $F_{X,Y}$ is a quasi-isomorphism. Moreover, the DG functor F is said to be *quasi essentially surjective* if $\mathbf{Ho}(F)$ is essentially surjective. A DG functor which is both quasi fully faithful and quasi essentially surjective is called a *quasiequivalence*.

Let F and G be two functors between two DG categories $\mathscr{C}$ and $\mathscr{D}$. We want to define the notion of an A_∞-natural transformation λ from F to G. A thorough discussion of this in connection with the theory of A_∞-categories is presented in Appendix B. Here, we want to be explicit, and motivate the definition as follows. If $X, Y \in \operatorname{Ob}\mathscr{C}$ and $f \in \operatorname{Hom}_{\mathscr{C}}(X, Y)$, we can consider the standard diagram

$$\begin{array}{ccc} F(X) & \xrightarrow{\lambda(X)} & G(X) \\ {\scriptstyle F(f)}\big\downarrow & & \big\downarrow{\scriptstyle G(f)} \\ F(Y) & \xrightarrow[\lambda(Y)]{} & G(Y) \end{array}$$

Normally one would require this diagram to commute. However, in our case we will only require this diagram to be commutative up to homotopy. To make precise what this means we need one piece of notation.

Let $\mathscr{C}$ be a DG category, and let $X_0, \dots, X_n$ be a collection of objects of $\mathscr{C}$. We endow

$$s\operatorname{Hom}_{\mathscr{C}}(X_{n-1}, X_n) \otimes_K \cdots \otimes_K s\operatorname{Hom}_{\mathscr{C}}(X_0, X_1)$$

with a differential b defined as

$$b(f_{n-1}\otimes\cdots\otimes f_0)=\sum_{i=0}^{n-1}(-1)^{\sum_{j=i+1}^{n-1}|f_j|+n-i-1}f_{n-1}\otimes\cdots\otimes df_i\otimes\cdots\otimes f_0$$
$$+\sum_{i=0}^{n-2}(-1)^{\sum_{j=i+2}^{n-1}|f_j|+n-i}f_{n-1}\otimes\cdots\otimes(f_{i+1}\circ f_i)\otimes\cdots\otimes f_0$$

for homogeneous elements $f_0\in s\mathrm{Hom}_{\mathscr{C}}(X_0,X_1),\ldots,f_{n-1}\in s\mathrm{Hom}_{\mathscr{C}}(X_{n-1},X_n)$. Here d denotes indistinctly the differential in any of the spaces $\mathrm{Hom}_{\mathscr{C}}(X_i,X_{i+1})$. A direct calculation shows that indeed $b^2=0$. Notice that the definition of b resembles that of the differential of the Hochschild chain complex of a DG algebra.

Armed with this notation, the formal definition of an A_∞-natural transformation is given as follows. Let $\mathscr{C}$ and $\mathscr{D}$ be DG categories, and let $F:\mathscr{C}\to\mathscr{D}$ and $G:\mathscr{C}\to\mathscr{D}$ be DG functors. An A_∞-*natural transformation* $\lambda:F\Rightarrow G$ is the datum of a closed morphism $\lambda_0(X)\in\mathrm{Hom}^0_{\mathscr{D}}(F(X),G(X))$ for each $X\in\mathrm{Ob}\,\mathscr{C}$ and a collection of K-linear maps of degree 0

$$\lambda_n: s\mathrm{Hom}_{\mathscr{C}}(X_{n-1},X_n)\otimes_K\cdots\otimes_K s\mathrm{Hom}_{\mathscr{C}}(X_0,X_1)\to\mathrm{Hom}_{\mathscr{D}}(F(X_0),G(X_n))$$

for every collection $X_0,\ldots,X_n\in\mathrm{Ob}\,\mathscr{C}$, such that for all composable chains of homogeneous morphisms $f_0\in s\mathrm{Hom}_{\mathscr{C}}(X_0,X_1),\ldots,f_{n-1}\in s\mathrm{Hom}_{\mathscr{C}}(X_{n-1},X_n)$ the relation

$$G(f_{n-1})\circ\lambda_{n-1}(f_{n-2}\otimes\cdots\otimes f_0)-(-1)^{\sum_{i=1}^{n-1}|f_i|-n+1}\lambda_{n-1}(f_{n-1}\otimes\cdots\otimes f_1)\circ F(f_0)$$
$$=\lambda(b(f_{n-1}\otimes\cdots\otimes f_0))+d(\lambda_n(f_{n-1}\otimes\cdots\otimes f_0))$$

is satisfied for any $n\geq 1$. The λ on the right denotes the direct sum of the various λ_n. For $n=1$ this yields the condition

$$G(f_0)\circ\lambda_0(X_0)-\lambda_0(X_1)\circ F(f_0)=\lambda_1(d(f_0))+d(\lambda_1(f_0)).$$

Since the map $\lambda_1: s\mathrm{Hom}_{\mathscr{C}}(X_0,X_1)\to\mathrm{Hom}_{\mathscr{D}}(F(X_0),G(X_1))$ has degree -1 when considered as a map defined over $\mathrm{Hom}_{\mathscr{C}}(X_0,X_1)$, this implies that the diagram

$$\begin{array}{ccc}
F(X_0) & \xrightarrow{\lambda_0(X_0)} & G(X_0)\\
{\scriptstyle F(f_0)}\downarrow & & \downarrow{\scriptstyle G(f_0)}\\
F(X_1) & \xrightarrow[\lambda_0(X_1)]{} & G(X_1)
\end{array}$$

commutes up to a homotopy given by λ_1. More generally, for $n\geq 2$, one may say that λ_{n-1} "commutes" with $G(f_{n-1})$ and $F(f_0)$ up to a homotopy given by λ_n.

As usual, A_∞-natural transformations can be composed: if $F:\mathscr{C}\to\mathscr{D}$, $G:\mathscr{C}\to\mathscr{D}$, and $H:\mathscr{C}\to\mathscr{D}$ are three DG functors from the DG category $\mathscr{C}$ to the DG category $\mathscr{D}$, and $\lambda : F \Rightarrow G$ and $\mu : G \Rightarrow H$ are two A_∞-natural transformations, then the formula

$$(\mu \circ \lambda)_n = \sum_{i=0}^{n} \mu_i \circ \lambda_{n-i}$$

defines a new A_∞-natural transformation $\mu \circ \lambda : F \Rightarrow H$. An A_∞*-natural isomorphism* between functors from $\mathscr{C}$ to $\mathscr{D}$ is an A_∞-natural transformation λ such that $\lambda_0(X)$ is an isomorphism for all $X \in \operatorname{Ob}\mathscr{C}$.

We close this section with the following observation.

Lemma 2.1. *Let $\mathscr{C}$ and $\mathscr{D}$ be DG categories, and let $F : \mathscr{C} \to \mathscr{D}$ be a DG functor. Suppose that there is a DG functor $G : \mathscr{D} \to \mathscr{C}$ together with A_∞-natural isomorphisms $\lambda : G \circ F \Rightarrow \mathrm{id}_{\mathscr{C}}$ and $\mu : F \circ G \Rightarrow \mathrm{id}_{\mathscr{D}}$. Then F is a quasiequivalence.*

Proof. Let us first prove that F is quasi essentially surjective. Given any object $Y \in \operatorname{Ob}\mathscr{D}$ the morphism $\mu_0(Y) \in \operatorname{Hom}^0_{\mathscr{D}}(F(G(Y)), Y)$ is an isomorphism. In particular it descends to an isomorphism in the homotopy category. Let us show that F is quasi fully faithful. By definition, if $f \in s\operatorname{Hom}_{\mathscr{C}}(X, Y)$ is a homogenous element, the A_∞-natural isomorphism $\lambda : G \circ F \Rightarrow \mathrm{id}_{\mathscr{C}}$ produces the relation

$$f \circ \lambda_0(X) - \lambda_0(Y) \circ G(F(f)) = \lambda_1(d(f)) + d(\lambda_1(f)).$$

This, in turn, may be written as

$$\lambda_0(X)^* \circ \mathrm{id}_{\mathscr{C}} - \lambda_0(Y)_* \circ (G \circ F) = \lambda_1 \circ d + d \circ \lambda_1,$$

for any pair of objects $X, Y \in \operatorname{Ob}\mathscr{C}$, where $\lambda_0(X)^*$ is the pullback of $\lambda_0(X)$ by X and $\lambda_0(Y)_*$ is the pushforward of $\lambda_0(Y)$ by $G(F(Y))$. Hence, the morphisms of cochain complexes $\lambda_0(X)^* \circ \mathrm{id}_{\mathscr{C}}$ and $\lambda_0(Y)_* \circ (G \circ F)$ are homotopic, and therefore, they induce the same morphism in cohomology. But clearly $\lambda_0(X)^*$, $\lambda_0(Y)_*$, and $\mathrm{id}_{\mathscr{C}}$ induce isomorphisms in cohomology, and thus so does $G \circ F$. It follows that $G \circ F$ is a quasi-isomorphism. By an entirely analogous argument, using the A_∞-natural isomorphism $\mu : F \circ G \Rightarrow \mathrm{id}_{\mathscr{D}}$, one may prove that $F \circ G$ is a quasi-isomorphism. The desired implication follows at once. □

2B. ∞-*local systems*. Let $E = \bigoplus_{k\in\mathbb{Z}} E^k$ be a $\mathbb{Z}$-graded vector bundle over a manifold M. We consider the space of E-valued differential forms $\Omega^\bullet(M, E)$ to be $\mathbb{Z}$-graded with respect to the total degree. A $\mathbb{Z}$*-graded superconnection* on E is an operator $D : \Omega^\bullet(M, E) \to \Omega^\bullet(M, E)$ of degree 1 which satisfies the Leibniz rule

$$D(\sigma \wedge \omega) = \mathrm{d}\sigma \wedge \omega + (-1)^k \sigma \wedge D\omega,$$

for all $\sigma \in \Omega^k(M)$ and $\omega \in \Omega^\bullet(M, E)$. The *curvature* of D is the operator D^2. This is an $\Omega^\bullet(M)$-linear operator on $\Omega^\bullet(M, E)$ of degree 2 which is given by multiplication by an element of $\Omega^\bullet(M, \operatorname{End}(E))$. If $D^2 = 0$, then we say that D is a *flat* $\mathbb{Z}$-graded superconnection. By an ∞-*local system* on M we mean a $\mathbb{Z}$-graded vector bundle E equipped with a flat $\mathbb{Z}$-graded superconnection D. We will denote such an ∞-local system by (E, D).

As a simple example, consider a trivial vector bundle $M \times V$ with fiber $V = \bigoplus_{k\in\mathbb{Z}} V^k$ a $\mathbb{Z}$-graded vector space. It is an easy matter to verify that the de Rham differential $\mathrm{d} : \Omega^\bullet(M) \to \Omega^\bullet(M)$ can be extended to an operator $\mathrm{d} : \Omega^\bullet(M, V) \to \Omega^\bullet(M, V)$ of degree 1. With the identification $\Omega^\bullet(M, V) = \Omega^\bullet(M, M \times V)$ in mind, one can readily show that $(M \times V, \mathrm{d})$ defines an ∞-local system on M. We will refer to it as a *constant* ∞-*local system* on M.

For convenience of reference, we make the following observation. Suppose that (E, D) is an ∞-local system on M. The Leibniz rule implies that D is completely determined by its restriction to $\Omega^0(M, E)$. Then we may decompose

$$D = \sum_{k\geq 0} D_k,$$

where D_k is of partial degree k with respect to the $\mathbb{Z}$-grading on $\Omega^\bullet(M)$. It is clear that each D_k for $k \neq 1$ is $\Omega^\bullet(M)$-linear and therefore it is given by multiplication by an element $-\alpha_k \in \Omega^k(M, \mathrm{End}(E)^{1-k})$ (the minus sign is only a matter of convention). On the contrary, D_1 satisfies the Leibniz rule on each of the vector bundles E^k, so it must be of the form d_∇, where ∇ is an ordinary connection on E which preserves the $\mathbb{Z}$-grading. We can thus write

$$D = \mathrm{d}_\nabla - \alpha_0 - \alpha_2 - \alpha_3 - \cdots .$$

From this formula, it is straightforward to check that the flatness condition becomes equivalent to

$$\begin{aligned} \alpha_0^2 &= 0, \\ \mathrm{d}_\nabla \alpha_0 &= 0, \\ [\alpha_0, \alpha_2] + F_\nabla &= 0, \\ [\alpha_0, \alpha_{n+1}] + \mathrm{d}_\nabla \alpha_n + \sum_{k=2}^{n-1} \alpha_k \wedge \alpha_{n+1-k} &= 0, \qquad n \geq 2, \end{aligned}$$

where F_∇ is the curvature of the connection ∇. The first identity implies that we have a cochain complex of vector bundles with differential α_0. The second equation expresses the fact that α_0 is covariantly constant with respect to the connection ∇. The third equation indicates that the connection ∇ fails to be flat up to terms involving the homotopy α_2 and the differential α_0.

Now let us assume that E is trivialized over M. This means $E = M \times V$ for some $\mathbb{Z}$-graded vector space $V = \bigoplus_{k\in\mathbb{Z}} V^k$. In this case, we have $\alpha_k \in \Omega^k(M, \mathrm{End}(V)^{1-k})$ for $k \neq 1$. Moreover, we can write $\mathrm{d}_\nabla = \mathrm{d} - \alpha_1$ for some $\alpha_1 \in \Omega^1(M, \mathrm{End}(V)^0)$.

Thus, the $\mathbb{Z}$-graded superconnection D may be expressed as $D = \mathrm{d} - \alpha$, where $\alpha \in \Omega^\bullet(M, \mathrm{End}(V))$ is the homogenous element of total degree 1 defined by $\alpha = \sum_{k\geq 0} \alpha_k$. In addition, a straightforward calculation gives

$$D^2 = \mathrm{d}\alpha - \alpha \wedge \alpha.$$

Consequently, the totality of equations of the flatness condition is equivalent to the single statement that α satisfies

$$\mathrm{d}\alpha - \alpha \wedge \alpha = 0.$$

This is known as the *Maurer–Cartan equation*.

Suppose we have another trivialization of E over M such that $E = M \times W$ for some $\mathbb{Z}$-graded vector space $W = \bigoplus_{k\in\mathbb{Z}} W^k$ and $D = \mathrm{d} - \beta$ for some homogenous element $\beta \in \Omega^\bullet(M, \mathrm{End}(W))$ of total degree 1 satisfying the Maurer–Cartan equation. Then, we have a transition isomorphism between the two trivializations, which is realized by a linear isomorphism $g : \Omega^0(M, V) \to \Omega^0(M, W)$ that commutes with the operators $\mathrm{d}-\alpha$ and $\mathrm{d}-\beta$. If we think of g as an element of $\Omega^0(M, \mathrm{Hom}(V, W))$, the latter condition is equivalent to the requirement that

$$\alpha = g^{-1}\beta g - g^{-1}\mathrm{d}g.$$

The change from β to α given in this equation goes by the name of a "gauge transformation".

For a pair of ∞-local systems (E, D) and (E', D') there is a natural notion of a morphism from (E, D) to (E', D'). Namely, such a morphism is a degree-0 linear map $\Phi : \Omega^\bullet(M, E) \to \Omega^\bullet(M, E')$ which is $\Omega^\bullet(M)$-linear and commutes with the $\mathbb{Z}$-graded superconnections D and D'. If both (E, D) and (E', D') are trivialized over M in such a way that $E = M \times V$ and $E' = M \times V'$ for some $\mathbb{Z}$-graded vector spaces V and V', and $D = \mathrm{d} - \alpha$ and $D' = \mathrm{d} - \alpha'$ for some homogeneous elements $\alpha \in \Omega^\bullet(M, \mathrm{End}(V))$ and $\alpha' \in \Omega^\bullet(M, \mathrm{End}(V'))$ of total degree 1 satisfying the Maurer–Cartan equation, then this condition is

$$(\mathrm{d} - \alpha') \circ \Phi = \Phi \circ (\mathrm{d} - \alpha)$$

or, interpreting Φ as an element of $\Omega^\bullet(M, \mathrm{Hom}(V, V'))$,

$$\mathrm{d}\Phi = \alpha' \wedge \Phi - \Phi \wedge \alpha.$$

A morphism from (E, D) to (E', D') is called an *isomorphism* if the underlying map $\Phi : \Omega^\bullet(M, E) \to \Omega^\bullet(M, E')$ is an isomorphism. Two ∞-local systems (E, D) and (E', D') are said to be *isomorphic* if there is an isomorphism from (E, D) to (E', D').

As mentioned in the introduction, all ∞-local systems on a manifold M can be naturally organized into a DG category, which we denote by $\mathbf{Loc}_\infty(M)$. Its objects are, of course, ∞-local systems (E, D) on M. Given two ∞-local systems (E, D) and (E', D') we define the space of morphisms to be the $\mathbb{Z}$-graded vector space $\Omega^\bullet(M, \mathrm{Hom}(E, E'))$ with the differential $\partial_{D,D'}$ acting as

$$\partial_{D,D'}\omega = D' \wedge \omega - (-1)^k \omega \wedge D,$$

for any homogenous element ω of degree k. If (E, D) and (E', D') are trivialized over M as in the previous paragraph, then $\partial_{D,D'}$ may be expressed by

$$\partial_{D,D'}\omega = \mathrm{d}\omega - \alpha' \wedge \omega + (-1)^k \omega \wedge \alpha.$$

Notice that what we call a morphism from (E, D) to (E', D') is simply a closed element of $\Omega^\bullet(M, \mathrm{Hom}(E, E'))$ of degree 0.

Finally, to close this section, let us briefly recall the pullback operation of ∞-local systems. For a smooth map $f : M \to N$ between two manifolds M and N, there is a DG functor $f^* : \mathbf{Loc}_\infty(N) \to \mathbf{Loc}_\infty(M)$ which sends E with structure superconnection

$$D = \mathrm{d}_\nabla - \alpha_0 - \alpha_2 - \alpha_3 - \cdots$$

to f^*E endowed with

$$f^*D = \mathrm{d}_{f^*\nabla} - f^*\alpha_0 - f^*\alpha_2 - f^*\alpha_3 - \cdots ,$$

where f^*E is the pullback of E and $f^*\nabla$ is the pullback connection on f^*E. One can easily check that (f^*E, f^*D) is indeed an ∞-local system on M, so the DG functor f^* is well defined. We refer to it as the *pullback functor* induced by f.

3. Some generalities on Chen's iterated integrals

In this section, we state some properties of the type of iterated integrals that appear in our study. We make use of the notation and conventions of Sections 2A and 2B.

Let M be a smooth manifold, and let $V = \bigoplus_{k\in\mathbb{Z}} V^k$ be a $\mathbb{Z}$-graded vector space. We denote by $\iota_s : M \to M \times [1, 0]$ the inclusion at height s given by $\iota_s(x) = (x, s)$. For an element ω of $\Omega^\bullet(M \times [0, 1], \mathrm{End}(V))$ we define for all $t \in [0, 1]$ the elements of $\Omega^\bullet(M, \mathrm{End}(V))$

$$\Phi_0^\omega(t) = \mathrm{id}_V,$$
$$\Phi_1^\omega(t) = \int_0^t \iota_{s_1}^* \mathrm{i}_{\frac{\partial}{\partial s_1}} \omega \, \mathrm{d}s_1,$$
$$\Phi_n^\omega(t) = \int_0^t \int_0^{s_1} \cdots \int_0^{s_{n-1}} \iota_{s_1}^* \mathrm{i}_{\frac{\partial}{\partial s_1}} \omega \wedge \iota_{s_2}^* \mathrm{i}_{\frac{\partial}{\partial s_2}} \omega \wedge \cdots \wedge \iota_{s_n}^* \mathrm{i}_{\frac{\partial}{\partial s_n}} \omega \, \mathrm{d}s_n \cdots \mathrm{d}s_2 \, \mathrm{d}s_1, \ n \geq 2,$$

where in the definition of $\Phi_n^\omega(t)$, $t \geq s_1 \geq \cdots \geq s_n \geq 0$. The following lemma is easy to verify.

Lemma 3.1. *The series*

$$\Phi^{\omega}(t)=\sum_{n=0}^{\infty}\Phi_n^{\omega}(t)$$

converges for all $t\in[0,1]$ *and defines a smooth map from* $[0,1]$ *to* $\Omega^{\bullet}(M,\mathrm{End}(V))$.

We call $\Phi^{\omega}(t)$ the *iterated integral* of the element ω. Compare this with the definitions of [Igusa 2009] and the more classical reference [Chen 1977].

These iterated integrals define solutions to differential equations we are interested in. More precisely, we have the following:

Proposition 3.2. *Consider an element* ω *of* $\Omega^{\bullet}(M\times[0,1],\mathrm{End}(V))$ *and the smooth map from* $[0,1]$ *to* $\Omega^{\bullet}(M,\mathrm{End}(V))$ *given by* $t\mapsto\Phi^{\omega}(t)$. *Then*

$$\frac{\mathrm{d}\Phi^{\omega}(t)}{\mathrm{d}t}=\iota_t^{*}\mathrm{i}_{\frac{\partial}{\partial t}}\omega\wedge\Phi^{\omega}(t),$$
$$\Phi^{\omega}(0)=\mathrm{id}_V,$$

for all $t\in[0,1]$.

Proof. It is clear that $\Phi^{\omega}(0)=\mathrm{id}_V$. Let us calculate the derivative with respect to t. According to Lemma 3.1, we have

$$\begin{aligned}\Phi^{\omega}(t)=\mathrm{id}_V+\int_0^t\iota_{s_1}^{*}\mathrm{i}_{\frac{\partial}{\partial s_1}}\omega\,\mathrm{d}s_1+\int_0^t\int_0^{s_1}\iota_{s_1}^{*}\mathrm{i}_{\frac{\partial}{\partial s_1}}\omega\wedge\iota_{s_2}^{*}\mathrm{i}_{\frac{\partial}{\partial s_2}}\omega\,\mathrm{d}s_2\,\mathrm{d}s_1\\+\int_0^t\int_0^{s_1}\int_0^{s_2}\iota_{s_1}^{*}\mathrm{i}_{\frac{\partial}{\partial s_1}}\omega\wedge\iota_{s_2}^{*}\mathrm{i}_{\frac{\partial}{\partial s_2}}\omega\wedge\iota_{s_3}^{*}\mathrm{i}_{\frac{\partial}{\partial s_3}}\omega\,\mathrm{d}s_3\,\mathrm{d}s_2\,\mathrm{d}s_1+\cdots.\end{aligned}$$

Therefore,

$$\begin{aligned}\frac{\mathrm{d}\Phi^{\omega}(t)}{\mathrm{d}t}&=\iota_t^{*}\mathrm{i}_{\frac{\partial}{\partial t}}\omega+\iota_t^{*}\mathrm{i}_{\frac{\partial}{\partial t}}\omega\wedge\int_0^t\iota_{s_2}^{*}\mathrm{i}_{\frac{\partial}{\partial s_2}}\omega\,\mathrm{d}s_2\\&\qquad+\iota_t^{*}\mathrm{i}_{\frac{\partial}{\partial t}}\omega\wedge\int_0^t\int_0^{s_2}\iota_{s_2}^{*}\mathrm{i}_{\frac{\partial}{\partial s_2}}\omega\wedge\iota_{s_3}^{*}\mathrm{i}_{\frac{\partial}{\partial s_3}}\omega\,\mathrm{d}s_3\,\mathrm{d}s_2+\cdots\\&=\iota_t^{*}\mathrm{i}_{\frac{\partial}{\partial t}}\omega\wedge\left(\mathrm{id}_V+\int_0^t\iota_{s_1}^{*}\mathrm{i}_{\frac{\partial}{\partial s_1}}\omega\,\mathrm{d}s_1+\int_0^t\int_0^{s_1}\iota_{s_1}^{*}\mathrm{i}_{\frac{\partial}{\partial s_1}}\omega\wedge\iota_{s_2}^{*}\mathrm{i}_{\frac{\partial}{\partial s_2}}\omega\,\mathrm{d}s_2\mathrm{d}s_1+\cdots\right)\\&=\iota_t^{*}\mathrm{i}_{\frac{\partial}{\partial t}}\omega\wedge\Phi^{\omega}(t),\end{aligned}$$

as asserted. □

Another important result that we need is the following gauge invariance property of iterated integrals.

Proposition 3.3. *Let* $W=\bigoplus_{k\in\mathbb{Z}}W^k$ *be another* $\mathbb{Z}$*-graded vector space, and let* $\omega\in\Omega^{\bullet}(M\times[0,1],\mathrm{End}(V))$ *and* $\eta\in\Omega^{\bullet}(M\times[0,1],\mathrm{End}(W))$. *Suppose that there is* *an invertible element* $g \in \Omega^0(M \times [0, 1], \mathrm{Hom}(V, W))$ *such that* $\omega = g^{-1}\eta g - g^{-1}\mathrm{d}g$. *Then*

$$\Phi^\omega(t) = (\iota_t^* g)^{-1}\Phi^\eta(t)\iota_0^* g,$$

for all $t \in [0, 1]$.

Proof. The strategy of the proof is to show that the right-hand side of the given formula satisfies the initial value problem of Proposition 3.2. Uniqueness will then tell us that both sides of the formula are equal. To start with, it is clear that $(\iota_t^* g)^{-1}\Phi^\eta(t)\iota_0^* g$ satisfies the initial condition. Let us calculate its derivative with respect to t. By Proposition 3.2, we have

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}[(\iota_t^* g)^{-1}\Phi^\eta(t)\iota_0^* g] &= \frac{\mathrm{d}}{\mathrm{d}t}(\iota_t^* g)^{-1}\Phi^\eta(t)\iota_0^* g + (\iota_t^* g)^{-1}\frac{\mathrm{d}\Phi^\eta(t)}{\mathrm{d}t}\iota_0^* g \\ &= \frac{\mathrm{d}}{\mathrm{d}t}(\iota_t^* g)^{-1}\Phi^\eta(t)\iota_0^* g + (\iota_t^* g)^{-1}(\iota_t^* \mathrm{i}_{\frac{\partial}{\partial t}}\eta \wedge \Phi^\eta(t))\iota_0^* g \\ &= \frac{\mathrm{d}}{\mathrm{d}t}(\iota_t^* g)^{-1}\Phi^\eta(t)\iota_0^* g + [(\iota_t^* g)^{-1}\iota_t^* \mathrm{i}_{\frac{\partial}{\partial t}}\eta\iota_t^* g] \wedge [(\iota_t^* g)^{-1}\Phi^\eta(t)\iota_0^* g].\end{aligned}$$

On the other hand, a straightforward calculation shows that

$$\frac{\mathrm{d}}{\mathrm{d}t}(\iota_t^* g)^{-1} = -(\iota_t^* g)^{-1}\frac{\mathrm{d}}{\mathrm{d}t}(\iota_t^* g)(\iota_t^* g)^{-1}.$$

Furthermore, using the assumption, we have

$$(\iota_t^* g)^{-1}\iota_t^* \mathrm{i}_{\frac{\partial}{\partial t}}\eta\iota_t^* g = \iota_t^* \mathrm{i}_{\frac{\partial}{\partial t}}\omega + (\iota_t^* g)^{-1}\frac{\mathrm{d}}{\mathrm{d}t}(\iota_t^* g).$$

Substituting into our previous equation we get

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}[(\iota_t^* g)^{-1}\Phi^\eta(t)\iota_0^* g] &= -(\iota_t^* g)^{-1}\frac{\mathrm{d}}{\mathrm{d}t}(\iota_t^* g)(\iota_t^* g)^{-1}\Phi^\eta(t)\iota_0^* g \\ &\qquad + \iota_t^* \mathrm{i}_{\frac{\partial}{\partial t}}\omega \wedge [(\iota_t^* g)^{-1}\Phi^\eta(t)\iota_0^* g] \\ &\qquad + (\iota_t^* g)^{-1}\frac{\mathrm{d}}{\mathrm{d}t}(\iota_t^* g)(\iota_t^* g)^{-1}\Phi^\eta(t)\iota_0^* g \\ &= \iota_t^* \mathrm{i}_{\frac{\partial}{\partial t}}\omega \wedge [(\iota_t^* g)^{-1}\Phi^\eta(t)\iota_0^* g],\end{aligned}$$

as required. □

It will be convenient for our purposes to give an equivalent alternative expression for $\Phi^\omega(t)$ in the special case in which ω is homogeneous. To do this we need some notation. For each $t \in [0, 1]$, we write $\Delta_n(t)$ for the n-simplex of width t. The geometric realization of $\Delta_n(t)$ that we take is

$$\Delta_n(t) = \{(s_1, \dots, s_n) \in \mathbb{R}^n \mid t \geq s_1 \geq \cdots \geq s_n \geq 0\}.$$

For any $i = 1, \dots, n$, we also denote by $\pi_i : M \times \Delta_n(t) \to M \times [0, t]$ the natural projection defined by $\pi_i(x, (s_1, \dots, s_n)) = (x, s_i)$ for all $x \in M$ and $(s_1, \dots, s_n) \in \Delta_n(t)$. Instead of $\Delta_n(1)$, we will simply write Δ_n.

With this notation, we have the following:

Proposition 3.4. *If ω is a homogeneous element of $\Omega^\bullet(M \times [0, 1], \mathrm{End}(V))$, then*

$$\Phi^\omega(t) = \mathrm{id}_V + \sum_{n=1}^{\infty} (-1)^{\varepsilon(n)|\omega|} \int_{\Delta_n(t)} \pi_1^*\omega \wedge \pi_2^*\omega \wedge \cdots \wedge \pi_n^*\omega,$$

where $\varepsilon(n) = \sum_{i=1}^{n-1}(n-i)$.

Proof. For each $(s_1, \dots, s_n) \in \Delta_n(t)$, let $\iota_{(s_1,\dots,s_n)} : M \to M \times \Delta_n(t)$ denote the natural inclusion given by $\iota_{(s_1,\dots,s_n)}(x) = (x, (s_1, \dots, s_n))$. Then, by definition,

$$\begin{aligned}&\int_{\Delta_n(t)} \pi_1^*\omega \wedge \pi_2^*\omega \wedge \cdots \wedge \pi_n^*\omega \\ &= \int_0^t \int_0^{s_1} \cdots \int_0^{s_{n-1}} \iota^*_{(s_1,\dots,s_n)} \mathrm{i}_{\frac{\partial}{\partial s_1}} \mathrm{i}_{\frac{\partial}{\partial s_2}} \cdots \mathrm{i}_{\frac{\partial}{\partial s_n}} (\pi_1^*\omega \wedge \pi_2^*\omega \wedge \cdots \wedge \pi_n^*\omega)\, \mathrm{d}s_n \cdots \mathrm{d}s_2\, \mathrm{d}s_1.\end{aligned}$$

But $\mathrm{i}_{\partial/\partial s_i}\pi_j^*\omega$ is equal to $\mathrm{i}_{\partial/\partial s_i}\pi_i^*\omega$ if $i = j$ and is equal to 0 otherwise. Moreover, since $\pi_i \circ \iota_{(s_1,\dots,s_n)} = \iota_{s_i}$, we also have that $\iota^*_{(s_1,\dots,s_n)} \mathrm{i}_{\partial/\partial s_i}\pi_i^*\omega = \iota^*_{s_i}\mathrm{i}_{\partial/\partial s_i}\omega$. Therefore, the integrand above becomes

$$\begin{aligned}&\iota^*_{(s_1,\dots,s_n)} \mathrm{i}_{\frac{\partial}{\partial s_1}} \mathrm{i}_{\frac{\partial}{\partial s_2}} \cdots \mathrm{i}_{\frac{\partial}{\partial s_n}} (\pi_1^*\omega \wedge \pi_2^*\omega \wedge \cdots \wedge \pi_n^*\omega) \\ &\qquad = (-1)^{(n-1)|\omega| + (n-2)|\omega| + \cdots + |\omega|} \iota^*_{s_1}\mathrm{i}_{\frac{\partial}{\partial s_1}}\omega \wedge \iota^*_{s_2}\mathrm{i}_{\frac{\partial}{\partial s_2}}\omega \wedge \cdots \wedge \iota^*_{s_n}\mathrm{i}_{\frac{\partial}{\partial s_n}}\omega.\end{aligned}$$

The desired conclusion now follows from the definition of $\Phi^\omega(t)$. □

We now provide a simple observation which will be useful in its own right.

Lemma 3.5. *If $\omega_1, \dots, \omega_n$ is a collection of homogeneous elements in $\Omega^\bullet(M \times [0, 1], \mathrm{End}(V))$, then*

$$\begin{aligned}&\mathrm{d}\int_{\Delta_n(t)} \pi_1^*\omega_1 \wedge \cdots \wedge \pi_n^*\omega_n \\ &= \sum_{i=1}^{n} (-1)^{n+\sum_{j=1}^{i-1}|\omega_j|} \int_{\Delta_n(t)} \pi_1^*\omega_1 \wedge \cdots \wedge \pi_{i-1}^*\omega_{i-1} \wedge \pi_i^*\mathrm{d}\omega_i \wedge \pi_{i+1}^*\omega_{i+1} \wedge \cdots \wedge \pi_n^*\omega_n \\ &+ \sum_{i=1}^{n-1} (-1)^i \int_{\Delta_{n-1}(t)} \pi_1^*\omega_1 \wedge \cdots \wedge \pi_{i-1}^*\omega_{i-1} \wedge \pi_i^*(\omega_i \wedge \omega_{i+1}) \wedge \pi_{i+1}^*\omega_{i+2} \wedge \cdots \wedge \pi_{n-1}^*\omega_n \\ &+ (-1)^n \left(\int_{\Delta_{n-1}(t)} \pi_1^*\omega_1 \wedge \cdots \wedge \pi_{n-1}^*\omega_{n-1} \right) \wedge \iota_0^*\omega_n \\ &+ (-1)^{(n-1)|\omega_1|} \iota_t^*\omega_1 \wedge \left(\int_{\Delta_{n-1}(t)} \pi_1^*\omega_2 \wedge \cdots \wedge \pi_{n-1}^*\omega_n \right).\end{aligned}$$

Proof. It is straightforward to check that

$$\int_{\Delta_n(t)} \pi_1^*\omega_1 \wedge \cdots \wedge \pi_n^*\omega_n = (-1)^{(n-1)|\omega_1|} \int_0^t \iota_s^* \mathrm{i}_{\frac{\partial}{\partial s}}\, \omega_1 \wedge \left(\int_{\Delta_{n-1}(s)} \pi_1^*\omega_2 \wedge \cdots \wedge \pi_{n-1}^*\omega_n \right) \mathrm{d}s,$$

so the result follows by induction on n. □

As a direct consequence of Lemma 3.5, we can prove the following formula, which will be used in what follows.

Proposition 3.6. *If ω is a homogeneous element of $\Omega^\bullet(M \times [0,1], \mathrm{End}(V))$, then*

$$\begin{aligned}
\mathrm{d}\Phi^\omega(t) &= \sum_{n=1}^{\infty}\sum_{i=1}^{n}(-1)^{n+(i-1+\varepsilon(n))|\omega|} \int_{\Delta_n(t)} \pi_1^*\omega\wedge\cdots\wedge\pi_{i-1}^*\omega\wedge\pi_i^*\mathrm{d}\omega\wedge\pi_{i+1}^*\omega\wedge\cdots\wedge\pi_n^*\omega \\
&+\sum_{n=2}^{\infty}\sum_{i=1}^{n-1}(-1)^{i+\varepsilon(n)|\omega|} \int_{\Delta_{n-1}(t)} \pi_1^*\omega\wedge\cdots\wedge\pi_{i-1}^*\omega\wedge\pi_i^*(\omega\wedge\omega)\wedge\pi_{i+1}^*\omega\wedge\cdots\wedge\pi_n^*\omega \\
&+\sum_{n=1}^{\infty}(-1)^{n+\varepsilon(n)|\omega|}\left(\int_{\Delta_{n-1}(t)} \pi_1^*\omega\wedge\cdots\wedge\pi_{n-1}^*\omega\right)\wedge\iota_0^*\omega \\
&+\sum_{n=1}^{\infty}(-1)^{(n-1+\varepsilon(n))|\omega|}\iota_t^*\omega\wedge\left(\int_{\Delta_{n-1}(t)} \pi_1^*\omega\wedge\cdots\wedge\pi_{n-1}^*\omega\right).
\end{aligned}$$

4. The A_∞-natural transformation and homotopy invariance

In this section we prove the main result of the paper, which is the construction of an A_∞-isomorphism between the pullback functors associated to homotopic maps. This may be thought of as a categorified version of what is called the homotopy invariance of the de Rham cohomology.

Let M be a smooth manifold, and let (E, D) be an ∞-local system on $M \times [0,1]$. Our first task is to show that there is an isomorphism of ∞-local systems between the restrictions of (E, D) to $M \times \{0\}$ and $M \times \{1\}$. The following two preliminary results will clear our path.

Lemma 4.1. *Suppose that the ∞-local system (E, D) is trivialized over $M \times [0,1]$, that is to say, $E = (M \times [0,1]) \times V$ for some $\mathbb{Z}$-graded vector space $V = \bigoplus_{k\in\mathbb{Z}} V^k$ and $D = \mathrm{d} - \alpha$ for some homogeneous element $\alpha \in \Omega^\bullet(M \times [0,1], \mathrm{End}(V))$ of total degree 1 satisfying the Maurer–Cartan equation. Then the iterated integral $\Phi^\alpha(1)$ of α defines an isomorphism of ∞-local systems from $\iota_0^*(E, D)$ onto $\iota_1^*(E, D)$.*

Proof. We first show that $\Phi^\alpha(1)$ is a morphism of ∞-local systems from $\iota_0^*(E, D)$ to $\iota_1^*(E, D)$. To this end, we need to check that $(\mathrm{d}-\iota_1^*\alpha)\circ\Phi^\alpha(1) = \Phi^\alpha(1)\circ(\mathrm{d}-\iota_0^*\alpha)$ or, what is the same,

$$\mathrm{d}\Phi^\alpha(1) = \iota_1^*\alpha \wedge \Phi^\alpha(1) - \Phi^\alpha(1) \wedge \iota_0^*\alpha.$$

Using the formula given in Proposition 3.6, we find

$$\begin{aligned}
\mathrm{d}\Phi^\alpha(1) = &\sum_{n=1}^{\infty}\sum_{i=1}^{n}(-1)^{n+i-1+\varepsilon(n)}\int_{\Delta_n}\pi_1^*\alpha\wedge\cdots\wedge\pi_{i-1}^*\alpha\wedge\pi_i^*\mathrm{d}\alpha\wedge\pi_{i+1}^*\alpha\wedge\cdots\wedge\pi_n^*\alpha\\
&+\sum_{n=2}^{\infty}\sum_{i=1}^{n-1}(-1)^{i+\varepsilon(n)}\int_{\Delta_{n-1}}\pi_1^*\alpha\wedge\cdots\wedge\pi_{i-1}^*\alpha\wedge\pi_i^*(\alpha\wedge\alpha)\wedge\pi_{i+1}^*\alpha\wedge\cdots\wedge\pi_n^*\alpha\\
&+\sum_{n=1}^{\infty}(-1)^{n+\varepsilon(n)}\left(\int_{\Delta_{n-1}}\pi_1^*\alpha\wedge\cdots\wedge\pi_{n-1}^*\alpha\right)\wedge\iota_0^*\alpha\\
&+\sum_{n=1}^{\infty}(-1)^{n-1+\varepsilon(n)}\iota_1^*\alpha\wedge\left(\int_{\Delta_{n-1}}\pi_1^*\alpha\wedge\cdots\wedge\pi_{n-1}^*\alpha\right).
\end{aligned}$$

Next, notice that $\varepsilon(n) = \varepsilon(n-1)+n-1$, from which we obtain $(-1)^{n-1+\varepsilon(n)} = (-1)^{\varepsilon(n-1)}$ and $(-1)^{n+\varepsilon(n)} = (-1)^{\varepsilon(n-1)+1}$. Therefore,

$$\begin{aligned}
\mathrm{d}\Phi^\alpha(1) = &\sum_{n=1}^{\infty}\sum_{i=1}^{n}(-1)^{i+\varepsilon(n-1)}\int_{\Delta_n}\pi_1^*\alpha\wedge\cdots\wedge\pi_{i-1}^*\alpha\wedge\pi_i^*\mathrm{d}\alpha\wedge\pi_{i+1}^*\alpha\wedge\cdots\wedge\pi_n^*\alpha\\
&-\sum_{n=2}^{\infty}\sum_{i=1}^{n-1}(-1)^{i+\varepsilon(n-1)}\int_{\Delta_{n-1}}\pi_1^*\alpha\wedge\cdots\wedge\pi_{i-1}^*\alpha\wedge\pi_i^*(\alpha\wedge\alpha)\wedge\pi_{i+1}^*\alpha\wedge\cdots\wedge\pi_n^*\alpha\\
&-\sum_{n=1}^{\infty}(-1)^{\varepsilon(n-1)}\left(\int_{\Delta_{n-1}}\pi_1^*\alpha\wedge\cdots\wedge\pi_{n-1}^*\alpha\right)\wedge\iota_0^*\alpha\\
&+\sum_{n=1}^{\infty}(-1)^{\varepsilon(n-1)}\iota_1^*\alpha\wedge\left(\int_{\Delta_{n-1}}\pi_1^*\alpha\wedge\cdots\wedge\pi_{n-1}^*\alpha\right).
\end{aligned}$$

But α satisfies the Maurer–Cartan equation, so that $\mathrm{d}\alpha-\alpha\wedge\alpha = 0$. Thus, the first and second terms on the right-hand side of this equality cancel out, leaving us with

$$\begin{aligned}
\mathrm{d}\Phi^\alpha(1) &= \iota_1^*\alpha\wedge\left(\sum_{n=1}^{\infty}(-1)^{\varepsilon(n-1)}\int_{\Delta_{n-1}}\pi_1^*\alpha\wedge\cdots\wedge\pi_{n-1}^*\alpha\right)\\
&\qquad\qquad -\left(\sum_{n=1}^{\infty}(-1)^{\varepsilon(n-1)}\int_{\Delta_{n-1}}\pi_1^*\alpha\wedge\cdots\wedge\pi_{n-1}^*\alpha\right)\wedge\iota_0^*\alpha\\
&= \iota_1^*\alpha\wedge\Phi^\alpha(1)-\Phi^\alpha(1)\wedge\iota_0^*\alpha,
\end{aligned}$$

as desired.

It remains to show that $\Phi^\alpha(1)$ is invertible. For this, we decompose $\Phi^\alpha(1) = \sum_{p\geq 0} \Phi^\alpha_p(1)$, where $\Phi^\alpha_p(1)$ is of partial degree p with respect to the total $\mathbb{Z}$-grading on $\Omega^\bullet(M, \mathrm{End}(V))$. From the definition, it is plain to see that $\Phi^\alpha_0(1) = \Phi^{\alpha_1}(1)$, with α_1 being the component of α of partial degree 1 with respect to the total $\mathbb{Z}$-grading on $\Omega^\bullet(M \times [0, 1], \mathrm{End}(V))$. Since the latter defines a connection which preserves the $\mathbb{Z}$-grading, $\Phi^\alpha_0(1)$ is nothing but the parallel transport with respect to such connection along the paths $t \mapsto M \times \{t\}$. Thus, as is well known, $\Phi^\alpha_0(1)$ is invertible. Therefore, $\Phi^\alpha(1)$ is the sum of an invertible element and a nilpotent element. From this it follows easily that $\Phi^\alpha(1)$ must necessarily be invertible. □

Lemma 4.2. *Suppose that the ∞-local system (E, D) is trivialized over $M \times [0, 1]$ as both $E = (M \times [0, 1]) \times V$ and $E = (M \times [0, 1]) \times W$ for some $\mathbb{Z}$-graded vector spaces $V = \bigoplus_{k\in\mathbb{Z}} V^k$ and $W = \bigoplus_{k\in\mathbb{Z}} W^k$ with $D = \mathrm{d} - \alpha$ and $D = \mathrm{d} - \beta$ for some homogenous elements $\alpha \in \Omega^\bullet(M \times [0, 1], \mathrm{End}(V))$ and $\beta \in \Omega^\bullet(M \times [0, 1], \mathrm{End}(W))$ of total degree 1 satisfying the Maurer–Cartan equation. Let $g \in \Omega^0(M \times [0, 1], \mathrm{Hom}(V, W))$ be a transition isomorphism associated with these trivializations. Then*

$$\Phi^\alpha(1) = (\iota_1^* g)^{-1} \Phi^\beta(1) \iota_0^* g.$$

Proof. As explained in Section 2B, the transformation rule from β to α can be expressed as $\alpha = g^{-1}\beta g - g^{-1}\mathrm{d}g$. Hence, the desired conclusion follows by applying Proposition 3.3 with $t = 1$. □

As an easy application of the above, we derive the following:

Proposition 4.3. *Let (E, D) be an ∞-local system over $M \times [0, 1]$. Then there is an isomorphism of ∞-local systems from $\iota_0^*(E, D)$ onto $\iota_1^*(E, D)$.*

Proof. Suppose that the ∞-local system (E, D) is trivialized on an open covering $\{U_i\}$ of M. Thus, $E|_{U_i} = (U_i \times [0, 1]) \times V_i$ for some $\mathbb{Z}$-graded vector space $V_i = \bigoplus_{k\in\mathbb{Z}} V_i^k$ and $D|_{U_i} = \mathrm{d} - \alpha_i$ for some homogeneous element $\alpha_i \in \Omega^\bullet(U_i \times [0, 1], \mathrm{End}(V_i))$ of total degree 1 satisfying the Maurer–Cartan equation. By virtue of Lemma 4.1, the iterated integral $\Phi^{\alpha_i}(1) \in \Omega^\bullet(U_i, \mathrm{End}(V_i))$ determines an isomorphism of ∞-local systems from $\iota_0^*(E|_{U_i}, D|_{U_i})$ onto $\iota_1^*(E|_{U_i}, D|_{U_i})$. On the other hand, if $U_i \cap U_j \neq \varnothing$ and $g_{ji} \in \Omega^0((U_i \cap U_j) \times [0, 1], \mathrm{Hom}(V_i, V_j))$ is the corresponding transition isomorphism, then by Lemma 4.2, we have

$$\Phi^{\alpha_i}(1) = (\iota_1^* g_{ji})^{-1} \Phi^{\alpha_j}(1) \iota_0^* g_{ji}.$$

Hence, the various $\Phi^{\alpha_i}(1)$ piece together to yield a well defined element $\Phi \in \Omega^\bullet(M, \mathrm{Hom}(\iota_0^* E, \iota_1^* E))$, which is an isomorphism of ∞-local systems from $\iota_0^*(E, D)$ onto $\iota_1^*(E, D)$. □

From this result it would seem reasonable to assume that there is a natural isomorphism between the pullback functors $\iota_0^*, \iota_1^* : \mathbf{Loc}_\infty(M \times [0, 1]) \to \mathbf{Loc}_\infty(M)$.

However, with a careful juggling we can show that this is not the case. In fact, something more precise holds.

Proposition 4.4. *There exists an* A_∞*-natural isomorphism* $\lambda : \iota_0^* \Rightarrow \iota_1^*$.

Proof. For every ∞-local system (E, D) on $M \times [0,1]$, we let $\lambda_0(E, D) \in \mathrm{Z}^0\Omega^\bullet(M, \mathrm{Hom}(\iota_0^* E, \iota_1^* E))$ be the isomorphism given by Proposition 4.3. We need to define linear maps of degree $-n$

$$\lambda_n : \Omega^\bullet(M \times [0,1], \mathrm{Hom}(E_{n-1}, E_n)) \otimes \cdots \otimes \Omega^\bullet(M \times [0,1], \mathrm{Hom}(E_0, E_1)) \\ \to \Omega^\bullet(M, \mathrm{Hom}(\iota_0^* E_0, \iota_1^* E_n))$$

for every collection of ∞-local systems $(E_0, D_0), \ldots, (E_n, D_n)$ on $M \times [0,1]$. As with the argument that led to the proof of Proposition 4.3, we construct such maps by assuming first that each ∞-local system (E_i, D_i) is trivialized over $M \times [0,1]$, that is, $E_i = (M \times [0,1]) \times V_i$ for some $\mathbb{Z}$-graded vector space $V_i = \bigoplus_{k\in\mathbb{Z}} V_i^k$ and $D_i = \mathrm{d} - \alpha_i$ for some homogeneous element $\alpha_i \in \Omega^\bullet(M \times [0,1], \mathrm{End}(V_i))$ of total degree 1 satisfying the Maurer–Cartan equation. On that account, let us take homogeneous elements $\xi_0 \in \Omega^\bullet(M \times [0,1], \mathrm{Hom}(V_0, V_1)), \ldots, \xi_{n-1} \in \Omega^\bullet(M \times [0,1], \mathrm{Hom}(V_{n-1}, V_n))$. If we put $V = \bigoplus_{i=0}^n V_i$, then both the elements $\alpha_0, \ldots, \alpha_n$ and the elements $\xi_0, \ldots, \xi_{n-1}$ may be seen as elements of $\Omega^\bullet(M \times [0,1], \mathrm{End}(V))$. Thus, if we set $\omega = \sum_{i=0}^n \alpha_i + \sum_{i=0}^{n-1} \xi_i$, the corresponding iterated integral $\Phi^\omega(1)$ determines an element of $\Omega^\bullet(M, \mathrm{End}(V))$. With this understood, we define $\lambda_n^{\{\alpha_v\}}(\xi_{n-1} \otimes \cdots \otimes \xi_0) \in \Omega^\bullet(M, \mathrm{Hom}(V_0, V_n))$ to be the $(0, n)$ block entry of $\Phi^\omega(1)$, and it is straightforward to verify that this prescription determines a linear map

$$\lambda_n^{\{\alpha_v\}} : \Omega^\bullet(M \times [0,1], \mathrm{Hom}(V_{n-1}, V_n)) \otimes \cdots \otimes \Omega^\bullet(M \times [0,1], \mathrm{Hom}(V_0, V_1)) \\ \to \Omega^\bullet(M, \mathrm{Hom}(V_0, V_n)).$$

We must check that this map has degree $-n$. To this end, notice $\lambda_n^{\{\alpha_v\}}(\xi_{n-1} \otimes \cdots \otimes \xi_0)$ is an infinite sum of terms that contain integrals of the form

$$\int_{\Delta_q} \Bigl(\bigwedge_{j=1}^{i_{n-1}-1} \pi_j^* \alpha_n \Bigr) \wedge \pi_{i_{n-1}}^* \xi_{n-1} \wedge \Bigl(\bigwedge_{j=i_{n-1}+1}^{i_{n-2}-1} \pi_j^* \alpha_{n-1} \Bigr) \\ \wedge \cdots \wedge \Bigl(\bigwedge_{j=i_1+1}^{i_0-1} \pi_j^* \alpha_1 \Bigr) \wedge \pi_{i_0}^* \xi_0 \wedge \Bigl(\bigwedge_{j=i_0+1}^{q} \pi_j^* \alpha_0 \Bigr)$$

where $q \geq n$ and $1 \leq i_{n-1} < i_{n-2} < \cdots < i_1 < i_0 \leq q$. Since the total degree of each of the integrands above is $\sum_{i=0}^{n-1} |\xi_i| + q - n$, it follows that the total degree of these terms is $\sum_{i=0}^{n-1} |\xi_i| - n$. From this we conclude that the map $\lambda_n^{\{\alpha_v\}}$ has degree $-n$.

Next, we must show that the linear maps $\lambda_n^{\{\alpha_v\}}$ satisfy the required relations to be an A$_\infty$-natural transformation. As indicated in Section 2A, these relations read

$$\iota_1^*\xi_{n-1}\wedge\lambda_{n-1}^{\{\alpha_v\}}(\xi_{n-2}\otimes\cdots\otimes\xi_0)-(-1)^{\sum_{j=1}^{n-1}|\xi_j|-n+1}\lambda_{n-1}^{\{\alpha_v\}}(\xi_{n-1}\otimes\cdots\otimes\xi_1)\wedge\iota_0^*\xi_0 \\ =\lambda^{\{\alpha_v\}}(b(\xi_{n-1}\otimes\cdots\otimes\xi_0))+\partial_{D_0,D_n}\lambda_n^{\{\alpha_v\}}(\xi_{n-1}\otimes\cdots\otimes\xi_0),$$

for every composable chain of homogenous elements

$$\xi_0\in\Omega^\bullet(M\times[0,1],\mathrm{Hom}(V_0,V_1)),\ldots,\xi_{n-1}\in\Omega^\bullet(M\times[0,1],\mathrm{Hom}(V_{n-1},V_n)),$$

where, bearing in mind the notations and definitions of Section 2B,

$$\begin{aligned}b(\xi_{n-1}\otimes\cdots\otimes\xi_0)&=\sum_{i=0}^{n-1}(-1)^{\sum_{j=i+1}^{n-1}|\xi_j|+n-i-1}\xi_{n-1}\otimes\cdots\otimes\xi_{i+1}\otimes\mathrm{d}\xi_i\otimes\xi_{i-1}\otimes\cdots\otimes\xi_0\\&\quad-\sum_{i=0}^{n-1}(-1)^{\sum_{j=i+1}^{n-1}|\xi_j|+n-i-1}\xi_{n-1}\otimes\cdots\otimes\xi_{i+1}\otimes(\alpha_{i+1}\wedge\xi_i)\otimes\xi_{i-1}\otimes\cdots\otimes\xi_0\\&\quad+\sum_{i=0}^{n-1}(-1)^{\sum_{j=i}^{n-1}|\xi_j|+n-i-1}\xi_{n-1}\otimes\cdots\otimes\xi_{i+1}\otimes(\xi_i\wedge\alpha_i)\otimes\xi_{i-1}\otimes\cdots\otimes\xi_0\\&\quad+\sum_{i=1}^{n-1}(-1)^{\sum_{j=i}^{n-1}|\xi_j|+n-i-1}\xi_{n-1}\otimes\cdots\otimes\xi_{i+1}\otimes(\xi_i\wedge\xi_{i-1})\otimes\xi_{i-2}\otimes\cdots\otimes\xi_0,\end{aligned}$$

and

$$\partial_{D_0,D_n}\lambda_n^{\{\alpha_v\}}(\xi_{n-1}\otimes\cdots\otimes\xi_0)=\mathrm{d}\lambda_n^{\{\alpha_v\}}(\xi_{n-1}\otimes\cdots\otimes\xi_0)-\iota_1^*\alpha_n\wedge\lambda_n^{\{\alpha_v\}}(\xi_{n-1}\otimes\cdots\otimes\xi_0) \\ +(-1)^{\sum_{j=0}^{n-1}|\xi_j|-n}\lambda_n^{\{\alpha_v\}}(\xi_{n-1}\otimes\cdots\otimes\xi_0)\wedge\iota_0^*\alpha_0.$$

Therefore, we are led to verify that

$$\begin{aligned}&\mathrm{d}\lambda_n^{\{\alpha_v\}}(\xi_{n-1}\otimes\cdots\otimes\xi_0)\\&\quad=\iota_1^*\alpha_n\wedge\lambda_n^{\{\alpha_v\}}(\xi_{n-1}\otimes\cdots\otimes\xi_0)-(-1)^{\sum_{j=0}^{n-1}|\xi_j|-n}\lambda_n^{\{\alpha_v\}}(\xi_{n-1}\otimes\cdots\otimes\xi_0)\wedge\iota_0^*\alpha_0\\&\qquad+\iota_1^*\xi_{n-1}\wedge\lambda_{n-1}^{\{\alpha_v\}}(\xi_{n-2}\otimes\cdots\otimes\xi_0)-(-1)^{\sum_{j=1}^{n-1}|\xi_j|-n+1}\lambda_{n-1}^{\{\alpha_v\}}(\xi_{n-1}\otimes\cdots\otimes\xi_1)\wedge\iota_0^*\xi_0\\&\qquad-\lambda^{\{\alpha_v\}}(b(\xi_{n-1}\otimes\cdots\otimes\xi_0)),\end{aligned}$$

for homogenous elements

$$\xi_0\in\Omega^\bullet(M\times[0,1],\mathrm{Hom}(V_0,V_1)),\ldots,\xi_{n-1}\in\Omega^\bullet(M\times[0,1],\mathrm{Hom}(V_{n-1},V_n)).$$

We relegate the proof of this identity to Appendix A.

We now examine what happens to the above construction when we change the trivialization of each ∞-local system (E_i,D_i). So assume that also $E_i=(M\times[0,1])\times W_i$ for some $\mathbb{Z}$-graded vector space $W_i=\bigoplus_{k\in\mathbb{Z}}W_i^k$ and $D_i=\mathrm{d}-\beta_i$

for some homogeneous element $\beta_i \in \Omega^\bullet(M \times [0,1], \mathrm{End}(W_i))$ of total degree 1 satisfying the Maurer–Cartan equation. We let $g_i \in \Omega^0(M \times [0,1], \mathrm{Hom}(V_i, W_i))$ denote the associated transition isomorphisms, so that the transformation rule from β_i to α_i is expressed as $\alpha_i = g_i^{-1}\beta_i g_i - g_i^{-1}\mathrm{d}g_i$. Consider a composable chain of homogenous elements $\xi_0 \in \Omega^\bullet(M \times [0,1], \mathrm{Hom}(V_0, V_1)), \dots, \xi_{n-1} \in \Omega^\bullet(M \times [0,1], \mathrm{Hom}(V_{n-1}, V_n))$, and set up another composable chain of homogenous elements $\zeta_0 \in \Omega^\bullet(M \times [0,1], \mathrm{Hom}(W_0, W_1)), \dots, \zeta_{n-1} \in \Omega^\bullet(M \times [0,1], \mathrm{Hom}(W_{n-1}, W_n))$ by means of the formula $\xi_i = g_{i+1}^{-1}\zeta_i g_i$ for $i = 0, \dots, n-1$. Similarly as above, we put $W = \bigoplus_{i=0}^n W_i$ and $\eta = \sum_{i=0}^n \beta_i + \sum_{i=0}^{n-1} \zeta_i$ and define $\lambda_n^{\{\beta_v\}}(\zeta_{n-1} \otimes \cdots \otimes \zeta_0) \in \Omega^\bullet(M, \mathrm{Hom}(W_0, W_n))$ to be the $(0, n)$ entry of the iterated integral $\Phi^\eta(1) \in \Omega^\bullet(M, \mathrm{End}(W))$. We claim that the following relation holds:

$$\lambda_n^{\{\alpha_v\}}(\xi_{n-1} \otimes \cdots \otimes \xi_0) = (\iota_1^* g_n)^{-1} \lambda_n^{\{\beta_v\}}(\zeta_{n-1} \otimes \cdots \otimes \zeta_0)\iota_0^* g_0.$$

To substantiate the claim, we set $g = \sum_{i=0}^n g_i \in \Omega^0(M \times [0,1], \mathrm{Hom}(V, W))$ and observe that, by definition, $\omega = g^{-1}\eta g - g^{-1}\mathrm{d}g$. Hence, by applying Proposition 3.3 with $t = 1$, we have that

$$\Phi^\omega(1) = (\iota_1^* g)^{-1}\Phi^\eta(1)\iota_0^* g.$$

By taking the $(0, n)$ entry to both sides of this equality, we get the desired relation.

Finally, to deal with the general situation, the foregoing argument shows that, just as with the proof of Proposition 4.3, the linear maps λ_n may be defined by piecing together linear maps defined locally on a trivializing cover for the (E_i, D_i). □

Finally, we can state and prove our main result.

Theorem 4.5. *Let M, N be smooth manifolds and h be a smooth homotopy between maps $f, g : M \to N$. Then there exists an A_∞-natural isomorphism* $\mathrm{hol} : f^* \Rightarrow g^*$ *between the pullback functors $f^*, g^* : \mathbf{Loc}_\infty(N) \to \mathbf{Loc}_\infty(M)$. Such A_∞-natural isomorphism depends only on h and is given explicitly by Chen's iterated integrals.*

Proof. By hypothesis, there is a smooth homotopy $h : M \times [0,1] \to N$ with $h(x, 0) = f(x)$ and $h(x, 1) = g(x)$ for all $x \in M$. So we have $h \circ \iota_0 = f$ and $h \circ \iota_1 = g$, and thus, $f^* = \iota_0^* \circ h^*$ and $g^* = \iota_1^* \circ h^*$. On the other hand, by Proposition 4.4, there is an A_∞-natural isomorphism $\lambda : \iota_0^* \Rightarrow \iota_1^*$. By restricting the latter to the full DG subcategory of $\mathbf{Loc}_\infty(M \times [0,1])$ consisting of objects of the form $h^*(E, D)$ with (E, D) an object of $\mathbf{Loc}_\infty(N)$, we obtain an A_∞-natural isomorphism between $f^*, g^* : \mathbf{Loc}_\infty(N) \to \mathbf{Loc}_\infty(M)$, as wished. □

Remark 4.6. Given a smooth manifold M, the usual de Rham map $\phi : \Omega^\bullet(M) \to \mathrm{C}^\bullet(M)$ from differential forms to singular cochains is not an algebra map. However, it does induce an algebra map in cohomology. This curiosity was clarified by Gugenheim [1977], who extended ϕ to an explicit A_∞-quasi-isomorphism given by certain iterated integrals. This map plays a crucial role in the higher Riemann–Hilbert correspondence [Block and Smith 2014]. As explained in [Arias Abad and Schätz 2013], the higher-dimensional holonomies that arise in the higher Riemann–Hilbert correspondence arise via pushforward of a Maurer–Cartan element along an A_∞-morphism constructed from that of Gugenheim. In the particular case where M is an interval I, the pushforward along the A_∞-morphism produces the ordinary solutions to the parallel transport equations and realizes an A_∞-morphism $q : \Omega^\bullet(I) \to C^\bullet(I)$. The differential equations for parallel transport that arise in the computations above are solved explicitly by Chen's iterated integrals. The solutions can also be regarded as arising from the map q, which allows one to replace $C^\bullet(I)$ in the definition of the path algebra by the algebra of differential forms. This can be regarded as the moral reason why the A_∞-natural transformation defined above arises.

5. The categorified Poincaré lemma

In this section we derive a series of corollaries of the results obtained in the previous section. Among other things we establish the categorified version of the Poincaré lemma for ∞-local systems.

Our first corollary is the following:

Corollary 5.1. *If $f : M \to N$ is a smooth homotopy equivalence, then the pullback functor $f^* : \mathbf{Loc}_\infty(N) \to \mathbf{Loc}_\infty(M)$ is a quasiequivalence.*

Proof. By definition, there exists a smooth map $g : N \to M$ such that $f \circ g$ and $g \circ f$ are smoothly homotopic to id_N and id_M, respectively. Hence, by Theorem 4.5, we obtain two A_∞-natural isomorphisms $\lambda : g^* \circ f^* \Rightarrow \mathrm{id}_{\mathbf{Loc}_\infty(N)}$ and $\mu : f^* \circ g^* \Rightarrow \mathrm{id}_{\mathbf{Loc}_\infty(M)}$. Therefore, the desired conclusion follows by appealing to Lemma 2.1. □

The above has as an immediate consequence the following:

Corollary 5.2 (categorified Poincaré lemma). *If M is contractible, then $\mathbf{Loc}_\infty(M)$ is quasiequivalent to $\mathbf{DGVect}_{\mathbb{R}}$.*

Proof. Since M is contractible, it has the same homotopy type as a point. Thus, according to Corollary 5.1, there is a quasiequivalence between $\mathbf{Loc}_\infty(M)$ and $\mathbf{Loc}_\infty(\{*\})$. Because $\mathbf{Loc}_\infty(\{*\}) = \mathbf{DGVect}_{\mathbb{R}}$, the desired assertion follows. □

It is now quite easy to see that the following result holds.

Corollary 5.3. *On a contractible manifold M, every ∞-local system (E, D) is isomorphic to a constant ∞-local system.*

We can strengthen the previous corollary and derive a local normal form for flat superconnections. The following result confirms that locally, all flat superconnections are isomorphic to a constant one.

Corollary 5.4. *For an arbitrary manifold M, any ∞-local system (E, D) is locally isomorphic to a constant ∞-local system, that is, every point has an open neighborhood U in which $(E|_U, D|_U)$ is isomorphic to a constant ∞-local system.*

Any contractible open neighborhood U will obviously work.

Remark 5.5. Some of the results of the paper apply to contexts more general than higher local systems on manifolds, for instance Block's cohesive modules [2010] or representations up to homotopy of Lie algebroids [Arias Abad and Crainic 2012]. For the sake of concreteness we have decided to remain in the context of ∞-local systems.

Appendix A: Calculation of $\mathrm{d}\lambda_n^{\{\alpha_v\}}(\xi_{n-1}\otimes\cdots\otimes\xi_0)$

In this appendix we embark on the calculation of $\mathrm{d}\lambda_n^{\{\alpha_v\}}(\xi_{n-1}\otimes\cdots\otimes\xi_0)$. The notation and symbols are as in the proof of Proposition 4.4.

To begin with, since $\lambda_n^{\{\alpha_v\}}(\xi_{n-1}\otimes\cdots\otimes\xi_0)$ is defined as the $(0, n)$ block entry of iterated integral $\Phi^{\omega}(1)$ of the element $\omega=\sum_{i=0}^{n}\alpha_i+\sum_{i=0}^{n-1}\xi_i$, it is an infinite sum of terms of the form

$$\int_0^1\int_0^{s_1}\cdots\int_0^{s_{q-1}}\iota_{s_1}^*\mathrm{i}_{\frac{\partial}{\partial s_1}}\omega_1\wedge\iota_{s_2}^*\mathrm{i}_{\frac{\partial}{\partial s_2}}\omega_2\wedge\cdots\wedge\iota_{s_q}^*\mathrm{i}_{\frac{\partial}{\partial s_q}}\omega_q\,\mathrm{d}s_q\cdots\mathrm{d}s_2\,\mathrm{d}s_1,$$

where $q\geq n$ and there is a strictly decreasing n-tuple $1\leq i_{n-1}<i_{n-2}<\cdots<i_1<i_0\leq q$ such that $\omega_{i_k}=\xi_k$ for $0\leq k\leq n-1$, $\omega_j=\alpha_n$ for $1\leq j\leq i_{n-1}-1$, $\omega_j=\alpha_{n-k}$ for $i_{n-k}+1\leq j\leq i_{n-k-1}-1$ with k running from 1 to $n-1$, and $\omega_j=\alpha_0$ for $i_0+1\leq j\leq q$. We want to compute the exterior derivative of each of these terms. For this purpose, by applying an argument similar to that presented in the proof of Proposition 3.4, we rewrite the latter as

$$(-1)^{\sum_{j=1}^{q-1}(q-j)|\omega_j|}\int_{\Delta_q}\pi_1^*\omega_1\wedge\pi_2^*\omega_2\wedge\cdots\wedge\pi_q^*\omega_q.$$

Next, we observe that, by virtue of Lemma 3.5, we have

$$\begin{aligned}
&\mathrm{d}\int_{\Delta_p}\pi_1^*\omega_1\wedge\cdots\wedge\pi_q^*\omega_q\\
&=\sum_{i=1}^{q}(-1)^{q+\sum_{j=1}^{i-1}|\omega_j|}\int_{\Delta_q}\pi_1^*\omega_1\wedge\cdots\wedge\pi_{i-1}^*\omega_{i-1}\wedge\pi_i^*\mathrm{d}\omega_i\wedge\pi_{i+1}^*\omega_{i+1}\wedge\cdots\wedge\pi_q^*\omega_q\\
&\quad+\sum_{i=1}^{q-1}(-1)^i\int_{\Delta_{q-1}}\pi_1^*\omega_1\wedge\cdots\wedge\pi_{i-1}^*\omega_{i-1}\wedge\pi_i^*(\omega_i\wedge\omega_{i+1})\wedge\pi_{i+1}^*\omega_{i+2}\wedge\cdots\wedge\pi_{q-1}^*\omega_q\\
&\quad+(-1)^q\left(\int_{\Delta_{q-1}}\pi_1^*\omega_1\wedge\cdots\wedge\pi_{q-1}^*\omega_{q-1}\right)\wedge\iota_0^*\omega_q\\
&\quad+(-1)^{(q-1)|\omega_1|}\iota_1^*\omega_1\wedge\left(\int_{\Delta_{q-1}}\pi_1^*\omega_2\wedge\cdots\wedge\pi_{q-1}^*\omega_q\right).
\end{aligned}$$

Therefore, by the foregoing, we find that

$$\begin{aligned}
&\mathrm{d}\int_0^1\int_0^{s_1}\cdots\int_0^{s_{q-1}} \iota_{s_1}^*\mathrm{i}_{\frac{\partial}{\partial s_1}}\omega_1\wedge\iota_{s_2}^*\mathrm{i}_{\frac{\partial}{\partial s_2}}\omega_2\wedge\cdots\wedge\iota_{s_q}^*\mathrm{i}_{\frac{\partial}{\partial s_q}}\omega_q\,\mathrm{d}s_q\cdots\mathrm{d}s_2\,\mathrm{d}s_1\\
&=\sum_{i=1}^{q}(-1)^{\sum_{j=1}^{i-1}|\omega_j|-i}\int_0^1\int_0^{s_1}\cdots\int_0^{s_{q-1}} \iota_{s_1}^*\mathrm{i}_{\frac{\partial}{\partial s_1}}\omega_1\wedge\iota_{s_2}^*\mathrm{i}_{\frac{\partial}{\partial s_2}}\omega_2\wedge\cdots\wedge\iota_{s_{i-1}}^*\mathrm{i}_{\frac{\partial}{\partial s_{i-1}}}\omega_{i-1}\\
&\qquad\wedge\iota_{s_i}^*\mathrm{i}_{\frac{\partial}{\partial s_i}}\mathrm{d}\omega_i\wedge\iota_{s_{i+1}}^*\mathrm{i}_{\frac{\partial}{\partial s_{i+1}}}\omega_{i+1}\wedge\cdots\wedge\iota_{s_q}^*\mathrm{i}_{\frac{\partial}{\partial s_q}}\omega_q\,\mathrm{d}s_q\cdots\mathrm{d}s_2\,\mathrm{d}s_1\\
&\quad+\sum_{i=1}^{q-1}(-1)^{\sum_{j=1}^{i}|\omega_j|+i}\int_0^1\int_0^{s_1}\cdots\int_0^{s_{q-2}} \iota_{s_1}^*\mathrm{i}_{\frac{\partial}{\partial s_1}}\omega_1\wedge\iota_{s_2}^*\mathrm{i}_{\frac{\partial}{\partial s_2}}\omega_2\wedge\cdots\wedge\iota_{s_{i-1}}^*\mathrm{i}_{\frac{\partial}{\partial s_{i-1}}}\omega_{i-1}\\
&\qquad\wedge\iota_{s_i}^*\mathrm{i}_{\frac{\partial}{\partial s_i}}(\omega_i\wedge\omega_{i+1})\wedge\iota_{s_{i+1}}^*\mathrm{i}_{\frac{\partial}{\partial s_{i+1}}}\omega_{i+2}\wedge\cdots\wedge\iota_{s_{q-1}}^*\mathrm{i}_{\frac{\partial}{\partial s_{q-1}}}\omega_q\,\mathrm{d}s_{q-1}\cdots\mathrm{d}s_2\,\mathrm{d}s_1\\
&\quad+(-1)^{\sum_{j=1}^{q-1}|\omega_j|+q}\Bigg(\int_0^1\int_0^{s_1}\cdots\int_0^{s_{q-2}} \iota_{s_1}^*\mathrm{i}_{\frac{\partial}{\partial s_1}}\omega_1\wedge\iota_{s_2}^*\mathrm{i}_{\frac{\partial}{\partial s_2}}\omega_2\\
&\qquad\wedge\cdots\wedge\iota_{s_{q-1}}^*\mathrm{i}_{\frac{\partial}{\partial s_{q-1}}}\omega_{q-1}\,\mathrm{d}s_{q-1}\cdots\mathrm{d}s_2\,\mathrm{d}s_1\Bigg)\wedge\iota_0^*\omega_q\\
&\quad+\iota_1^*\omega_1\wedge\Bigg(\int_0^1\int_0^{s_1}\cdots\int_0^{s_{q-2}} \iota_{s_1}^*\mathrm{i}_{\frac{\partial}{\partial s_1}}\omega_2\wedge\iota_{s_2}^*\mathrm{i}_{\frac{\partial}{\partial s_2}}\omega_3\\
&\qquad\wedge\cdots\wedge\iota_{s_{q-1}}^*\mathrm{i}_{\frac{\partial}{\partial s_{q-1}}}\omega_q\,\mathrm{d}s_{q-1}\cdots\mathrm{d}s_2\,\mathrm{d}s_1\Bigg).
\end{aligned}$$

Let us analyze each of the terms on the right-hand side of this relation separately.

Consider the term inside the first sum. We distinguish two cases. First, assume that $\omega_i=\alpha_i$. Then the sign in front is

$$(-1)^{\sum_{j=1}^{i-1}|\omega_j|-i}=(-1)^{\sum_{j=i}^{n-1}|\xi_j|-n+i-1},$$

and so the term reduces to

$$\begin{aligned}
\text{(A-1)}\quad &(-1)^{\sum_{j=i}^{n-1}|\xi_j|-n+i-1}\int_0^1\int_0^{s_1}\cdots\int_0^{s_{q-1}} \iota_{s_1}^*\mathrm{i}_{\frac{\partial}{\partial s_1}}\omega_1\wedge\iota_{s_2}^*\mathrm{i}_{\frac{\partial}{\partial s_2}}\omega_2\\
&\wedge\cdots\wedge\iota_{s_{i-1}}^*\mathrm{i}_{\frac{\partial}{\partial s_{i-1}}}\omega_{i-1}\wedge\iota_{s_i}^*\mathrm{i}_{\frac{\partial}{\partial s_i}}\mathrm{d}\alpha_i\wedge\iota_{s_{i+1}}^*\mathrm{i}_{\frac{\partial}{\partial s_{i+1}}}\omega_{i+1}\wedge\cdots\wedge\iota_{s_q}^*\mathrm{i}_{\frac{\partial}{\partial s_q}}\omega_q\,\mathrm{d}s_q\cdots\mathrm{d}s_2\,\mathrm{d}s_1.
\end{aligned}$$

Second, suppose that $\omega_i=\xi_i$. Then the sign turns out to be

$$(-1)^{\sum_{j=1}^{i-1}|\omega_j|-i}=(-1)^{\sum_{j=i+1}^{n-1}|\xi_j|-n+i},$$

and consequently the term becomes

$$\begin{aligned}
&(-1)^{\sum_{j=i+1}^{n-1}|\xi_j|-n+i}\int_0^1\int_0^{s_1}\cdots\int_0^{s_{q-1}} \iota_{s_1}^*\mathrm{i}_{\frac{\partial}{\partial s_1}}\omega_1\wedge\iota_{s_2}^*\mathrm{i}_{\frac{\partial}{\partial s_2}}\omega_2\wedge\cdots\wedge\iota_{s_{i-1}}^*\mathrm{i}_{\frac{\partial}{\partial s_{i-1}}}\omega_{i-1}\\
&\qquad\wedge\iota_{s_i}^*\mathrm{i}_{\frac{\partial}{\partial s_i}}\mathrm{d}\xi_i\wedge\iota_{s_{i+1}}^*\mathrm{i}_{\frac{\partial}{\partial s_{i+1}}}\omega_{i+1}\wedge\cdots\wedge\iota_{s_q}^*\mathrm{i}_{\frac{\partial}{\partial s_q}}\omega_q\,\mathrm{d}s_q\cdots\mathrm{d}s_2\,\mathrm{d}s_1.
\end{aligned}$$

If we add these over all $q \geq n$ and all $1 \leq i_{n-1} < i_{n-2} < \cdots < i_1 < i_0 \leq q$, we get

$$(-1)^{\sum_{j=i+1}^{n-1}|\xi_j|-n+i}\lambda_n^{\{\alpha_v\}}(\xi_{n-1}\otimes\cdots\otimes\xi_{i+1}\otimes \mathrm{d}\xi_i\otimes\xi_{i-1}\otimes\cdots\otimes\xi_0). \tag{A-2}$$

We now turn to the term inside the second sum. We have four cases to consider. In the first case, $\omega_i = \omega_{i+1} = \alpha_i$. Then the sign in front is

$$(-1)^{\sum_{j=1}^{i}|\omega_j|+i} = (-1)^{\sum_{j=i}^{n-1}|\xi_j|-n+i},$$

and thus, the term becomes

$$(-1)^{\sum_{j=i}^{n-1}|\xi_j|-n+i}\int_0^1\int_0^{s_1}\cdots\int_0^{s_{q-2}} \iota_{s_1}^*\mathrm{i}_{\frac{\partial}{\partial s_1}}\omega_1\wedge\iota_{s_2}^*\mathrm{i}_{\frac{\partial}{\partial s_2}}\omega_2\wedge\cdots\wedge\iota_{s_{i-1}}^*\mathrm{i}_{\frac{\partial}{\partial s_{i-1}}}\omega_{i-1} \\ \wedge\iota_{s_i}^*\mathrm{i}_{\frac{\partial}{\partial s_i}}(\alpha_i\wedge\alpha_{i+1})\wedge\iota_{s_{i+1}}^*\mathrm{i}_{\frac{\partial}{\partial s_{i+1}}}\omega_{i+2}\wedge\cdots\wedge\iota_{s_{q-1}}^*\mathrm{i}_{\frac{\partial}{\partial s_{q-1}}}\omega_q\,\mathrm{d}s_{q-1}\cdots\mathrm{d}s_2\,\mathrm{d}s_1. \tag{A-3}$$

In the second case, $\omega_i = \alpha_{i+1}$ and $\omega_i = \xi_i$. Then the sign comes out to be

$$(-1)^{\sum_{j=1}^{i}|\omega_j|+i} = (-1)^{\sum_{j=i+1}^{n-1}|\xi_j|-n+i-1},$$

and as a result the term becomes

$$(-1)^{\sum_{j=i+1}^{n-1}|\xi_j|-n+i-1}\int_0^1\int_0^{s_1}\cdots\int_0^{s_{q-2}} \iota_{s_1}^*\mathrm{i}_{\frac{\partial}{\partial s_1}}\omega_1\wedge\iota_{s_2}^*\mathrm{i}_{\frac{\partial}{\partial s_2}}\omega_2\wedge\cdots\wedge\iota_{s_{i-1}}^*\mathrm{i}_{\frac{\partial}{\partial s_{i-1}}}\omega_{i-1} \\ \wedge\iota_{s_i}^*\mathrm{i}_{\frac{\partial}{\partial s_i}}(\alpha_{i+1}\wedge\xi_i)\wedge\iota_{s_{i+1}}^*\mathrm{i}_{\frac{\partial}{\partial s_{i+1}}}\omega_{i+2}\wedge\cdots\wedge\iota_{s_{q-1}}^*\mathrm{i}_{\frac{\partial}{\partial s_{q-1}}}\omega_q\,\mathrm{d}s_{q-1}\cdots\mathrm{d}s_2\,\mathrm{d}s_1.$$

Adding these over all $q \geq n$ and all $1 \leq i_{n-1} < i_{n-2} < \cdots < i_1 < i_0 \leq q$, we obtain

$$(-1)^{\sum_{j=i+1}^{n-1}|\xi_j|-n+i-1}\lambda_n^{\{\alpha_v\}}(\xi_{n-1}\otimes\cdots\otimes\xi_{i+1}\otimes(\alpha_{i+1}\wedge\xi_i)\otimes\xi_{i-1}\otimes\cdots\otimes\xi_0). \tag{A-4}$$

For the third case, we take $\omega_i = \xi_i$ and $\omega_{i+1} = \alpha_i$. Then the sign in front is

$$(-1)^{\sum_{j=1}^{i}|\omega_j|+i} = (-1)^{\sum_{j=i}^{n-1}|\xi_j|-n+i},$$

and hence, the term becomes

$$(-1)^{\sum_{j=i}^{n-1}|\xi_j|-n+i}\int_0^1\int_0^{s_1}\cdots\int_0^{s_{q-2}} \iota_{s_1}^*\mathrm{i}_{\frac{\partial}{\partial s_1}}\omega_1\wedge\iota_{s_2}^*\mathrm{i}_{\frac{\partial}{\partial s_2}}\omega_2\wedge\cdots\wedge\iota_{s_{i-1}}^*\mathrm{i}_{\frac{\partial}{\partial s_{i-1}}}\omega_{i-1} \\ \wedge\iota_{s_i}^*\mathrm{i}_{\frac{\partial}{\partial s_i}}(\xi_i\wedge\alpha_i)\wedge\iota_{s_{i+1}}^*\mathrm{i}_{\frac{\partial}{\partial s_{i+1}}}\omega_{i+2}\wedge\cdots\wedge\iota_{s_{q-1}}^*\mathrm{i}_{\frac{\partial}{\partial s_{q-1}}}\omega_q\,\mathrm{d}s_{q-1}\cdots\mathrm{d}s_2\,\mathrm{d}s_1.$$

Once again, adding over all $q \geq n$ and all $1 \leq i_{n-1} < i_{n-2} < \cdots < i_1 < i_0 \leq q$, this yields

$$(-1)^{\sum_{j=i}^{n-1}|\xi_j|-n+i}\lambda_n^{\{\alpha_v\}}(\xi_{n-1}\otimes\cdots\otimes\xi_{i+1}\otimes(\xi_i\wedge\alpha_i)\otimes\xi_{i-1}\otimes\cdots\otimes\xi_0). \tag{A-5}$$

In the fourth and last case, $\omega_i = \xi_i$ and $\omega_{i+1} = \xi_{i-1}$. Then the sign results in

$$(-1)^{\sum_{j=1}^{i}|\omega_j|+i} = (-1)^{\sum_{j=i}^{n-1}|\xi_j|-n+i},$$

and the term becomes

$$(-1)^{\sum_{j=i}^{n-1}|\xi_j|-n+i}\int_0^1\int_0^{s_1}\cdots\int_0^{s_{q-2}}\iota_{s_1}^*\mathrm{i}_{\frac{\partial}{\partial s_1}}\omega_1\wedge\iota_{s_2}^*\mathrm{i}_{\frac{\partial}{\partial s_2}}\omega_2\wedge\cdots\wedge\iota_{s_{i-1}}^*\mathrm{i}_{\frac{\partial}{\partial s_{i-1}}}\omega_{i-1}$$
$$\wedge\,\iota_{s_i}^*\mathrm{i}_{\frac{\partial}{\partial s_i}}(\xi_i\wedge\xi_{i-1})\wedge\iota_{s_{i+1}}^*\mathrm{i}_{\frac{\partial}{\partial s_{i+1}}}\omega_{i+2}\wedge\cdots\wedge\iota_{s_{q-1}}^*\mathrm{i}_{\frac{\partial}{\partial s_{q-1}}}\omega_q\,\mathrm{d}s_{q-1}\cdots\mathrm{d}s_2\,\mathrm{d}s_1.$$

Thus, adding over all $q\geq n$ and all $1\leq i_{n-1}<i_{n-2}<\cdots<i_1<i_0\leq q$, we obtain

(A-6) $$(-1)^{\sum_{j=i}^{n-1}|\xi_j|-n+i}\lambda_n^{\{\alpha_v\}}(\xi_{n-1}\otimes\cdots\otimes\xi_{i+1}\otimes(\xi_i\wedge\xi_{i-1})\otimes\xi_{i-2}\otimes\cdots\otimes\xi_0).$$

Finally, let us consider the two remaining terms. Here we identify two cases. First, assume that $\omega_1=\alpha_n$ and $\omega_q=\alpha_0$. Then the sign in front of the first summand is

$$(-1)^{\sum_{j=1}^{q-1}|\omega_j|+q}=(-1)^{\sum_{j=0}^{n-1}|\xi_j|-n+1},$$

and therefore, these two terms become

$$(-1)^{\sum_{j=0}^{n-1}|\xi_j|-n+1}\Bigg(\int_0^1\int_0^{s_1}\cdots\int_0^{s_{q-2}}\iota_{s_1}^*\mathrm{i}_{\frac{\partial}{\partial s_1}}\omega_1\wedge\iota_{s_2}^*\mathrm{i}_{\frac{\partial}{\partial s_2}}\omega_2$$
$$\wedge\cdots\wedge\iota_{s_{q-1}}^*\mathrm{i}_{\frac{\partial}{\partial s_{q-1}}}\omega_{q-1}\,\mathrm{d}s_{q-1}\cdots\mathrm{d}s_2\,\mathrm{d}s_1\Bigg)\wedge\iota_0^*\alpha_0$$
$$+\iota_1^*\alpha_n\wedge\Bigg(\int_0^1\int_0^{s_1}\cdots\int_0^{s_{q-2}}\iota_{s_1}^*\mathrm{i}_{\frac{\partial}{\partial s_1}}\omega_2\wedge\iota_{s_2}^*\mathrm{i}_{\frac{\partial}{\partial s_2}}\omega_3\wedge\cdots\wedge\iota_{s_{q-1}}^*\mathrm{i}_{\frac{\partial}{\partial s_{q-1}}}\omega_q\,\mathrm{d}s_{q-1}\cdots\mathrm{d}s_2\,\mathrm{d}s_1\Bigg).$$

Thus, if we add these over all $q\geq n$ and all $1\leq i_{n-1}<i_{n-2}<\cdots<i_1<i_0\leq q$, we get

(A-7) $$\iota_1^*\alpha_n\wedge\lambda_n^{\{\alpha_v\}}(\xi_{n-1}\otimes\cdots\otimes\xi_0)+(-1)^{\sum_{j=0}^{n-1}|\xi_j|-n+1}\lambda_n^{\{\alpha_v\}}(\xi_{n-1}\otimes\cdots\otimes\xi_0)\wedge\iota_0^*\alpha_0.$$

Second, suppose that $\omega_1=\xi_{n-1}$ and $\omega_q=\xi_0$. Then the relevant sign is

$$(-1)^{\sum_{j=1}^{q-1}|\omega_j|+q}=(-1)^{\sum_{j=1}^{n-1}|\xi_j|-n},$$

and so these two terms become

$$(-1)^{\sum_{j=1}^{n-1}|\xi_j|-n}\Bigg(\int_0^1\int_0^{s_1}\cdots\int_0^{s_{q-2}}\iota_{s_1}^*\mathrm{i}_{\frac{\partial}{\partial s_1}}\omega_1\wedge\iota_{s_2}^*\mathrm{i}_{\frac{\partial}{\partial s_2}}\omega_2$$
$$\wedge\cdots\wedge\iota_{s_{q-1}}^*\mathrm{i}_{\frac{\partial}{\partial s_{q-1}}}\omega_{q-1}\mathrm{d}s_{q-1}\cdots\mathrm{d}s_2\mathrm{d}s_1\Bigg)\wedge\iota_0^*\xi_0$$
$$+\iota_1^*\xi_{n-1}\wedge\Bigg(\int_0^1\int_0^{s_1}\cdots\int_0^{s_{q-2}}\iota_{s_1}^*\mathrm{i}_{\frac{\partial}{\partial s_1}}\omega_2\wedge\iota_{s_2}^*\mathrm{i}_{\frac{\partial}{\partial s_2}}\omega_3\wedge\cdots\wedge\iota_{s_{q-1}}^*\mathrm{i}_{\frac{\partial}{\partial s_{q-1}}}\omega_q\mathrm{d}s_{q-1}\cdots\mathrm{d}s_2\mathrm{d}s_1\Bigg).$$

Adding these over all $q\geq n$ and all $1\leq i_{n-1}<i_{n-2}<\cdots<i_1<i_0\leq q$, yields

(A-8) $$\iota_1^*\xi_{n-1}\wedge\lambda_{n-1}^{\{\alpha_v\}}(\xi_{n-2}\otimes\cdots\otimes\xi_0)+(-1)^{\sum_{j=1}^{n-1}|\xi_j|-n}\lambda_{n-1}^{\{\alpha_v\}}(\xi_{n-1}\otimes\cdots\otimes\xi_1)\wedge\iota_0^*\xi_0.$$

Having paved the way, we are at last in a position to explicitly give the full expression for $\mathrm{d}\lambda_n^{\{\alpha_v\}}(\xi_{n-1}\otimes\cdots\otimes\xi_0)$. The first thing to notice is that, owing to the Maurer–Cartan equation satisfied by each α_i, when we add over all $q\geq n$ and all $1\leq i_{n-1}<i_{n-2}<\cdots<i_1<i_0\leq q$, the terms associated with the contributions (A-1) and (A-3) cancel out. Next, observe that, thanks to the definition of the differential b, if we add together the contributions (A-2), (A-4), (A-5), and (A-6), the result of exactly $-\lambda^{\{\alpha_v\}}(b(\xi_{n-1}\otimes\cdots\otimes\xi_0))$. Taking into account the two remaining contributions (A-7) and (A-8), we thus obtain

$$\begin{aligned}&\mathrm{d}\lambda_n^{\{\alpha_v\}}(\xi_{n-1}\otimes\cdots\otimes\xi_0)\\&\quad=\iota_1^*\alpha_n\wedge\lambda_n^{\{\alpha_v\}}(\xi_{n-1}\otimes\cdots\otimes\xi_0)-(-1)^{\sum_{j=0}^{n-1}|\xi_j|-n}\lambda_n^{\{\alpha_v\}}(\xi_{n-1}\otimes\cdots\otimes\xi_0)\wedge\iota_0^*\alpha_0\\&\qquad+\iota_1^*\xi_{n-1}\wedge\lambda_{n-1}^{\{\alpha_v\}}(\xi_{n-2}\otimes\cdots\otimes\xi_0)-(-1)^{\sum_{j=1}^{n-1}|\xi_j|-n+1}\lambda_{n-1}^{\{\alpha_v\}}(\xi_{n-1}\otimes\cdots\otimes\xi_1)\wedge\iota_0^*\xi_0\\&\qquad-\lambda^{\{\alpha_v\}}(b(\xi_{n-1}\otimes\cdots\otimes\xi_0)),\end{aligned}$$

which is the relation we wanted to verify.

Appendix B: A_∞-categories, A_∞-functors, and A_∞-natural transformations

In this appendix, we review the basic notions of the theory of A_∞-categories. A full treatment of the subject can be found in [Seidel 2008].

An *nonunital* A_∞*-category* $\mathscr{C}$ over a field K consists of a set of objects $\operatorname{Ob}\mathscr{C}$, a $\mathbb{Z}$-graded K-vector space $\operatorname{Hom}_{\mathscr{C}}(X,Y)$ for any pair of objects $X,Y\in\operatorname{Ob}\mathscr{C}$, and composition maps of degree 2

$$m_n^{\mathscr{C}}: s\operatorname{Hom}_{\mathscr{C}}(X_{n-1},X_n)\otimes_K\cdots\otimes_K s\operatorname{Hom}_{\mathscr{C}}(X_0,X_1)\to\operatorname{Hom}_{\mathscr{C}}(X_0,X_n)$$

for every collection $X_0,\ldots,X_n\in\operatorname{Ob}\mathscr{C}$, such that for all chains of homogeneous elements $a_1\in s\operatorname{Hom}_{\mathscr{C}}(X_0,X_1),\ldots,a_n\in s\operatorname{Hom}_{\mathscr{C}}(X_{n-1},X_n)$ the A_∞*-associativity equation*

$$\begin{aligned}&\sum_{i=1}^{n}\sum_{j=0}^{n-i}(-1)^{\sum_{k=0}^{n-1}|a_k|-j}m_{n-i+1}^{\mathscr{C}}\\&\qquad\times(a_n\otimes\cdots\otimes a_{i+j+1}\otimes m_i^{\mathscr{C}}(a_{i+j}\otimes\cdots\otimes a_{i+1})\otimes a_i\otimes\cdots\otimes a_1)=0\end{aligned}$$

is satisfied for any $n\geq 1$.

The first two A_∞-associativity equations say that $m_1^{\mathscr{C}}$ squares to zero and is a derivation with respect to the composition on $\mathscr{C}$ defined via $m_2^{\mathscr{C}}$. One may hence consider the associated *homotopy category* $\mathbf{Ho}(\mathscr{C})$, with the same objects as $\mathscr{C}$, morphisms spaces the 0-th cohomology group $H^0(\operatorname{Hom}_{\mathscr{C}}(X,Y),m_1^{\mathscr{C}})$, and composition given by

$$[b]\circ[a]=(-1)^{|b|}[m_2^{\mathscr{C}}(a\otimes b)].$$

Along the same lines, in the case that all higher compositions vanish, the third A_∞-associativity equation simply says that $m_2^{\mathscr{C}}$ is associative. We thus find that a nonunital DG category is a special case of a nonunital A_∞-category $\mathscr{C}$ with $m_n^{\mathscr{C}} = 0$ for all $n > 2$.

If $\mathscr{C}$ and $\mathscr{D}$ are nonunital A_∞-categories, a *nonunital* A_∞*-functor* $F : \mathscr{C} \to \mathscr{D}$ consists of a map $F_0 : \operatorname{Ob}\mathscr{C} \to \operatorname{Ob}\mathscr{D}$ and K-linear maps of degree 1

$$F_n : s\mathrm{Hom}_{\mathscr{C}}(X_{n-1}, X_n) \otimes_K \cdots \otimes_K s\mathrm{Hom}_{\mathscr{C}}(X_0, X_1) \to \mathrm{Hom}_{\mathscr{D}}(F(X_0), F(X_n))$$

for every collection $X_0, \dots, X_n \in \operatorname{Ob}\mathscr{C}$, such that for all chains of homogeneous elements $a_1 \in s\mathrm{Hom}_{\mathscr{C}}(X_0, X_1), \dots, a_n \in s\mathrm{Hom}_{\mathscr{C}}(X_{n-1}, X_n)$ the polynomial equation

$$\sum_{i=1}^{n}\sum_{j=0}^{n-i}(-1)^{\sum_{k=0}^{n-1}|a_k|-j} F_{n-i+1}(a_n\otimes\cdots\otimes a_{i+j+1}\otimes m_i^{\mathscr{C}}(a_{i+j}\otimes\cdots\otimes a_{i+1})\otimes a_i\otimes\cdots\otimes a_1)$$
$$= \sum_{r\geq 1}\sum_{s_1+\cdots+s_r=n} m_r^{\mathscr{D}}(F_{s_r}(a_n\otimes\cdots\otimes a_{n-s_r+1})\otimes\cdots\otimes F_{s_1}(a_{s_1}\otimes\cdots\otimes a_1))$$

is satisfied for any $n \geq 1$. If $\mathscr{C}$, $\mathscr{D}$, and $\mathscr{E}$ are three nonunital A_∞-categories, and $F : \mathscr{C} \to \mathscr{D}$ and $G : \mathscr{D} \to \mathscr{E}$ are two nonunital A_∞-functors, then F and G can be composed as

$$(G\circ F)_n(a_n\otimes\cdots\otimes a_1)$$
$$= \sum_{r\geq 1}\sum_{s_1+\cdots+s_r=n} G_r(F_{s_r}(a_n\otimes\cdots\otimes a_{n-s_r+1})\otimes\cdots\otimes F_{s_1}(a_{s_1}\otimes\cdots\otimes a_1)).$$

Composition is strictly associative, and the identity functor is a neutral element. Any nonunital A_∞-functor $F : \mathscr{C} \to \mathscr{D}$ induces an ordinary nonunital functor

$$\mathbf{Ho}(F) : \mathbf{Ho}(\mathscr{C}) \to \mathbf{Ho}(\mathscr{D})$$

between the corresponding homotopy categories, acting in the same way on objects and on morphisms by $\mathbf{Ho}(F)([a]) = (-1)^{|a|}[F_1(a)]$.

Nonunital A_∞-functors between two nonunital A_∞-categories $\mathscr{C}$ and $\mathscr{D}$ can be naturally organized into a nonunital A_∞-category $\mathscr{P} = \mathsf{A}_\infty\text{-}\mathbf{Fun}(\mathscr{C}, \mathscr{D})$. An element $\lambda \in \mathrm{Hom}_{\mathscr{P}}^d(F, G)$ of the $\mathbb{Z}$-graded K-vector space in this A_∞-category is a family of K-linear maps of degree d

$$\lambda_n : s\mathrm{Hom}_{\mathscr{C}}(X_{n-1}, X_n) \otimes_K \cdots \otimes_K s\mathrm{Hom}_{\mathscr{C}}(X_0, X_1) \to \mathrm{Hom}_{\mathscr{D}}(F(X_0), G(X_n))$$

for all $X_0, \dots, X_n \in \operatorname{Ob}\mathscr{C}$. In particular, λ_0 is a family of elements in $\mathrm{Hom}_{\mathscr{D}}^d(F(X), G(X))$ for each object $X \in \operatorname{Ob}\mathscr{C}$. We call such λ an A_∞*-prenatural transformation* of degree d from F to G. The derivation $m_1^{\mathcal{P}}$ is given by

$$[m_1^{\mathcal{P}}(\lambda)]_n(a_n\otimes\cdots\otimes a_1)=\sum_{r\geq 1}\sum_{i=1}^{r}\sum_{s_1+\cdots+s_r=n}(-1)^{(d-1)(\sum_{k=1}^{s_1+\cdots+s_{i-1}}|a_k|-\sum_{k=1}^{i-1}s_k)}$$
$$\times m_r^{\mathcal{D}}\big(G_{s_r}(a_n\otimes\cdots\otimes a_{n-s_r+1})\otimes\cdots\otimes G_{s_{i+1}}(a_{s_1+\cdots+s_{i+1}}\otimes\cdots\otimes a_{s_1+\cdots+s_i+1})$$
$$\otimes\lambda_{s_i}(a_{s_1+\cdots+s_i}\otimes\cdots\otimes a_{s_1+\cdots+s_{i-1}+1})$$
$$\otimes F_{s_{i-1}}(a_{s_1+\cdots s_{i-1}}\otimes\cdots\otimes a_{s_1+\cdots+s_{i-2}+1})\otimes\cdots\otimes F_{s_1}(a_{s_1}\otimes\cdots\otimes a_1)\big)$$
$$-\sum_{i=1}^{n}\sum_{j=0}^{n-i}(-1)^{\sum_{k=0}^{n-1}|a_k|-j+d-1}$$
$$\times\lambda_{d-i+1}(a_n\otimes\cdots\otimes a_{i+j+1}\otimes m_i^{\mathcal{C}}(a_{i+j}\otimes\cdots\otimes a_{j+1})\otimes a_j\otimes\cdots\otimes a_1).$$

The formulae for the $m_n^{\mathcal{P}}$ with $n\geq 2$ follow a much simpler pattern and can be consulted in [Seidel 2008].

With the above understood, an A_∞-*natural transformation* between two nonunital A_∞-functors $F:\mathcal{C}\to\mathcal{D}$ and $G:\mathcal{C}\to\mathcal{D}$ is a closed A_∞-prenatural transformation $\lambda\in\mathrm{Hom}_{\mathcal{P}}(F,G)$ of degree 0. We simply write $\lambda:F\Rightarrow G$ to indicate that we have such a transformation.

Given an A_∞-natural transformation $\lambda:F\Rightarrow G$ between nonunital A_∞-functors $F,G:\mathcal{C}\to\mathcal{D}$, consider the elements $[\lambda_0(X)]\in\mathrm{Hom}_{\mathbf{Ho}(\mathcal{D})}(F(X),G(X))$ for each $X\in\mathrm{Ob}\,\mathcal{C}$. These satisfy the natural condition

$$[\lambda_0(Y)]\circ[F_1(a)]=[G_1(a)]\circ[\lambda_0(X)]$$

for all $[a]\in\mathrm{Hom}_{\mathbf{Ho}(\mathcal{C})}(X,Y)$. Hence, they constitute a natural transformation, which we may denote by $\mathbf{Ho}(\lambda)$, between the ordinary nonunital functors $\mathbf{Ho}(F)$ and $\mathbf{Ho}(G)$.

To close we would like to clarify the connection between the previous definition and the one given in Section 2A. Suppose that $\mathcal{C}$ and $\mathcal{D}$ are nonunital A_∞-categories with $m_n^{\mathcal{C}}=0$ and $m_n^{\mathcal{D}}=0$ for all $n>2$. Thus, as already remarked, both $\mathcal{C}$ and $\mathcal{D}$ are nonunital DG categories, where the differential and composition in $\mathcal{C}$ are given by $da=(-1)^{|a|}m_1^{\mathcal{C}}(a)$ and $b\circ a=(-1)^{|a|}m_2^{\mathcal{C}}(a,b)$, respectively, and similarly for $\mathcal{D}$. If $F:\mathcal{C}\to\mathcal{D}$ and $G:\mathcal{C}\to\mathcal{D}$ are two nonunital DG functors, then the closeness condition for an A_∞-natural transformation $\lambda:F\Rightarrow G$ is equivalent to the defining relation presented in Section 2A, with the replacements $f_0=a_1,\ldots,f_{n-1}=a_n$.

Remark B.1. As suggested by the referee, in the latter context, the definition of an A_∞-natural transformation can be described in terms of the path algebra. For simplicity, we discuss the case of DG algebras. So let us assume that $\mathcal{C}$ and $\mathcal{D}$ are DG algebras, and let $F:\mathcal{C}\to\mathcal{D}$ and $G:\mathcal{C}\to\mathcal{D}$ be DG maps. If we denote by Λ the DG algebra of cellular cochains on the interval $I=[0,1]$, the inclusion of the endpoints induces natural maps $\pi_0:\Lambda\to\mathbb{R}$ and $\pi_1:\Lambda\to\mathbb{R}$. Moreover, if $\mathbf{B}$

denotes the bar construction functor, the DG maps F and G induce maps of DG coalgebras $\mathbf{B}(F):\mathbf{B}(\mathscr{C})\to\mathbf{B}(\mathscr{D})$ and $\mathbf{B}(G):\mathbf{B}(\mathscr{C})\to\mathbf{B}(\mathscr{D})$. Then, an alternative definition of an A_∞-natural transformation from F to G is a DG coalgebra map

$$\eta:\mathbf{B}(\mathscr{C})\to\mathbf{B}(\mathscr{D}\otimes\Lambda),$$

such that the map $\mathbf{B}(\mathrm{id}_{\mathscr{D}}\otimes\pi_0)\circ\eta$ is equal to $\mathbf{B}(F)$, and the map $\mathbf{B}(\mathrm{id}_{\mathscr{D}}\otimes\pi_1)\circ\eta$ is equal to $\mathbf{B}(G)$. The reason that this definition is equivalent to the previous one is the following. As described in Section 2A, an A_∞-natural transformation $\lambda:F\Rightarrow G$ is given by a sequence K-linear maps of degree 0

$$\lambda_n:(s\mathscr{C})^{\otimes n}\to\mathscr{D},$$

satisfying the defining relations. Given such a sequence of K-linear maps, one can construct a DG coalgebra map $\eta:\mathbf{B}(\mathscr{C})\to\mathbf{B}(\mathscr{D}\otimes\Lambda)$ as follows. Since $\mathbf{B}(\mathscr{D}\otimes\Lambda)$ is cofree, η is determined by a K-linear map

$$\bar\eta:\mathbf{B}(\mathscr{C})\to s(\mathscr{D}\otimes\Lambda).$$

If we denote by $\langle 0\rangle$, $\langle 1\rangle$, $\langle 0,1\rangle$ the three natural generators in Λ so that

$$\mathscr{D}\otimes\Lambda=(\mathscr{D}\otimes\langle 0\rangle)\oplus(\mathscr{D}\otimes\langle 1\rangle)\oplus(\mathscr{D}\otimes\langle 0,1\rangle),$$

then the projections of $\bar\eta$ onto $s(\mathscr{D}\otimes\langle 0\rangle)$ and $s(\mathscr{D}\otimes\langle 1\rangle)$ are determined by F and G, respectively, while the maps $\bar\eta:(s\mathscr{C})^{\otimes n}\to(\mathscr{D}\otimes\langle 0,1\rangle)$ are determined by the λ_n. The relations satisfied by the maps λ_n guarantee that η is indeed a map of DG coalgebras. Reciprocally, it is clear that the maps λ_n can be recovered from η so that the two definitions are equivalent.

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WONDERFUL COMPACTIFICATION OF CHARACTER VARIETIES

INDRANIL BISWAS, SEAN LAWTON AND DANIEL RAMRAS
APPENDIX BY ARLO CAINE AND SAMUEL EVENS

Using the wonderful compactification of a semisimple adjoint affine algebraic group G defined over an algebraically closed field $\Bbbk$ of arbitrary characteristic, we construct a natural compactification $\overline{\mathfrak{X}_\Gamma(G)}$ of the G-character variety of any finitely generated group Γ. When Γ is a free group, we show that this compactification is always simply connected with respect to the étale fundamental group, and when $\Bbbk = \mathbb{C}$ it is also topologically simply connected. For other groups Γ, we describe conditions for the compactification of the moduli space to be simply connected and give examples when these conditions are satisfied, including closed surface groups and free abelian groups when $G = \mathrm{PGL}_n(\mathbb{C})$. Additionally, when Γ is a free group we identify the boundary divisors of $\overline{\mathfrak{X}_\Gamma(G)}$ in terms of previously studied moduli spaces, and we construct a family of Poisson structures on $\overline{\mathfrak{X}_\Gamma(G)}$ and its boundary divisors arising from Belavin–Drinfeld splittings of the double of the Lie algebra of G. In the appendix, we explain how to put a Poisson structure on a quotient of a Poisson algebraic variety by the action of a reductive Poisson algebraic group.

1. Introduction

To understand how groups Γ act on spaces X one considers homomorphisms $\Gamma \to \mathrm{Aut}(X)$. When $\mathrm{Aut}(X)$ is an algebraic group G, the collection of homomorphisms $\mathrm{Hom}(\Gamma, G)$ is an algebraic variety and so deformation techniques are available. From the associated study of G-local systems, two homomorphisms are equivalent when they are conjugate via an element of G. In this case, the quotient space $\mathrm{Hom}(\Gamma, G)/G$ is naturally considered. Unfortunately this quotient space is not generally algebraic and so deformation techniques are not available. An approximation to this space, that often has better properties, is called the G-character variety of Γ. It will be denoted by $\mathfrak{X}_\Gamma(G)$.

When G is a reductive algebraic group over an algebraically closed field $\Bbbk$, the above mentioned space $\mathfrak{X}_\Gamma(G)$ is precisely the geometric invariant theoretic (GIT)

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quotient $\mathrm{Hom}(\Gamma, G)/\!\!/G$; in other words, it is the spectrum of the ring of invariants $\Bbbk[\mathrm{Hom}(\Gamma, G)]^G$.

Considering families lying in $\mathfrak{X}_\Gamma(G)$ demands an understanding of (geometrically meaningful) boundary divisors, and as such compactifications of $\mathfrak{X}_\Gamma(G)$ arise naturally.

For example, in [Morgan and Shalen 1984], a compactification of $\mathrm{SL}_2(\mathbb{C})$-character varieties by actions on $\mathbb{R}$-trees gave a new proof of Thurston's theorem that projective measured geodesic laminations give a compactification of Teichmüller space; the latter gives a classification of surface group automorphisms. Extensions of these ideas to real Lie groups were considered by Parreau [2012]. More recently, in [Manon 2015], it was shown that each quiver-theoretic avatar of a free group character variety developed in [Florentino and Lawton 2013] determines a natural compactification, under the assumption that G is simple and simply connected over $\mathbb{C}$. And in [Komyo 2015], compactifications of relative character varieties of punctured spheres are considered in order to understand the relationship between the Dolbeault moduli space of Higgs bundles and the Betti moduli space of representations.

In this paper, we prove the following theorem:

Theorem 1.1. *Let G be a semisimple algebraic group of adjoint type defined over an algebraically closed field $\Bbbk$. Then the wonderful compactification of G determines a compactification of $\mathfrak{X}_\Gamma(G)$ for any finitely generated group Γ. If Γ is a free group, then this compactification is étale simply connected. Moreover, when $\Bbbk = \mathbb{C}$ there exists a compactification of $\mathfrak{X}_\Gamma(G)$ that is both topologically and étale simply connected whenever $\mathfrak{X}_\Gamma(G)$ is simply connected and normal.*

This result follows from Theorem 3.5, Corollary 4.2 and Lemma 4.3. Let $\overline{\mathfrak{X}_\Gamma(G)}$ denote the compactification of $\mathfrak{X}_\Gamma(G)$ from Theorem 1.1. In Proposition 4.5, we apply Theorem 1.1 to prove the following corollary.

Corollary 1.2. *Let G be a semisimple algebraic group of adjoint type over $\mathbb{C}$. Then $\overline{\mathfrak{X}_\Gamma(G)}$ is both topologically and étale simply connected if*:

(1) Γ *is a free group*,

(2) Γ *is a surface group and* $G = \mathrm{PGL}_n(\mathbb{C})$, *or*

(3) Γ *is free abelian and G does not have exceptional factors.*

In Sections 5 and 6 we further study the case in which Γ is a free group. We identify the boundary divisors of $\overline{\mathfrak{X}_\Gamma(G)}$ (Theorem 5.2) in terms of the *parabolic character varieties* studied by Biswas, Florentino, Lawton and Logares [Biswas et al. 2014], and we construct a Poisson structure on $\overline{\mathfrak{X}_\Gamma(G)}$ and on its boundary divisors (Theorem 6.5) using work of Evens and Lu [2001; 2006], who constructed a Poisson structure on $\overline{G}$. To show there is a Poisson structure on $\overline{\mathfrak{X}_\Gamma(G)}$, we utilize recent work of Lu and Mouquin [2017] to equip $\overline{G}^r$ with a Poisson structure for which the diagonal conjugation action of G is a Poisson action (for an appropriate Poisson Lie group structure on G). To show that this Poisson structure descends to $\overline{\mathfrak{X}_\Gamma(G)}$, we use the fact that when a reductive algebraic Poisson group acts on a projective Poisson variety and the action is Poisson, then the GIT quotient inherits a Poisson structure. This fact, although known to experts, does not appear in the literature. The Appendix, written by Arlo Caine and Sam Evens, provides a proof of this fact.

2. Wonderful compactification of groups

Let G be a connected affine algebraic group defined over an algebraically closed field $\Bbbk$; there is no condition on its characteristic. Let $\mathfrak{g} = \mathrm{Der}_{\Bbbk}(\Bbbk[G], \Bbbk)^G$ be the Lie algebra of G, where G acts on the derivations via the left-translation action of G on itself. The group G is said to be of *adjoint type* if the adjoint representation

$$\rho : G \to \mathrm{GL}(\mathfrak{g}) \tag{2-1}$$

is an embedding. The center of a group of adjoint type is trivial.

We will always assume that G is semisimple of adjoint type. Therefore, G is of the form $\prod_{i=1}^{m}(G_i/Z_i)$, where each G_i is a simple simply connected group and Z_i is the center of G_i.

A *compactification* of a variety X is a complete variety Y with X as a dense open subset. In [De Concini and Procesi 1983], assuming the base field is of characteristic 0, a compactification of G is constructed, called the *wonderful compactification*. In [Strickland 1987] the construction is generalized to arbitrary characteristic. Denote the wonderful compactification of G by $\overline{G}$. In [Evens and Lu 2001; 2006], a Poisson structure on $\overline{G}$ is constructed when the characteristic of the base field is zero.

We now describe the construction of $\overline{G}$, following the exposition in [Evens and Lu 2001; Evens and Jones 2008]. Let n be the dimension of G. The general linear group $\mathrm{GL}(\mathfrak{g}\oplus\mathfrak{g})$ acts on the space of n-dimensional subspaces of $\mathfrak{g}\oplus\mathfrak{g}$ transitively with the stabilizer of a point being a parabolic subgroup P. The Grassmannian $\mathrm{Gr}(n, \mathfrak{g}\oplus\mathfrak{g}) = \mathrm{GL}(\mathfrak{g}\oplus\mathfrak{g})/P$ of dimension $(2n)^2 - 3n^2 = n^2$ parametrizes the n-dimensional subspaces of $\mathfrak{g}\oplus\mathfrak{g}$. Consider the composition homomorphism

$$G \times G \xrightarrow{\rho\times\rho} \mathrm{GL}(\mathfrak{g}) \times \mathrm{GL}(\mathfrak{g}) \hookrightarrow \mathrm{GL}(\mathfrak{g}\oplus\mathfrak{g}),$$

where ρ is the homomorphism in (2-1) and $\mathrm{GL}(\mathfrak{g}) \times \mathrm{GL}(\mathfrak{g})$ is the subgroup of automorphisms of $\mathfrak{g}\oplus\mathfrak{g}$ that preserves its decomposition. This homomorphism produces an action of $G \times G$ on $\mathrm{Gr}(n, \mathfrak{g}\oplus\mathfrak{g})$. Let

$$\mathfrak{g}_\Delta := \{(x, x) \mid x \in \mathfrak{g}\} \subset \mathfrak{g}\oplus\mathfrak{g}$$

be the diagonal subalgebra, which is an n-dimensional subspace and hence a point in $\mathrm{Gr}(n, \mathfrak{g}\oplus\mathfrak{g})$. The stabilizer of $\mathfrak{g}_\Delta$ with respect to the above action of $G \times G$ on

$\mathrm{Gr}(n, \mathfrak{g} \oplus \mathfrak{g})$ is

$$G_\Delta := \{(g, g) \mid g \in G\}.$$

Therefore, the orbit of $\mathfrak{g}_\Delta$ is

$$(G \times G) \cdot \mathfrak{g}_\Delta = (G \times G)/G_\Delta \cong G.$$

The wonderful compactification of G is then $\overline{G} = \overline{(G \times G) \cdot \mathfrak{g}_\Delta}$, where the closure is taken inside $\mathrm{Gr}(n, \mathfrak{g} \oplus \mathfrak{g})$, making $\overline{G}$ an irreducible projective variety containing $G = (G \times G) \cdot \mathfrak{g}_\Delta$ as a Zariski open subvariety.

Theorem 2.1 [Strickland 1987; De Concini and Procesi 1983]. *The following properties hold for the wonderful compactification $\overline{G}$:*

(1) *The action of $G \times G$ on G, defined by $(g_1, g_2) \cdot x = g_1 x g_2^{-1}$, extends to a $G \times G$ action on $\overline{G}$ with 2^r orbits, where $r = \mathrm{rank}(G)$;*

(2) *$\overline{G}$ is smooth, as is each $G \times G$ orbit closure in $\overline{G}$;*

(3) *The complement $\overline{G} \setminus G$ consists of r smooth divisors $D_1, \ldots, D_r$ with simple normal crossings, each of which is the closure of a single $G \times G$ orbit.*

Remark 2.2. In [De Concini and Procesi 1983], a canonical compactification (called the wonderful compactification) is constructed for certain homogeneous spaces H/K called symmetric varieties, where K is the fixed locus of an involution. The wonderful compactification of G above is a special case of this more general construction since the diagonal copy of G inside $G \times G$, denoted G_Δ, is the fixed locus of the involution $(a, b) \mapsto (b, a)$. Then $G \cong (G \times G)/G_\Delta$, and the left action of H on H/K extends to the wonderful compactification of H/K and becomes the $G \times G$ action on $\overline{G}$ after passing through this isomorphism. We note this generalization since we will be referring to properties about this more general construction later.

Note that the diagonal $G_\Delta \cong G$ acts by conjugation on $\overline{G}$. We now show that $\overline{G}$ is simply connected, after reminding the reader of requisite terms.

A morphism of irreducible normal projective varieties $f : Y \to X$ is *étale* if the induced map $\widehat{\mathcal{O}_{f(y)}} \to \widehat{\mathcal{O}_y}$ between complete local rings is an isomorphism for all points $y \in Y$. An étale morphism f is *Galois* if the induced injection on quotient fields $\Bbbk(X) \to \Bbbk(Y)$ is a Galois extension. The Galois group for this extension acts on Y with X being the quotient. A *Galois covering* of X is a finite Galois étale map $Y \to X$. We say X is *étale simply connected* if it does not admit any nontrivial Galois coverings. Over $\mathbb{C}$, if the topological fundamental group of X (in the strong topology) is trivial, then the étale fundamental group is trivial [Milne 1980].

Corollary 2.3. *The variety $\overline{G}$ is étale simply connected. When $\Bbbk = \mathbb{C}$, the topological fundamental group of $\overline{G}$ is trivial.*

Proof. Recall that G is an open dense affine subvariety of $\overline{G}$. Since we are over an algebraically closed field, the Bruhat decomposition gives an affine cell in G that is open and dense [Borel 1991]. So $\overline{G}$ is birational to affine space, which itself is birational to projective space. Therefore, $\overline{G}$ is a rational variety. In general a projective, smooth, rational variety over an algebraically closed field is étale simply connected [Kollár 2003]. Thus, $\overline{G}$ is étale simply connected.

When $\Bbbk = \mathbb{C}$, the topological fundamental group of $\overline{G}$ is trivial, because $\overline{G}$ is a rational variety [Serre 1959, p. 483, Proposition 1]. □

Remark 2.4. Our proof of Corollary 2.3 shows that any smooth compactification of G is étale simply connected, and topologically simply connected over $\mathbb{C}$.

Example 2.5. In the case of $G = \mathrm{PSL}_2(\mathbb{C}) = \mathrm{PGL}_2(\mathbb{C})$, we have that $\overline{G} = \mathbb{P}(M_2(\mathbb{C})) = \mathbb{C}P^3$ where $M_2(\mathbb{C})$ is the monoid of 2×2 complex matrices. Naturally $\mathrm{PSL}_2(\mathbb{C}) \subset \mathbb{P}(M_2(\mathbb{C}))$ and the action of $\mathrm{PSL}_2(\mathbb{C}) \times \mathrm{PSL}_2(\mathbb{C})$ on $\mathrm{PSL}_2(\mathbb{C})$ defined by $(g_1, g_2)\cdot x = g_1 x g_2^{-1}$ extends to an action on $\mathbb{P}(M_2(\mathbb{C}))$. The complement $D = \mathbb{P}(M_2(\mathbb{C})) \setminus \mathrm{PGL}_2(\mathbb{C})$ is the divisor

$$(\{X \in M_2(\mathbb{C}) \mid \det(X) = 0\} \setminus \{\mathbf{0}\})/\mathbb{C}^* = (\{(a, b, c, d) \in \mathbb{C}^4 \mid ad = bc\} \setminus \{\mathbf{0}\})/\mathbb{C}^*$$

which is the image of $\mathbb{C}P^1 \times \mathbb{C}P^1$ under the Segre embedding. In this divisor, the locus of $a \neq 0$ is an affine open $\mathbb{C}^2$, and when $a = 0$ we have two copies of $\mathbb{C}P^1$ intersecting at the point $[(0, 0, 0, 1)]$.

3. Wonderful compactification of character varieties

In this section, given a finitely generated group Γ and a semisimple algebraic group G of adjoint type we construct a compactification of the G-character variety of Γ. There is no assumption on the characteristic of the algebraically closed base field $\Bbbk$.

First however we remind the reader of the basic terms and theorems of projective GIT. A G-linearized line bundle over a G-variety X is a line bundle L over X such that the projection map $L \to X$ is G-equivariant, and where the zero section of L is G-invariant. A point $x \in X$ is *semistable* with respect to L if there exists a G-invariant section $s : X \to L^{\otimes m}$ so $s(x) \neq 0$ and the principal open U_s defined by s is affine. If additionally the stabilizer at x is finite and all G-orbits in U_s are closed then x is called *stable*. Any point that is not semistable is called *unstable*. If there exists a basis $\{s_0, \dots, s_n\}$ for the space of sections of L over X such that the map $x \mapsto (s_0(x), \dots, s_n(x))$ is a closed embedding into $\mathbb{P}^n$ then we say L is *very ample*. If $L^{\otimes m}$ is very ample for some positive m, then we say L is *ample*. An algebraic variety X is isomorphic to a quasiprojective variety if and only if there exists an ample line bundle over X. Given a G-linearized line bundle L over X, there always exists a GIT quotient $X^{ss}_L \to X /\!\!/_L G := X^{ss}_L /\!\!/ G$, where X^{ss}_L is the set of semistable points in X. Moreover, $X/\!\!/_L G$ is in general quasiprojective (see [Mumford et al. 1994, Theorem 1.10] or [Dolgachev 2003, Theorem 8.1]) and is projective if X was projective and L was ample to begin with (see [Dolgachev 2003, Proposition 8.1]).

We begin constructing our compactifications with the case of a free group. Let $\Gamma = F_r$ be the free group of rank r (we call the *standard* presentation of F_r the one with no relations). With respect to the standard presentation, the evaluation map gives a bijection $\mathrm{Hom}(F_r, G) \cong G^r$. Therefore, as the adjoint action of G on G extends to $\overline{G}$, the diagonal adjoint action of G on G^r also extends to the product $\overline{G}^r$. Precisely, the action of $g \in G$ sends any $(x_1, \ldots, x_r) \in \overline{G}^r$ to $(gx_1g^{-1}, \ldots, gx_rg^{-1})$. Thus, $\mathrm{Hom}(F_r, G)$ is an affine Zariski open G-invariant subset of the G-variety $\overline{G}^r$; that is, $\overline{G}^r$ is a compactification of $\mathrm{Hom}(F_r, G)$.

With respect to an ample line bundle L, the GIT quotient $\overline{G}^r/\!\!/_L G$ is a projective variety. We claim there is a line bundle that makes it a compactification of $\mathfrak{X}_{F_r}(G)$.

To establish this we prove a lemma that will also be relevant in Section 5, where we discuss divisors.

Lemma 3.1. *Let G be a semisimple algebraic group of adjoint type, and let $\overline{G}$ be the wonderful compactification of G. Then there is an ample line bundle L on $\overline{G}$ so the divisors $\overline{G} \setminus G$ are the zero locus of a $G \times G$-invariant section of L.*

Proof. We follow the discussion in Section 3 of [De Concini et al. 2008], making some slight notational changes.

Let H be a semisimple adjoint-type algebraic group over a field $\Bbbk$ of arbitrary characteristic (not equal to 2) and let $\widetilde{H}$ be a simply-connected cover of H. Let $\iota : \widetilde{H} \to H$ be the corresponding central isogeny. Let σ be an involution of H and let $K = \iota^{-1}(H^\sigma)$, where H^σ is the fixed locus of σ. Define $X := \widetilde{H}/K$; a *symmetric variety*. In [De Concini and Procesi 1983; De Concini and Springer 1999], a compactification of X, denoted $\overline{X}$, is constructed called the *wonderful compactification*. It is a compactification of X that is a $\widetilde{H}$-wonderful variety in the sense of Luna [2001].

As noted in Remark 2.2, we can think of $\overline{G}$ as an example of the wonderful compactification of a symmetric variety where $\widetilde{H} = \widetilde{G} \times \widetilde{G}$, σ is the involution $(a, b) \mapsto (b, a)$, $H^\sigma = G_\Delta$, and K is the inverse image of G_Δ by the central isogeny $\iota : \widetilde{G} \times \widetilde{G} \to G \times G$. Then $\widetilde{H}/K = (\widetilde{G} \times \widetilde{G})/\iota^{-1}(G_\Delta) \cong (G \times G)/G_\Delta \cong G$.

Returning to the more general setting, let S be a maximal torus in $\widetilde{H}$ such that $\sigma(s) = s^{-1}$ for all $s \in S$. Denote $\Lambda_A = \mathrm{Hom}(A, \Bbbk^*)$ for any abelian group A, and let $S_K = S/(S \cap K)$. In [De Concini et al. 2008, Sections 2.2 and 3.1], the authors construct a basis for Λ_{S_K} consisting of *simple restricted roots* $\tilde{\Delta} = \{\tilde{\alpha}_1, \ldots, \tilde{\alpha}_\ell\}$, where ℓ is the dimension of S. Let $\Delta_{\overline{X}}$ be the irreducible components of codimension 1 in $\overline{X} \setminus X$ (i.e., the divisors). They show (Theorem 3.2 of the same work) that there is a bijection between $\Delta_{\overline{X}}$ and $\tilde{\Delta}$ given by $D \mapsto j(\mathcal{O}(D))$, where $j : \mathrm{Pic}(\overline{X}) \to \Lambda_{S_K}$ is a monomorphism and $\mathcal{O}(D)$ is the line bundle over $\overline{X}$ with section whose zero locus is D. This correspondence extends to a bijection between subsets $\Gamma \subset \tilde{\Delta}$ and the set of $\widetilde{H}$-orbit closures defined by $X_\Gamma := \bigcap_{\{D \mid j(\mathcal{O}(D)) \in \Gamma\}} D$.

From this, for each $\tilde{\alpha} \in \tilde{\Delta}$ there is a line bundle $\mathcal{L}_{\tilde{\alpha}}$ over $\overline{X}$ and an $\widetilde{H}$-invariant section $s_{\tilde{\alpha}}$ of $\mathcal{L}_{\tilde{\alpha}}$ whose divisor is $X_{\tilde{\alpha}}$. In our setting, $\overline{G}$ and each of its divisors are embedded in a Grassmannian, and so we may take $\mathcal{L}_{\tilde{\alpha}}$ to be ample. Therefore, $\mathcal{L}_{\tilde{\alpha}_1} \otimes \cdots \otimes \mathcal{L}_{\tilde{\alpha}_\ell}$ is an ample line bundle over $\overline{X}$ whose section $s_{\tilde{\alpha}_1} \otimes \cdots \otimes s_{\tilde{\alpha}_\ell}$ is $\widetilde{H}$-invariant and whose nonzero locus is exactly X.

Therefore, the same holds for the special case when $\overline{X} = \overline{G}$. We note that the $\widetilde{G} \times \widetilde{G}$-action on $\overline{G}$ factors through the $G \times G$-action we consider given the isomorphism $(\widetilde{G} \times \widetilde{G})/\iota^{-1}(G_\Delta) \cong (G \times G)/G_\Delta$. □

Theorem 3.2. *There exists an ample line bundle $\mathcal{L}$ on $\overline{G}^r$ so that $\overline{G}^r /\!\!/_{\mathcal{L}} G$ is a compactification of $\mathfrak{X}_{F_r}(G)$.*

Proof. Let L be the line bundle on $\overline{G}$ and s the invariant section from Lemma 3.1. Then $\mathcal{L} := L^{\boxtimes r}$ is an ample line bundle on $\overline{G}^r$ with a $G \times G$-invariant section $s^{\boxtimes r}$ whose nonvanishing locus is G^r. Therefore the GIT quotient $\overline{G}^r /\!\!/_{\mathcal{L}} G$, which is a projective variety, is a compactification of $\mathfrak{X}_{F_r}(G)$. □

Remark 3.3. As in [He and Starr 2011], which concerned the case of $r = 1$, we suspect the above construction is independent of $\mathcal{L}$. Regardless, we will always use the line bundle $\mathcal{L}$ in our constructions, even if the notation is suppressed.

Now let Γ be a finitely generated group, say with r generators. Fixing r generators, there is a surjection $\varphi : F_r \to \Gamma$ that induces an inclusion $\varphi_\# : \mathfrak{X}_\Gamma(G) \hookrightarrow \mathfrak{X}_{F_r}(G)$.

Definition 3.4. The *wonderful compactification of* $\mathfrak{X}_\Gamma(G)$ is the closure of $\mathfrak{X}_\Gamma(G)$ in $\overline{G}^r /\!\!/_{\mathcal{L}} G$ with respect to the above inclusion $\varphi_\#$. This compactification will be denoted by $\overline{\mathfrak{X}_\Gamma(G)}$.

Up to isomorphism $\mathfrak{X}_\Gamma(G)$ does not depend on $\varphi_\#$, however the compactification $\overline{\mathfrak{X}_\Gamma(G)}$ does depend on the choice of φ; see [Martin 2011] for example. In other words, since a presentation of Γ is equivalent to φ, the compactification depends on a choice of a presentation for Γ.

It would be interesting to explore how different presentations of Γ change the geometry of the resulting divisors (the Zariski open subvariety $\mathfrak{X}_\Gamma(G)$ does not change up to isomorphism).

With that said, it is perhaps surprising that some of our theorems concerning $\overline{\mathfrak{X}_\Gamma(G)}$ do not depend on the presentation of Γ. Because of this, we will not always specify the presentation of Γ in the statement of our theorems.

Theorem 3.5. *With respect to the standard presentation of F_r, the wonderful compactification $\overline{\mathfrak{X}_{F_r}(G)}$ is normal and étale simply connected. When $\Bbbk = \mathbb{C}$ it is topologically simply connected.*

Proof. Since the GIT quotient of a smooth variety is normal, and $\overline{G}^r$ is smooth, it follows that $\overline{\mathfrak{X}_{F_r}(G)} \cong \overline{G}^r /\!\!/_{\mathcal{L}} G$ is normal.

The quotient map $\overline{G}^r \to \overline{G}^r /\!\!/_{\mathcal{L}} G$ induces an isomorphism of étale fundamental groups (and topological fundamental groups when $\Bbbk = \mathbb{C}$) by [Biswas et al. 2015a, Theorem 1]. From Corollary 2.3 we know that $\overline{G}$ is étale simply connected and therefore the product $\overline{G}^r$ is also étale simply connected. Consequently, $\overline{\mathfrak{X}_{F_r}(G)} \cong \overline{G}^r /\!\!/_{\mathcal{L}} G$ is étale simply connected.

If $\Bbbk = \mathbb{C}$, then $\overline{G}^r$ is topologically simply connected by Corollary 2.3. Hence $\overline{\mathfrak{X}_{F_r}(G)}$ is topologically simply connected when $\Bbbk = \mathbb{C}$. □

Example 3.6. By [He and Starr 2011, Theorem 0.7], in arbitrary characteristic $\overline{\mathfrak{X}_{F_1}(G)} \cong \overline{T} /\!\!/ W$, where $\overline{T}$ is the closure of a maximal torus $T \subset G$ in $\overline{G}$, $W \subset G$ is the Weyl group, and the quotient is independent of the line bundle.

Example 3.7. Let $\mathcal{K} := \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}$ be the Klein 4-group. Consider

$$\mathfrak{X}_{F_2}(\mathrm{PSL}_2(\mathbb{C})) \cong \mathfrak{X}_{F_2}(\mathrm{SL}_2(\mathbb{C})) /\!\!/ \mathcal{K}.$$

By [Sikora 2015],

$$\mathfrak{X}_{F_2}(\mathrm{PSL}_2(\mathbb{C})) \cong \mathbb{C}^3 /\!\!/ \mathcal{K} \cong \mathrm{Spec}(\mathbb{C}[g_1, g_2, g_3, g_4]/(g_1 g_2 g_3 - g_4^2)),$$

where

$$\mathfrak{X}_{F_2}(\mathrm{SL}_2(\mathbb{C})) \cong \{(\mathrm{tr}(A), \mathrm{tr}(B), \mathrm{tr}(AB)) \mid A, B \in \mathrm{SL}_2(\mathbb{C})\} \cong \mathbb{C}^3,$$

and g_1 corresponds to $\mathrm{tr}(A)^2$, g_2 to $\mathrm{tr}(B)^2$, g_3 to $\mathrm{tr}(AB)^2$, and g_4 to $\mathrm{tr}(A)\mathrm{tr}(B)\mathrm{tr}(AB)$. Given Example 2.5, $\overline{\mathfrak{X}_{F_2}(\mathrm{PSL}_2(\mathbb{C}))} \cong (\mathbb{C}P^3 \times \mathbb{C}P^3) /\!\!/_{\mathcal{L}} \mathrm{PSL}_2(\mathbb{C})$.

Remark 3.8. In [Florentino and Lawton 2013, Theorem 3.4] it is shown that to each connected quiver Q and connected reductive complex algebraic group G, there is an algebraic variety $\mathcal{M}_Q(G)$ isomorphic to $\mathfrak{X}_{F_r}(G)$, where r is the first Betti number of Q. In [Manon 2015, Theorem 1.1] it is shown, in the case where G is simple and simply connected, that each such $\mathcal{M}_Q(G)$ determines a generally distinct compactification of $\mathfrak{X}_{F_r}(G)$. When Q has exactly one vertex the compactification in [Manon 2015] reduces to the GIT quotient of a product of compactifications of G, similar to the construction considered here for $\Gamma = F_r$. Now the compactification of the group G considered in [Manon 2015] comes from its so-called Rees algebra. As shown in [Kaveh and Manon 2019, Example 8.1], this compactification of G coincides with the wonderful compactification of G. Therefore, our construction is a special case of the construction in [Manon 2015] in the overlapping situation when Γ is free, and G is a simple, simply connected, complex algebraic group of adjoint type (exactly if G is one of G_2, F_4, or E_8; see [Hu 2013] for example).

Remark 3.9. In [Senthamarai Kannan 1999, Remark 4.6] it is shown that there is a natural isomorphism $\overline{G}^r \to \overline{G^r}$. For any semisimple algebraic group H of adjoint type over an algebraically closed field, Lusztig [2004a; 2004b] introduced a partition of $\overline{H}$ into finitely many H-stable pieces (where H acts by conjugation). Applied to the group $H = G^r \cong \mathrm{Hom}(F_r, G)$, this gives a partition of $\overline{G^r} \cong \overline{G}^r$ into G^r-stable pieces, which are automatically stable under the diagonal conjugation action of the diagonal subgroup $G \cong G_\Delta \subset G^r$. The closures of these G^r-stable pieces were investigated by He [2007]. It would be interesting to understand the images of these sets in $\overline{\mathfrak{X}_{F_r}(G)}$.

4. Simply connected compactifications over $\mathbb{C}$

In this section we work over $\mathbb{C}$, and argue that in some cases we can normalize the wonderful compactification of $\mathfrak{X}_\Gamma(G)$ and obtain simply connected compactifications of character varieties when Γ is not free.

We need the following standard result; see [Arapura et al. 2016].

Proposition 4.1. *If Z is a normal projective variety, and $A \subsetneq Z$ is a closed subvariety, then the natural homomorphism $\pi_1(Z \setminus A) \to \pi_1(Z)$ is surjective.*

Corollary 4.2. *Let G be a semisimple algebraic group of adjoint type over $\mathbb{C}$, and let Γ be either a finitely generated free or free abelian group of rank r, or the fundamental group of a closed, orientable surface. If $\overline{\mathfrak{X}_\Gamma(G)}$ is a normal compactification of $\mathfrak{X}_\Gamma(G)$, then $\overline{\mathfrak{X}_\Gamma(G)}$ is simply connected. Consequently, $\overline{\mathfrak{X}_\Gamma(G)}$ is also étale simply connected.*

Proof. For the allowed G and Γ, it is shown in [Biswas and Lawton 2015; Biswas et al. 2015b] that $\pi_1(\mathfrak{X}_\Gamma(G)) = 1$. The result now follows from Proposition 4.1. □

The following two lemmas are standard.

Lemma 4.3. *If $A \subset Z$ is a nonempty Zariski open normal subset of an irreducible projective variety Z, then the normalization $\widetilde{Z}$ of Z contains an open subset isomorphic to A. In particular, $\widetilde{Z}$ is still a compactification of A.*

Lemma 4.4. *Let X and Y be normal varieties over an algebraically closed field $\Bbbk$. Then $X \times Y$ is also normal.*

With the above lemmas and corollary in mind, we define the normalized wonderful compactification of a normal character variety $\mathfrak{X}_\Gamma(G)$ to be the normalization of $\overline{\mathfrak{X}_\Gamma(G)}$.

Proposition 4.5. *Let $\mathfrak{X}^0_\Gamma(G)$ denote the component of $\mathfrak{X}_\Gamma(G)$ that contains the trivial representation. In the following cases, the normalized wonderful compactification of $\mathfrak{X}^0_\Gamma(G)$ is a simply connected compactification of $\mathfrak{X}^0_\Gamma(G)$ independent of the presentation of* Γ:

(1) $\Gamma = \mathbb{Z}^r$ *and G is any semisimple algebraic adjoint group with no exceptional factors*;

(2) $\Gamma = \pi_1(\Sigma)$, *with Σ a closed orientable surface*, *and* $G = \mathrm{PGL}_n$.

Proof. We will show that in both these cases, the character variety $\mathfrak{X}_\Gamma(G)$ is normal. The result will then follow from Corollary 4.2 and Lemma 4.3.

When $G = \mathrm{SL}_n, \mathrm{GL}_n$, SO_n, or Sp_{2n}, Sikora [2014, Theorem 2.1] has shown that $\mathfrak{X}^0_{\mathbb{Z}^r}(G)$ is normal. Now since the left action of the center of G, denoted $Z(G)$, commutes with the conjugation action of G on $\mathrm{Hom}(\mathbb{Z}^r, G)$, we conclude $\mathfrak{X}_{\mathbb{Z}^r}(G/Z(G)) \cong \mathfrak{X}_{\mathbb{Z}^r}(G)/Z(G)^r$. In view of this, since normality is preserved under GIT quotients $\mathfrak{X}_{\mathbb{Z}^r}(G)$ is likewise normal for $G = \mathrm{PSL}_n \cong \mathrm{PGL}_n$, PSO_n, or PSp_{2n}.

Now let G be a semisimple algebraic adjoint group with no exceptional factors. Then $G \cong G_1 \times \cdots \times G_n$, where each G_i is isomorphic to a simple algebraic adjoint group of type $A_n,\ B_n,\ C_n,\ D_n$. By Lemma 4.4 and the previous paragraph $\mathfrak{X}_{\mathbb{Z}^r}(G_1 \times \cdots \times G_n) \cong \mathfrak{X}_{\mathbb{Z}^r}(G_1) \times \cdots \times \mathfrak{X}_{\mathbb{Z}^r}(G_n)$ is normal.

In the second case, Simpson [1994a; 1994b] has shown that $\mathrm{Hom}(\pi_1(\Sigma), \mathrm{GL}_n)$ is a normal variety. The group $\mathcal{Z} = \mathrm{Hom}(\pi_1(\Sigma), Z(\mathrm{GL}_n))$, which is isomorphic to $\mathbb{G}_m^{b_1(\Sigma)}$, acts on $\mathrm{Hom}(\pi_1(\Sigma), \mathrm{GL}_n)$ by left multiplication, and we have

$$\mathrm{Hom}(\pi_1\Sigma, \mathrm{GL}_n)/\!\!/\mathcal{Z} \cong \mathrm{Hom}^0(\pi_1(\Sigma), \mathrm{PGL}_n),$$

where the right-hand side denotes the identity component. Since the GIT quotient of a normal variety is normal, we find $\mathrm{Hom}^0(\pi_1(\Sigma), \mathrm{PGL}_n)$, and consequently $\mathfrak{X}^0_{\pi_1(\Sigma)}(\mathrm{PGL}_n)$, are normal. □

We have conjectured that for certain groups Γ whose abelianization is free abelian (which we call *exponent canceling groups*), that $\mathfrak{X}^0_\Gamma(G)$ is simply connected; see [Biswas et al. 2015b, Conjecture 2.7]. We also expect that $\mathfrak{X}^0_\Gamma(G)$ is normal in these cases. Consequently, we now make:

Conjecture 4.6. *The normalized wonderful compactification of $\mathfrak{X}^0_\Gamma(G)$ is a simply connected compactification of $\mathfrak{X}^0_\Gamma(G)$ for all exponent canceling Γ and any semisimple adjoint type complex algebraic group G.*

5. Boundary divisors

In this section we continue to work over $\mathbb{C}$. Given a complex projective variety X with a distinguished dense open affine subvariety $A \subset X$, we will use the term *boundary divisor* to refer to hypersurfaces of X (that is, irreducible codimension 1 subvarieties) contained in $X \setminus A$. By Theorem 2.1, the complement $\overline{G} \setminus G$ is a union of $r = \operatorname{rank}(G)$ smooth boundary divisors, and each of these divisors is the closure of a $G \times G$-orbit.

Now let D_i be a boundary divisor of $\overline{G}$. Then there exist

$$\mathfrak{m}_{I_1}, \ldots, \mathfrak{m}_{I_{m_i}} \in \operatorname{Gr}(n, \mathfrak{g} \times \mathfrak{g}),$$

where each $I_j \subset \{1, \ldots, r\}$, so that

$$D_i = \bigcup_j (G \times G) \cdot \mathfrak{m}_{I_j} \cong \bigcup_j (G \times G)/\operatorname{Stab}(\mathfrak{m}_{I_j}).$$

In particular, each boundary divisor is isomorphic to a union of homogeneous spaces, each a quotient by a closed subgroup (since stabilizers of algebraic group actions are always algebraic subgroups).

Given a surjective, continuous map $q : X \to Y$, we say that $A \subset X$ is saturated with respect to q if $A = q^{-1}(q(A))$.

Lemma 5.1. *Let V be an affine G-variety and W a compactification of V on which the G-action extends. Let L be an ample line bundle with a G-invariant section whose nonzero locus is exactly V. Assume that each boundary divisor of W is saturated with respect to the GIT quotient map $W \to W /\!\!/_L G$. Then the boundary divisors of $W /\!\!/_L G$, with respect to the open subvariety $V /\!\!/ G$, are exactly the components of $(W \setminus V) /\!\!/_L G$.*

Proof. As the G-action extends to W, we see that V is a G-stable affine open subset of W, and the boundary divisors in $W \setminus V$ are unions of G-orbits. The usual gluing construction for the GIT quotient (see [Dolgachev 2003, Section 8.2]) shows that $V /\!\!/ G$ is an affine open subvariety in $W /\!\!/_L G$. Since the boundary divisors in $W \setminus V$ are saturated, $W \setminus V$ is itself saturated, so we find that $(W /\!\!/_L G) \setminus (V /\!\!/ G)$ is exactly $\left(\bigcup_i D_i\right) /\!\!/_L G$ where the D_i's are the boundary divisors in $W \setminus V$. □

In [Biswas et al. 2014] parabolic character varieties of free groups are defined and studied. We recall their definition. Let G be a complex reductive group, and let $G_1, \ldots, G_m$ be closed subgroups. Then G acts on the product

$$G^n \times \prod_{1 \le j \le m} G/G_j$$

by

$$g \cdot (h_1, \ldots, h_n, g_1 G_1, \ldots, g_m G_m) = (g h_1 g^{-1}, \ldots, g h_n g^{-1}, g g_1 G_1, \ldots, g g_m G_m).$$

The quotient $(G^n \times \prod_{1 \le j \le m} G/G_j) /\!\!/ G$ is the parabolic character variety of the free group of rank n with parabolic data $\{G/G_j\}_{j=1}^m$. We note that when the G_i's are reductive, as assumed in [Biswas et al. 2014], the homogeneous spaces G/G_i are affine, and when the G_i's are parabolic, the homogeneous spaces G/G_i are projective. In general, the homogeneous spaces G/G_i are quasiprojective [Borel 1991, Theorem 6.8].

Theorem 5.2. *The boundary divisors in $\overline{G}^r /\!\!/_{\mathcal{L}} G$ are unions of parabolic character varieties of free groups.*

Proof. As noted above the boundary divisors in $\overline{G}$ are unions of homogeneous spaces of $G \times G$, and by Theorem 2.1 each boundary divisor is the closure of a single $G \times G$-orbit. Therefore, $\overline{G}^r \setminus G^r$ consists of unions of products of $G \times G$-homogeneous spaces. Since the conjugation action is a restriction of the $G \times G$-action and by Lemma 3.1 there exists a $G \times G$-equivariant section s to $\mathcal{L}$ such that G^r is the nonvanishing locus of s, the boundary divisors of $\overline{G}^r$ are saturated with respect to the GIT quotient map for the conjugation action. The action of conjugation on an orbit corresponds, under the isomorphism between the orbit and the corresponding homogeneous space, to the left action on the homogeneous space. Thus, by Lemma 5.1 and the definition of parabolic character variety of free groups, the result follows. □

Remark 5.3. As shown in [Esposito 2012], the closure of an orbit in $\overline{G}$ under the conjugation action need not be a finite union of suborbits. Therefore, the boundary divisors in Theorem 5.2 need not be finite unions of parabolic character varieties.

Example 5.4. In Example 2.5 we see that the sole boundary divisor of the wonderful compactification of $\mathrm{PSL}_2(\mathbb{C})$ is isomorphic to $\mathbb{C}P^1 \times \mathbb{C}P^1$, a product of homogeneous spaces. Therefore, in Example 3.7, given Theorem 5.2, we have that $\overline{\mathfrak{X}_{F_2}(\mathrm{PSL}_2(\mathbb{C}))} \setminus \mathfrak{X}_{F_2}(\mathrm{PSL}_2(\mathbb{C}))$ consists of GIT quotients of the diagonal left multiplication action of $\mathrm{PSL}_2(\mathbb{C})$ on products of $\mathbb{C}P^1 \times \mathbb{C}P^1$. This is an example of a parabolic character variety as it is a left diagonal quotient of a product of homogeneous spaces.

It would be interesting to work out more examples (especially when Γ is not free), or the above examples in more detail. We leave this to future work.

6. Poisson structures

Recall that a Poisson algebra is a Lie algebra in which the Lie bracket is also a derivation in each variable. We call a quasiprojective variety X over $\mathbb{C}$ a Poisson variety if the sheaf of regular functions on X, denoted $\mathcal{O}(X)$, is equipped with the structure of a sheaf of Poisson algebras. In this case, the sheaf of *holomorphic* functions on X^{sm} (where X^{sm} is the smooth locus of X) becomes a sheaf of Poisson algebras as well, making X^{sm} a complex Poisson manifold.

The Poisson bracket on the algebra of holomorphic functions $\mathcal{O}(X^{\mathrm{sm}})$ is induced by an exterior bivector field $\Lambda \in \Lambda^2(T^{1,0}X^{\mathrm{sm}})$, see for instance [Polishchuk 1997].

In other words, if $f, g \in \mathcal{O}(X^{\mathrm{sm}})$, then the bracket is given by $\{f, g\} = \Lambda(df, dg)$. In local (complex) coordinates $(z_1, \ldots, z_k)$ the bivector takes the form

$$\Lambda = \sum_{i,j} \Lambda_{i,j} \frac{\partial}{\partial z_i} \wedge \frac{\partial}{\partial z_j}$$

and so

$$\begin{aligned} \{f, g\} &= \sum_{i,j} \left(\Lambda_{i,j} \frac{\partial}{\partial z_i} \wedge \frac{\partial}{\partial z_j} \right) \cdot \left(\frac{\partial f}{\partial z_i} dz_i \otimes \frac{\partial g}{\partial z_j} dz_j \right) \\ &= \sum_{i,j} \Lambda_{i,j} \left(\frac{\partial f}{\partial z_i} \frac{\partial g}{\partial z_j} - \frac{\partial f}{\partial z_j} \frac{\partial g}{\partial z_i} \right). \end{aligned} \tag{6-1}$$

In general, complex Poisson manifolds admit (2, 0)-symplectic foliations; see [Laurent-Gengoux et al. 2013]. For $f, g \in \mathcal{O}(X^{\mathrm{sm}})$, the Hamiltonian vector field H_f associated to f is defined by $H_f(g) = \{f, g\}$. Restricting the bivector Λ to symplectic leaves gives the symplectic form $\omega(H_g, H_f) = \{f, g\}$.

For the rest of the section, G will denote a semisimple algebraic group of adjoint type over $\mathbb{C}$, with Lie algebra $\mathfrak{g}$. Let $\langle\langle\ ,\ \rangle\rangle$ denote the Killing form on $\mathfrak{g}$. Following [Evens and Lu 2006], we give the *double* $\mathfrak{d} := \mathfrak{g} \oplus \mathfrak{g}$ the symmetric, nondegenerate, and Ad-invariant bilinear form

$$\langle (x_1, x_2), (y_1, y_2) \rangle = \langle\langle x_1, y_1 \rangle\rangle - \langle\langle x_2, y_2 \rangle\rangle. \tag{6-2}$$

A Lie subalgebra $\mathfrak{l} \subset \mathfrak{d}$ is said to be *Lagrangian* if $\mathfrak{l}$ is maximal isotropic with respect to the form (6-2). In other words, $\mathfrak{l}$ is Lagrangian if $\dim_{\mathbb{C}} \mathfrak{l} = \dim_{\mathbb{C}} \mathfrak{g}$ and $\langle x, y \rangle = 0$ for all $x, y \in \mathfrak{l}$.

A *Lagrangian splitting* of $\mathfrak{d} = \mathfrak{g} \oplus \mathfrak{g}$ is a vector space decomposition $\mathfrak{d} = \mathfrak{l}_1 + \mathfrak{l}_2$ in which both $\mathfrak{l}_1$ and $\mathfrak{l}_2$ are Lagrangian (note that it is not assumed that $\mathfrak{d}$ is isomorphic to $\mathfrak{l}_1 \oplus \mathfrak{l}_2$ as Lie algebras). It will be helpful to observe that the form (6-2) yields an isomorphism $\mathfrak{l}_2 \xrightarrow{\cong} (\mathfrak{l}_1)^*$. It is clear that the diagonal Lie subalgebra $\mathfrak{g}_\Delta = \{(x, y) \in \mathfrak{d} \mid x = y\}$ is Lagrangian in $\mathfrak{d}$. A *Belavin–Drinfeld splitting*, or just BD splitting, is a Lagrangian splitting $\mathfrak{d} = \mathfrak{l}_1 + \mathfrak{l}_2$ where $\mathfrak{l}_1 = \mathfrak{g}_\Delta$. In [Evens and Lu 2006, Example 4.4] BD splittings are classified via [Belavin and Drinfeld 1998]. There is always at least one such splitting, namely the *standard Lagrangian splitting* $\mathfrak{l}_2 \subset \mathfrak{b} \oplus \mathfrak{b}^-$ where $\mathfrak{b}, \mathfrak{b}^-$ are opposite Borel subalgebras of $\mathfrak{g}$ (see [Evens and Lu 2006] for details).

Evens and Lu [2001; 2006] show that each Lagrangian splitting of $\mathfrak{d}$ endows $\overline{G}$ with a Poisson structure. Moreover, they show that each of these Poisson structures restricts to a Poisson structure on each $(G \times G)$-orbit, and hence to each boundary divisor in $\overline{G}$. We now review this construction.

For a complex manifold M, a bracket on the ring of holomorphic functions is a Poisson bracket if and only if the associated bivector Λ satisfies $[\Lambda, \Lambda] = 0$, where $[\Lambda, \Lambda] \in \Lambda^3(T^{1,0}M)$ is the Schouten bracket of Λ with itself; see [Dufour and Zung 2005, Theorem 1.8.5]. We will say that Λ is a Poisson bivector when $[\Lambda, \Lambda] = 0$. To simplify notation, given a holomorphic map $f : M \to N$ of complex manifolds, we write f_* to denote both the derivative Df of f and the maps on higher-order tensor fields induced by Df.

Let $\mathcal{L}_{\mathfrak{d}} \subset \mathrm{Gr}(n, \mathfrak{d})$ be the space of Lagrangians in $\mathfrak{d} = \mathfrak{g} \oplus \mathfrak{g}$. Clearly $\mathcal{L}_{\mathfrak{d}}$ is a subvariety of the Grassmannian $\mathrm{Gr}(n, \mathfrak{d})$. Following the construction in [Evens and Lu 2001; 2006], the Evens–Lu bivector Λ on $\mathcal{L}_{\mathfrak{d}}$ is defined by choosing a basis $\{x_i\}_i$ for $\mathfrak{l}_1$, and letting $\{y_i\}$ be the dual basis for $\mathfrak{l}_2 \cong \mathfrak{l}_1^*$ (that is, $\{y_i\}$ is the basis satisfying $\langle x_i, \xi_j\rangle = \delta_{ij}$). Now define

$$r = \tfrac{1}{2}\sum_i x_i \wedge y_i \in \Lambda^2(\mathfrak{g} \oplus \mathfrak{g})$$

and

$$\Lambda_{\mathfrak{l}} = (\rho_{\mathfrak{l}})_*(r) = \tfrac{1}{2}\sum_i (\rho_{\mathfrak{l}})_*(x_i) \wedge (\rho_{\mathfrak{l}})_*(y_i) \in \Lambda^2(T_{\mathfrak{l}}\mathcal{L}_{\mathfrak{d}}),$$

where $\rho_{\mathfrak{l}}$ is defined below. We note $\Lambda_{\mathfrak{l}}$ is independent of the choice of basis $\{x_i\}_i$: for instance, using the form (6-2), we may view $r = \frac{1}{2}\sum_i x_i \wedge y_i$ as an element of $(\Lambda^2\mathfrak{d})^*$, and evaluating r on an element $(v_1, f_1) \wedge (v_2, f_2) \in \Lambda^2(\mathfrak{l}_1 \oplus \mathfrak{l}_1^*) \cong \Lambda^2(\mathfrak{d})$ gives $f_1(v_2) - f_2(v_2)$, as can be checked on the basis for $\Lambda^2(\mathfrak{l}_1 \oplus \mathfrak{l}_1^*)$ constructed from $\{x_i\}_i$.

As discussed in [Evens and Lu 2006, Examples 4.3 and 4.4], this bivector induces a Poisson structure on $\mathcal{L}_{\mathfrak{d}}$ and on each $G \times G$ orbit in $\mathcal{L}_{\mathfrak{d}}$, as well as on the closure of each orbit. In particular, Λ induces a Poisson structure on $\overline{G}$, which is the closure of the orbit $(G \times G) \cdot \mathfrak{g}_\Delta$ of the diagonal $\mathfrak{g}_\Delta \in \mathcal{L}_{\mathfrak{d}}$.

Our next goal is to understand how the Evens–Lu Poisson structure interacts with the action of $G \times G$ on $\overline{G}$, which is induced by the inclusion

$$G \times G \hookrightarrow \mathrm{Aut}(\mathfrak{g}) \times \mathrm{Aut}(\mathfrak{g}) \subset \mathrm{Aut}(\mathfrak{g} \oplus \mathfrak{g}).$$

We recall some terminology regarding Poisson Lie groups and Poisson actions. Let M_1 and M_2 be two Poisson varieties. A morphism $M_1 \to M_2$ is called a *Poisson morphism* (or ichthyomorphism) if the dual morphism $\mathcal{O}(M_2) \to \mathcal{O}(M_1)$ is a morphism of Poisson sheaves. A Poisson algebraic group is an algebraic group G, equipped with a Poisson structure for which the group multiplication $G \times G \to G$ is a Poisson map. The action of a Poisson algebraic group G on a Poisson variety M is a *Poisson action* when the action map $\alpha : G \times M \to M$ is a Poisson map, where $G \times M$ has the product Poisson structure (defined by the sum of bivectors).

We introduce some notation that will be needed in the next lemma. Consider the (left) action of $G \times G$ on $\mathcal{L}_{\mathfrak{d}}$. For each $\mathfrak{l} \in \mathcal{L}_{\mathfrak{d}}$, let

$$\rho_{\mathfrak{l}} : G \times G \to \mathcal{L}_{\mathfrak{d}}$$

be the map

$$\rho_{\mathfrak{l}}(g, h) = (g, h) \cdot \mathfrak{l}.$$

For each $(g,h) \in G \times G$, let

$$\rho_{(g,h)} : \mathcal{L}_{\mathfrak{d}} \to \mathcal{L}_{\mathfrak{d}}$$

be the map

$$\rho_{(g,h)} = (g,h) \cdot \mathfrak{l},$$

and let

$$\mu^R_{(g,h)} : G \times G \to G \times G \quad \text{and} \quad \mu^L_{(g,h)} : G \times G \to G \times G$$

be the maps given by right- and left-multiplication by (g,h) (respectively).

Define the BD-bivector on $G \times G$ associated to the data $\{x_i\}_i$, $\{y_i\}_i$ by

$$\Pi_{(h,k)} = \tfrac{1}{2} \sum_i \big[(\mu^R_{(h,k)})_*(x_i \wedge y_i) - (\mu^L_{(h,k)})_*(x_i \wedge y_i)\big]. \tag{6-3}$$

Similar to the discussion of the Evens–Lu bivector, the BD-bivector is independent of the choice of basis and so only depends on the BD splitting.

We will need the following standard fact.

Lemma 6.1. *The bivector Π is Poisson, and induces a Poisson–Lie group structure on $G \times G$ called the BD–Poisson structure.*

This fact is discussed in various places in the literature. As discussed in [Lu and Mouquin 2017, Section 2], the element $\frac{1}{2} \sum_i x_i \otimes y_i \in \mathfrak{d} \otimes \mathfrak{d}$ is a *quasitriangular r-matrix*, and a quasitriangular r-matrix always induces a Poisson Lie group structure via the construction (6-3); see [Kosmann-Schwarzbach 1997, pp. 46–47]. Another discussion of this fact can be found in [Korogodski and Soibelman 1998, Proposition 3.4.1].

The next lemma is a version of Proposition 2.17 in [Evens and Lu 2001].

Lemma 6.2. *For any BD-splitting of $\mathfrak{g} \oplus \mathfrak{g}$, the action of $G \times G$ on $\mathcal{L}_{\mathfrak{d}}$ is a Poisson action, where $G \times G$ has the BD–Poisson structure and $\mathcal{L}_{\mathfrak{d}}$ has the Evens–Lu Poisson structure.*

Proof. Written in terms of bivectors, the condition for the action to be Poisson is

$$\Lambda_{(g,h)\cdot\mathfrak{l}} = (\rho_{(g,h)})_*(\Lambda_{\mathfrak{l}}) + (\rho_{\mathfrak{l}})_*(\Pi_{(g,h)}) \tag{6-4}$$

(see, for instance, [Dufour and Zung 2005, 5.4.5]).

To prove (6-4), observe that

$$\rho_{(g,h)\cdot\mathfrak{l}} = \rho_{\mathfrak{l}} \circ \mu^R_{(g,h)} \quad \text{and} \quad \rho_{(g,h)} \circ \rho_{\mathfrak{l}} = \rho_{\mathfrak{l}} \circ \mu^L_{(g,h)}.$$

We now have

$$\begin{aligned}
\Lambda_{(g,h)\cdot\mathfrak{l}} - (\rho_{(g,h)})_*(\Lambda_{\mathfrak{l}}) &= (\rho_{(g,h)\cdot\mathfrak{l}})_*(r) - (\rho_{(g,h)})_*((\rho_{\mathfrak{l}})_*(r)) \\
&= (\rho_{\mathfrak{l}})_*((\mu^R_{(g,h)})_*(r)) - (\rho_{\mathfrak{l}})_*((\mu^L_{(g,h)})_*(r)) \\
&= (\rho_{\mathfrak{l}})_*(\Pi_{(g,h)}).
\end{aligned}$$

□

We now turn to the conjugation action of G on $\overline{G}$, which extends the conjugation action of G on itself. Recall that $\overline{G}$ is the closure of $(G\times G)\cdot\mathfrak{g}_\Delta$ inside $\mathcal{L}_{\mathfrak{d}}$. The map

$$G \to (G\times G)\cdot\mathfrak{g}_\Delta$$

defined by $g\mapsto (g,e)\cdot\mathfrak{g}_\Delta$ is a diffeomorphism. If we give G the $G\times G$ action

$$(h,k)\cdot g = hgk^{-1},$$

then this diffeomorphism is $G\times G$-equivariant. In particular, the action of the subgroup $G_\Delta\subset G\times G$ on $\overline{G}$ corresponds, under this diffeomorphism, to the (left) conjugation action of G on itself; $h\cdot g = hgh^{-1}$.

We wish to study the conjugation action of G on $\overline{G}^n$ and its interaction with the Evens–Lu Poisson structure. However, a subtlety arises: if we equip $\overline{G}^n$ and $(G\times G)^n$ with the direct product Poisson structures arising from a BD-splitting of $\mathfrak{d}$, then the action of $(G\times G)^n$ on $\overline{G}^n$ is Poisson, but this does not imply that the action of the diagonal subgroup $\{(g,g,\dots,g)\}\subset (G\times G)^n$ is Poisson, as this diagonal subgroup need not be a Poisson Lie subgroup.

Recent work of Lu and Mouquin [2017] provides a way to avoid this problem by using the *mixed product* Poisson structure on $\overline{G}^n$. We briefly explain the setup, specialized to our situation. Details may be found in Section 6 of the same work. Let G be as above, and equip $D = G\times G$ with the above Poisson structure. Given a Poisson D-space (Z,π_Z), let $\lambda:\mathfrak{d}\to\mathcal{V}^1(Z)$ be the map induced by the action, sending $x\in\mathfrak{d}$ to the vector field $(d/dt)|_{t=0}\exp(tx)y$; see [Lu and Mouquin 2017, Section 1.4].

Lu and Mouquin define the mixed product Poisson bivector on Z^n by the formula

$$\pi_{Z^n} = (\pi_Z,\dots,\pi_Z) + \sum_{1\le j<k\le n}\sum_i (i_j)_*\lambda(y_i)\wedge (i_k)_*(\lambda(x_i)),$$

where $r=\sum_i x_i\otimes y_i$ is the r-matrix defining the Poisson structure on D and $i_l : Z\to Z^n$ is the inclusion into the l-th factor of the product. By [Lu and Mouquin 2017, Theorem 6.8 and Lemma 2.13], the diagonal action of D on (Z^n,π_{Z^n}) is a Poisson action. In particular, letting $Z=\overline{G}$ with $\pi_Z=\Lambda$ (the Evens–Lu Poisson bracket), we find that the diagonal action of D on $(\overline{G}^n,\Lambda_n)$ is Poisson, where Λ_n is the mixed product Poisson structure on $\overline{G}^n$ associated to Λ. The diagonal subgroup $G_\Delta\subset D$ (corresponding to the Lagrangian subalgebra $\mathfrak{g}_\Delta\subset\mathfrak{d}=\mathfrak{g}\oplus\mathfrak{g}$) is a Poisson Lie subgroup of D, as explained (for instance) in [Evens and Lu 2007, Appendix]. Returning to the general setting above, this implies that the diagonal action of D on Z^n restricts to a Poisson action of $G=G_\Delta$ on (Z^n,π_{Z^n}); note that this is precisely the action of G given by the diagonal embedding of G into $D^n=G^{2n}$. In our case, these facts lead to the following result:

Proposition 6.3. *Let G be a semisimple group of adjoint type, and fix a BD-splitting of $\mathfrak{g} \oplus \mathfrak{g}$, with associated quasitriangular r-matrix $r \in \Lambda^2(\mathfrak{g} \oplus \mathfrak{g})$. Equip G with the Poisson structure induced by r, and equip $\overline{G}^n$ with the mixed product Poisson structure associated to the Evens–Lu Poisson structure on $\overline{G}$. Then the diagonal action of G on $\overline{G}^n$ is Poisson, and restricts to the diagonal conjugation action of G on $G^n \subset \overline{G}^n$.*

It is well known that if X is a Poisson manifold and a Lie group G acts on X through Poisson maps, then the G-invariant functions on X form a Poisson algebra; see for instance [Dufour and Zung 2005, p. 24]. The following proposition is a version of this statement.

Proposition 6.4. *Let X be a quasiprojective Poisson variety and let G be a reductive algebraic group that is a Poisson Lie group. If G acts on X and the action map $X \times G \to X$ is Poisson, then with respect to any G-linearized ample line bundle L, the GIT quotient $X/\!\!/_L G$ is a Poisson variety and the quotient map $X \to X/\!\!/_L G$ is a Poisson map.*

Proof. This is a consequence of Property (1) of Lemma 5.4.5 in [Dufour and Zung 2005] which characterizes Poisson actions in terms of bivectors. The explicit statement, in the affine case, is given in [Laurent-Gengoux et al. 2013, Proposition 5.33]. In the quasiprojective case, $X/\!\!/_L G$ is built from open affine subvarieties; see [Dolgachev 2003, Section 8.2], so one can apply the affine case locally. A detailed discussion is provided in the Appendix. □

Theorem 6.5. *There exists a Poisson structure on the wonderful compactification of a free group character variety over $\mathbb{C}$, and also on its boundary divisors.*

Proof. The Poisson structure on $\overline{\mathfrak{X}_{F_r}(G)}$ follows directly from Propositions 6.3 and 6.4.

Since each boundary divisor of $\overline{G}^r$ is a union of products of orbits where each admits a Poisson structure (restricted from that on $\overline{G}$), the same argument as above shows that the Poisson structures on the boundary divisors of $\overline{G}^r$ descend to the boundary divisors of $\overline{\mathfrak{X}_{F_r}(G)}$. □

Since the boundary divisors of $\overline{\mathfrak{X}_{F_r}(G)}$ are unions of parabolic free group character varieties, we immediately conclude:

Corollary 6.6. *There exists a Poisson structure on those parabolic character varieties of free groups that lie inside the boundary divisors of $\overline{\mathfrak{X}_{F_r}(G)}$.*

We call the Poisson structures shown to exist above the *wonderful Poisson structures.*

In [Goldman 1984; 1986] it was shown that there is a Poisson structure on $\mathrm{Hom}(\pi_1(\Sigma_{g,n}), G)/\!\!/G$ where $\Sigma_{g,n}$ is an orientable surface of genus g with n disjoint boundary components; see also [Lawton 2009]. Moreover, the Casimirs (those functions that Poisson commute) are exactly the invariant functions restricted to the boundary components.

Question 6.7. *How does Goldman's Poisson structure on $G^r /\!\!/ G$ relate to the wonderful Poisson structures on $G^r /\!\!/_{\mathcal{L}} G$, and $\overline{G}^r /\!\!/ G$?*

Remark 6.8. Given an affine Poisson variety V, the Poisson bracket $\{\ ,\ \}_V$ is determined by its action on the coordinate ring $\mathbb{C}[V]$ by the Stone–Weierstrass theorem. Suppose V has Casimirs $\{c_1, \dots, c_m\}$. Then the algebra

$$A := \mathbb{C}[V]/(c_1 - \lambda_1, \dots, c_k - \lambda_k),$$

where $\lambda_1, \dots, \lambda_k \in \mathbb{C}$, is a Poisson algebra with bracket defined by $\{f+I, g+I\} = \{f, g\}_V + I$ where I is the ideal $(c_1 - \lambda_1, \dots, c_k - \lambda_k)$. Therefore, the variety $\operatorname{Spec}(A)$ is an affine Poisson variety.

Now applying Remark 6.8 to the setting of parabolic character varieties of free groups we see that whenever the parabolic data $\{G/H_i\}$ are isomorphic to G-conjugation orbits (equivalently H_i's are isomorphic to conjugation stabilizers), then the Goldman Poisson bracket on $G^r /\!\!/ G$ with some set of its Casimirs fixed (fixing some set of the boundaries up to conjugation is equivalent to fixing some set of the Casimirs) determines a Poisson structure on the parabolic character variety of a free group resulting from fixing some (but not all) the boundaries to conjugation orbits. Therefore, we have a Goldman-type Poisson structure on certain parabolic character varieties of free groups.

Question 6.9. *How does this Goldman-type Poisson structure compare to the wonderful Poisson structures from Corollary 6.6?*

Appendix: Poisson structures on GIT quotients by Arlo Caine and Sam Evens

We explain how to put a Poisson structure on a quotient of a linearized irreducible Poisson algebraic variety by the action of a reductive Poisson algebraic group G. We discuss the affine setting, and then we apply the affine case to the general situation.

Quotient of an affine variety. We explain how to put a Poisson structure on the quotient of an affine variety. These results are in [Yang 2002] and in [Laurent-Gengoux et al. 2013].

As above, let (G, π_G) be a reductive Poisson linear algebraic group. Denote the Poisson Lie algebra structure on the coordinate ring $\Bbbk[G]$ by $\{\phi_1, \phi_2\}_G$ for $\phi_1, \phi_2 \in \Bbbk[G]$.

Let $(X, \{\ ,\ \}_X)$ be a Poisson algebraic variety, i.e., $\{\ ,\ \}$ makes the sheaf of regular functions $\mathcal{O}_X$ into a Poisson algebra. Assume that X is a G-variety with action map $a : G \times X \to X$, and denote by $p : G \times X \to X$ the projection $p(g, x) = x$. The sheaf of functions $\mathcal{O}_{G\times X} = \mathcal{O}_G \otimes_{\Bbbk} \mathcal{O}_X$ then acquires the structure of a Poisson Lie algebra, which is uniquely determined by the property (see [Korogodski and Soibelman 1998], Proposition 1.2.10, p. 9):

$$(*)\quad \{\phi_1 \otimes f_1, \phi_2 \otimes f_2\} = \{\phi_1, \phi_2\}_G \otimes f_1 f_2 + \phi_1\phi_2 \otimes \{f_1, f_2\}_X, \qquad \phi_i \in \mathcal{O}_G,\ f_i \in \mathcal{O}_X.$$

Suppose for the remainder of this subsection that X is affine, so we may work with regular functions $\Bbbk[G \times X] \cong \Bbbk[G] \otimes_{\Bbbk} \Bbbk[X]$. Note that $p^*(f) = 1 \otimes f$ using this identification. By formula $(*)$, it follows that $p : G \times X \to X$ is Poisson.

Remark A.1. Let $f \in \Bbbk[X]$, and $\Bbbk[X]^G$ the ring of G-invariant functions on X. Then $f \in \Bbbk[X]^G$ if and only if $p^*(f) = a^*(f)$.

Lemma A.2. *Let X be an affine Poisson G-variety. If $a : G \times X \to X$ is a Poisson morphism, then $\Bbbk[X]^G$ is a Poisson subalgebra of $\Bbbk[X]$.*

Proof. Since a is a Poisson morphism, we have $a^*\{f_1, f_2\}_X = \{a^* f_1, a^* f_2\}_{G\times X}$ for $f_1, f_2 \in \Bbbk[X]$. Suppose $f_1, f_2 \in \Bbbk[X]^G$. Using Remark A.1, $a^*(f_i) = p^*(f_i) = 1 \otimes f_i$. It follows that

$$a^*\{f_1, f_2\}_X = \{1 \otimes f_1, 1 \otimes f_2\}_{G\times X} = 1 \otimes \{f_1, f_2\}_X = p^*\{f_1, f_2\}_X.$$

Again by Remark A.1, $\{f_1, f_2\}_X \in \Bbbk[X]^G$. □

Now assume that G is reductive. Then $\Bbbk[X]^G$ is a finitely generated $\Bbbk$-algebra, and by definition the geometric invariant theory quotient $X/\!\!/G = \operatorname{Spec}(\Bbbk[X]^G)$, or in other words, $X/\!\!/G$ is the affine variety with ring of regular functions $\Bbbk[X/\!\!/G] = \Bbbk[X]^G$. There is a quotient morphism $q : X \to X/\!\!/G$ with the property that $q^* : \Bbbk[X/\!\!/G] \to \Bbbk[X]$ is the inclusion of invariant functions.

By Lemma A.2, $\Bbbk[X/\!\!/G]$ is a Poisson algebra, so $X/\!\!/G$ is a Poisson algebraic variety. Since the inclusion $q^* : \Bbbk[X/\!\!/G] \to \Bbbk[X]$ is Poisson, it follows that $q : X \to X/\!\!/G$ is Poisson. Therefore we have proved the following proposition:

Proposition A.3. *If (G, π_G) is a reductive Poisson linear algebraic group and $(X, \{\ ,\ \}_X)$ is an affine Poisson algebraic variety, and the action map $G \times X \to X$ is Poisson, then $X/\!\!/G$ is a Poisson algebraic variety, and the morphism $q : X \to X/\!\!/G$ is Poisson.*

Quotient of a G-linearized variety. In this section, we explain how to put a Poisson structure on a GIT quotient of a linearized irreducible G-variety X. Recall the notions of G-linearized line bundle L on X and semistable locus from Section 3. The semistable locus $X^{ss}_L = \bigcup_{s_i} X_{s_i}$ is a finite union of open affine G-stable subsets U_{s_i} of X, where U_{s_i} is the nonvanishing locus of the section s_i of a power of L. Let $Y_{s_i} := U_{s_i}/\!\!/G$ be the quotient of the affine G-variety U_{s_i}. Then the quotient $X/\!\!/_L G$ has an open affine cover $X/\!\!/_L G = \bigcup Y_{s_i}$; see [Dolgachev 2003, Theorem 8.1].

We remark that if we are given a Poisson structure on a variety Z, there is an induced Poisson structure on any open set U of Z. Indeed, we may assume that Z is affine and U is covered by affine open sets $Z_f := \{x \in Z : f(x) \neq 0\}$. The Poisson structure on Z induces a Poisson Lie algebra structure on $\Bbbk[Z]$, and we can define a Poisson Lie algebra structure on $\Bbbk[Z_f]$ by the formula given in the proof of Lemma 1.3 in [Kaledin 2009]. These Poisson structures glue together on $Z_f \cap Z_g = Z_{fg}$ and hence define a Poisson structure on the open set U.

Proposition A.4. *Let X be an irreducible Poisson G-variety with G-linearization L, where (G, π_G) is a reductive Poisson algebraic group and the action morphism $a : G \times X \to X$ is a Poisson morphism. Then X_L^{ss} and $X/\!\!/_L G$ are Poisson and $q : X_L^{ss} \to X/\!\!/_L G$ is a Poisson morphism.*

Proof. There is a finite set of G-invariant sections s_i with the property that the nonvanishing locus X_{s_i} of s_i, is open, affine and G-stable. Hence by Proposition A.3, $Y_i := U_{s_i} /\!\!/ G$ is an affine Poisson variety. Thus, we have a Poisson structure π_i on each open set Y_i in the open cover $X/\!\!/_L G = \bigcup Y_i$. The functions on the intersections $Y_i \cap Y_j$ form a subring in the fraction field $\Bbbk(Y_i)$, and the above formula from [Kaledin 2009] implies that π_i and π_j coincide on the sheaf of functions on $Y_i \cap Y_j$ and thus glue to give an induced Poisson structure on $X/\!\!/_L G$. Since the morphism $q : X \to Y$ is Poisson on the affine cover $U_i \to Y_i$ for each of our invariant sections s_i, it follows that q is a Poisson morphism. □

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WHAT DO FROBENIUS'S, SOLOMON'S, AND IWASAKI'S THEOREMS ON DIVISIBILITY IN GROUPS HAVE IN COMMON?

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Our result contains as special cases the Frobenius theorem (1895) on the number of solutions to the equation $x^n = 1$ in a group, the Solomon theorem (1969) on the number of solutions in a group to a system of equations having fewer equations than unknowns, and the Iwasaki theorem (1985) on roots of subgroups. There are other curious corollaries on groups and rings.

0. Introduction

The following result was proved in the nineteenth century.

Frobenius theorem [1895]. *The number of solutions to the equation $x^n = 1$ in a finite group is divisible by* $\mathrm{GCD}(|G|, n)$ *for any integer n.*

This theorem was generalized in different directions; see, e.g., [Hall 1936; Kulakoff 1938; Sehgal 1962; Brown and Thévenaz 1988; Yoshida 1993; Asai and Takegahara 2001; Asai et al. 2013], and references therein. For example, Frobenius [1903] himself obtained the following generalization:

> *for any positive integer n and any element g of a finite group G, the number of solutions to the equation $x^n = g$ in G is divisible by the greatest common divisor of n and the order of the centralizer of g.*

P. Hall [1936, Theorem II] showed that

> *in any finite group, the number of solutions to a system of equations in one unknown is divisible by* $\mathrm{GCD}(|C|, n_1, n_2, \dots)$*, where C is the centralizer of the set of all coefficients and n_i are exponent sums of the unknown in the i-th equation.*

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Here as usual, an equation over a group G is an expression of form $v(x_1, \ldots, x_m) = 1$, where v is a word whose letters are unknowns, their inverses, and elements of G (called *coefficients*). In other terms, the left-hand side of an equation is an element of the free product $G * F(x_1, \ldots, x_m)$ of G and the free group $F(x_1, \ldots, x_m)$ of rank m (where m is the number of unknowns).

The following theorem is also about equations in groups and divisibility, but on first view, it is not similar to the Frobenius theorem and its generalizations.

Solomon theorem [1969]. *In any group, the number of solutions to a system of coefficient-free equations is divisible by the order of the group provided the number of equations is less than the number of unknowns.*

This theorem was also generalized in different directions; see [Isaacs 1970; Strunkov 1995; Amit and Vishne 2011; Gordon and Rodriguez-Villegas 2012; Klyachko and Mkrtchyan 2014; 2017], and references therein. For instance, in [Klyachko and Mkrtchyan 2014], it was shown that

> *in any group, the number of solutions to a system of equations (with coefficients from this group) is divisible by the order of the intersection of centralizers of all coefficients provided the rank of the matrix composed of the exponent sums of the j-th unknown in the i-th equation is less than the number of unknowns.*

Solomon [1969] himself wrote:

> "*There seems to be no connection between this theorem and the Frobenius theorem on solutions of $x^k = 1$.*"

Nevertheless, a connection between the Frobenius and Solomon theorems exists.

Theorem 0. *In any (not necessarily finite) group, the number of solutions to a (not necessarily finite) system of equations in m unknowns is a multiple of the greatest common divisor of the centralizer of the set of coefficients and the number $\frac{\Delta_m}{\Delta_{m-1}}$, where Δ_i is the greatest common divisor of all minors of order i of the matrix of the system, and the following conventions are assumed: $\Delta_i = 0$ if i is larger than the number of equations, $\Delta_0 = 1$, and $\frac{0}{0} = 0$.*

We define the *greatest common divisor* $\mathrm{GCD}(G, n)$ of a group G and an integer n as the least common multiple of orders of subgroups of G dividing n. The divisibility is always understood in the sense of cardinal arithmetic: each infinite cardinal is divisible by all smaller nonzero cardinals (and surely zero is divisible by all cardinals and divides only zero). This means that $\mathrm{GCD}(G, 0) = |G|$ for any group G and, e.g., $\mathrm{GCD}(\mathrm{SL}_2(\mathbb{Z}), 2018) = 2$. Although, the reader will not lose much by assuming all group to be finite; in this case, $\mathrm{GCD}(G, n) = \mathrm{GCD}(|G|, n)$ by the Sylow theorem (and because a finite p-group contains subgroups of all possible orders).

The *matrix of a system of equations over a group* is the integer matrix $A = (a_{ij})$, where a_{ij} is the exponent sum of the j-th unknown in the i-th equation. For example, the matrix of the system

$$\begin{cases} xay^2[x, y]^{2019}(xby)^3 = 1, \\ bx^3y[x, y]^{100}(xby)^4 = 1, \\ [x, y^5]x^{-2} = 1 \end{cases}$$

(where x and y are unknowns, and a and b are coefficients, i.e., some fixed group elements) has the form

$$\begin{pmatrix} 4 & 5 \\ 7 & 5 \\ -2 & 0 \end{pmatrix}.$$

As usual, the *minors of order i* are determinants of submatrices composed of entries at the intersections of some i rows and i columns. In the example above, there are three minors of order m (up to signs),

$$\det\begin{pmatrix} 4 & 5 \\ 7 & 5 \end{pmatrix} = -15, \qquad \det\begin{pmatrix} 4 & 5 \\ -2 & 0 \end{pmatrix} = 10, \qquad \det\begin{pmatrix} 7 & 5 \\ -2 & 0 \end{pmatrix} = 10,$$

and six minors of order $m-1$: 4, 5, 7, 5, -2, 0. Thus, the theorem asserts that (in this example) the number of solutions is divisible by

$$\mathrm{GCD}\left(\frac{\mathrm{GCD}(-15, 10, 10)}{\mathrm{GCD}(4, 5, 7, 5, -2, 0)}, |C(a) \cap C(b)|\right) = \mathrm{GCD}(5, |C(a) \cap C(b)|).$$

Note that the agreements about boundary cases in Theorem 0 are natural. Indeed, we always can add a fictitious equation $1 = 1$ to make the number of equations larger than m. We can also add a new variable z and the equation $z = 1$ (this does not affect the number of solutions and makes $m > 1$). As for the philosophical question on the interpretation of the fraction $\frac{0}{0}$, it can be understood arbitrarily, e.g., the reader may assume that $\frac{0}{0} = 2019$; in any case, Theorem 0 remains valid (but weaker than under the suggested interpretation).

The meaning of the value $\frac{\Delta_m}{\Delta_{m-1}}$ is as follows. It is well known (see, e.g., [Vinberg 2003]) that invertible integer elementary transformations of rows and columns can transform any integer matrix A into a diagonal matrix, where the diagonal entries divide each other (each diagonal entry divides the next one). This diagonal matrix is uniquely determined up to the signs of diagonal elements (and is sometimes called the *Smith form* of A); the diagonal elements of the Smith form (sometimes called the *invariant factors* of A) equal the ratios $\frac{\Delta_i}{\Delta_{i-1}}$. Thus, in these terms, $\frac{\Delta_m}{\Delta_{m-1}}$ is the m-th invariant factor of the matrix of the system of equations. One can also say that *the absolute value of* $\frac{\Delta_m}{\Delta_{m-1}}$ *is the period (exponent) of the quotient of the free abelian group* $\mathbb{Z}^m$ *by the subgroup generated by the rows of the matrix of the system of equations*

(with the stipulation that this ratio vanishes if and only if the period is infinite).

The Frobenius and Solomon theorems as well as their generalizations stated above are special cases of Theorem 0.

The following theorem is on first view similar to neither the Frobenius theorem nor the Solomon theorem.

Iwasaki theorem [1982]. *For any integer* n, *the number of elements of a finite group* G *whose* n*-th powers lie in a subgroup* $H \subseteq G$ *is divisible by* $|H|$.

This beautiful theorem remains (for some reason) not widely known. In [Sato and Sakurai 2007], it was noticed that the divisibility by $|H|$ still holds for the number of solutions to the "equation" $x^n \in HgH$, where HgH is any double coset of a subgroup H. Clearly, the Iwasaki theorem and its generalizations deal with predicates that are not equations in the usual sense. Let us say that a *generalized equation* over a group G is an expression of the form $w(x_1, \dots, x_n) \in HgH$, where H is a subgroup of $G \ni g$, and $w(x_1, \dots, x_m)$ is an element of the free product $G * F(x_1, \dots, x_m)$ of G and a free group; in other terms, w is a word in the alphabet $G \sqcup \{x_1^{\pm 1}, \dots, x_m^{\pm 1}\}$. The elements of G occurring in this word are called the *coefficients* of the generalized equation. A system of generalized equations, a solution to this system, and a matrix of this system are defined in a natural way.

In [Klyachko and Mkrtchyan 2017], the following generalization of the Iwasaki theorem was obtained:

the number of solutions to a system of generalized coefficient-free equations whose right-hand sides are double cosets of the same subgroup H (e.g., $\{x^{100}y^{2019}[x, y]^4 \in Hg_1H,\ [x^5, y^6]^7(xy)^8 \in Hg_2H,\ \dots\}$) *is divisible by* $|H|$.

The following theorem includes all results stated above.

Theorem 1. *Let* S *be a (not necessarily finite) system of generalized equations in finitely many unknowns* $x_1, \dots, x_m$ *over a group* G *and let* P *be its subsystem*:

$$S = \{u_i(x_1, \dots, x_m) \in H_i g_i H_i \mid i \in I\} \supseteq P = \{u_j(x_1, \dots, x_m) \in H_j g_j H_j \mid j \in J\},$$

(*where* $J \subseteq I$, $u_i \in G * F(x_1, \dots, x_m)$, $g_i \in G$, *and* H_i *are subgroups of* G). *Then the number of solutions to* S *in* G *is divisible by the greatest common divisor of the subgroup*

$$\widetilde{H} = \Big(\bigcap_{j \in J} N(H_j g_j H_j)\Big) \cap \Big(\bigcap_{i \in I \setminus J} H_i\Big) \cap (\text{the centralizer of the set of coefficients of } S)$$

and the number $\frac{\Delta_m}{\Delta_{m-1}}$, *where* Δ_k *is the greatest common divisor of all minors of order k of the matrix of the subsystem* P. Henceforth, $N(A) := \{g \in G \mid g^{-1}Ag = A\}$ is the normalizer of a subset A in a group G.

To deduce Theorem 0 from Theorem 1, we rewrite the system of equations in the "generalized" form, i.e., we put $S = P = \{u_1(x_1, \dots, x_m) \in \{1\}1\{1\}$ and $u_2(x_1, \dots, x_m) \in \{1\}1\{1\}, \dots\}$ and note that the normalizer of the trivial subgroup is the whole group.

On the other hand, setting

$$S = \{u_1(x_1, \dots, x_m) \in Hg_1H,\ u_2(x_1, \dots, x_m) \in Hg_2H,\ \dots\}$$
$$\text{(where } u_i \in F(x_1, \dots, x_m)\text{)},$$
$$P = \varnothing,$$

we obtain the above-mentioned generalization (from [Klyachko and Mkrtchyan 2017]) of the Iwasaki theorem.

As a matter of fact, a relation between Solomon's and Iwasaki's theorems was established in [Klyachko and Mkrtchyan 2014; 2017]; our achievement consists only of adding "Frobeniusness". The main theorem of [Klyachko and Mkrtchyan 2017] says that, if we have a group F with a fixed epimorphism onto $\mathbb{Z}$ and some set of homomorphisms from F into another group G, and this set is invariant with respect to some natural transformations (depending on the epimorphism $F \to \mathbb{Z}$ and a subgroup H of G), then the number of these homomorphisms $F \to G$ is divisible by $|H|$. Choosing suitable sets of homomorphisms, the Klyachko and Mkrtchyan [2017] obtained Solomon's and Iwasaki's theorems as special cases of their main theorem.

Our main theorem (see Section 1) is a modular analogue of the main theorem of [Klyachko and Mkrtchyan 2017]: we take an epimorphism $F \to \mathbb{Z}/n\mathbb{Z}$ instead of $F \to \mathbb{Z}$. One can say that the main theorem of this paper is related to the main theorem of [Klyachko and Mkrtchyan 2017] in the same way as Theorem 0 to the generalization (from [Klyachko and Mkrtchyan 2014]) of the Solomon theorem mentioned in the beginning of this paper. An important role in our argument is played by an elementary (but nontrivial) lemma due to Brauer [1969]. Actually, we need this lemma not to prove the main theorem but rather to explain that its statement per se makes some sense. For readers' convenience, we give a proof of the Brauer lemma. Section 5 contains the proof of the main theorem.

In Section 2, we deduce Theorem 1 from the main theorem. As another corollary, we obtain a theorem on equations in rings (Theorem 4 in Section 3) that implies, e.g., the following fact, which can be considered as a generalization of the Frobenius theorem in another direction:

for any representation $\rho : G \to \mathrm{GL}(V)$ of a group G and any words $u_i(x_1, \dots, x_m) \in F(x_1, \dots, x_m)$, the number of solutions to the equation

$$\sum_{i=1}^{k} (\rho(u_i(x_1, \dots, x_m)))^{l_i} = \mathrm{id}$$

is divisible by

$$\begin{cases} \mathrm{GCD}(G, \mathrm{GCD}\{l_i\}) & \textit{always}, \\ \mathrm{GCD}(G, \mathrm{LCM}\{l_i\}) & \textit{if } k \le m, \\ |G| & \textit{if } k < m. \end{cases}$$

In Section 4, we show that the main theorem implies some fact about the number of crossed homomorphisms, generalizing earlier known results. In the last section, we discuss open questions.

Notations and conventions. We use mainly standard notations and conventions. Note only that, if $k \in \mathbb{Z}$ and x and y are elements of a group, then x^y, x^{ky}, and x^{-y} denote $y^{-1}xy$, $y^{-1}x^k y$, and $y^{-1}x^{-1}y$, respectively. The commutator subgroup of a group G is denoted by G' or $[G, G]$. If X is a subset of a group, then $|X|$, $\langle X \rangle$, $\langle\langle X \rangle\rangle$, $C(X)$, and $N(X)$ are the cardinality of X, subgroup generated by X, normal closure of X, centralizer of X, and normalizer of X. The index of a subgroup H of a group G is denoted by $|G : H|$. The letter $\mathbb{Z}$ denotes the set of integers. If R is an associative ring with unity, then R^* denotes the group of units of this ring. GCD and LCM are the greatest common divisor and least common multiple. The symbol $\exp G$ denotes the period (exponent) of a group G if this period is finite; we assume $\exp G = 0$ if the period is infinite. The symbol $\langle g \rangle_n$ denotes the cyclic group of order n generated by an element g. The free group of rank n is denoted by $F(x_1, \dots, x_n)$ or F_n. The symbol $A * B$ denotes the free product of groups A and B.

Let us recall once again that the finiteness of groups is not assumed by default; the divisibility is always understood in the sense of cardinal arithmetic (an infinite cardinal is divisible by all nonzero cardinals not exceeding it), and $\mathrm{GCD}(G, n) := \mathrm{LCM}\{|H| \mid H \text{ is a subgroup of } G, \text{ and } |H| \text{ divides } n\}$.

1. Main theorem

A group F equipped with an epimorphism $F \to \mathbb{Z}/n\mathbb{Z}$ (where $n \in \mathbb{Z}$) is called an *n-indexed* group. This epimorphism $F \to \mathbb{Z}/n\mathbb{Z}$ is called *degree* and denoted deg. Thus, to any element f of an indexed group F, an element $\deg f \in \mathbb{Z}/n\mathbb{Z}$ is assigned; the group F contains elements of all degrees and $\deg(fg) = \deg f + \deg g$ for any $f, g \in F$.

Suppose that $\phi : F \to G$ is a homomorphism from an n-indexed group F to a group G and H is a subgroup of G. The subgroup

$$H_\phi = \bigcap_{f \in F} H^{\phi(f)} \cap C(\phi(\ker \deg))$$

is called the *ϕ-core* of H [Klyachko and Mkrtchyan 2017]. In other words, the ϕ-core H_ϕ of H consists of elements h such that $h^{\phi(f)} \in H$ for all f, and $h^{\phi(f)} = h$ if $\deg f = 0$.

Main theorem. *Suppose that an integer n is a multiple of the order of a subgroup H of group G and a set Φ of homomorphisms from an n-indexed group F to G satisfies the following conditions.*

(I) *Φ is invariant with respect to conjugation by elements of H:*

if $h \in H$ and $\phi \in \Phi$, then the homomorphism $\psi : f \mapsto \phi(f)^h$ lies in Φ.

(II) *For any $\phi \in \Phi$ and any element h of the ϕ-core H_ϕ of H, the homomorphism ψ defined by*

$$\psi(f) = \begin{cases} \phi(f) & \text{for all elements } f \in F \text{ of degree zero,} \\ \phi(f)h & \text{for some element } f \in F \text{ of degree one} \\ & \qquad\text{(and, hence, for all degree-one elements)} \end{cases}$$

belongs to Φ too.

Then $|\Phi|$ is divisible by $|H|$.

Note that the mapping ψ from condition (I) is a homomorphism for any $h \in G$, and the formula for ψ from condition (II) defines a homomorphism for any $h \in H_\phi$ (as explained below). Thus, conditions (I) and (II) only require these homomorphisms to belong to Φ.

Lemma 2. *Suppose that $\phi : F \to G$ is a homomorphism from an n-indexed group F to a group G, $f_1 \in F$ is an element of degree one, and $g \in G$. Then the homomorphism $\psi : F \to G$ such that $\psi(f) = \phi(f)$ for all $f \in F$ of degree zero and $\psi(f_1) = \phi(f_1)g$ exists if and only if $g \in C(\phi(\ker \deg))$ and $(\phi(f_1)g)^n = (\phi(f_1))^n$.*

Proof. The group F can be presented in the form

$$F \simeq (F_0 * \langle x \rangle_\infty) / \langle\!\langle \{u^x u^{-f_1} \mid u \in F_0\} \cup \{x^n f_1^{-n}\} \rangle\!\rangle, \quad \text{where } F_0 = \ker \deg.$$

Therefore, the mapping $\psi : F_0 \cup \{x\} \to G$ can be extended to a homomorphism if and only if its restriction to F_0 is a homomorphism and the relations $u^x = u^{f_1}$ (for $u \in F_0$) and $x^n = f_1^n$ are mapped to true equalities in G:

$$(*) \qquad \psi(u)^{\psi(x)} = \psi(u^{f_1}) \quad \text{and} \quad \psi(x)^n = \psi(f_1^n).$$

If the restrictions of ψ and ϕ to F_0 coincide and $\psi(x) = \phi(f_1)g$, then the first equality of $(*)$ says that g commutes with $\phi(u)$ (for all $u \in F_0$), while the second equality of $(*)$ takes the form $(\phi(f_1)g)^n = (\phi(f_1))^n$. □

Recall also the following beautiful (but not widely known) fact.

Brauer lemma [1969]. *If U is a finite normal subgroup of a group V, then, for all $v \in V$ and $u \in U$, the elements $v^{|U|}$ and $(vu)^{|U|}$ are conjugate by an element of U.*

Proof. The group $\mathbb{Z}$ acts by permutations on the subgroup U:

$$a \circ i = v^{-i} a (vu)^i \quad \text{(where } i \in \mathbb{Z} \text{ and } a \in U).$$

Let m be the minimum length of an orbit. In other words, m is the minimum length of a cycle in the decomposition of the permutation $a \mapsto v^{-1}avu$ (of U) into the product of independent cycles. The set $X = \{a \in U \mid a \circ m = a\}$ is the union of all orbits of length m; therefore, $|X|$ is divisible by m. On the other hand, (by definition of the action) $X = \{a \in U \mid v^{-m}a(vu)^m = a\} = \{a \in U \mid a^{-1}v^m a = (vu)^m\}$ and, hence, $|X|$ is the order of the centralizer of v^m in U (because, in any group, a nonempty set of the form $\{x \mid x^{-1}yx = z\}$ is a coset of the centralizer of y). Thus, $|X|$ divides $|U|$ and, therefore, m divides $|U|$ and $a \circ |U| = a$ (if a lies in an orbit of length m). □

These two lemmata imply immediately that the mapping ψ from condition (II) is a homomorphism for any $h \in H_\phi$ because $(\phi(f)h)^n = (\phi(f))^n$ by the Brauer lemma applied to $U = H_\phi \subset V = H_\phi \cdot \langle \phi(f_1) \rangle \ni \phi(f_1) = v$. Indeed, we obtain the equality $(\phi(f_1)h)^{|H_\phi|} = (\phi(f_1))^{|H_\phi| u}$ for some $u \in H_\phi$ and, hence, $(\phi(f_1)h)^n = (\phi(f_1))^{nu} = (\phi(f_1^n))^u$ (because $|H_\phi|$ divides n). It remains to note that $u \in H_\phi$ commutes with $\phi(f_1^n)$ because $\deg f_1^n = n = 0 \in \mathbb{Z}/n\mathbb{Z}$. Thus, we obtain the equality $(\phi(f_1)h)^n = (\phi(f_1))^n$. It remains to refer to Lemma 2.

In the case $n = 0$ the main theorem was proved by Klyachko and Mkrtchyan [2017]. So, our theorem is a "modular analogue" of their main result. On the other hand, our main theorem is deduced (in Section 5) from this special case $n = 0$.

Lemma 3. *In condition* (II) *of the main theorem, $\psi(f) \in \phi(f)H_\phi$ for all $f \in F$.*

Proof. Indeed, if $\deg f = d$, then $f = f_1^d f_0$, where f_1 is the (fixed) element of degree one (from condition (II)) and f_0 is an element of degree zero. Then

$$\psi(f) = \psi(f_1)^d \psi(f_0) = (\phi(f_1)h)^d \phi(f_0) \overset{(E)}{=} \phi(f_1)^d \phi(f_0) h' = \phi(f_1^d f_0) h' = \phi(f) h',$$

where the equality (E) is valid for some $h' \in H_\phi$ because $h \in H_\phi$ and $\phi(F)$ normalizes H_ϕ. □

2. Proof of Theorem 1

Let $L \subseteq G$ be the subgroup generated by all coefficients of the system S. Take as H any subgroup of the group $\widetilde{H}$ whose order divides $n := \frac{\Delta_m}{\Delta_{m-1}}$, and put

$$F = L * F(x_1, \dots, x_m),$$
$$\Phi = \{\phi : F \to G \mid \phi(f) = f \text{ for } f \in L \text{ and } \phi(u_i) \in H_i g_i H_i \text{ for } i \in I\}.$$

As the indexing $\deg : F \to \mathbb{Z}/n\mathbb{Z}$, take an epimorphism whose kernel contains L and all u_j, where $j \in J$. Such an epimorphism exists because n is the period of the finitely generated abelian group $F/([F, F] \cdot L \cdot \langle\{u_j \mid j \in J\}\rangle)$.

Let us verify that the conditions of the main theorem hold. Condition (I) holds obviously for all $h \in H$ (and even for all $h \in \widetilde{H}$) because (by definition) $\widetilde{H}$ centralizes L and normalizes double cosets $H_i g_i H_i$.

Condition (II) holds also for all $h \in H_\phi$ because

- on L, the homomorphism ψ coincides with ϕ as L consists of zero-degree elements,
- $\psi(u_j) = \phi(u_j)$ for $j \in J$ because again $\deg u_j = 0$, and
- for $i \in I \setminus J$, we have $\psi(u_i) \in \phi(u_i) H_\phi \subseteq \phi(u_i) H_i$ (where the inclusion $\in$ follows from Lemma 3).

Thus, the main theorem implies that $|\Phi|$ is divisible by the order of any subgroup $H \subseteq \widetilde{H}$ whose order divides n, i.e., $|\Phi|$ is divisible by $\mathrm{GCD}(\widetilde{H}, n)$. It remains to note that $|\Phi|$ is the number of solutions to S.

3. Rings and representations

A *generalized homogeneous modulo n* equation with a set of unknowns X over an associative unital ring R is a finite expression of the form

$$\sum_i \prod_j c_{ij} x_{ij}^{k_{ij}} = 0,$$

where *coefficients* $c_{ij} \in R$, *unknowns* $x_{ij} \in X$, and *exponents* $k_{ij} \in \mathbb{Z}$,

such that, for some mapping $\deg : X \to \mathbb{Z}/n\mathbb{Z}$, the value $\sum_j k_{ij} \deg x_{ij}$ (called the *degree of the equation*) does not depend on i (i.e., the "polynomial" in the left-hand side of the equation is homogeneous with respect to some assigning of degrees to variables), and $\langle\{\deg x \mid x \in X\}\rangle = \mathbb{Z}/n\mathbb{Z}$. (This means that the free group $F(X)$ is n-indexed with respect to the map deg.)

A system of equations is called generalized homogeneous modulo n if all equations of this system are generalized homogeneous modulo n (of possibly different degrees) with respect to the same function $\deg : X \to \mathbb{Z}/n\mathbb{Z}$.

As we explain below, the set $M = \{n \in \mathbb{Z} \mid$ a given system is generalized homogeneous modulo $n\}$ consists of all divisors of a number n_0, called the *homogeneity modulus* of the system. In other words, the homogeneity modulus is the maximal number from M or zero if M is infinite.

To find the homogeneity modulus, consider a homogenous system of linear equations, where unknowns are degrees of variables and also (the negations of) degrees of equations; these linear equations say that the degree of each monomial equals the degree of the corresponding equation. The matrix of this system (called the *homogeneity matrix* of the initial system of equations) has the following form. Suppose that $X = \{x_1, \dots, x_m\}$. The *homogeneity matrix of p-th equation* is the integer matrix $A_p = (a_{kl})$ of size

(the total number of monomials in the system) $\times$ ($m+$(the number of equations)),

where, for $l \le m$, the (k,l)-th entry is the exponent sum of the l-th unknown in the k-th monomial, the $(m+p)$-th column consists of ones, and the remaining columns are zero for $l > m$. The homogeneity matrix of the system of equations is composed from the matrices A_p written one under another: $A = \begin{pmatrix} A_1 & A_2 & \cdots \end{pmatrix}^T$. For example, the system of equations $\{ax^3y^2 + y^7bx - 1 = 0,\ xy^2x + y^7x^5 = 0\}$ (where x and y are unknowns and $a, b \in R$ are coefficients) has the homogeneity matrix

$$A = \begin{pmatrix} 3 & 2 & 1 & 0 \\ 1 & 7 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 2 & 2 & 0 & 1 \\ 5 & 7 & 0 & 1 \end{pmatrix} = \begin{pmatrix} A_1 \\ A_2 \end{pmatrix}, \quad \text{where } A_1 = \begin{pmatrix} 3 & 2 & 1 & 0 \\ 1 & 7 & 1 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \text{ and } A_2 = \begin{pmatrix} 2 & 2 & 0 & 1 \\ 5 & 7 & 0 & 1 \end{pmatrix}.$$

Homogeneity-modulus lemma. *The homogeneity modulus of a system of s equations in m unknowns over an associative ring with unity is* $\frac{\Delta_{m+s}}{\Delta_{m+s-1}}$, *where* Δ_i *is the greatest common divisor of all minors of order i of the homogeneity matrix of the system. As always, the following conventions are assumed*: $\Delta_i = 0$ *if the total number of monomials in all equations is less than i*, $\Delta_0 = 1$, *and* $\frac{0}{0} = 0$.

Proof. Let A be the homogeneity matrix. We have to find the maximal number n such that the system of linear homogeneous equations $AX = 0$ (in $m + s$ variables) has a solution in $\mathbb{Z}/n\mathbb{Z}$ whose components generate $\mathbb{Z}/n\mathbb{Z}$ as an additive group (or, equivalently, the first m components of the solution generate $\mathbb{Z}/n\mathbb{Z}$, because the equations say that the last s components are combinations of the first m ones). In other words, n is the largest order of cyclic quotient of the finitely generated group $\mathbb{Z}^{m+s}/N$, where N is the subgroup generated by rows of A. As noted already, the largest cyclic quotient n of $\mathbb{Z}^{m+s}/N$ is $\frac{\Delta_{m+s}}{\Delta_{m+s-1}}$, as required. □

Theorem 4. *Let R be an associative ring with unity and let G be a subgroup of the multiplicative group of this ring. Then, for each system of equations over R in*

m unknowns, the number of its solutions lying in G^m is divisible by the greatest common divisor of the homogeneity modulus of the system and the intersection of G with the centralizer of the set of coefficients of the system.

Proof. Let G_0 be the intersection of G and the centralizer of the set of coefficients and let n be the homogeneity modulus. Consider the free group $F = F(X)$ (where X is the set of unknowns) and an epimorphism $\deg : F \to \mathbb{Z}/n\mathbb{Z}$.

Let us apply the main theorem taking Φ to be the set of all homomorphisms $\phi : F \to G$ such that the tuple $(\phi(x_1), \dots, \phi(x_m))$ is a solution to the system of equations (so, the number of solutions is $|\Phi|$). Take H to be any subgroup of G_0 of order dividing n. Condition (I) of the main theorem obviously holds. To verify condition (II), choose an element $t \in F$ of degree one and write each variable x_i in the form $x_i = t^{\deg x_i} y_i$, where $y_i = t^{-\deg x_i} x_i$ has degree zero. In new notation, each equation $w(x_1, \dots, x_m) = 0$ takes the form $v(t, y_1, \dots, y_m) = 0$ and the exponent sum of t in each term of this equation is the same (modulo n). Now, note that, if $v(\phi(t), \phi(y_1), \dots, \phi(y_m)) = 0$ and $h \in H_\phi$, then $v(\phi(t)h, \phi(y_1), \dots, \phi(y_m)) = 0$. This result follows from the (right) divisibility of $v(\phi(t)h, \phi(y_1), \dots, \phi(y_m))$ by $v(\phi(t), \phi(y_1), \dots, \phi(y_m))$ due to the following fact.

Fact [Klyachko and Mkrtchyan 2017, Lemma 1]. *If M is a monoid, $b_i, a, h \in M$, elements a and h are invertible, and the elements $a^{-s}ha^s$, where $s \in \mathbb{Z}$, commute with all b_i, then, for any expression of the form $u(t) = b_0 t^{m_1} b_1 \cdots t^{m_l} b_l$, where $m_i \in \mathbb{Z}$, we have*

$$u(ah) = \begin{cases} h^{a^{-1}} h^{a^{-2}} \cdots h^{a^{-k}} u(a) & \textit{if } k = \sum m_i > 0, \\ h^{-1} h^{-a} \cdots h^{-a^{-1-k}} u(a) & \textit{if } k = \sum m_i < 0, \\ u(a), & \textit{if } k = \sum m_i = 0. \end{cases}$$

We apply this fact to each term of v; we also use that t^n has degree zero and $(\phi(t)h)^n = (\phi(t))^n$ according to Lemma 2.

Thus, the main theorem implies that $|\Phi|$ (i.e., the number of solutions to the system of equations) is divisible by $|H|$ as required (because H is an arbitrary subgroup of G_0 whose order divides the homogeneity modulus). □

Example. If $\rho : G \to R^*$ is a homomorphism from a finite group G to the multiplicative group of an associative ring R with unity (e.g., $\rho : G \to \mathrm{GL}(V)$ is a linear representation of G), then, for any words $u_i(x_1, \dots, x_m) \in F(x_1, \dots, x_m)$,

the number of solutions to the equation $\displaystyle\sum_{i=1}^{k} (\rho(u_i(x_1, \dots, x_m)))^{l_i} = 1$

$$\text{is divisible by } \begin{cases} \mathrm{GCD}(G, \mathrm{GCD}\{l_i\}) & \text{always}, \\ \mathrm{GCD}(G, \mathrm{LCM}\{l_i\}) & \text{if } k \le m, \\ |G| & \text{if } k < m. \end{cases}$$

To show this, it suffices to apply Theorem 4 to the subgroup $\rho(G) \subseteq R^*$. The homogeneity matrix of this equation has the form

$$B = \begin{pmatrix} & & & 1 \\ & A & & \vdots \\ 0 & \cdots & 0 & 1 \end{pmatrix},$$

where the last row corresponds to 1 in the right-hand side of the equation, and the i-th row of the matrix A corresponds to the i-th term in the left-hand side of the equation and, therefore, all elements of this row are divisible by l_i. It remains to note that the j-th invariant factor of the matrix B coincides with the $(j-1)$-th invariant factor of A and use the following fact, which we leave to readers as an easy exercise:

if the i-th row of an integer matrix $k \times m$ is divisible by l_i, then the m-th invariant factor of this matrix

$$\begin{cases} \textit{is divisible by } \mathrm{GCD}\{l_i\} & \textit{always}, \\ \textit{is divisible by } \mathrm{LCM}\{l_i\} & \textit{for } k = m, \\ \textit{vanishes} & \textit{for } k < m. \end{cases}$$

Note that Theorem 0 can be obtained as a corollary of Theorem 4. Indeed, take $R = \mathbb{Z}G$; the group ring contains G as a subgroup of the multiplicative group. Any system of equations over G can be rewritten in "ring" form: $\{w_i(x_1, \dots) - 1 = 0\}$. It remains to note that the value $\frac{\Delta_m}{\Delta_{m-1}}$ from Theorem 0 becomes exactly the homogeneity modulus from the homogeneity-modulus lemma.

4. Crossed homomorphisms

Suppose a group F acts (on the right) on a group B by automorphisms: $(f, b) \mapsto b^f$. Recall that a *crossed homomorphism* from F to B with respect to this action is a mapping $\alpha : F \to B$ such that $\alpha(ff') = \alpha(f)^{f'}\alpha(f')$ for all $f, f' \in F$. Saveliy Skresanov noted that the main theorem easily implies the following fact proved in [Asai et al. 2013] (using character theory) for finite groups F and B.

Theorem 5. *If a group F admitting an epimorphism onto $\mathbb{Z}/n\mathbb{Z}$ acts by automorphisms on a group B, then the number of crossed homomorphisms $F \to B$ is divisible by* $\mathrm{GCD}(B, n)$.

Proof. The set of crossed homomorphisms is in one-to-one correspondence with the set Φ of (usual) homomorphisms from F to the semidirect product $G = F \leftthreetimes B$ (with respect to the given action) such that their compositions with the projection $\pi : F \leftthreetimes B \to F$ is the identity mapping $F \to F$. We have to show that $|\Phi|$ is a multiple of $|H|$ for any subgroup $H \subseteq B$ whose order divides n (by definition of $\mathrm{GCD}(B, n)$).

The group F is n-indexed by the hypothesis of Theorem 5. Therefore, the assertion follows immediately from the main theorem. Conditions of the main theorem hold by trivial reasons: condition (I) is fulfilled because $\pi(h^{-1}gh) = \pi(g)$, and condition (II) follows immediately from Lemma 3 because $\pi(gh) = \pi(g)$ (for $g \in G$ and $h \in H$). $\square$

5. Proof of the main theorem

Take an element $f_1 \in F$ of degree one, put $F_0 = \ker \deg \subset F$, and consider the semidirect product $\widetilde{F} = \langle a \rangle_\infty \leftthreetimes F_0$, where a acts on F_0 as f_1 does: $u^a = u^{f_1}$ for $u \in F_0$. The group $\widetilde{F}$ admits a natural indexing (0-indexing) $\deg : \widetilde{F} \to \mathbb{Z}$ (denoted by the same symbol deg). The kernel of this map is F_0 and $\deg a = 1$. Moreover, there is a natural epimorphism $\alpha : \widetilde{F} \to F$ mapping a to f_1 and identity on F_0. Let us verify that the conditions of the main theorem hold for the set $\widetilde{\Phi} = \{\phi \circ \alpha \mid \phi \in \Phi\}$ of homomorphisms from $\widetilde{F}$ to G.

Condition (I) holds obviously. To verify condition (II), take the degree-one element $a \in \widetilde{F}$ and some homomorphism $\tilde{\phi} = \phi \circ \alpha \in \widetilde{\Phi}$ (where $\phi \in \Phi$). Then the homomorphism $\tilde{\psi}$ from condition (II) has the form

$$(**) \quad \tilde{\psi}(\tilde{f}) = \begin{cases} \phi(\tilde{f}) & \text{for all elements } \tilde{f} \in F_0, \\ \phi(f_1)h & \text{for } \tilde{f} = a, \end{cases} \quad \text{where } \phi \in \Phi \text{ and } h \in H_{\tilde{\varphi}}.$$

We have to show that $\tilde{\psi}$ lies in $\widetilde{\Phi}$, i.e., has the form $\tilde{\psi} = \phi' \circ \alpha$, where $\phi' \in \Phi$. Note that $H_{\tilde{\varphi}} = H_\phi$, because the images of $\tilde{\phi} = \phi \circ \alpha$ and ϕ coincide, and the images of zero-degree elements for these homomorphisms coincide: $\tilde{\phi}(\ker \deg) = \tilde{\phi}(F_0) = \phi(F_0)$. Equation $(**)$ takes the form

$$\tilde{\psi}(\tilde{f}) = \begin{cases} \phi(\tilde{f}) & \text{for } \tilde{f} \in F_0, \\ \phi(f_1)h & \text{for } \tilde{f} = a, \end{cases} \quad \text{where } \phi \in \Phi \text{ and } h \in H_\phi.$$

This means that $\tilde{\psi} = \psi \circ \alpha$, where

$$\psi(f) = \begin{cases} \phi(f) & \text{for } f \in F_0, \\ \phi(f_1)h & \text{for } f = f_1, \end{cases} \quad \text{where } \phi \in \Phi \text{ and } h \in H_\phi.$$

The homomorphism $\psi : F \to G$ lies in Φ by condition (II) of the theorem we are proving. Therefore, $\tilde{\psi} \in \widetilde{\Phi}$. Thus, the conditions of the main theorem hold for the set $\widetilde{\Phi}$ of homomorphisms from the 0-indexed group $\widetilde{F}$ to G. Therefore, $|\widetilde{\Phi}|$ is divisible on $|H|$ by virtue of the main theorem of [Klyachko and Mkrtchyan 2017]. It remains to note that $|\Phi| = |\widetilde{\Phi}|$ since α is surjective. This completes the proof.

Note that we do not verify here that ψ defines a homomorphism; this is non-obvious but true; see Section 1.

6. Open questions

Theorems 0, 1, 4, and 5 assert that some numbers are multiples of the ratios of two integers. Oddly, we do not know *whether these ratios can be replaced by their numerators*.

Questions 6 and 7. *Is it possible to replace the ratio* Δ_m/Δ_{m-1} *by its numerator* Δ_m *in Theorems 0 and 1*?

For coefficient-free systems of equations, Question 6 is equivalent to the following question posed in [Asai and Yoshida 1993] (for finite groups F and G):

> *is the number of homomorphisms from a finitely generated group* F *to a group* G *divisible by* $\mathrm{GCD}(|F/F'|, G)$?

This problem remains unsolved even for finite groups (as far as we know). A survey of some results can be found in [Asai and Takegahara 2001]; e.g., the answer is positive if F is abelian [Yoshida 1993].

Theorem 4 suggests a similar question.

Question 8. *Is it possible*, *in Theorem 4*, *to replace the homogeneity modulus by its numerator* Δ_{m+s} (see the homogeneity-modulus lemma)?

As for Theorem 5, it also leads us to a similar question. Indeed, Theorem 5 implies, in particular, the following corollary.

Corollary. *If a finitely generated group* F *acts by automorphisms on a group* B, *then* $\mathrm{GCD}(\exp(F/F'), B)$ *divides the number of crossed homomorphisms* $F \to B$.

Question 9. *Is it possible*, *in this corollary*, *to replace the period* $\exp(F/F')$ *by the order of this quotient group*?

This question was posed for the first time in [Asai and Yoshida 1993] (for finite groups F and B). To show the similarity of Questions 9 and 6, we recall that the absolute value of the ratio Δ_m/Δ_{m-1} in Question 6 is the period of the quotient group of the free abelian group $\mathbb{Z}^m$ by the subgroup generated by the rows of the matrix of the system of equations, while the absolute value of the numerator Δ_m is the order of this quotient group.

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ON HOMOGENEOUS AND INHOMOGENEOUS DIOPHANTINE APPROXIMATION OVER THE FIELDS OF FORMAL POWER SERIES

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We prove over fields of power series the analogues of several Diophantine approximation results obtained over the field of real numbers. In particular we establish the power series analogue of Kronecker's theorem for matrices, together with a quantitative form of it, which can also be seen as a transference inequality between uniform approximation and inhomogeneous approximation. Special attention is devoted to the one-dimensional case. Namely, we give a necessary and sufficient condition on an irrational power series α which ensures that, for some positive ε, the set

$$\liminf_{Q\in\mathbb{F}_q[z],\ \deg Q\to\infty} \|Q\|\cdot\min_{y\in\mathbb{F}_q[z]}\|Q\alpha-\theta-y\|\geq\varepsilon$$

has full Hausdorff dimension.

1. Introduction

Let q be a power of a prime number p and $\mathbb{F}_q$ the finite field of order q. Recall that $\mathbb{F}_q[z]$ and $\mathbb{F}_q(z)$ denote the ring of polynomials and the field of rational functions over $\mathbb{F}_q$, respectively. Let $\mathbb{F}_q((z^{-1}))$ denote the field of formal power series $x=\sum_{i=-n}^{\infty}a_iz^{-i}$ over the field $\mathbb{F}_q$. We equip $\mathbb{F}_q((z^{-1}))$ with the norm $\|x\|=q^n$, where $a_{-n}\neq 0$ is the first nonzero coefficient in the expansion of the nonzero power series x. This integer n is called the degree of x and denoted by $\deg x$.

The sets $\mathbb{F}_q[z]$, $\mathbb{F}_q(z)$, and $\mathbb{F}_q((z^{-1}))$ play the roles of $\mathbb{Z}$, $\mathbb{Q}$, and $\mathbb{R}$, respectively. A power series x in $\mathbb{F}_q((z^{-1}))$ but not in $\mathbb{F}_q(z)$ is called irrational. We denote by $[x]$ and $\{x\}$ the "integral part" and the "fractional part" of the power series $x=\sum_{i=-n}^{\infty}a_iz^{-i}$ in $\mathbb{F}_q((z^{-1}))$, defined as

$$[x]=\sum_{i=-n}^{0}a_iz^{-i},\quad \{x\}=\sum_{i=1}^{\infty}a_iz^{-i}.$$

In particular, $[x]$ is a polynomial in z.

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Let $\mathbb{I} = \{x \in \mathbb{F}_q((z^{-1})) : \|x\| < 1\}$ be the open unit ball. A natural measure on $\mathbb{I}$ is the normalized Haar measure on $\prod_{n=1}^{\infty} \mathbb{F}_q$, which we denote by μ. Observe that $\mu(\mathbb{I}) = 1$. If $B(x, q^{-r})$ is the open ball of center x in $\mathbb{I}$ and radius q^{-r}, namely,

$$B(x, r) = \{y \in \mathbb{I} : \|y - x\| < q^{-r}\},$$

then $\mu(B(x, q^{-r})) = q^{-r}$. Since the norm $\|\cdot\|$ is non-Archimedean, any two balls C_1 and C_2 satisfy either $C_1 \cap C_2 = \varnothing$, $C_1 \subset C_2$, or $C_2 \subset C_1$. This is sometimes referred to as *the ball intersection property*. Moreover, the distance between any two disjoint balls is not less than the maximal radius of the two balls.

For any (column) vector $\underline{\theta}$ in $\mathbb{F}_q((z^{-1}))^n$, we denote by $\|\underline{\theta}\|$ the maximum of the norm of its coordinates and by

$$|\langle\underline{\theta}\rangle| = \min_{\underline{y} \in \mathbb{F}_q[z]^n} \|\underline{\theta} - \underline{y}\|$$

the maximum of the distances of its coordinates to their integral parts.

There are numerous results on Diophantine approximation in the fields of formal power series, see [Lasjaunias 2000] and Chapter 9 of [Bugeaud 2004] for references; more recent works include [Bank et al. 2017; Ganguly and Ghosh 2017; 2019; Kristensen 2003; Zhang 2012; Zheng 2017]. However, few results are known on the relation between homogenous and inhomogeneous Diophantine approximation. Our first result is the analogue of Kronecker's theorem over fields of formal power series. As far as we are aware, it has not yet been proved in such a generality (see, however, [Carlitz 1952; Mahler 1941] for the case of column matrices). The transposed matrix of a matrix A is denoted by A^T.

Theorem 1.1. *Let m, n be positive integers. Let A be in $\mathcal{M}_{n,m}(\mathbb{F}_q((z^{-1})))$ and $\underline{\theta}$ in $\mathbb{F}_q((z^{-1}))^n$. Then the following two statements are equivalent*:

(1) *For every $\varepsilon > 0$, there exists a polynomial vector $\underline{x}$ in $\mathbb{F}_q[z]^m$ such that*

$$|\langle A\underline{x} - \underline{\theta}\rangle| \le \varepsilon.$$

(2) *If $\underline{u} = (u_1, \dots, u_n)^T$ is any polynomial vector such that $A^T\underline{u}$ is in $\mathbb{F}_q[z]^m$, then*

$$u_1\theta_1 + \cdots + u_n\theta_n \in \mathbb{F}_q[z].$$

As in [Bugeaud and Laurent 2005], which deals with the real case, our aim is to give a quantitative version of Theorem 1.1. Following [Bugeaud and Laurent 2005], we introduce several exponents of homogeneous and inhomogeneous Diophantine approximation. Let n and m be positive integers and A a matrix in $\mathcal{M}_{n,m}(\mathbb{F}_q((z^{-1})))$. Let $\underline{\theta}$ be in $\mathbb{F}_q((z^{-1}))^n$. We denote by $\omega(A, \underline{\theta})$ the supremum of the real numbers ω for which, for arbitrarily large real numbers H, the inequalities

$$|\langle A\underline{x} - \underline{\theta}\rangle| \le H^{-\omega} \quad \text{and} \quad \|\underline{x}\| \le H \tag{1}$$

have a solution $\underline{x}$ in $\mathbb{F}_q[z]^m$. Let $\widehat{\omega}(A,\underline{\theta})$ be the supremum of the real numbers ω for which, for all sufficiently large positive real numbers H, the inequalities (1) have a solution $\underline{x}$ in $\mathbb{F}_q[z]^m$. It is obvious that

$$\omega(A,\underline{\theta}) \geq \widehat{\omega}(A,\underline{\theta}) \geq 0.$$

We define furthermore two homogeneous exponents $\omega(A)$ and $\widehat{\omega}(A)$ as in (1) when $\underline{\theta}$ is the zero vector, requiring moreover that the polynomial solution $\underline{x}$ should be nonzero.

Our second result is the power series analogue of the main result of [Bugeaud and Laurent 2005]. Throughout this paper, the quantity $1/+\infty$ is understood to be 0.

Theorem 1.2. *Let m,n be positive integers. Let A be in $\mathcal{M}_{n,m}(\mathbb{F}_q((z^{-1})))$ and $\underline{\theta}$ in $\mathbb{F}_q((z^{-1}))^n$. Then, we have the lower bounds*

$$\omega(A,\underline{\theta}) \geq \frac{1}{\widehat{\omega}(A^T)} \quad \text{and} \quad \widehat{\omega}(A,\underline{\theta}) \geq \frac{1}{\omega(A^T)}, \tag{2}$$

with equalities in (2) *for almost all $\underline{\theta}$ with respect to the Haar measure on $\mathbb{F}_q((z^{-1}))^n$. If $\underline{\theta}$ is not in $A\mathbb{F}_q[z]^m+\mathbb{F}_q[z]^n$, then we also have the upper bound*

$$\widehat{\omega}(A,\underline{\theta}) \leq \omega(A).$$

If the subgroup $G_A = A^T\mathbb{F}_q[z]^n + \mathbb{F}_q[z]^m$ of $\mathbb{F}_q((z^{-1}))^m$ has rank $\mathrm{rk}_{\mathbb{F}_q[z]}(G_A)$ smaller than $m+n$, then there exists $\underline{x}$ in $\mathbb{F}_q[z]^n$ with arbitrarily large norm such that $|\langle A^T\underline{x}\rangle| = 0$ and we have

$$\widehat{\omega}(A^T) = \omega(A^T) = +\infty.$$

Throughout the paper, we avoid this degenerate case and consider only matrices A for which $\mathrm{rk}_{\mathbb{F}_q[z]}(G_A) = m+n$.

Kim and Nakada [2011] proved that, for any α in $\mathbb{I}$, we have

$$\liminf_{n\to\infty}(q^n \min_{\deg Q=n} \|\{Q\alpha\}-\beta\|) = 0$$

for almost all β in $\mathbb{I}$. In a subsequent paper [Kim et al. 2013], the authors complemented this result in showing that, for any irrational power series α in $\mathbb{I}$, the set

$$\{\beta\in\mathbb{I} : \liminf_{n\to\infty}(q^n \min_{\deg Q=n} \|\{Q\alpha\}-\beta\|) > 0\}$$

has full Hausdorff dimension. Our next result generalizes this statement to matrices of arbitrary dimension. Before stating it, we introduce the following notation.

Let m,n be positive integers and A in $\mathcal{M}_{n,m}(\mathbb{F}_q((z^{-1})))$. For $\varepsilon>0$, we define the set

$$\mathrm{Bad}^{\varepsilon}(A) := \{\underline{\theta}\in\mathbb{I}^n : \liminf_{\underline{x}\in\mathbb{F}_q[z]^m,\ \|\underline{x}\|\to\infty} \|\underline{x}\|^{m/n}\cdot|\langle A\underline{x}-\underline{\theta}\rangle| \geq \varepsilon\}$$

and we put

$$\mathrm{Bad}(A) := \bigcup_{\varepsilon>0} \mathrm{Bad}^{\varepsilon}(A) = \{\underline{\theta} \in \mathbb{I}^n : \liminf_{\underline{x}\in\mathbb{F}_q[z]^m,\ \|\underline{x}\|\to\infty} \|\underline{x}\|^{m/n} \cdot |\langle A\underline{x} - \underline{\theta}\rangle| > 0\}.$$

When $n = m = 1$ and $A = (\alpha)$ we simply write $\mathrm{Bad}^{\varepsilon}(\alpha)$ and $\mathrm{Bad}(\alpha)$ instead of $\mathrm{Bad}^{\varepsilon}(A)$ and $\mathrm{Bad}(A)$.

Theorem 1.3. *Let m, n be positive integers. For any matrix A in $\mathcal{M}_{n,m}(\mathbb{F}_q((z^{-1})))$, the set* $\mathrm{Bad}(A)$ *has full Hausdorff dimension. More precisely, there exists a continuous function $f : \mathbb{R}_+ \to \mathbb{R}_+$ such that $f(0) = 0$ and the Hausdorff dimension of the set* $\mathrm{Bad}^{\varepsilon}(A)$ *is at least $n - f(\varepsilon)$, for every positive $\varepsilon \le q^{-m/n-6}$.*

If the sequence of the norms of the best approximation vectors associated to A (see Definition 3.3) increases sufficiently rapidly, then the above results can be strengthened as follows. Similar results in the real case have been established in [Bugeaud et al. 2019].

Theorem 1.4. *Let m, n be positive integers. Let A be in $\mathcal{M}_{n,m}(\mathbb{F}_q((z^{-1})))$ and $(\underline{y}_k)_{k\ge1}$ the sequence of best approximation vectors associated to A. If $\|\underline{y}_k\|^{1/k}$ tends to infinity with k, then there exists a positive real number ε such that the set* $\mathrm{Bad}^{\varepsilon}(A)$ *has full Hausdorff dimension. More precisely, ε can be taken to be any positive real number less than $q^{-4-m/n}$. Moreover, if $m = n = 1$, $A = (\alpha)$, and the degree of the partial quotients in the continued fraction expansion of α in $\mathbb{F}_q((z^{-1}))$ tends to infinity, then the set* $\mathrm{Bad}^{\varepsilon}(\alpha)$ *has full Hausdorff dimension for every $\varepsilon \le q^{-2}$.*

Except for $(m, n) = (1, 1)$ (see the next section), we do not know whether the condition "$\|\underline{y}_k\|^{1/k}$ tends to infinity with k" is necessary to ensure that $\mathrm{Bad}^{\varepsilon}(A)$ has full Hausdorff dimension for some positive ε.

The present paper is organized as follows. In Section 2, we give additional results in the one-dimensional case, including necessary and sufficient conditions to ensure that the set $\mathrm{Bad}^{\varepsilon}(\alpha)$ has full Hausdorff dimension. In Section 3, we present some auxiliary results. A transference lemma is established in Section 4, where we also give the proof of Theorem 1.1. The proofs of Theorem 1.2, Theorem 1.3, and Theorem 1.4 are given in Sections 5, 6, and 7, respectively. We use similar arguments to those in the real case. In Section 8, we prove Theorem 2.3. The proofs of Theorem 2.1 and Theorem 2.2 are postponed to Sections 9 and 10.

2. One-dimensional case

In the one-dimensional case, Theorem 1.4 can be complemented as follows.

Theorem 2.1. *Let α be an irrational power series in $\mathbb{F}_q((z^{-1}))$ and Q_k the denominator of its k-th convergent for $k \ge 1$. Then, there exists $\varepsilon > 0$ such that the set* $\mathrm{Bad}^{\varepsilon}(\alpha)$ *has full Hausdorff dimension if and only if* $\lim_{k\to\infty} \|Q_k\|^{1/k} = \infty$.

In addition, we give a third condition equivalent to those occurring in Theorem 2.1. For an irrational power series α in $\mathbb{I}$ and a positive real number c, let $\Delta_{N,c}(\alpha)$ denote the number of integers l in $\{1, \dots, N\}$ for which the inequality $\|\{Q\alpha\}\| \le c2^{-l}$ has a solution Q in $\mathbb{F}_q[z]$ with $0 < \|Q\| \le 2^l$. Then, the power series α is called singular on average if, for every $c > 0$, we have $\lim_{N\to\infty} \frac{1}{N}\Delta_{N,c}(\alpha) = 1$. As far as we are aware, this notion was introduced in [Kadyrov et al. 2017].

Theorem 2.2. *Let α be an irrational power series. There exists $\varepsilon > 0$ such that the set* $\mathrm{Bad}^{\varepsilon}(\alpha)$ *has full Hausdorff dimension if and only if α is singular on average.*

Theorems 2.1 and 2.2 are the power series analogues of Theorem 1.1 of [Bugeaud et al. 2019]. In the proof of Theorem 2.1, our method is different: we replace the use of the three-distance theorem in [Bugeaud et al. 2019] by that of Ostrowski expansions; see Theorem 9.1 and its proof. Theorem 2.2 is proved in a similar way to that in the real case.

Our last result gives additional information about the relation between the exponents of homogeneous and inhomogeneous Diophantine approximation in dimension one. Its first statement has already been established in Theorem 1.2.

Theorem 2.3. *Let ξ in $\mathbb{F}_q((z^{-1}))$ be an irrational power series. For any element θ in $\mathbb{F}_q((z^{-1}))$ not in $\mathbb{F}_q[z] + \xi\mathbb{F}_q[z]$, we have*

$$\frac{1}{\omega((\xi))} \le \widehat{\omega}((\xi), \theta) \le \omega((\xi)).$$

Let ω denote $+\infty$ or a real number greater than or equal to 1; *then there exists a ξ in $\mathbb{F}_q((z^{-1}))$ for which $\omega((\xi)) = \omega$ and the set of values taken by the function $\widehat{\omega}((\xi), \cdot)$ is equal to the interval* $\left[\frac{1}{\omega}, \omega\right]$.

Theorem 2.3 is the power series analogue of Proposition 8 of [Bugeaud and Laurent 2005] and its proof uses similar arguments.

3. Preliminaries

In this section, we briefly recall some notation and classical results which will be used later in the proofs of our theorems.

In the setting of formal power series, every irrational element α in $\mathbb{I}$ has a unique infinite continued fraction expansion over the field $\mathbb{F}_q((z^{-1}))$, which is induced by the map

$$T\alpha = \frac{1}{\alpha} - \left[\frac{1}{\alpha}\right].$$

The reader is referred to Artin [1924a; 1924b] or Berthé and Nakada [2000] for more details. For every irrational power series α in $\mathbb{I}$, we denote by $\alpha = [0; A_1, A_2, \dots]$ its continued fraction expansion, where $A_k = A_k(\alpha) := [1/(T^{k-1}\alpha)]$ is called the k-th partial quotient of α. For each $k \ge 1$, $P_k(\alpha)/Q_k(\alpha) = [0, A_1, A_2, \dots, A_k]$ is the

k-th convergent of α. This defines $P_k(\alpha)$ and $Q_k(\alpha)$ up to a common multiplicative factor. To define numerator and denominator of the k-th convergent of α, we set $P_{-1}(\alpha) = Q_0(\alpha) = 1$ and $Q_{-1}(\alpha) = P_0(\alpha) = 0$, and, for any $k \geq 0$,

$$P_{k+1}(\alpha) = A_{k+1}(\alpha) P_k(\alpha) + P_{k-1}(\alpha),$$
$$Q_{k+1}(\alpha) = A_{k+1}(\alpha) Q_k(\alpha) + Q_{k-1}(\alpha).$$

The following elementary properties of continued fraction expansions of formal power series are well known (see Fuchs [2002] for details).

Lemma 3.1 [Fuchs 2002]. *Under the above notation, we have for $k \geq 1$:*

(1) $(P_k(\alpha), Q_k(\alpha)) = 1$.

(2) $1 = \|Q_0(\alpha)\| < \|Q_1(\alpha)\| < \|Q_2(\alpha)\| < \cdots$.

(3) $\|Q_k(\alpha)\| = \prod_{i=1}^{k} \|A_i(\alpha)\|$.

(4) $P_{k-1}(\alpha) Q_k(\alpha) - P_k(\alpha) Q_{k-1}(\alpha) = (-1)^k$.

We also need a version of Dirichlet's theorem in the fields of formal power series. The next statement follows from Theorem 2.1 of [Ganguly and Ghosh 2017].

Theorem 3.2. *Let m, n be positive integers. Let A be in $\mathcal{M}_{n,m}(\mathbb{F}_q((z^{-1})))$. Then, for any positive integer c, there is a nonzero polynomial vector $\underline{u}$ such that*

$$|\langle A\underline{u}\rangle| < q^{-c\frac{m}{n}} \quad \textit{and} \quad 1 \leq \|\underline{u}\| \leq q^c.$$

In dimension greater than one, we deal with sequences of vectors having similar properties to the sequence of convergents in dimension one. For this purpose, for a matrix $A = (\alpha_{i,j})_{1 \leq i \leq n, 1 \leq j \leq m}$, we denote by

$$M_j(\underline{y}) = \sum_{i=1}^{n} \alpha_{ij} y_i, \quad \underline{y} = (y_1, \ldots, y_n)^T, \quad 1 \leq j \leq m,$$

the linear forms determined by its columns. Then, for $\underline{y}$ in $\mathbb{F}_q((z^{-1}))^n$, we set

$$M(\underline{y}) = \max_{1 \leq j \leq m} |\langle M_j(\underline{y})\rangle| = |\langle A^T \underline{y}\rangle|.$$

Definition 3.3. For a sequence of polynomial vectors $(\underline{y}_i)_{i \geq 1}$, write

$$\|\underline{y}_i\| = Y_i, \quad M_i = M(\underline{y}_i).$$

If the sequence satisfies

$$1 = Y_1 < Y_2 < \cdots, \qquad M_1 > M_2 > \cdots$$

and $M(\underline{y}) \geq M_i$ for all nonzero polynomial vectors $\underline{y}$ of norm $\|\underline{y}\| < Y_{i+1}$, then it is called a sequence of best approximations related to the matrix A^T (or to the linear forms $M_1, M_2, \ldots, M_m$).

Now we construct inductively a sequence of best approximations related to the matrix A^T.

Let $Y_1 = \|\underline{y_1}\| = 1$, and $M(\underline{y}) \geq M(\underline{y_1}) = M_1$ for any polynomial vector $\underline{y}$ in $\mathbb{F}_q[z]^n$ with $\|\underline{y}\| = 1$.

Suppose that $\underline{y_1}, \ldots, \underline{y_i}$ have already been constructed in such a way that $M(\underline{y}) \geq M_i$ for all nonzero polynomial vectors $\underline{y}$ with $\|\underline{y}\| \leq Y_i$. Let Y be the smallest integer power of q greater than Y_i and for which there exists a polynomial vector $\underline{z}$ with $\|\underline{z}\| = Y$ and $M(\underline{z}) < M_i$. Since M_i is positive, the integer Y does exist by Theorem 3.2. Among those points $\underline{z}$, we select an element $\underline{y}$ for which $M(\underline{z})$ is minimal. Then we set

$$\underline{y}_{i+1} = \underline{y}, \; Y_{i+1} = Y, \quad \text{and} \quad M_{i+1} = M(\underline{y}).$$

The sequence $(\underline{y}_i)_{i\geq 1}$ constructed in this way enjoys the desired properties.

The following two lemmas collect some properties of the sequence of best approximations.

Lemma 3.4. *Let $(\underline{y}_i)_{i\geq 1}$ be the sequence of best approximations related to the linear forms $M_1, \ldots, M_m$. Then we have*:

(i) *$Y_i \geq q^i$ for $i \geq 1$.*

(ii) *$M_i < q^{\frac{n}{m}} Y_{i+1}^{-\frac{n}{m}}$ for $i \geq 1$.*

(iii) *For $\omega < \widehat{\omega}(A^T)$, $M_i \leq Y_{i+1}^{-\omega}$ holds for any sufficiently large i.*

(iv) *For $\omega < \omega(A^T)$, $M_i \leq Y_i^{-\omega}$ holds for infinitely many i.*

Remark. In the special case $m = 1$, (ii) can be replaced by the large inequality $M_i \leq q^{n-1} Y_{i+1}^{-n}$.

Proof. (i). This is immediate since $Y_{i+1} \geq qY_i$.

(ii). It follows from Theorem 3.2 that the system of inequalities

$$M(\underline{y}) < q^{-c\frac{n}{m}} \quad \text{and} \quad \|\underline{y}\| \leq q^c$$

has a nonzero polynomial $\underline{y}$ for $q^c = q^{-1}Y_{i+1}$. This implies $M_i < (q^{-1}Y_{i+1})^{-n/m}$, as asserted.

(iii). Let ω with $0 < \omega < \widehat{\omega}(A^T)$. Then, the system of inequalities

$$M(\underline{y}) \leq H^{-\omega} \quad \text{and} \quad \|\underline{y}\| \leq H$$

has a nonzero solution for any sufficiently large real number H. In particular, for every sufficiently large integer i, the system of inequalities

$$M(\underline{y}) \leq Y_{i+1}^{-\omega} \quad \text{and} \quad \|\underline{y}\| < Y_{i+1}$$

has a nonzero solution $\underline{z}_i$, satisfying

$$M_i \le M(\underline{z}_i) \le Y_{i+1}^{-\omega}.$$

(iv). For $\omega < \omega(A^T)$, there are infinitely many polynomial vectors $\underline{h}$ in $\mathbb{F}_q((z^{-1}))^n$ such that $M(\underline{h}) \le \|\underline{h}\|^{-\omega}$. For every such $\underline{h}$ in $\mathbb{F}_q((z^{-1}))^n$, there exists an index i such that $Y_i \le \|\underline{h}\| < Y_{i+1}$. Then, $M_i \le M(\underline{h}) \le \|\underline{h}\|^{-\omega} \le Y_i^{-\omega}$. □

Lemma 3.5. *Let $(\underline{y}_i)_{i\ge1}$ be the sequence of best approximations related to the linear forms $M_1, \dots, M_m$. Then, for almost all $\underline{\theta} = (\theta_1, \dots, \theta_n)^T$ in $\mathbb{F}_q((z^{-1}))^n$, we have*

$$|\langle \underline{y}_i\, \underline{\theta}\rangle| \ge Y_i^{-\delta},$$

for any $\delta > 0$ and any index i which is sufficiently large in terms of δ and $\underline{\theta}$.

Proof. For any $\delta > 0$ and any $i \ge 1$, consider the set

$$B(\underline{y}_i) = \{\underline{\theta} = (\theta_1, \dots, \theta_n)^T : |\langle \underline{y}_i\, \underline{\theta}\rangle| < Y_i^{-\delta}\}.$$

It follows from equality (2.3) in [Kristensen 2003] that the Haar measure of $B(\underline{y}_i)$ is bounded from above by $Y_i^{-\delta}$ times some absolute, positive constant. Combined with the fact that $Y_i \ge q^i$ for $i \ge 1$, which ensures that the series $\sum_{i\ge1} Y_i^{-\delta}$ converges, we deduce from the Borel–Cantelli lemma that the set of $\underline{\theta}$ which belong to infinitely many sets $B(\underline{y}_i)$ has Haar measure zero. This implies the lemma. □

Let α be in $\mathbb{I}$. Denote by $[0\,; A_1, A_2, \dots]$ its continued fraction expansion and by $(P_k)/(Q_k)$ its k-th convergent, for $k \ge 0$. Set

$$D_k = Q_k\alpha - P_k \quad \text{for } k \ge 1.$$

Lemma 3.6 [Fuchs 2002]. *Under the above notation, we have*

(1) $D_{k+1} = A_{k+1}D_k + D_{k-1}$,

(2) $\|D_k\| = \|Q_k\alpha - P_k\| = \|\{Q_k\alpha\}\| = \frac{1}{\|Q_{k+1}\|}$.

In addition to continued fractions, we also make use of the Ostrowski expansion of the elements of $\mathbb{I}$ with respect to an irrational power series α.

Lemma 3.7 [Kim and Nakada 2011]. *Under the above notation, for every positive integer k and every Q in $\mathbb{F}_q[z]$ with* $\deg Q < \deg Q_{k+1}$, *there is a unique decomposition*

$$Q = B_1Q_0 + B_2Q_1 + \cdots + B_{k+1}Q_k,$$

where B_i is in $\mathbb{F}_q[z]$ and $\deg B_i < \deg A_i$ *for $1 \le i \le k+1$.*

Lemma 3.8 [Kim et al. 2013]. *Under the above notation, for every β in $\mathbb{I}$, there is a representation of β under the form*

$$\beta = \sum_{k=0}^{\infty} \sigma_{k+1}(\beta) D_k = \sigma_1(\beta) D_0 + \sigma_2(\beta) D_1 + \cdots, \tag{3}$$

where $\sigma_i(\beta)$ is in $\mathbb{F}_q[z]$ and $\deg \sigma_i(\beta) < \deg A_i(\alpha)$ for $i \geq 1$. The representation (3) *is called the Ostrowski expansion of β with respect to α or an α-expansion for β.*

For simplicity, we write

$$\beta = [\sigma_1(\beta), \sigma_2(\beta), \ldots, \sigma_n(\beta), \ldots]_\alpha$$

and call the sequence $(\sigma_n(\beta))_{n\geq 1}$ the sequence of digits of β. To facilitate the exposition, we make use of a kind of symbolic space defined as follows.

For any $n \geq 1$, set

$$\mathbb{L}_n(\alpha) = \{(\sigma_1, \ldots, \sigma_n) : \sigma_i \in \mathbb{F}_q[z] \text{ and } \deg \sigma_i < \deg A_i(\alpha) \text{ for } 1 \leq i \leq n\}$$

$$\mathbb{L}(\alpha) = \bigcup_{n=1}^{\infty} \mathbb{L}_n(\alpha).$$

Then, for any $(\sigma_1, \ldots, \sigma_n)$ in $\mathbb{L}_n(\alpha)$, there exists an element β in $\mathbb{I}$ whose sequence of digits begins with $(\sigma_1, \ldots, \sigma_n)$.

For an n-tuple $\sigma = (\sigma_1, \ldots, \sigma_n)$ in $\mathbb{L}_n(\alpha)$, we call

$$I_n(\sigma_1, \ldots, \sigma_n) = \{\beta \in \mathbb{I} : \sigma_k(\beta) = \sigma_k \text{ for } 1 \leq k \leq n\}$$

a cylinder of order n; this is the set of formal power series in $\mathbb{I}$ which have an α-expansion beginning with $\sigma_1, \ldots, \sigma_n$.

For the size of the cylinder, we have the following lemma.

Lemma 3.9 [Kim et al. 2013]. *For any $\sigma = (\sigma_1, \ldots, \sigma_n)$ in $\mathbb{L}_n(\alpha)$, the n-th cylinder $I_n(\sigma_1, \ldots, \sigma_n)$ is a closed disc centered at $\sum_{k=0}^{n-1} \sigma_{k+1} D_k$ and of diameter $q^{-\deg Q_n - 1}$.*

4. A transference lemma and the proof of Theorem 1.1

Recall that

$$M_j(\underline{y}) = \sum_{i=1}^{n} \alpha_{i,j} y_i, \quad \underline{y} = (y_1, \ldots, y_n)^T, \qquad 1 \leq j \leq m,$$

are the linear forms determined by the columns of the matrix $A = (\alpha_{i,j})$, and

$$L_i(\underline{x}) = \sum_{j=1}^{m} \alpha_{i,j} x_j, \quad \underline{x} = (x_1, \ldots, x_m)^T, \qquad 1 \leq i \leq n,$$

are the linear forms determined by its rows.

In this section, by using a similar method to that in the real case (see [Cassels 1957]), we prove a transference lemma, which establishes a relation between inhomogeneous simultaneous approximation and homogeneous approximation. To give the proof, we need some auxiliary results. We first state a power series analogue of Theorem XVI on page 97 of [Cassels 1957].

Theorem 4.1. *Let l be a positive integer and $f_k(\underline{\theta})$, $g_k(\underline{\xi})$ for $1 \le k \le l$ be linear forms in $\underline{\theta} = (\theta_1, \dots, \theta_l)$ and $\underline{\xi} = (\xi_1, \dots, \xi_l)$, respectively. Suppose that*

$$\sum_{k=1}^{l} f_k(\underline{\theta}) g_k(\underline{\xi}) = \sum_{k=1}^{l} \theta_k \xi_k \tag{4}$$

identically. Let $\underline{\beta} = (\beta_1, \dots, \beta_l)$ be a vector in $\mathbb{F}_q((z^{-1}))^l$. If

$$\left| \left\langle \sum_{k=1}^{l} g_k(\underline{\xi}) \beta_k \right\rangle \right| \le \max_{1 \le k \le l} \|g_k(\underline{\xi})\| \tag{5}$$

holds for all polynomial vectors $\underline{\xi}$, then there exists a polynomial vector $\underline{b}$ in $\mathbb{F}_q[z]^l$ such that

$$|\langle \beta_k - f_k(\underline{b}) \rangle| \le 1, \qquad 1 \le k \le l. \tag{6}$$

Proof. We regard $\underline{\xi}$ as a row vector and $\underline{\theta}$ and $\underline{\beta}$ as column vectors. Let $G = (g_{i,j})$ be the $l \times l$ square matrix whose k-th column is the coefficients of g_k and $F = (f_{i,j})$ be the $l \times l$ square matrix whose k-th row is the coefficients of f_k. Then, (4) becomes

$$(\xi_1, \xi_2, \dots, \xi_l) \begin{pmatrix} g_{11} & g_{21} & \cdots & g_{l1} \\ g_{12} & g_{22} & \cdots & g_{l2} \\ \vdots & \vdots & \ddots & \vdots \\ g_{1l} & g_{2l} & \cdots & g_{ll} \end{pmatrix} \begin{pmatrix} f_{11} & f_{12} & \cdots & f_{1l} \\ f_{21} & f_{22} & \cdots & f_{2l} \\ \vdots & \vdots & \ddots & \vdots \\ f_{l1} & f_{l2} & \cdots & f_{ll} \end{pmatrix} \begin{pmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_l \end{pmatrix} = \sum_{k=1}^{l} \theta_k \xi_k.$$

This implies that

$$G = F^{-1}. \tag{7}$$

By the analogue of Minkowski's theorem in $\mathbb{F}_q((z^{-1}))$ proved in Section 9 of [Mahler 1941] and applied to the convex body $\max_{1 \le j \le l} \|g_j(\underline{\xi})\| \le 1$, there is a polynomial $l \times l$ matrix W with $\|\det W\| = 1$ whose k-th row $\underline{w}^{(k)}$ satisfies

$$\max_{1 \le j \le l} \|g_j(\underline{w}^{(k)})\| = \mu_k, \qquad \prod_{k=1}^{l} \mu_k = \|\det G\|, \tag{8}$$

where the positive real numbers μ_k, $1 \le k \le l$, are the successive minima for the function $\max_{1 \le j \le l} \|g_j(\underline{\xi})\|$.

By (5), (8), and the definition of $g_k(\underline{\xi})$, we have

$$
\begin{aligned}
WG\underline{\beta} &= \begin{pmatrix} \underline{w}^{(1)}G \\ \underline{w}^{(2)}G \\ \vdots \\ \underline{w}^{(l)}G \end{pmatrix} \underline{\beta} \\
&= \begin{pmatrix} g_1(\underline{w}^{(1)}) & g_2(\underline{w}^{(1)}) & \cdots & g_l(\underline{w}^{(1)}) \\ g_1(\underline{w}^{(2)}) & g_2(\underline{w}^{(2)}) & \cdots & g_l(\underline{w}^{(2)}) \\ \vdots & \vdots & \ddots & \vdots \\ g_1(\underline{w}^{(l)}) & g_2(\underline{w}^{(l)}) & \cdots & g_l(\underline{w}^{(l)}) \end{pmatrix} \begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_l \end{pmatrix} \\
&= \begin{pmatrix} \sum_{j=1}^{l} \beta_j g_j(\underline{w}^{(1)}) \\ \sum_{j=1}^{l} \beta_j g_j(\underline{w}^{(2)}) \\ \vdots \\ \sum_{j=1}^{l} \beta_j g_j(\underline{w}^{(l)}) \end{pmatrix} = \underline{a} + \underline{\delta},
\end{aligned}
$$

where $\underline{a}$ is polynomial vector and

(9) $$\|\underline{\delta_k}\| \le \mu_k \quad \text{for } 1 \le k \le l.$$

Hence, by (7), we get

(10) $$\underline{\beta} = F\underline{b} + \underline{\gamma},$$

where $\underline{b} = W^{-1}\underline{a}$ and $\underline{\delta} = WG\underline{\gamma}$. Here, $\underline{b}$ is also a polynomial vector since $\|\det W\| = 1$. By the matrix operation on the ring of matrices whose coordinates are in the fields of power series, we get

$$\gamma_j = \frac{\det((WG)_j)}{\det(WG)^{-1}},$$

where

$$(WG)_j = \begin{pmatrix} g_1(\underline{w}^{(1)}) & \cdots & g_{j-1}(\underline{w}^{(1)}) & \delta_1 & g_{j+1}(\underline{w}^{(1)}) & \cdots & g_l(\underline{w}^{(1)}) \\ g_1(\underline{w}^{(2)}) & \cdots & g_{j-1}(\underline{w}^{(2)}) & \delta_2 & g_{j+1}(\underline{w}^{(2)}) & \cdots & g_l(\underline{w}^{(2)}) \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ g_1(\underline{w}^{(l)}) & \cdots & g_{j-1}(\underline{w}^{(l)}) & \delta_l & g_{j+1}(\underline{w}^{(l)}) & \cdots & g_l(\underline{w}^{(l)}) \end{pmatrix}.$$

By (8), the norm of the k-th row of the WG is at most μ_k. Combined with (9), we get

(11) $$\|\gamma_j\| \le \|\det G\|^{-1} \prod_{k=1}^{l} \mu_k \le 1,$$

which gives

$$|\langle \beta_k - f_k(\underline{b}) \rangle| \le 1, \qquad 1 \le k \le l. \qquad \square$$

Corollary 4.2. *Let $L_j(\underline{x})$ and $M_i(\underline{u})$ be as above and set $l = m + n$. Let $\underline{\alpha} = (\alpha_1, \dots, \alpha_n)$ in $\mathbb{F}_q((z^{-1}))^n$, and s and t be positive integers. Suppose that*

$$|\langle u_1\alpha_1 + \cdots + u_n\alpha_n\rangle| \le \max\{q^t \max_{1\le i\le m} |\langle M_i(\underline{u})\rangle|, q^{-s} \max_{1\le j\le n} \|u_j\|\} \tag{12}$$

holds for all polynomial vectors $\underline{u}$. Then, there exists a polynomial vector $\underline{b} = (b_1, \dots, b_m)$ with

$$|\langle L_j(\underline{b}) - \alpha_j\rangle| \le q^{-s}, \quad \|b_j\| \le q^t, \qquad j = 1, \dots, m.$$

Proof. This is a special case of Theorem 4.1. Let C and X be in $\mathbb{F}_q((z^{-1}))$ with $\|C\| = q^{-s}$ and $\|X\| = q^t$. Let

$$\underline{\theta} = (\underline{x}, \underline{z}) = (x_1, \dots, x_m, z_1, \dots, z_n),$$
$$\underline{\xi} = (\underline{v}, \underline{u}) = (v_1, \dots, v_m, u_1, \dots, u_n),$$
$$f_k(\underline{\theta}) = \begin{cases} C^{-1}(L_k(\underline{x}) + z_k) & \text{for } k \le n, \\ X^{-1}x_{k-n} & \text{for } n < k \le l, \end{cases}$$
$$g_k(\underline{\xi}) = \begin{cases} Cu_k & \text{for } k \le n, \\ X(v_{k-n} - M_{k-n}(\underline{u})) & \text{for } n < k \le l, \end{cases}$$

and $\underline{\beta} = (C^{-1}\underline{\alpha}, \underline{0})$. The corollary then follows from Theorem 4.1. □

Lemma 4.3 (transference lemma). *Let s and t be positive integers. Suppose that the inequality*

$$M(\underline{y}) \ge q^{-t}$$

holds for any nonzero polynomial n-tuple $\underline{y}$ of norm $\|\underline{y}\| \le q^s$. Then, for all n-tuples $(\theta_1, \dots, \theta_n)$ in $\mathbb{F}_q((z^{-1}))^n$, there exists a polynomial vector $\underline{x}$ with $\|\underline{x}\| \le q^t$ such that

$$\max_{1\le i\le n} |\langle L_i(\underline{x}) - \theta_i\rangle| \le q^{-s}.$$

Proof. We apply Corollary 4.2 with $\underline{u} = \underline{y}$ and $\underline{\alpha} = \underline{\theta}$. If $\|\underline{y}\| > q^s$, then the inequality (12) holds, since the left-hand side of inequality (12) is not greater than $\frac{1}{q}$. If $\|\underline{y}\| \le q^s$, then, since $M(\underline{y}) \ge q^{-t}$, the right-hand side of (12) is greater than 1 and (12) holds. By Corollary 4.2, the proof is established. □

Proof of Theorem 1.1. First of all, we suppose that for every $\varepsilon > 0$, there is a polynomial vector $\underline{x}$ such that simultaneously $|\langle L_i(\underline{x}) - \theta_i\rangle| \le \varepsilon$, $(1 \le i \le n)$. If $\underline{u} = (u_1, \dots, u_n)^T$ is any polynomial vector such that $A^T\underline{u}$ is in $\mathbb{F}_q[z]^m$, then

$$u_1L_1(\underline{x}) + \cdots + u_nL_n(\underline{x}) = \underline{u}^T A\underline{x} \in \mathbb{F}_q[z].$$

It follows that

$$\begin{aligned}|\langle u_1\theta_1+\cdots+u_n\theta_n\rangle| &= |\langle u_1(L_1(\underline{x})-\theta_1)+\cdots+u_n(L_n(\underline{x})-\theta_n)\rangle|\\ &\le \max\{|\langle u_1(L_1(\underline{x})-\theta_1)\rangle|,\ldots,|\langle u_n(L_n(\underline{x})-\theta_n)\rangle|\}\\ &\le \|\underline{u}\|\varepsilon.\end{aligned}$$

Since ε is arbitrary, we have

$$|\langle u_1\theta_1+\cdots+u_n\theta_n\rangle| = 0.$$

Thus,

$$u_1\theta_1+\cdots+u_n\theta_n \in \mathbb{F}_q[z].$$

Now we turn to proving that (2) implies (1), with the help of Corollary 4.2.

For every $\varepsilon > 0$, there is a positive integer s such that $q^{-s} \le \varepsilon$.

If $|\langle u_1\theta_1+\cdots+u_n\theta_n\rangle| = 0$, then the inequality (12) obviously holds. Otherwise, we have $\max_{1\le i\le m}|\langle M_i(\underline{u})\rangle| > 0$ by the assumption.

Since $|\langle u_1\theta_1+\cdots+u_n\theta_n\rangle| \le q^{-1}$, (12) is satisfied if $\|\underline{u}\| \ge q^s$. For the finitely many polynomial vectors $\underline{u}$ whose norm is less than q^s, (12) still holds if we choose the integer t large enough. Then the proof is completed by using Corollary 4.2. □

5. Proof of the Theorem 1.2

We begin by proving that the inequalities

$$\omega(A,\underline{\theta}) \ge \frac{1}{\widehat{\omega}(A^T)} \quad \text{and} \quad \widehat{\omega}(A,\underline{\theta}) \ge \frac{1}{\omega(A^T)} \tag{13}$$

hold for all vectors $\underline{\theta} = (\theta_1,\ldots,\theta_n)^T$ in $\mathbb{F}_q((z^{-1}))^n$.

For the first inequality, we can clearly assume that $\widehat{\omega}(A^T)$ is finite. Let $\omega > \widehat{\omega}(A^T)$ be a real number. By the definition of the exponent $\widehat{\omega}(A^T)$, there exists a real number H, which may be chosen arbitrarily large, such that

$$M(\underline{y}) \ge H^{-\omega} \tag{14}$$

for any nonzero polynomial vector $\underline{y}$ of norm at most equal to H. Let s, t be positive integers such that $H^{-\omega} \ge q^{-t} > q^{-1}H^{-\omega}$ and $q^s \le H < q^{s+1}$. Then we have $M(\underline{y}) \ge H^{-\omega} \ge q^{-t}$ for any nonzero polynomial vector $\underline{y}$ of norm at most equal to q^s. By Lemma 4.3, there exists a polynomial n-tuple $\underline{x}$ with $\|\underline{x}\| \le q^t$ such that

$$\max_{1\le i\le n}|\langle L_i(\underline{x})-\theta_i\rangle| \le q^{-s} \le qH^{-1} < q^{1+\frac{1}{\omega}}q^{-t\frac{1}{\omega}} < q^{1+\frac{1}{\omega}}\|\underline{x}\|^{-\frac{1}{\omega}}.$$

This shows that $\omega(A,\underline{\theta}) \ge \frac{1}{\omega}$.

For the second inequality of (13), we can clearly assume that $\omega(A^T)$ is finite. For $\omega > \omega(A^T)$ and all real numbers H with sufficiently large, the inequality (14) is satisfied for any nonzero polynomial vector $\underline{y}$ of norm $\|\underline{y}\| \le H$. We argue in a similar way as in the proof of the first inequality. We omit the details.

We now prove that

$$\omega(A, \underline{\theta}) \le \frac{1}{\widehat{\omega}(A^T)} \quad \text{and} \quad \widehat{\omega}(A, \underline{\theta}) \le \frac{1}{\omega(A^T)} \tag{15}$$

hold for almost all vectors $\underline{\theta} = (\theta_1, \ldots, \theta_n)^T$ in $\mathbb{F}_q((z^{-1}))^n$.

By the formula $\underline{y}^T A \underline{x} = \underline{x}^T A^T \underline{y}$, it is easily seen that

$$y_1\theta_1 + \cdots + y_n\theta_n = \sum_{j=1}^{m} x_j M_j(y_1, \ldots, y_n) - \sum_{i=1}^{n} y_i (L_i(x_1, \ldots, x_m) - \theta_i),$$

from which it follows that

$$|\langle y_1\theta_1 + \cdots + y_n\theta_n \rangle| \le \max\{\|\underline{y}\| \max_{1\le i\le n} |\langle L_i(\underline{x}) - \theta_i\rangle|, \|\underline{x}\| M(\underline{y})\} \tag{16}$$

for all polynomial vectors $\underline{x} = (x_1, \ldots, x_m)^T$ and $\underline{y} = (y_1, \ldots, y_n)^T$.

We follow the notation in Section 3 and denote by

$$\underline{y}_i = (y_{i1}, \ldots, y_{in})^T \quad \text{and} \quad Y_i = \|\underline{y}_i\|, \qquad i \ge 1,$$

the sequence of best approximations associated with the matrix A^T.

By Lemma 3.5, for almost all $\underline{\theta}$ in $\mathbb{F}_q((z^{-1}))^n$, the inequality

$$|\langle y_{i1}\theta_1 + \cdots + y_{in}\theta_n \rangle| \ge Y_i^{-\delta} \tag{17}$$

holds for all $\delta > 0$ and any index i large enough. Let us fix two real numbers δ and ω such that

$$0 < \delta < \omega < \widehat{\omega}(A^T).$$

Let $\underline{x}$ be a polynomial m-tuple with sufficiently large norm $\|\underline{x}\|$, and let k be the index defined by the inequality

$$Y_k \le \|\underline{x}\|^{\frac{1}{\omega-\delta}} < Y_{k+1}.$$

This gives

$$Y_{k+1}^{\omega} > \|\underline{x}\|^{\frac{\omega}{\omega-\delta}} \ge \|\underline{x}\| Y_k^{\delta}.$$

By (iii) of Lemma 3.4, we have

$$\|\underline{x}\| M(\underline{y}_k) \le \|\underline{x}\| Y_{k+1}^{-\omega} < Y_k^{-\delta}.$$

Using (16) with $\underline{y} = \underline{y}_k$ and (17) with $i = k$, we deduce that

$$Y_k^{-\delta} \le \|\underline{y}_k\| \max_{1\le i\le n} |\langle L_i(\underline{x}) - \theta_i\rangle| \le Y_k \max_{1\le i\le n} |\langle L_i(\underline{x}) - \theta_i\rangle|,$$

which gives

$$|\langle A\underline{x}-\underline{\theta}\rangle| = \max_{1\le i\le n} |\langle L_i(\underline{x})-\theta_i\rangle| \ge Y_k^{-1-\delta} \ge \|\underline{x}\|^{-\frac{1+\delta}{\omega-\delta}}.$$

This implies

$$\omega(A,\underline{\theta}) \le \frac{1+\delta}{\omega-\delta}.$$

Let δ and ω be arbitrarily close to 0 and to $\widehat{\omega}(A^T)$, respectively. Then, it is immediate that the first inequality of (15) holds.

The second upper bound can be handled in the same manner. Let us fix now two real numbers δ and ω such that

$$0<\delta<\omega<\omega(A^T).$$

Let $\underline{x}$ be a polynomial m-tuple with $\|\underline{x}\| \le H_k := Y_k^{\omega-\delta}/2$. By (iv) of Lemma 3.4, there exist infinitely many integers $k\ge 1$ such that $M(\underline{y}_k) \le Y_k^{-\omega}$, thus, for which,

$$\|\underline{x}\| M(\underline{y}_k) \le \|\underline{x}\| Y_k^{-\omega} \le \frac{Y_k^{-\delta}}{2}.$$

Applying again inequality (16), we obtain

$$Y_k^{-\delta} \le \|\underline{y}_k\| \max_{1\le i\le n} |\langle L_i(\underline{x})-\theta_i\rangle| \le Y_k \max_{1\le i\le n} |\langle L_i(\underline{x})-\theta_i\rangle|,$$

which yields

$$|\langle A\underline{x}-\underline{\theta}\rangle| = \max_{1\le i\le n} |\langle L_i(\underline{x})-\theta_i\rangle| \ge Y_k^{-1-\delta} = 2^{-\frac{1+\delta}{\omega-\delta}} H_k^{-\frac{1+\delta}{\omega-\delta}}.$$

Since the above lower bound holds for any polynomial $\underline{x}$ whose norm is less than H_k and for infinitely many $k\ge 1$, noting that the sequence $(H_i)_{i\ge 1}$ tends to infinity, it follows that

$$\widehat{\omega}(A,\underline{\theta}) \le \frac{1+\delta}{\omega-\delta}.$$

Choosing δ and ω arbitrarily close to 0 and to $\omega(A^T)$, respectively, we get the second inequality of (15), and the proof of the first assertion is completed.

It only remains to prove that

$$\widehat{\omega}(A,\underline{\theta}) \le \omega(A),$$

when $\underline{\theta}=(\theta_1,\dots,\theta_n)^T$ is not in $A\mathbb{F}_q[z]^m+\mathbb{F}_q[z]^n$.

For any $\underline{x}$ in $\mathbb{F}_q[z]^m$, set $L(\underline{x}) = |\langle A\underline{x}-\underline{\theta}\rangle|$. By the denseness of $A\mathbb{F}_q[z]^m$ in $\mathbb{F}_q((z^{-1}))^n$ (which is implied by Theorem 1.1) and following the same method as in the homogeneous case, we can construct a sequence of polynomial vectors $\underline{x}_i,\ i\ge 1,$

in $\mathbb{F}_q[z]^m$ associated with $L(\underline{x}_1), L(\underline{x}_2), \dots$ which satisfy the following properties. Set $\|\underline{x}_i\| = H_i$ and $L_i = L(\underline{x}_i)$, then we have

$$1 = H_1 < H_2 < \cdots \quad \text{and} \quad L_1 > L_2 > \cdots$$

and $L(\underline{x}) \geq L_i$ for all polynomial vectors $\underline{x}$ with $\|\underline{x}\| < H_{i+1}$. Here we also call the above sequence $(\underline{x}_i)_{i\geq 1}$ a sequence of best approximations related to $L_1, L_2, \dots$. By definition of $\widehat{\omega}(A, \underline{\theta})$ and best approximation, for any $\omega < \widehat{\omega}(A, \underline{\theta})$, the inequality

$$0 < |\langle A\underline{x}_i - \underline{\theta}\rangle| \leq H_{i+1}^{-\omega}$$

holds for any index i sufficiently large in terms of ω. By using the triangle inequality, we conclude that

$$\begin{aligned}|\langle A(\underline{x}_i - \underline{x}_{i-1})\rangle| &= |\langle A\underline{x}_i - \underline{\theta} - (A\underline{x}_{i-1} - \underline{\theta})\rangle| \\ &\leq \max\{|\langle A\underline{x}_i - \underline{\theta}\rangle|, |\langle A\underline{x}_{i-1} - \underline{\theta}\rangle|\} \\ &\leq H_i^{-\omega},\end{aligned}$$

which gives that $\omega(A) \geq \omega$. Choosing ω arbitrarily close to $\widehat{\omega}(A, \underline{\theta})$, we complete the proof.

6. Proof of Theorem 1.3

Before proving Theorem 1.3 we establish an auxiliary lemma.

Lemma 6.1. *Let $l \geq 2$ be an integer. For a sequence $(\underline{h}_k)_{k\geq 1}$ of polynomial vectors such that $\|\underline{h}_k\| \geq q^l \|\underline{h}_{k-1}\|$ for $k \geq 2$, set*

$$S_{\{\underline{h}_k\}} = \{\underline{\theta} \in \mathbb{I}^n : \text{ there exists } k_0(\underline{\theta}) \text{ such that } |\langle \underline{h}_k\, \underline{\theta}\rangle| \geq q^{-1} \text{ for all } k \geq k_0(\underline{\theta})\}.$$

Then we have $\dim_H S_{\{\underline{h}_k\}} \geq n - \frac{1}{l}$.

Proof. Our strategy to prove this lemma is as follows. First, we define some partitions of $\mathbb{I}^n$ and construct a family of balls covering the points which do not satisfy the condition in the definition of the set $S_{\{\underline{h}_k\}}$. Then we delete the family of balls from the partitions to construct a Cantor subset contained in $S_{\{\underline{h}_k\}}$.

For any $i \geq 1$, define d_i by $\|\underline{h}_i\| = q^{d_i}$ and set

$$\Gamma_i = z^{-d_i-1}\mathbb{F}_q[z]^n \cap \mathbb{I}^n.$$

It is clear that all distinct elements $\underline{x}, \underline{y}$ in Γ_i satisfy

$$\|\underline{x} - \underline{y}\| \geq q^{-d_i-1}. \tag{18}$$

Now we define a partition of $\mathbb{I}^n$. For each $i \geq 1$, let $\mathscr{C}_i$ be the family of balls $B(\underline{c}, q^{-d_i-1})$ centered at some point $\underline{c}$ in Γ_i, i.e.,

$$\mathscr{C}_i = \{B(\underline{c}, q^{-d_i-1}) : \underline{c} \in \Gamma_i\}.$$

By (18) and the ball intersection property, any two distinct balls in $\mathscr{C}_i$ have empty intersection. Each ball in $\mathscr{C}_i$ has measure $q^{(-d_i-1)n}$. Since there are exactly $q^{(d_i+1)n}$ of these balls, they do indeed define a partition of $\mathbb{I}^n$.

For any $i \geq 1$, we consider the resonant set

$$R_i = \{\underline{x} \in \mathbb{I}^n : \underline{h}_i\, \underline{x} = p \text{ for some } p \in \mathbb{F}_q[z]\}.$$

Since $\underline{x}$ is in $\mathbb{I}^n$, each resonant set R_i is contained in one of the affine spaces

$$R_i(r) = \{\underline{x} \in \mathbb{I}^n : \underline{h}_i\, \underline{x} = r\}, \quad \text{where } r \text{ is in } \mathbb{F}_q[z] \text{ with } \|r\| \leq \|\underline{h}_i\|.$$

In each $R_i(r)$, we choose a subset $\Lambda_i(r)$ such that the distance between any two different points in $\Lambda_i(r)$ is at least q^{-d_i-1} and such that, for any point $\underline{\xi}$ in $R_i(r)$, there is a point $\underline{\eta}$ in $\Lambda_i(r)$ at a distance to $\underline{\xi}$ less than q^{-d_i-1}. Let Λ_i be the union of the sets $\Lambda_i(r)$ where $\|r\| \leq \|\underline{h}_i\|$. Set

$$\mathcal{G}_i = \{B(\underline{c}, q^{-d_i-1}) : \underline{c} \in \Lambda_i\}.$$

If $\underline{\theta}$ in $\mathbb{I}^n$ satisfies $|\langle \underline{h}_i\, \underline{\theta} \rangle| < \frac{1}{q}$, then we have

$$\|\underline{h}_i\| \operatorname{dist}_\infty(\underline{\theta}, R_i) \leq |\langle \underline{h}_i \underline{\theta} \rangle| < \frac{1}{q},$$

where $\operatorname{dist}_\infty$ denotes the distance associated with the supremum norm. Then,

$$\operatorname{dist}_\infty(\underline{\theta}, R_i) < q^{-d_i-1},$$

which implies that there exists $\underline{\xi}$ in R_i such that

$$\|\underline{\theta} - \underline{\xi}\| < q^{-d_i-1},$$

and, consequently, $\underline{\theta}$ is contained in some ball which belongs to $\mathcal{G}_i$.

Let $\mathcal{D}_i = \{B \in \mathscr{C}_i : B \cap \mathcal{G}_i = \varnothing\}$. Define

$$E_i = \bigcup_{B \in \mathcal{D}_i} B \quad \text{and} \quad E = \bigcap_{i=1}^{\infty} E_i.$$

Then, $E \subset S_{\{\underline{h}_k\}}$.

Now we determine the Hausdorff dimension of the set E. By the ball intersection property, the distance between any two balls in $\mathcal{D}_i$ is $\epsilon_i = q^{-d_i-1}$. Since $\mathscr{C}_i$ is a partition of $\mathbb{I}^n$, for any ball B in $\mathcal{D}_i$, the number of balls of $\mathscr{C}_{i+1}$ contained in B is $q^{(d_{i+1}-d_i)n}$.

For any $\underline{\xi}$ in $R_{i+1}(r)$, $\underline{\theta}$ in $R_{i+1}(t)$, where r and t are in $\mathbb{F}_q[z]$, we obtain

$$1 \leq \|r - t\| \leq \|\underline{h}_{i+1}\underline{\xi} - \underline{h}_{i+1}\underline{\theta}\| \leq \|\underline{h}_{i+1}\| \|\underline{\xi} - \underline{\theta}\|;$$

hence

$$\|\underline{\xi} - \underline{\theta}\| \geq \frac{1}{\|\underline{h}_{i+1}\|}.$$

Consequently, the number of affine spaces which can intersect a ball B in $\mathcal{D}_i$ is at most $q^{d_{i+1}-d_i-1}$. Since every such affine space contains $q^{(d_{i+1}-d_i)(n-1)}$ points of $\Lambda_{i+1} \cap B$, the number of balls of $\mathcal{D}_{i+1}$ contained in the ball B is at least

$$m_{i+1} = q^{(d_{i+1}-d_i)n} - q^{(d_{i+1}-d_i)n-1} = q^{(d_{i+1}-d_i)n}(1-q^{-1}) \geq 2^{-1}q^{(d_{i+1}-d_i)n}.$$

Since $\|\underline{h}_k\| \geq q^l \|\underline{h}_{k-1}\|$ for $k \geq 2$, we have $d_k \geq (k-1)l$. By this fact and Example 4.6 of [Falconer 1990], we have

$$\begin{aligned}
\dim_H E &\geq \liminf_{k\to+\infty} \frac{\log m_1 m_2 \cdots m_{k-1}}{-\log m_k \epsilon_k^n} \cdot n \\
&\geq \liminf_{k\to+\infty} \frac{k \log \frac{1}{2} + n d_{k-1} \log q}{-\log \frac{1}{2} + n(d_{k-1}+1)\log q} \cdot n \\
&\geq \liminf_{k\to+\infty} \frac{n d_{k-1} - k}{n(d_{k-1}+2)} \cdot n \\
&\geq \liminf_{k\to+\infty} \frac{n d_{k-1} - \frac{1}{l}(d_{k-1}) - 2}{n(d_{k-1}+2)} \cdot n \geq n - \frac{1}{l}.
\end{aligned}$$

□

Now we prove Theorem 1.3.

For a positive integer $l \geq 2$, we extract a subsequence $(\underline{y}_{\varphi_l(k)})_{k\geq 1}$ from the sequence of best approximations $(\underline{y}_k)_{k\geq 1}$, where the index function is an increasing function $\varphi_l : \mathbb{Z}_{\geq 1} \to \mathbb{Z}_{\geq 1}$ satisfying $\varphi_l(1) = 1$ and, for any integer $i \geq 2$,

$$Y_{\varphi_l(i)} \geq q^l Y_{\varphi_l(i-1)} \quad \text{and} \quad Y_{\varphi_l(i-1)+1} \geq q^{-2l} Y_{\varphi_l(i)}. \tag{19}$$

Let

$$\mathcal{J}_0 = \{j : Y_{j+1} \geq q^l Y_j\}.$$

To define the function φ_l we distinguish two cases, according to whether the set $\mathcal{J}_0$ is finite or not.

If $\mathcal{J}_0$ is an infinite set, then set $\varphi_l(1) = 1$. Suppose that $\varphi_l(i)$ has already been defined for $1 \leq i \leq h'$, and define $\varphi_l(h)$ to be the smallest element of $\mathcal{J}_0$ greater than $\varphi_l(h')$. We let $\varphi_l(h-1)$ be the largest index $t \geq \varphi_l(h')$ for which $Y_{\varphi_l(h)} \geq q^l Y_t$, we let $\varphi_l(h-2)$ be the largest index $t \geq \varphi_l(h')$ for which $Y_{\varphi_l(h-1)} \geq q^l Y_t$, and so on until an index t as above does not exist. We have just defined $\varphi_l(h), \varphi_l(h-1), \ldots, \varphi_l(h-h_0)$. Then, we set $h = h' + h_0 + 1$, and the inequalities (19) are satisfied for $i = h'+1, \ldots, h'+h_0+1$.

If $\mathcal{J}_0$ is a finite set, we denote by g the largest of its elements, putting $g = 1$ if $\mathcal{J}_0$ is empty. We apply the above process to construct the initial values of the function φ up to $g = \varphi_l(h)$. Then, we define $\varphi_l(h+1)$ as the smallest index t for which $Y_t \geq q^l Y_{\varphi_l(h)}$. We observe that $Y_{\varphi_l(h+1)-1} < q^l Y_{\varphi_l(h)}$ and $Y_{\varphi_l(h)+1} \geq Y_{\varphi_l(h)} > q^{-l} Y_{\varphi_l(h+1)-1} > q^{-2l} Y_{\varphi_l(h+1)}$, as required. We continue in this way, by defining $\varphi_l(h+2)$ as the smallest index t for which $Y_t \geq q^l Y_{\varphi_l(h+1)}$, and so on. The inequalities (19) are then satisfied.

By Lemma 6.1, for any $\underline{\theta}$ in $S_{\{\underline{y}_{\varphi_l(i)}\}}$, it follows that

$$|\langle y_{\varphi_l(i),1}\theta_1 + \cdots + y_{\varphi_l(i),n}\theta_n\rangle| \geq \frac{1}{q} \quad \text{for sufficiently large } i.$$

Let $\underline{x}$ be a nonzero polynomial m-tuple whose norm is sufficiently large and let k be the index defined by the inequalities

$$Y_{\varphi_l(k)} \leq q^{(2l+1)} q^{\frac{m}{n}} \|\underline{x}\|^{\frac{m}{n}} < Y_{\varphi_l(k+1)}.$$

By Lemma 3.4 and inequality (16) with $\underline{y} = y_{\varphi_l(k)}$, we have

$$\frac{1}{q} \leq \max\bigl\{q^{(2l+1)} q^{\frac{m}{n}} \|\underline{x}\|^{\frac{m}{n}} |\langle A\underline{x} - \underline{\theta}\rangle|,\ \|\underline{x}\| q^{\frac{n}{m}} Y_{\varphi_l(k)+1}^{-\frac{n}{m}}\bigr\}.$$

By construction of the subsequence $(Y_{\varphi_l(i)})_{i\geq 1}$, we have $Y_{\varphi_l(k)+1}^{-1} Y_{\varphi_l(k+1)} \leq q^{2l}$, so

$$\|\underline{x}\| q^{\frac{n}{m}} Y_{\varphi_l(k)+1}^{-\frac{n}{m}} < q^{-1} q^{-\frac{(2l+1)n}{m}} q^{\frac{n}{m}} q^{\frac{2ln}{m}} = q^{-1},$$

then

$$\frac{1}{q} \leq q^{(2l+1)} q^{\frac{m}{n}} \|\underline{x}\|^{\frac{m}{n}} |\langle A\underline{x} - \underline{\theta}\rangle|,$$

which gives

$$|\langle A\underline{x} - \underline{\theta}\rangle| \geq q^{-(2l+2)} q^{-\frac{m}{n}} \|\underline{x}\|^{-\frac{m}{n}}.$$

From this, we deduce that $S_{\{\underline{y}_{\varphi_l(i)}\}} \subset \mathrm{Bad}^{\varepsilon}(A)$ with $\varepsilon = q^{-(2l+2)} q^{-m/n}$, and then

$$\dim_H \mathrm{Bad}^{\varepsilon}(A) \geq n - \frac{1}{l},$$

which implies the second assertion.

Recall that

$$\mathrm{Bad}(A) := \bigcup_{\varepsilon>0} \mathrm{Bad}^{\varepsilon}(A) = \{\underline{\theta} \in \mathbb{I}^n : \liminf_{\underline{x}\in\mathbb{F}_q[z]^m,\, \|\underline{x}\|\to\infty} \|\underline{x}\|^{m/n} \cdot |\langle A\underline{x} - \underline{\theta}\rangle| > 0\}.$$

We have just proved that, for any integer $l \geq 2$, we have

$$S_{\{\underline{y}_{\varphi_l(i)}\}} \subset \mathrm{Bad}(A).$$

Letting l tend to infinity, we obtain

$$\dim_H \mathrm{Bad}(A) = n.$$

This completes the proof of the theorem.

7. Proof of Theorem 1.4

We use the same method as in the last section. The next lemma can be seen as a sharpening of Lemma 6.1 when the sequence of norms of the polynomial vectors increases very rapidly.

Lemma 7.1. *For any δ in $(0, q^{-1}]$, let $(\underline{h}_k)_{k\geq 1}$ be a sequence of polynomial vectors such that $\|\underline{h}_{k+1}\|/\|\underline{h}_k\| \geq q\delta^{-1}$ for $k \geq 1$ and $\lim_{k\to\infty} \|\underline{h}_k\|^{1/k} = \infty$. Then, the set*

$$S_\delta = \{\underline{\theta} \in \mathbb{I}^n : \text{ there exists } k_0(\underline{\theta}) \text{ such that } |\langle \underline{h}_k \underline{\theta}\rangle| \geq \delta \text{ for all } k \geq k_0(\underline{\theta})\}$$

has full Hausdorff dimension.

Proof. Since the proof is very similar to that of Lemma 6.1, we just give the necessary modifications here.

Let δ be in $(0, q^{-1}]$. For any $k \geq 1$, set $\|\underline{h}_k\| = q^{d_k}$. We note that δ plays the role of q^{-1} in the proof of Lemma 6.1. The remaining part of the construction of a suitable subset can be done in a similar way. Notice that, since d_k/k tends to infinity with k, we have

$$\begin{aligned}\dim_H E &\geq \liminf_{k\to+\infty} \frac{\log m_1 m_2 \cdots m_{k-1}}{-\log m_k \varepsilon_k^n} \cdot n \\ &= \liminf_{k\to+\infty} \frac{k \log \frac{1}{2} + n d_{k-1} \log q}{-\log \frac{1}{2} + n(d_{k-1}+1)\log q} \cdot n = n,\end{aligned}$$

which completes the proof. □

Let us begin the proof of Theorem 1.4.

Let

$$\underline{y}_k = (y_{k1}, \dots, y_{kn})^T, \qquad k \geq 1,$$

be the sequence of best approximations associated to the matrix A^T, and set $Y_k := \|\underline{y}_k\|$ for $k \geq 1$.

Let δ be in $(0, q^{-1}]$ and set $R = q\delta^{-1}$. Since $Y_k^{1/k}$ tends to infinity with k, the set

$$\mathcal{J}_R = \{j : Y_{j+1} \geq RY_j\}.$$

is an infinite set. In the same way as in the proof of Theorem 1.3, we can extract a subsequence $(\underline{y}_{\varphi(k)})_{k\geq 1}$ of $(\underline{y}_k)_{k\geq 1}$ with the property that

$$Y_{\varphi(k)} \geq RY_{\varphi(k-1)}, \quad Y_{\varphi(k-1)+1} \geq R^{-1} Y_{\varphi(k)}, \qquad \text{for } k \geq 2. \tag{20}$$

We apply Lemma 7.1 to $(\underline{y}_{\varphi(k)})_{k\geq 1}$ and take $\underline{\theta} = (\theta_1, \dots, \theta_n)$ in the corresponding set S_δ, that is, satisfying

$$|\langle y_{\varphi(k)1}\theta_1 + \cdots + y_{\varphi(k)n}\theta_n\rangle| \geq \delta \quad \text{for sufficiently large } k. \tag{21}$$

Let $\underline{h}$ be a nonzero polynomial m-tuple whose norm is sufficiently large and let k be the index defined by the inequality

$$Y_{\varphi(k)} \le qR\delta^{-\frac{m}{n}} \|\underline{h}\|^{\frac{m}{n}} < Y_{\varphi(k+1)}.$$

By (16), (20), and (ii) of Lemma 3.4 with $\underline{y} = \underline{y}_{\varphi(k)}$ and $\underline{x} = \underline{h}$, since

$$\|\underline{h}\| M(\underline{y}_{\varphi(k)}) \le \|\underline{h}\| q^{\frac{n}{m}} Y_{\varphi(k)+1}^{-\frac{n}{m}} < \delta(qR)^{-\frac{n}{m}} q^{\frac{n}{m}} Y_{\varphi(k)+1}^{-\frac{n}{m}} Y_{\varphi(k+1)}^{\frac{n}{m}} \le \delta,$$

we have

$$\delta \le Y_{\varphi(k)} |\langle A\underline{h} - \underline{\theta}\rangle| \le qR\delta^{-\frac{m}{n}} \|\underline{h}\|^{\frac{m}{n}} |\langle A\underline{h} - \underline{\theta}\rangle|.$$

Consequently, we get

$$\|\underline{h}\|^{\frac{m}{n}} |\langle A\underline{h} - \underline{\theta}\rangle| \ge \frac{\delta^{1+\frac{m}{n}}}{qR} = \frac{\delta^{2+\frac{m}{n}}}{q^2}.$$

By letting $\delta = q^{-1}$, this gives the first assertion of Theorem 1.4.

If $m = n = 1$, $A = (\alpha)$, and the degrees of the partial quotients of α tend to infinity, then the assumption of Lemma 7.1 is satisfied for $h_k = Q_{k+N}$ for some constant $N \ge 0$. For any $0 < \delta \le \frac{1}{q}$, the set S_δ has full Hausdorff dimension. Let x be in $\mathbb{I}$ and let h be a polynomial. Then, for every y in $\mathbb{F}_q[z]$, we have

$$|\langle yx\rangle| = |\langle yx - y\alpha h + y\alpha h\rangle| \le \max\{\|y\| |\langle h\alpha - x\rangle|, \|h\| |\langle y\alpha\rangle|\}. \tag{22}$$

Now we assume that $\|h\|$ is large enough and let l be the integer with $\|Q_l\| \le \delta^{-1}\|h\| < \|Q_{l+1}\|$. For any θ in S_δ, letting $y = Q_l$ and $x = \theta$ in the inequality (22), since $\|h\| \|\{Q_l\alpha\}\| = \|h\|/\|Q_{l+1}\| < \delta$, we have

$$\delta \le |\langle Q_l\theta\rangle| \le \|Q_l\| |\langle h\alpha - \theta\rangle| \le \delta^{-1}\|h\| |\langle h\alpha - \theta\rangle|.$$

This gives $\|h\| |\langle h\alpha - \theta\rangle| \ge \delta^2$. Setting $\delta = \frac{1}{q}$, the proof is complete.

8. Proof of Theorem 2.3

Since we always have $\omega((\xi)) = 1$ for any irrational power series ξ whose partial quotients have bounded degree, we may assume that $\omega > 1$.

If $\omega((\xi))$ is finite and equal to ω, then let $(\omega_n)_{n\ge 0}$ be the constant sequence equal to ω, otherwise, put $\omega_n = n$ for any $n \ge 0$. Let ξ be an element in $\mathbb{F}_q((z^{-1}))$ such that the sequence of the denominators $(Q_n)_{n\ge 0}$ of its convergents P_n/Q_n satisfies the growth condition

$$\|Q_n\|^{\omega_n} \le \|Q_{n+1}\| < q\|Q_n\|^{\omega_n}.$$

By Theorem 1.2, we have $\widehat{\omega}((\xi), \theta) = 1/\omega((\xi))$ for almost all θ in $\mathbb{F}_q((z^{-1}))$. Let ν be a nonnegative real number. If $\omega((\xi))$ is finite, then assume furthermore that $\frac{1}{\omega} \le \nu \le \omega$. We construct an element θ in $\mathbb{F}_q((z^{-1}))$ for which $\widehat{\omega}((\xi), \theta) = \nu$. When

$\omega((\xi)) = +\infty$, our process furnishes moreover some θ not in $\mathbb{F}_q[z] + \xi\mathbb{F}_q[z]$ with $\widehat{\omega}((\xi), \theta) = +\infty$.

Let $(u_n)_{n\geq 0}$ be a sequence of polynomials with

$$\|Q_n\|^{\frac{\omega_n-\nu}{\nu+1}} \leq \|u_n\| < q\|Q_n\|^{\frac{\omega_n-\nu}{\nu+1}}, \quad \text{for } n \geq 1.$$

Set

$$\theta = \sum_{k\geq 0} u_k(Q_k\xi - P_k).$$

For any $n \geq 0$, set

$$V_n = \sum_{k=0}^{n} u_k Q_k \quad \text{and} \quad W_n = \sum_{k=0}^{n} u_k P_k.$$

Then we have

$$\|V_n\| = \|u_n\|\|Q_n\| \quad \text{and} \quad \|V_n\xi - W_n - \theta\| = \|u_{n+1}\|\|Q_{n+2}\|^{-1},$$

so

$$\|Q_n\|^{\frac{\omega_n+1}{\nu+1}} \leq \|V_n\| < q\|Q_n\|^{\frac{\omega_n+1}{\nu+1}}$$

and

$$q^{-1}\|Q_{n+1}\|^{-\frac{\nu(\omega_{n+1}+1)}{\nu+1}} < \|V_n\xi - W_n - \theta\| < q\|Q_{n+1}\|^{-\frac{\nu(\omega_{n+1}+1)}{\nu+1}};$$

hence

$$\|V_n\xi - W_n - \theta\| < q\|Q_{n+1}\|^{-\frac{\nu(\omega_{n+1}+1)}{\nu+1}} \leq q^{1+\nu}\|V_{n+1}\|^{-\nu} \tag{23}$$

which implies that $\widehat{\omega}((\xi), \theta) \geq \nu$. When $\omega((\xi)) = +\infty$, we construct θ in $\mathbb{F}_q((z^{-1}))$ not in $\mathbb{F}_q[z] + \xi\mathbb{F}_q[z]$ and with $\widehat{\omega}((\xi), \theta) = +\infty$ exactly in the same way, by taking $u_n = 1$ for any $n \geq 0$.

Next we prove that for infinitely many n and all polynomials x and y with $\|x\| \leq \frac{1}{q}\|V_n\|$, we have

$$\|x\xi - y - \theta\| \geq q^{-2}\|V_n\|^{-\nu}. \tag{24}$$

It follows that $\widehat{\omega}((\xi), \theta) \leq \nu$, and therefore that $\widehat{\omega}((\xi), \theta) = \nu$.

To obtain a contradiction, we suppose inequality (24) does not hold for some polynomials x and y with $\|x\| \leq \frac{1}{q}\|V_n\|$. Then we deduce from (23) and the triangle inequality that

$$\begin{aligned}\|(x - V_{n-1})\xi - (y - W_{n-1})\| &= \|x\xi - y - \theta - (V_{n-1}\xi - W_{n-1} - \theta)\| \\ &\leq \max\{\|x\xi - y - \theta\|, \|V_{n-1}\xi - W_{n-1} - \theta\|\} \\ &\leq q^{1+\nu}\|V_n\|^{-\nu}.\end{aligned}$$

Set

$$a = -P_n(x - V_{n-1}) + Q_n(y - W_{n-1}) \quad \text{and} \quad b = P_{n-1}(x - V_{n-1}) - Q_{n-1}(y - W_{n-1})$$

if n is even (the case n is odd can be handled in the same way). Then we have

$$x - V_{n-1} = aQ_{n-1} + bQ_n \quad \text{and} \quad y - W_{n-1} = aP_{n-1} + bP_n.$$

A trivial verification shows that

$$\begin{aligned} b &= (x - V_{n-1})P_{n-1} - Q_{n-1}(y - W_{n-1}) \\ &= (x - V_{n-1})(P_{n-1} - \xi Q_{n-1}) - Q_{n-1}(y - W_{n-1} - (x - V_{n-1})\xi). \end{aligned}$$

This gives

$$\begin{aligned} \|b\| &\le \max\{q^{1+\nu}\|Q_{n-1}\|\|V_n\|^{-\nu}, q^{-1}\|V_n\|\|Q_n\|^{-1}\} \\ &= q^{-1}\|V_n\|\|Q_n\|^{-1} \le q^{-1}\|u_n\|. \end{aligned}$$

Now we use the formula

$$x\xi - y - \theta = a(Q_{n-1}\xi - P_{n-1}) - (u_n - b)(Q_n\xi - P_n) - \sum_{k \ge n+1} u_k(Q_k\xi - P_k).$$

When $a \neq 0$, we bound from below

$$\|x\xi - y - \theta\| = \|a(Q_{n-1}\xi - P_{n-1})\| \ge \frac{q}{\|Q_n\|} \ge \|Q_n\|^{-\frac{\nu(\omega_n+1)}{\nu+1}} \ge \|V_n\|^{-\nu}.$$

When $a = 0$, we obtain

$$\begin{aligned} \|x\xi - y - \theta\| &= \|(u_n - b)(Q_n\xi - P_n)\| = \|u_n\|\|Q_{n+1}\|^{-1} \\ &> q^{-1}\|Q_n\|^{-\omega_n}\|Q_n\|^{\frac{\omega_n - \nu}{\nu+1}} \\ &\ge q^{-1}\|V_n\|^{-\nu}. \end{aligned}$$

We have reached the expected contradiction.

9. Proof of Theorem 2.1

We only need to establish the implication "⇒" in Theorem 2.1 and it can be restated as follows.

Theorem 9.1. *Under the assumption that* $\liminf_{k\to\infty} \frac{1}{k} \log \|Q_k\| < \infty$, *we have*

$$\dim_H \mathrm{Bad}^{\varepsilon}(\alpha) < 1 \quad \textit{for any } \varepsilon > 0.$$

Proof. For positive integers K and t, set

$$\mathrm{Bad}_K^t(\alpha) = \{\theta \in \mathbb{I} : \|Q\|\|\{Q\alpha\} - \theta\| \ge q^{-t} \text{ for all } Q \text{ in } \mathbb{F}_q[z] \text{ with } \|Q\| \ge \|Q_K\|\}.$$

For $k \ge 1$, set $n_k = \deg Q_k$.

We define a sequence $(k_i)_{i\geq 0}$ as follows. Set $k_0 = K$ and, for $i \geq 1$, let k_{i+1} be the smallest integer k for which $n_k - n_{k_i} > t+4$. Since $\|Q_{k+1}\| \geq q\|Q_k\|$, the sequence $(k_{i+1}-k_i)_{i\geq 0}$ is uniformly bounded from above by an absolute constant and we deduce from our assumption on the growth of the sequence $((\log\|Q_k\|)/k)_{k\geq 1}$ that

$$\lambda := \liminf_{i\to\infty} \frac{1}{i} \log\|Q_{k_i}\| < +\infty.$$

Setting $\Omega(i) = \bigcup_{\deg Q=n,\, n_{k_i}\leq n\leq n_{k_{i+1}}-t} B(\{Q\alpha\}, q^{-n_{k_{i+1}}})$, we have

$$\bigcup_{\deg Q=n,\, n_{k_i}\leq n<n_{k_{i+1}}} B(\{Q\alpha\}, q^{-t}\|Q\|^{-1}) = \bigcup_{\deg Q=n,\, n_{k_i}\leq n<n_{k_{i+1}}} B(\{Q\alpha\}, q^{-n-t}) \supset \Omega(i).$$

Write

$$\mathcal{C}(k) = \{I(\sigma_1, \dots, \sigma_k) : (\sigma_1, \dots, \sigma_k) \in \mathbb{L}_k(\alpha)\},$$

where $I(\sigma_1, \dots, \sigma_k)$ is the cylinder of order n with respect to the α-expansion (see the end of Section 3), and

$$\mathcal{H}_i = \{B \in \mathcal{C}(k_{i+1}) : B \cap \Omega(i) = \varnothing\}.$$

Let

$$E_i = \bigcup_{B\in\mathcal{H}_i} B \quad \text{and} \quad E = \bigcap_{i\geq 1} E_i.$$

Then we have

$$\mathrm{Bad}_K^t(\alpha) \subset E.$$

Every ball B in $\mathcal{C}(k_i)$ can be written as $B = I(\sigma_1, \dots, \sigma_{k_i})$ for some $(\sigma_1, \dots, \sigma_{k_i})$ in $\mathbb{L}_{k_i}(\alpha)$. For any Q with $\deg Q = n$ where $n_{k_i} \leq n \leq n_{k_{i+1}} - t$, it follows from Lemma 3.7 that

$$\{Q\alpha\} = \sigma_1 D_0 + \sigma_2 D_1 + \cdots + \sigma_{k_i} D_{k_i-1} + \cdots + \sigma_{k_i+d} D_{k_i+d-1}, \tag{25}$$

where d is defined by $\|Q_{k_i+d-1}\| \leq q^{n_{k_{i+1}}-t} < \|Q_{k_i+d}\|$. Then, the element of such $\{Q\alpha\}$ contained in the ball B is at least $q^{\deg A_{k_i+1}+\cdots+\deg A_{k_i+d}}$, which is greater than $q^{n_{k_{i+1}}-n_{k_i}-t}$. In the same way as one gets (25), we deduce that, for any distinct Q and Q' in $\mathbb{F}_q[z]$ with $\deg Q$ and $\deg Q' < n_{k_{i+1}}$, we have

$$\|\{Q\alpha\} - \{Q'\alpha\}\| \geq \|D_{k_{i+1}-1}\| = q^{-n_{k_{i+1}}}.$$

Thus the number of balls $B(\{Q\alpha\}, q^{-n_{k_{i+1}}})$ with $\deg Q = n$ and $n_{k_i} \leq n \leq n_{k_{i+1}} - t$ which are contained in the ball B is at least $q^{n_{k_{i+1}}-n_{k_i}-t}$.

Then the number of balls in E_{i+1} contained in a ball of E_i is at most

$$q^{n_{k_{i+1}}-n_{k_i}} - q^{n_{k_{i+1}}-n_{k_i}-t} = (1-q^{-t})q^{n_{k_{i+1}}-n_{k_i}}.$$

For a real number s in (0, 1), let H^s denote the Hausdorff s-measure. For any M satisfying $\log M > \lambda$, for any s with $1 > s > 1 + \log(1 - q^{-t})/\log M$, we have

$$\begin{aligned} H^s(E) &\le \sum_{B \in \bigcap_{j=1}^{i} E_j} |B|^s \le (1 - q^{-t})^i q^{n_{k_i}} (q^{-n_{k_i}})^s \\ &\le (1 - q^{-t})^i M^{(1-s)i} \le 1. \end{aligned}$$

Then $\dim_H(E) \le 1 + \log(1 - q^{-t})/\log M < 1$; this completes the proof. □

10. Proof of Theorem 2.2

By Theorem 2.1, we only need to prove the following statement.

Theorem 10.1. *Let α in $\mathbb{F}_q((z^{-1}))$ be an irrational power series and $(P_k/Q_k)_{k\ge 1}$ the sequence of its convergents. Then α is singular on average if and only if $\|Q_k\|^{1/k}$ tends to infinity with k.*

Proof. First, we prove that α is singular on average under the condition that $\|Q_k\|^{1/k}$ tends to infinity with k.

Let $0 < c < \frac{1}{q}$ and $k \ge 3$ be an integer. By Lemmas 3.6 and 3.7, for any Q in $\mathbb{F}_q[z]$ with $0 < \|Q\| < \|Q_{k+1}\|$, we have $Q = B_1 Q_0 + B_2 Q_1 + \cdots + B_{k+1} Q_k$. Then

$$\{Q\alpha\} = B_1 D_0 + B_2 D_1 + \cdots + B_{k+1} D_k,$$

which gives

$$\|\{Q\alpha\}\| = \|B_1 D_0 + B_2 D_1 + \cdots + B_{k+1} D_k\| \ge \|D_k\| = \|\{Q_k\alpha\}\| = |\langle Q_k\alpha\rangle|.$$

In this way, for each integer X with $\|Q_k\| \le X < \|Q_{k+1}\|$, the inequalities

$$\|\{h\alpha\}\| \le cX^{-1} \quad \text{and} \quad 0 < \|h\| \le X \tag{26}$$

have a solution in $\mathbb{F}_q[z]$ if and only if $\|\{Q_k\alpha\}\| \le cX^{-1}$.

Thus for each integer l in $[\log_2 \|Q_k\|, \log_2 \|Q_{k+1}\|)$, inequalities (26) have no solution for $X = 2^l$ if and only if

$$-\log_2 \frac{\|\{Q_k\alpha\}\|}{c} < l < \log_2 \|Q_{k+1}\|.$$

Since $\|\{Q_k\alpha\}\| = \|Q_{k+1}\|^{-1}$, the number of integers l in $[\log_2 \|Q_k\|, \log_2 \|Q_{k+1}\|)$ such that inequalities (26) have no solution for $X = 2^l$ is at most

$$\log_2 \|Q_{k+1}\| + \log_2 \frac{\|\{Q_k\alpha\}\|}{c} + 1 \le \log \frac{1}{c} + 1.$$

Therefore, for an integer N with $\log_2 \|Q_k\| \le N < \log_2 \|Q_{k+1}\|$, the number of integers l in $\{1, 2, \ldots, N\}$ such that inequalities (26) have no solution for X is not greater than $\big(\log \frac{1}{c} + 1\big)(k+1)$. Recalling that $\Delta_{N,c}(\alpha)$ denote the number of integers l in $\{1, \dots, N\}$ for which the inequality $\|\{Q\alpha\}\| \le c2^{-l}$ has a solution with $0 < \|Q\| \le 2^l$, we have

$$\frac{N-\Delta_{N,c}(\alpha)}{N} \le \frac{\left(\log\frac{1}{c}+1\right)(k+1)}{N} \le \frac{\left(\log\frac{1}{c}+1\right)(k+1)}{\log_2\|Q_k\|}.$$

Using the assumption that $\|Q_k\|^{1/k}$ tends to infinity with k, we can deduce that $\frac{1}{N}(N-\Delta_{N,c}(\alpha))$ converges to 0. Therefore, α is singular on average.

Suppose that α is singular on average, and choose $c = q^{-3}$. Let l be an integer satisfying $q^{-2}\|Q_{k+1}\| \le 2^l < \|Q_{k+1}\|$ for some $k \ge 1$. Then, we have

$$\|\{Q_k\alpha\}\| = \|Q_{k+1}\|^{-1} \ge \frac{q^{-2}}{2^l} > \frac{c}{2^l}.$$

Since $\|\{h\alpha\}\| \ge \|\{Q_k\alpha\}\|$ for any polynomial h with $0 < \|h\| < \|Q_{k+1}\|$, we conclude that inequalities (26) have no solution for $X = 2^l$, if l is an integer in $[\log_2\|Q_{k+1}\| - 2\log_2 q, \log_2\|Q_{k+1}\|)$.

By Lemma 3.6, $\|Q_{k+1}\| = \prod_{i=1}^{k+1}\|A_i\|$ and $\deg A_k \ge 1$, we have that

$$\|Q_{k+1}\| \ge q^2\|Q_{k-1}\|,$$

which implies that

$$[\log_2\|Q_{k-1}\| - 2\log_2 q, \log_2\|Q_{k-1}\|) \quad \text{and} \quad [\log_2\|Q_{k+1}\| - 2\log_2 q, \log_2\|Q_{k+1}\|)$$

are disjoint for $k \ge 1$. Let N be an integer with $\log_2\|Q_{2k}\| \le N < \log_2\|Q_{2k+2}\|$; it follows that the number of integers l in $\{1, 2, \dots, N\}$ such that inequalities (26) have no solution for $X = 2^l$ and $c = q^{-3}$ is at least $2k$. In this way,

$$\frac{2k}{\log_2\|Q_{2k+2}\|} \le \frac{2k}{N} \le \frac{N-\Delta_{N,c}(\alpha)}{N}.$$

The condition of singularity on average implies that the right-hand side of the above inequality goes to 0 as N tends to infinity. By the monotonicity of $(\|Q_k\|)_{k\ge1}$, we conclude that $(\|Q_k\|^{1/k})_{k\ge1}$ tends to infinity. □

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TORSION OF RATIONAL ELLIPTIC CURVES OVER THE MAXIMAL ABELIAN EXTENSION OF $\mathbb{Q}$

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Let E be an elliptic curve defined over $\mathbb{Q}$, and let $\mathbb{Q}^{\mathrm{ab}}$ be the maximal abelian extension of $\mathbb{Q}$. In this article we classify the groups that can arise as $E(\mathbb{Q}^{\mathrm{ab}})_{\mathrm{tors}}$ up to isomorphism. The method illustrates techniques for finding explicit models of modular curves of mixed level structure. Moreover, we provide an explicit algorithm to compute $E(\mathbb{Q}^{\mathrm{ab}})_{\mathrm{tors}}$ for any elliptic curve $E/\mathbb{Q}$.

1. Introduction and notation

Let K denote a number field, and let E be an elliptic curve over K. The Mordell–Weil theorem states that the group of K-rational points on E form a finitely generated abelian group. In particular, letting $E(K)$ denote the K-rational points on E, we have that

$$E(K) \cong \mathbb{Z}^{r_K} \oplus E(K)_{\mathrm{tors}}$$

for some finite group $E(K)_{\mathrm{tors}}$, called the torsion of E over K. In fact, due to a theorem of Merel [1996], there is a bound on the size of the torsion subgroup that depends only on the degree of K over $\mathbb{Q}$. Thus, there is a finite list of torsion subgroups that appear as $E(K)_{\mathrm{tors}}$ as K varies over number fields of a fixed degree d and E/K varies. Let $\Phi(d)$ denote the set of torsion subgroups (up to isomorphism) that appear as $E(K)_{\mathrm{tors}}$ for some elliptic curve E/K as K ranges over all number fields of a fixed degree d over $\mathbb{Q}$. In particular, Mazur [1978] determined $\Phi(1)$. Not many other values of $\Phi(d)$ have been determined. The set $\Phi(2)$ was classified by Kamienny [1992] and Kenku and Momose [1988], and the set $\Phi(3)$ was classified by Derickx, Etropolski, Morrow, van Hoeij, and Zureick-Brown [Derickx et al. $\geq$ 2019].

Classifying torsion subgroups of elliptic curves over number fields is equivalent to classifying points on the modular curves $X_1(M, N)$ defined over these number fields. Thus, the classification of $\Phi(d)$ involves determining all such modular curves with K-rational points for any number field K of degree d over $\mathbb{Q}$.

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One may also ask a more refined question. Let $\Phi_{\mathbb{Q}}(d)$ denote the set of torsion subgroups (up to isomorphism) that appear as $E(K)_{\text{tors}}$ for some elliptic curve $E/\mathbb{Q}$ as K ranges over all number fields of degree d over $\mathbb{Q}$. Notice that necessarily $\Phi_{\mathbb{Q}}(d) \subseteq \Phi(d)$ since we are restricting the set of elliptic curves we are considering. Of course, $\Phi_{\mathbb{Q}}(1) = \Phi(1)$. The sets $\Phi_{\mathbb{Q}}(2)$ and $\Phi_{\mathbb{Q}}(3)$ were determined by Najman [2016]. A subset of $\Phi_{\mathbb{Q}}(4)$, namely $E(K)_{\text{tors}}$ for $[K:\mathbb{Q}] = 4$ and $K/\mathbb{Q}$ abelian, was classified by the author [Chou 2016], and $\Phi_{\mathbb{Q}}(4)$ has been determined by González-Jiménez and Najman [2016]. For a more in-depth summary of what is known about torsion of elliptic curves over number fields of a fixed degree d, see for instance the introduction of [Chou 2016].

In the setting of modular curves, these torsion subgroups can be viewed as K-rational points for some $[K:\mathbb{Q}] = d$ on $X_1(M, N)$ whose image under the j-map is in $\mathbb{Q}$. These elliptic curves obtain the torsion structure $\mathbb{Z}/M\mathbb{Z} \oplus \mathbb{Z}/N\mathbb{Z}$ over a degree-d number field as they correspond to a K-rational point on $X_1(M, N)$, but their j-invariants are in $\mathbb{Q}$, as each elliptic curve can be defined over $\mathbb{Q}$.

One can also consider torsion over an infinite extension L of $\mathbb{Q}$. For a fixed algebraic extension L of $\mathbb{Q}$, let $\Phi_{\mathbb{Q}}(L)$ denote the set of torsion subgroups $E(L)_{\text{tors}}$ up to isomorphism that appear as $E/\mathbb{Q}$ varies. The Mordell–Weil theorem no longer applies, and so a priori it is not guaranteed that the size of $E(L)_{\text{tors}}$ is finite, let alone uniformly bounded as E varies. Even so, in certain infinite extensions the number of torsion points is finite and, in fact, uniformly bounded as E varies. Fujita determined $\Phi_{\mathbb{Q}}(\mathbb{Q}(2^\infty))$ where $\mathbb{Q}(2^\infty)$ is the compositum of all degree-2 extensions of $\mathbb{Q}$, i.e., $\mathbb{Q}(2^\infty) := \mathbb{Q}(\{\sqrt{m} : m \in \mathbb{Z}\})$.

Theorem 1.1 [Fujita 2005, Theorem 2].

$$\Phi_{\mathbb{Q}}(\mathbb{Q}(2^\infty)) = \begin{cases} \mathbb{Z}/N_1\mathbb{Z}, & N_1 = 1, 3, 5, 7, 9, 15, \\ \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2N_2\mathbb{Z}, & N_2 = 1, 2, 3, 4, 5, 6, 8, \\ \mathbb{Z}/4\mathbb{Z} \times \mathbb{Z}/4N_4\mathbb{Z}, & N_4 = 1, 2, 3, 4, \\ \mathbb{Z}/3\mathbb{Z} \times \mathbb{Z}/3\mathbb{Z}, & \\ \mathbb{Z}/6\mathbb{Z} \times \mathbb{Z}/6\mathbb{Z}, & \\ \mathbb{Z}/8\mathbb{Z} \times \mathbb{Z}/8\mathbb{Z}. & \end{cases}$$

Torsion over a similar infinite extension, $\mathbb{Q}(3^\infty)$, the compositum of all cubic number fields, was studied by Daniels, Lozano-Robledo, Najman, and Sutherland [Daniels et al. 2018]. They classify $\Phi_{\mathbb{Q}}(\mathbb{Q}(3^\infty))$. Moreover, they determine which of these torsion structures appear infinitely often and which appear for only finitely many isomorphism classes of elliptic curves.

Here is some notation that will be used throughout the paper: $E[p^\infty]$ denotes torsion points of order a power of p and $\mathbb{Q}^{\text{ab}}$ denotes the maximal abelian extension of $\mathbb{Q}$. By the Kronecker–Weber theorem we have that $\mathbb{Q}^{ab} = \mathbb{Q}(\{\zeta_n : n \in \mathbb{Z}^+\})$ where ζ_n denotes a primitive n-th root of unity.

Given an abelian variety $A/\mathbb{Q}$, the torsion subgroup of $A(\mathbb{Q}^{ab})$ is finite (this is due to a theorem of Ribet [1981]). Thus, one can ask if there is a uniform bound for the size of such a torsion subgroup or whether there are possibly infinitely many torsion structures that appear. If we restrict to genus-1 abelian varieties, we prove there are only finitely many groups that appear as $E(\mathbb{Q}^{ab})_{\text{tors}}$ for any elliptic curve $E/\mathbb{Q}$. In fact, we completely determine $\Phi_{\mathbb{Q}}(\mathbb{Q}^{ab})$.

Theorem 1.2. *Let $E/\mathbb{Q}$ be an elliptic curve. Then $E(\mathbb{Q}^{ab})_{\text{tors}}$ is isomorphic to one of the following groups*:

$$
\begin{array}{ll}
\mathbb{Z}/N_1\mathbb{Z}, & N_1 = 1,3,5,7,9,11,13,15,17,19,21,25,27,37,43,67,163,\\
\mathbb{Z}/2\mathbb{Z}\times\mathbb{Z}/2N_2\mathbb{Z}, & N_2 = 1,2,\ldots,9,\\
\mathbb{Z}/3\mathbb{Z}\times\mathbb{Z}/3N_3\mathbb{Z}, & N_3 = 1,3,\\
\mathbb{Z}/4\mathbb{Z}\times\mathbb{Z}/4N_4\mathbb{Z}, & N_4 = 1,2,3,4,\\
\mathbb{Z}/5\mathbb{Z}\times\mathbb{Z}/5\mathbb{Z}, & \\
\mathbb{Z}/6\mathbb{Z}\times\mathbb{Z}/6\mathbb{Z}, & \\
\mathbb{Z}/8\mathbb{Z}\times\mathbb{Z}/8\mathbb{Z}. &
\end{array}
$$

Each of these groups appears as $E(\mathbb{Q}^{ab})_{\text{tors}}$ for some elliptic curve over $\mathbb{Q}$.

A uniform bound on the size of $E(\mathbb{Q}^{ab})_{\text{tors}}$ for all elliptic curves $E/\mathbb{Q}$ is an easy corollary of the classification.

Corollary 1.3. *Let $E/\mathbb{Q}$ be an elliptic curve. Then $\#E(\mathbb{Q}^{ab})_{\text{tors}} \leq 163$. This bound is sharp*, *as the curve* 26569a1 *has a point of order* 163 *over* $\mathbb{Q}^{ab}$.

In Section 2 we discuss what is known about isogenies of elliptic curves over $\mathbb{Q}$. We then discuss the intimate connection between isogenies and torsion points over $\mathbb{Q}^{ab}$. In Section 4 we use the results from Section 2 to prove bounds on the group $E(\mathbb{Q}^{ab})_{\text{tors}}$ based on the isogenies E has over $\mathbb{Q}$. In Section 5 we further refine the bounds to eliminate the possibility of any group not appearing in Theorem 1.2. In Section 6 we construct an algorithm to determine $E(\mathbb{Q}^{ab})_{\text{tors}}$ for any elliptic curve $E/\mathbb{Q}$. Finally, Section 7 has, for each subgroup T appearing in Theorem 1.2, an example of an elliptic curve $E/\mathbb{Q}$ such that $E(\mathbb{Q}^{ab})_{\text{tors}} \cong T$, completing the proof of Theorem 1.2. We use Cremona labels for our elliptic curves, and more information on each curve can be found on the LMFDB [2013].

2. Isogenies

In the rest of the paper, when we refer to an isogeny, we will mean a cyclic $\mathbb{Q}$-rational isogeny. The classification of $\mathbb{Q}$-rational n-isogenies is an integral part of the classification of torsion of elliptic curves $E/\mathbb{Q}$ over $\mathbb{Q}^{ab}$.

Theorem 2.1 (Fricke, Kenku, Klein, Kubert, Ligozat, Mazur, and Ogg, among others). *If $E/\mathbb{Q}$ has an n-isogeny, $n \leq 19$ or $n \in \{21, 25, 27, 37, 43, 67, 163\}$. If E does not have complex multiplication, then $n \leq 18$ or $n \in \{21, 25, 37\}$.*

See [Lozano-Robledo 2013, §9] for a more detailed discussion of this theorem. Moreover, there is a detailed bound on the number of $\mathbb{Q}$-isogenies an elliptic curve can have. The following theorem is from [Kenku 1982], combining Theorem 2 and the surrounding discussion.

Theorem 2.2 [Kenku 1982]. *There are at most eight $\mathbb{Q}$-isomorphism classes of elliptic curves in each $\mathbb{Q}$ isogeny class.*

Let $C_p(E)$ denote the number of distinct $\mathbb{Q}$-rational cyclic subgroups of order p^n for any $n \geq 0$ of E. Then, we have the following table for bounds on C_p for any elliptic curve over $\mathbb{Q}$:

p	2	3	5	7	11	13	17	19	37	43	67	163	*else*
C_p	8	4	3	2	2	2	2	2	2	2	2	2	1

In particular, fix a $\mathbb{Q}$-isogeny class and a representative E of that class. Let $C(E) = \prod_p C_p(E)$.

- *If $C_p(E) = 2$ for some prime $p \geq 11$, then $C_q(E) = 1$ for all other primes. So $C(E) = 2$.*
- *If $C_7(E) = 2$, then $C_5(E) = 1$ and either $C_3(E) \leq 2$ and $C_2(E) = 1$ or $C_3(E) = 1$ and $C_2(E) \leq 2$. All these yield $C(E) \leq 4$.*
- *If $C_5(E) = 3$, then $C_p(E) = 1$ for all primes $p \neq 5$.*
- *If $C_5(E) = 2$, then either $C_3(E) \leq 2$ and $C_2(E) = 1$ or $C_3(E) = 1$ and $C_2(E) \leq 2$. Hence, $C(E) \leq 4$.*
- *If $C_3(E) = 4$, then there exists a representative of the class of E with a $\mathbb{Q}$-rational cyclic subgroup of order 27, and $C_2(E) = 1$ so $C(E) \leq 4$.*
- *If $C_3(E) = 3$, then $C_2(E) \leq 2$ so that $C(E) \leq 6$.*
- *If $C_3(E) \leq 2$, then $C_2(E) \leq 4$ so that $C(E) \leq 8$.*

Note the fact that $C(E) = 8$ is possible only if $C_2(E) = 8$ or $C_3(E) = 2$ and $C_2(E) = 4$.

The first connection between isogenies and points over $\mathbb{Q}^{\text{ab}}$ is shown in the following lemma.

Lemma 2.3. *If $E/\mathbb{Q}$ has an n-isogeny defined over $\mathbb{Q}$, then $E(\mathbb{Q}^{\text{ab}})$ has a point of order n.*

Proof. Let φ denote the n-isogeny over $\mathbb{Q}$. Then $\ker(\varphi) = \langle P \rangle$ for some point $P \in E(\overline{\mathbb{Q}})$ of order n such that $\langle P \rangle^\sigma = \langle P \rangle$ for all $\sigma \in \mathrm{Gal}(\overline{\mathbb{Q}}/\mathbb{Q})$. This induces a character

$$\psi : \mathrm{Gal}(\overline{\mathbb{Q}}/\mathbb{Q}) \to (\mathbb{Z}/n\mathbb{Z})^\times$$

defined by $\sigma \mapsto a \bmod n$ where a is given by $\sigma(P) = aP$. The kernel of ψ is precisely $\mathrm{Gal}(\overline{\mathbb{Q}}/\mathbb{Q}(P))$, and thus, we have that $\mathrm{Gal}(\mathbb{Q}(P)/\mathbb{Q})$ is isomorphic to a subgroup of $(\mathbb{Z}/n\mathbb{Z})^\times$, and hence abelian. Therefore, $P \in E(\mathbb{Q}^{\mathrm{ab}})$. □

Given an elliptic curve $E/\mathbb{Q}$, due to Ribet's theorem we know that there exists $m, n \in \mathbb{Z}^{\geq 0}$ such that $E(\mathbb{Q}^{\mathrm{ab}})_{\mathrm{tors}} \cong \mathbb{Z}/m\mathbb{Z} \times \mathbb{Z}/mn\mathbb{Z}$. We wish to understand what possible m and n can occur together.

In regards to the values of m, normally one could use an argument via the Weil pairing which implies that our field must contain ζ_m; however, this is not very restrictive when looking at torsion over $\mathbb{Q}^{\mathrm{ab}}$. Instead, we have the following theorem.

Theorem 2.4 [González-Jiménez and Lozano-Robledo 2016, Theorem 1.1]. *Let $E/\mathbb{Q}$ be an elliptic curve. If there is an integer $n \geq 2$ such that $\mathbb{Q}(E[n]) = \mathbb{Q}(\zeta_n)$, then $n = 2, 3, 4,$ or 5. More generally, if $\mathbb{Q}(E[n])/\mathbb{Q}$ is abelian, then $n = 2, 3, 4, 5, 6,$ or 8. Moreover,* $\mathrm{Gal}(\mathbb{Q}(E[n]/\mathbb{Q}))$ *is isomorphic to one of the following groups*:

n	2	3	4	5	6	8
$\mathrm{Gal}(\mathbb{Q}(E[n]/\mathbb{Q}))$	$\{0\}$ $\mathbb{Z}/2\mathbb{Z}$ $Z/3\mathbb{Z}$	$\mathbb{Z}/2\mathbb{Z}$ $(\mathbb{Z}/2\mathbb{Z})^2$	$\mathbb{Z}/2\mathbb{Z}$ $(\mathbb{Z}/2\mathbb{Z})^2$ $(\mathbb{Z}/2\mathbb{Z})^3$ $(\mathbb{Z}/2\mathbb{Z})^4$	$\mathbb{Z}/4\mathbb{Z}$ $\mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/4\mathbb{Z}$ $(\mathbb{Z}/4\mathbb{Z})^2$	$(\mathbb{Z}/2\mathbb{Z})^2$ $(\mathbb{Z}/2\mathbb{Z})^3$	$(\mathbb{Z}/2\mathbb{Z})^4$ $(\mathbb{Z}/2\mathbb{Z})^5$ $(\mathbb{Z}/2\mathbb{Z})^6$

Furthermore, each possible Galois group occurs for infinitely many distinct j-invariants.

In fact, if $E(\mathbb{Q}^{\mathrm{ab}})_{\mathrm{tors}} \cong \mathbb{Z}/m\mathbb{Z} \times \mathbb{Z}/mn\mathbb{Z}$, both values m and n are controlled primarily by isogenies. For instance, in the proof of Theorem 2.4, González-Jiménez and Lozano-Robledo make use of a key corollary relating full-p-torsion over $\mathbb{Q}^{\mathrm{ab}}$ to $\mathbb{Q}$-rational p-isogenies.

Corollary 2.5 [González-Jiménez and Lozano-Robledo 2016, Corollary 3.9]. *Let $E/\mathbb{Q}$ be an elliptic curve, let $p > 2$ be a prime, and suppose that $\mathbb{Q}(E[p])/\mathbb{Q}$ is abelian. Then, the $\mathbb{Q}$-isogeny class of E contains at least three distinct $\mathbb{Q}$-isomorphism classes, and $C_p(E) \geq 3$. In particular $p \leq 5$.*

In particular, the proof of Corollary 2.4 in [González-Jiménez and Lozano-Robledo 2016] shows that for all $p > 2$, if $\mathbb{Q}(E[p])/\mathbb{Q}$ is abelian for some $E/\mathbb{Q}$, then E has two independent p-isogenies over $\mathbb{Q}$. Note that the converse is also true.

Lemma 2.6. *Let $E/\mathbb{Q}$ be an elliptic curve, let p be a prime, and suppose that E has two distinct p-isogenies over $\mathbb{Q}$. Then $\mathbb{Q}(E[p])/\mathbb{Q}$ is abelian.*

Proof. Let $\rho_{E,p} : \mathrm{Gal}(\overline{\mathbb{Q}}/\mathbb{Q}) \to \mathrm{Aut}(E[p]) \cong \mathrm{GL}(2, p)$ denote the mod p Galois representation associated to E. Since E has two independent p-isogenies, there exists a basis $\{P, Q\}$ of $E[p]$ so that the image of $\rho_{E,p}$ is contained in a split Cartan subgroup of $\mathrm{GL}(2, p)$. Now, since $\ker \rho_{E,p} = \mathrm{Gal}(\overline{\mathbb{Q}}/\mathbb{Q}(E[p]))$, it follows that

$$\mathrm{Gal}(\mathbb{Q}(E[p])/\mathbb{Q}) = \mathrm{Gal}(\mathbb{Q}(P, Q)/\mathbb{Q}) \cong \rho_{E,p}(\mathrm{Gal}(\overline{\mathbb{Q}}/\mathbb{Q}))$$

which is contained in split Cartan subgroup and thus abelian. □

Note that we can see in [González-Jiménez and Lozano-Robledo 2016, Table 1] a complete table showing which elliptic curves with complex multiplication (CM) can have $\mathbb{Q}(E[n])$ abelian for which n. We also have the following lemma to help understand the possible values of n.

Lemma 2.7. *Let K be a Galois extension of $\mathbb{Q}$ and E an elliptic curve over $\mathbb{Q}$. If $E(K)_{\mathrm{tors}} \cong \mathbb{Z}/m\mathbb{Z} \times \mathbb{Z}/mn\mathbb{Z}$, then E has an n-isogeny over $\mathbb{Q}$.*

Proof. Suppose $E(K)_{\mathrm{tors}} \cong \mathbb{Z}/m\mathbb{Z} \times \mathbb{Z}/mn\mathbb{Z} = \langle P, Q\rangle$ where P has order m and Q has order mn. Then $[m]E(K)_{\mathrm{tors}} = \langle mP, mQ\rangle = \langle mQ\rangle \cong \mathbb{Z}/n\mathbb{Z}$. Let $\sigma \in \mathrm{Gal}(\overline{\mathbb{Q}}/\mathbb{Q})$. Since K is Galois over $\mathbb{Q}$ and E is defined over $\mathbb{Q}$, we have

$$Q^\sigma \in E(K)_{\mathrm{tors}},$$

and since the action of Galois commutes with multiplication by m,

$$(mQ)^\sigma = m(Q^\sigma) \in [m]E(K)_{\mathrm{tors}} = \langle mQ\rangle.$$

Thus, $\langle mQ\rangle$ is a cyclic subgroup of order n that is stable under the action of $\mathrm{Gal}(\overline{\mathbb{Q}}/\mathbb{Q})$, which implies E has an n-isogeny over $\mathbb{Q}$. □

Thus, the possible values for m (up to a power of 2) and n are controlled by the $\mathbb{Q}$-isogenies of the elliptic curve.

3. Points of order 2^n

In order to understand $E(\mathbb{Q}_{\mathrm{ab}})[2^\infty]$ and its connection to isogenies, we will use the database of Rouse and Zureick-Brown [2015]. First we prove a simple lemma concerning quadratic twists.

Lemma 3.1. *Let $E/\mathbb{Q}$ be an elliptic curve, let d be a square-free integer, and let E_d denote the quadratic twist of E by d. Then $E(\mathbb{Q}^{\mathrm{ab}})_{\mathrm{tors}} \cong E_d(\mathbb{Q}^{\mathrm{ab}})_{\mathrm{tors}}$.*

Proof. Since E and E_d become isomorphic over $\mathbb{Q}(\sqrt{d})$ and $\mathbb{Q}(\sqrt{d}) \subseteq \mathbb{Q}^{\mathrm{ab}}$ for any d, the lemma follows immediately. □

Note that the minimal field of definition of the torsion for E and E_d may differ, but by the previous lemma their torsion over $\mathbb{Q}^{ab}$ will always be isomorphic. In particular, when examining elliptic curves with j-invariant not equal to 0 or 1728, it suffices to fix a specific curve E, and examine $E(\mathbb{Q}^{ab})_{tors}$.

The following lemma gives a criterion for a point to be halved which will be handy to explicitly compute $\mathbb{Q}(E[2^k])$ for various k:

Lemma 3.2 [Knapp 1992, Theorem 4.2, p. 85]. *Let K be a field of characteristic not equal to 2 or 3 and E an elliptic curve over K given by $y^2 = (x-\alpha)(x-\beta)(x-\gamma)$ with α, β, γ in K. For $P = (x, y) \in E(K)$, there exists a K-rational point $Q = (x', y')$ on E such that $[2]Q = P$ if and only if $x-\alpha$, $x-\beta$, and $x-\gamma$ are all squares in K. In this case, if we fix the sign of $\sqrt{x-\alpha}$, $\sqrt{x-\beta}$, and $\sqrt{x-\gamma}$, then x' equals one of*

$$\sqrt{x-\alpha}\sqrt{x-\beta} \pm \sqrt{x-\alpha}\sqrt{x-\gamma} \pm \sqrt{x-\beta}\sqrt{x-\gamma} + x$$

or

$$-\sqrt{x-\alpha}\sqrt{x-\beta} \pm \sqrt{x-\alpha}\sqrt{x-\gamma} \mp \sqrt{x-\beta}\sqrt{x-\gamma} + x$$

where the signs are taken simultaneously.

In particular, we can prove a nice criterion for an elliptic curve having a point of order 4 over $\mathbb{Q}^{ab}$, but not full 4-torsion. We will make use of the following proposition describing the Galois group of various degree-4 polynomials.

Proposition 3.3 [Conrad 2012, Corollary 4.5]. *Let $f(X) = X^4 + bX^2 + d$ be irreducible in $K[X]$, where K does not have characteristic 2. Its Galois group over K, denoted G_f, is $\mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}$, $\mathbb{Z}/4\mathbb{Z}$, or D_4 according to the following conditions*:

(1) *If $d \in (K^\times)^2$, then $G_f = \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}$.*

(2) *If $d \notin (K^\times)^2$ and $(b^2-4d)d \in (K^\times)^2$, then $G_f = \mathbb{Z}/4\mathbb{Z}$.*

(3) *If $d \notin (K^\times)^2$ and $(b^2-4d)d \notin (K^\times)^2$, then $G_f = D_4$.*

We combine this result with Lemma 3.2 to prove the following lemma.

Lemma 3.4. *Suppose E is an elliptic curve over $\mathbb{Q}$ that has a point of order 4 over $\mathbb{Q}^{ab}$ but does not have full 4-torsion defined over $\mathbb{Q}^{ab}$. Then, either $C_2(E) \geq 4$, or there is a model of E of the form*

$$E : y^2 = x(x^2 + bx + d)$$

and either d or $(b^2-4d)d$ is a nonzero perfect square in $\mathbb{Q}$.

Proof. Suppose that $C_2(E) < 4$. By Lemma 2.7 if E has a point of order 4 but not full 4-torsion defined over $\mathbb{Q}^{ab}$, then E has at least one 2-isogeny over $\mathbb{Q}$. Thus, there exists a point P of order 2 defined over $\mathbb{Q}$, and by moving that point to $P = (0, 0)$

we obtain a model for E of the form $y^2 = x(x^2+bx+d) = x(x-\alpha)(x-\bar{\alpha})$ with $b, d \in \mathbb{Q}$ and $\alpha, \bar{\alpha} \notin \mathbb{Q}$. If $\alpha, \bar{\alpha} \in \mathbb{Q}$, then $E(\mathbb{Q})[2] \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}$, which would imply $C_2(E) \geq 4$.

Over $\mathbb{Q}^{\mathrm{ab}}$ we have a point of order 4, say Q. Suppose first that this point lies above a rational point of order 2. Without loss of generality we have $2Q = P = (0, 0)$. Writing $E : y^2 = x(x-\alpha)(x-\bar{\alpha})$, Lemma 3.2 says that we have that $\sqrt{-\alpha}$ and $\sqrt{-\bar{\alpha}}$ must be elements in $\mathbb{Q}^{\mathrm{ab}}$. Notice that $\sqrt{-\alpha}$ and $\sqrt{-\bar{\alpha}}$ satisfy the polynomial

$$f = x^4 - bx^2 + d.$$

We prove that this polynomial is irreducible, and hence the minimal polynomial of $\sqrt{-\alpha}$ and $\sqrt{-\bar{\alpha}}$ over $\mathbb{Q}$.

Suppose f is reducible; then $[\mathbb{Q}(x(Q)) : \mathbb{Q}] = 1$ or 2. If $[\mathbb{Q}(x(Q)) : \mathbb{Q}] = 1$, then there is a quadratic twist of E, say E', with $E'(\mathbb{Q})_{\mathrm{tors}}$ having a point of order 4. Then, E' has a 4-isogeny, so E' is 2-isogenous to an elliptic curve E'' with full 2-torsion over $\mathbb{Q}$ by [González-Jiménez and Najman 2016, Lemma 8.14]. Since E'' has full 2-torsion over $\mathbb{Q}$, it has isogenies of degrees 1, 2, 2, and 2, with one of those curves being E'. Therefore, E' has isogenies of degrees 1, 2, 4, and 4. Since E is a quadratic twist of E', it also has isogenies of degrees 1, 2, 4, and 4. This contradicts the assumption that $C_2(E) < 4$. If $[\mathbb{Q}(x(Q)) : \mathbb{Q}] = 2$, then f factors over $\mathbb{Q}[x]$ as

$$f = (x^2+\alpha)(x^2+\bar{\alpha}),$$

which implies $\alpha \in \mathbb{Q}$. As mentioned above, this contradicts $C_2(E) < 4$. Thus, f is irreducible, and is the minimal polynomial of $\sqrt{-\alpha}$ and $\sqrt{-\bar{\alpha}}$ over $\mathbb{Q}$.

Since $Q \in E(\mathbb{Q}^{\mathrm{ab}})$, the Galois group of f over $\mathbb{Q}$ is abelian. Therefore, $G_f = \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}$ or $\mathbb{Z}/4\mathbb{Z}$. Now by Proposition 3.3 the two cases above follow.

Suppose instead that our point of order 4 is halving a point of order 2 that is not rational. Without loss of generality we may assume $2Q = (\alpha, 0)$. By Lemma 3.2 we have that α and $\alpha - \bar{\alpha}$ are squares in $\mathbb{Q}^{\mathrm{ab}}$. However, since $\sqrt{-1} \in \mathbb{Q}^{\mathrm{ab}}$ it also follows that $-\alpha$ and $-\bar{\alpha}$ are squares in $\mathbb{Q}^{\mathrm{ab}}$. Thus, the point $(0, 0)$ is also halved in $\mathbb{Q}^{\mathrm{ab}}$, contradicting our original assumption that E does not have full 4-torsion over $\mathbb{Q}^{\mathrm{ab}}$. □

We now prove our proposition relating 2-powered torsion to the isogenies of an elliptic curve.

Proposition 3.5. *Let $E/\mathbb{Q}$ be an elliptic curve. Table 1 gives the possibilities for $E(\mathbb{Q}^{\mathrm{ab}})[2^\infty]$, the 2-powered isogenies attached to each case, and also $C_2(E)$.*

Proof. If E does not have CM, it must be in one of the families given in the Rouse–Zureick-Brown database [2015]. We compute for each family the 2-powered

$E(\mathbb{Q}^{ab})[2^\infty]$	isogeny degrees	$C_2(E)$
$\{\mathbb{O}\}$	1	1
$\mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}$	1	1
	1, 2	2
$\mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/4\mathbb{Z}$	1, 2	2
	1, 2, 4, 4	4
$\mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/8\mathbb{Z}$	1, 2, 4, 4	4
	1, 2, 4, 4, 8, 8	6
$\mathbb{Z}/4\mathbb{Z} \times \mathbb{Z}/4\mathbb{Z}$	1, 2, 2, 2	4
	1, 2, 4, 4	4
$\mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/16\mathbb{Z}$	1, 2, 4, 4, 8, 8, 16, 16	8
$\mathbb{Z}/4\mathbb{Z} \times \mathbb{Z}/8\mathbb{Z}$	1, 2, 2, 2, 4, 4	6
	1, 2, 4, 4, 8, 8, 8, 8	8
$\mathbb{Z}/4\mathbb{Z} \times \mathbb{Z}/16\mathbb{Z}$	1, 2, 2, 2, 4, 4, 8, 8	8
$\mathbb{Z}/8\mathbb{Z} \times \mathbb{Z}/8\mathbb{Z}$	1, 2, 2, 2, 4, 4, 4, 4	8

Table 1. Possible 2-primary torsion over $\mathbb{Q}^{ab}$.

torsion over $\mathbb{Q}^{ab}$. We do this as follows: for each family let G be the image of $\rho_{E,32}$, that is $G = \rho_{E,32}(\mathrm{Gal}(\overline{\mathbb{Q}}/\mathbb{Q}))$. In fact,

$$G = \rho_{E,32}(\mathrm{Gal}(\overline{\mathbb{Q}}/\mathbb{Q})) \cong \mathrm{Gal}(\mathbb{Q}(E[32])/\mathbb{Q})$$

since $\ker \rho_{E,32} = \mathrm{Gal}(\overline{\mathbb{Q}}/\mathbb{Q}(E[32]))$. Then the commutator subgroup $[G, G]$ has fixed field equal to $\mathbb{Q}(E[32]) \cap \mathbb{Q}^{ab}$. We fix a $\mathbb{Z}/32\mathbb{Z}$-basis $\{P, Q\}$ of $E[32]$ and identify G with a subgroup of $\mathrm{GL}(2, 32)$. We then compute the vectors fixed in $(\mathbb{Z}/32\mathbb{Z})^2$ by $[G, G]$, which gives the structure of the points on E defined over $\mathbb{Q}(E[32]) \cap \mathbb{Q}^{ab}$, that is the structure of $E(\mathbb{Q}^{ab})[32]$. Here, a vector $[a, b] \in (\mathbb{Z}/32\mathbb{Z})^2$ corresponds to a point $aP + bQ \in E[32]$. Since the largest-order point found in $E(\mathbb{Q}^{ab})[32]$ has order 16, we see that $E(\mathbb{Q}^{ab})[2^\infty] = E(\mathbb{Q}^{ab})[16]$.

For elliptic curves with CM we examine the finitely many j-invariants over $\mathbb{Q}$ [González-Jiménez and Lozano-Robledo 2016, Table 1]. The table is broken up into quadratic twist families by j-invariant. For $j \neq 0, 1728$, there are only finitely many quadratic twist families, and so by Lemma 3.1 it suffices to fix a single curve within each family and examine its torsion over $\mathbb{Q}^{ab}$.

Let E be such a curve. From that table we can see the largest m such that $\mathbb{Q}(E[2^m])$ is abelian, as well as the isogenies each $\mathbb{Q}$-isomorphism class has. Let 2^n denote the largest degree-2-powered isogeny E has. Then from Lemma 2.7 it follows that $E(\mathbb{Q}^{ab})[2^\infty] \subseteq \mathbb{Z}/2^m\mathbb{Z} \times \mathbb{Z}/2^{n+m}\mathbb{Z}$.

Thus, to find the structure of $E(\mathbb{Q}^{ab})[2^\infty]$ it simply remains to find the largest 2-powered torsion E has over some abelian number field, up to 2^{n+m}. We do this by using the division polynomial method. For each $0 < k \le n+m$ we use Magma [Bosma et al. 1997] to compute the (2^k)-th-division polynomial of E, whose roots are the x-coordinates of the points of order 2^k on E. From the x-coordinates, we can compute the corresponding y-coordinates and get a list of all points of order 2^k on E. Now we simply compute the field of definition of these points and check whether each field is abelian or not. If k_0 is the first value where no points of order 2^{k_0} are defined over an abelian extension, then $E(\mathbb{Q}^{ab})[2^\infty] \cong \mathbb{Z}/2^m\mathbb{Z} \times \mathbb{Z}/2^{k_0-1}\mathbb{Z}$.

We run through each quadratic twist family. Once computed we find that we do not gain any new groups nor do we add any new 2-powered isogeny degree combinations to the list originally found for non-CM curves. Note that the code used to do these computations is available at https://sites.tufts.edu/michaelchou/research/.

For $j = 0$, the cases $y^2 = x^3 + t^3$ and $y^2 = x^3 + 16t^3$, where $t \in \mathbb{Q}$, are single quadratic twist families, so may be treated as above. For the case $y^2 = x^3 + s$ with $s \neq t^3$, $16t^3$, [González-Jiménez and Lozano-Robledo 2016, Table 1] already shows that $E(\mathbb{Q}^{ab})[2] = \{\mathbb{O}\}$ for any of these quadratic twist families.

Similarly for $j = 1728$, the cases $y^2 = x^3 \pm t^2 x$ for $t \in \mathbb{Q}$ are in two separate quadratic twist families, so may be treated as before. Finally, we consider the case $E : y^2 = x^3 + sx$, with $s \neq \pm t^2$ for any $t \in \mathbb{Q}$. We see from [González-Jiménez and Lozano-Robledo 2016, Table 1] that the largest division field that is abelian is $\mathbb{Q}(E[2])$. Suppose that E has a point of order 4 over $\mathbb{Q}^{ab}$; then since $C_2(E) < 4$, Lemma 3.4 gives that s is a square in $\mathbb{Q}$ or $-4s^2$ is a square in $\mathbb{Q}$, contradicting our assumption that $s \neq \pm t^2$ for any $t \in \mathbb{Q}$. Thus, $E(\mathbb{Q}^{ab})[2^\infty] \equiv \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}$. Thus, the table above is complete. □

From Table 1 we can make a simple observation:

Lemma 3.6. *Let $E/\mathbb{Q}$ be an elliptic curve and suppose that $E(\mathbb{Q}^{ab})[2^\infty] \ncong \{\mathbb{O}\}$ or $\mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}$. Then E has at least one 2-isogeny over $\mathbb{Q}$, that is, $C_2(E) \ge 2$.*

4. Bounding torsion

We begin with a proposition that bounds $E(\mathbb{Q}^{ab})[p^\infty]$ for all primes p.

Proposition 4.1. *Let $E/\mathbb{Q}$ be an elliptic curve, and $\mathbb{Q}^{ab}$ be the maximal abelian extension of $\mathbb{Q}$. Then the following table gives a bound on $E(\mathbb{Q}^{ab})[p^\infty]$ for all primes p, i.e., the p-power torsion is contained in the following subgroups*:

p	2	3	5	7, 11, 13, 17, 19, 37, 43, 67, 163	else
$E(\mathbb{Q}^{ab})[p^\infty] \subseteq$	$\mathbb{Z}/4\mathbb{Z} \times \mathbb{Z}/16\mathbb{Z}$ $\mathbb{Z}/8\mathbb{Z} \times \mathbb{Z}/8\mathbb{Z}$	$\mathbb{Z}/3\mathbb{Z} \times \mathbb{Z}/27\mathbb{Z}$	$\mathbb{Z}/5\mathbb{Z} \times \mathbb{Z}/25\mathbb{Z}$	$\mathbb{Z}/p\mathbb{Z}$	$\{\mathbb{O}\}$

Proof. Note that $E(\overline{\mathbb{Q}})[p^n] \cong \mathbb{Z}/p^n\mathbb{Z} \times \mathbb{Z}/p^n\mathbb{Z}$; thus, $E(\mathbb{Q}^{\mathrm{ab}})[p^n] \subseteq \mathbb{Z}/p^n\mathbb{Z} \times \mathbb{Z}/p^n\mathbb{Z}$ for any n. However, by Theorem 2.4, if $\mathbb{Q}(E[p^n])$ is abelian, then $p = 2$, 3, or 5, and therefore, for any prime except 2, 3, and 5, we must have that E does not have full p torsion defined over $\mathbb{Q}^{\mathrm{ab}}$. Thus, if $p > 5$, then $E(\mathbb{Q}^{\mathrm{ab}})[p^\infty] \subseteq \mathbb{Z}/p^n\mathbb{Z}$ for some n. However, since $\mathbb{Q}^{\mathrm{ab}}$ is a Galois extension of $\mathbb{Q}$, Lemma 2.7 combined with Theorem 2.1 shows that $E(\mathbb{Q}^{\mathrm{ab}})[p^\infty] \subseteq \mathbb{Z}/p\mathbb{Z}$ for $p = 7$, 11, 13, 17, 19, 37, 43, 67, and 163, and for all other primes l larger than 5, $E(\mathbb{Q}^{\mathrm{ab}})[l^\infty] \cong \{\mathbb{O}\}$.

For the prime $p = 2$, we simply refer to Table 1.

For the prime $p = 3$, first notice that E cannot have full 9-torsion over $\mathbb{Q}^{\mathrm{ab}}$ because of Theorem 2.4. Thus, $E(\mathbb{Q}^{\mathrm{ab}})[3^\infty] \subseteq \mathbb{Z}/3\mathbb{Z} \times \mathbb{Z}/3^e\mathbb{Z}$ for some natural number e. By Lemma 2.7 if $E(\mathbb{Q}^{\mathrm{ab}})[3^\infty] \cong \mathbb{Z}/3\mathbb{Z} \times \mathbb{Z}/3^e\mathbb{Z}$, then E has a 3^{e-1} isogeny. By Theorem 2.1, the largest 3-power degree rational isogeny is 27, and so $e - 1 \leq 3$, i.e., $E(\mathbb{Q}^{\mathrm{ab}})[3^\infty] \subseteq \mathbb{Z}/3\mathbb{Z} \times \mathbb{Z}/81\mathbb{Z}$. However, suppose that in fact $E(\mathbb{Q}^{\mathrm{ab}})[3^\infty] \cong \mathbb{Z}/3\mathbb{Z} \times \mathbb{Z}/81\mathbb{Z}$. Then by the above argument, E has a rational 27-isogeny. However, the only elliptic curves over $\mathbb{Q}$ that have a 27-isogeny are CM curves (those with j-invariant $-2^{15} \cdot 3 \cdot 5^3$ [Lozano-Robledo 2013, Table 4]). By [González-Jiménez and Lozano-Robledo 2016, Table 1] we see that such a curve does not have $\mathbb{Q}(E[n])$ abelian for any $n \geq 2$. Thus, $E(\mathbb{Q}^{\mathrm{ab}})[3^\infty] \subseteq \mathbb{Z}/3\mathbb{Z} \times \mathbb{Z}/27\mathbb{Z}$.

For the prime $p = 5$, first notice that E cannot have full 25-torsion over $\mathbb{Q}^{\mathrm{ab}}$ because of Theorem 2.4. By an identical argument as in the $p = 3$ case, we have that $E(\mathbb{Q}^{\mathrm{ab}})[5^\infty] \subseteq \mathbb{Z}/5\mathbb{Z} \times \mathbb{Z}/125\mathbb{Z}$, since the largest 5-power degree rational isogeny is 25. However, suppose that $\mathbb{Z}/5\mathbb{Z} \times \mathbb{Z}/25\mathbb{Z} \hookrightarrow E(\mathbb{Q}^{\mathrm{ab}})[5^\infty]$. Consider the Galois representation $\rho_{E,25} : \mathrm{Gal}(\overline{\mathbb{Q}}/\mathbb{Q}) \to \mathrm{Aut}(E[25]) \cong \mathrm{GL}(2, 25)$. Let G denote the image of $\rho_{E,25}$. Since full 5-torsion is defined over $\mathbb{Q}^{\mathrm{ab}}$, Corollary 2.5 says there is a basis of $E[5]$ such that G mod 5 is contained in a split Cartan subgroup of GL(2, 5). Thus, we have that

$$G \leq \mathcal{G} := \left\{ \begin{bmatrix} a & 5b \\ 5c & d \end{bmatrix} : a, d \in (\mathbb{Z}/25\mathbb{Z})^\times,\ b, c \in \mathbb{Z}/5\mathbb{Z} \right\}.$$

Now, let H denote the image $\rho_{E,25}(\mathrm{Gal}(\overline{\mathbb{Q}}/\mathbb{Q}(E[25]) \cap \mathbb{Q}^{\mathrm{ab}}))$. Notice that $H = [G, G]$, the commutator subgroup of G. Since E has a point of order 25 over $\mathbb{Q}^{\mathrm{ab}}$, we have that H must fix a vector of order 25 in $(\mathbb{Z}/25\mathbb{Z})^2$, and therefore, $[G, G]$ must also fix a vector of order 25 in $(\mathbb{Z}/25\mathbb{Z})^2$.

By the Weil pairing the image of $\rho_{E,25}$ must have determinant equal to the full group $(\mathbb{Z}/25\mathbb{Z})^\times$, and therefore, G must be a subgroup of $\mathcal{G}$ with full determinant, and whose commutator subgroup fixes a vector of order 25 in $(\mathbb{Z}/25\mathbb{Z})^2$. Using Magma we can compute all such subgroups of GL(2, 25), and further we can also compute, given a subgroup of GL(2, 25), the isogenies of an elliptic curve associated with that image.

We thus compute that in fact all subgroups of $\mathcal{G}$ with the described properties all yield a 25-isogeny, and thus, any elliptic curve with such an image must in fact have a 25-isogeny. However, since full 5-torsion was defined over $\mathbb{Q}^{ab}$, Corollary 2.5 gives two isogenies of degree 5 and thus it is impossible for E to have a 25-isogeny, otherwise $C_5(E) = 4$ contradicting Theorem 2.2. Thus, $E(\mathbb{Q}^{ab})[5^\infty] \subseteq \mathbb{Z}/5\mathbb{Z} \times \mathbb{Z}/5\mathbb{Z}$. □

To prove bounds on the structure of $E(\mathbb{Q}^{ab})_{tors}$ we will need a lemma about full 6-torsion.

Lemma 4.2 [González-Jiménez and Lozano-Robledo 2016, Lemma 3.12]. *Let $E/\mathbb{Q}$ be an elliptic curve. If $\mathbb{Q}(E[6])/\mathbb{Q}$ is abelian, then* $\mathrm{Gal}(\mathbb{Q}(E[2])/\mathbb{Q}) \cong \mathbb{Z}/2\mathbb{Z}$.

As has been noted in Section 2, the structure of torsion over $\mathbb{Q}^{ab}$ is closely tied to the $\mathbb{Q}$-isogenies an elliptic curve has. We now prove bounds on $E(\mathbb{Q}^{ab})_{tors}$ based on these isogenies.

Proposition 4.3. *Let $E/\mathbb{Q}$ be an elliptic curve. Suppose $C_p(E) = 1$ for all primes $p \neq 2$. Then $E(\mathbb{Q}^{ab})_{tors} = E(\mathbb{Q}^{ab})[2^\infty]$ and is contained in either $\mathbb{Z}/4\mathbb{Z} \times \mathbb{Z}/16\mathbb{Z}$ or $\mathbb{Z}/8\mathbb{Z} \times \mathbb{Z}/8\mathbb{Z}$*

Proof. By Corollary 2.5 and Lemma 2.7 it follows that $E(\mathbb{Q}^{ab})_{tors} = E(\mathbb{Q}^{ab})[2^\infty]$. Thus, $E(\mathbb{Q}^{ab})_{tors}$ is one of the groups on Table 1 from Proposition 3.5. □

Proposition 4.4. *Let $E/\mathbb{Q}$ be an elliptic curve. Suppose E has a 3-isogeny and $C_p(E) = 1$ for all primes $p > 3$. Then*

$$E(\mathbb{Q}^{ab})_{tors} \subseteq \begin{cases} \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2N_2\mathbb{Z}, & N_2 = 12, 18, \\ \mathbb{Z}/3\mathbb{Z} \times \mathbb{Z}/27\mathbb{Z}, & \\ \mathbb{Z}/4\mathbb{Z} \times \mathbb{Z}/4N_4\mathbb{Z}, & N_4 = 1, 3, \textit{or} \\ \mathbb{Z}/6\mathbb{Z} \times \mathbb{Z}/12\mathbb{Z}. & \end{cases}$$

Proof. By Theorem 2.2 we have either

- $C_3(E) = 4$ and $C_p(E) = 1$ for all primes $p \neq 3$,
- $C_3(E) = 3$ and $C_2(E) \leq 2$, or
- $C_3(E) = 2$ and $C_2(E) \leq 4$.

Suppose $C_3(E) = 4$ and $C_p(E) = 1$ for all primes $p \neq 3$. Then by Proposition 4.1 we know that $E(\mathbb{Q}^{ab})[3^\infty] \subseteq \mathbb{Z}/3\mathbb{Z} \times \mathbb{Z}/27\mathbb{Z}$. Suppose E has full 3-torsion over $\mathbb{Q}^{ab}$. If E also has full 2-torsion over $\mathbb{Q}^{ab}$, then it has full 6-torsion over $\mathbb{Q}^{ab}$. Thus, by Lemma 4.2 we must have $\mathrm{Gal}(\mathbb{Q}(E[2])/\mathbb{Q}) \cong \mathbb{Z}/2\mathbb{Z}$. This is possible only if E has a point of order 2 defined over $\mathbb{Q}$, but that would give a Galois stable subgroup of order 2, and hence $C_2(E) \geq 2$, a contradiction. Therefore, by Lemma 3.6 we have that $E(\mathbb{Q}^{ab})[2^\infty] \cong \{\mathcal{O}\}$ and so $E(\mathbb{Q}^{ab})_{tors} \subseteq \mathbb{Z}/3\mathbb{Z} \times \mathbb{Z}/27\mathbb{Z}$. Suppose instead that E does not have full 3-torsion over $\mathbb{Q}^{ab}$. Then $E(\mathbb{Q}^{ab})[3^\infty] \subseteq \mathbb{Z}/27\mathbb{Z}$. If

$E(\mathbb{Q}^{ab})[3^\infty] \cong \mathbb{Z}/27\mathbb{Z}$, then E has a 27-isogeny and all such curves have CM (for instance see [Lozano-Robledo 2013, Table 4]). By [González-Jiménez and Lozano-Robledo 2016, Table 1] we see that such a curve does not have full n torsion defined over $\mathbb{Q}^{ab}$ for any n. Thus, $E(\mathbb{Q}^{ab})_{tors} = E(\mathbb{Q}^{ab})[3^\infty] \cong \mathbb{Z}/27\mathbb{Z}$ or $E(\mathbb{Q}^{ab})[3^\infty] \subseteq \mathbb{Z}/9\mathbb{Z}$ and $E(\mathbb{Q}^{ab})[2^\infty] \subseteq \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}$, which yields $E(\mathbb{Q}^{ab})_{tors} \subseteq \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/18\mathbb{Z}$.

Suppose $C_3(E) = 3$ and $C_2(E) \leq 2$. Then we have that $E(\mathbb{Q}^{ab})[3^\infty] \cong \mathbb{Z}/3\mathbb{Z} \times \mathbb{Z}/3\mathbb{Z}$ or $\mathbb{Z}/9\mathbb{Z}$. From Table 1 the largest $E(\mathbb{Q}^{ab})[2^\infty]$ can be so that $C_2(E) = 2$ is $\mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/4\mathbb{Z}$. Therefore, $E(\mathbb{Q}^{ab})_{tors} \subseteq \mathbb{Z}/6\mathbb{Z} \times \mathbb{Z}/12\mathbb{Z}$ or $\mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/36\mathbb{Z}$.

Suppose that $C_3(E) = 2$ and $C_2(E) \leq 4$. Then $E(\mathbb{Q}^{ab})[3^\infty] \cong \mathbb{Z}/3\mathbb{Z}$. From Proposition 3.5 the largest $E(\mathbb{Q}^{ab})[2^\infty]$ can be so that $C_2(E) = 4$ is $\mathbb{Z}/4\mathbb{Z} \times \mathbb{Z}/4\mathbb{Z}$ or $\mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/8\mathbb{Z}$. Thus, $E(\mathbb{Q}^{ab})_{tors} \subseteq \mathbb{Z}/4\mathbb{Z} \times \mathbb{Z}/12\mathbb{Z}$ or $\mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/24\mathbb{Z}$. □

Proposition 4.5. *Let $E/\mathbb{Q}$ be an elliptic curve. Suppose E has a 5-isogeny. Then*

$$E(\mathbb{Q}^{ab})_{tors} \subseteq \begin{cases} \mathbb{Z}/5\mathbb{Z} \times \mathbb{Z}/5\mathbb{Z}, \\ \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/50\mathbb{Z}, \\ \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/30\mathbb{Z}, \textit{ or} \\ \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/20\mathbb{Z}. \end{cases}$$

Proof. By Theorem 2.2 we have either

- $C_5(E) = 3$ and $C_p(E) = 1$ for all primes $p \neq 5$,
- $C_5(E) = 2$, $C_3(E) \leq 2$, and $C_2(E) = 1$, or
- $C_5(E) = 2$, $C_3(E) = 1$, and $C_2(E) \leq 2$.

Suppose $C_5(E) = 3$ and $C_p(E) = 1$ for all primes $p \neq 5$. By Corollary 2.5 we see that E does not have full 3-torsion over $\mathbb{Q}^{ab}$. By Lemma 3.6 we have $E(\mathbb{Q}^{ab})[2^\infty] \cong \{\mathcal{O}\}$ or $\mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}$. If $E(\mathbb{Q}^{ab})[5^\infty] \cong \mathbb{Z}/5\mathbb{Z} \times \mathbb{Z}/5\mathbb{Z}$, then $E(\mathbb{Q}^{ab})[2^\infty] \cong \{\mathcal{O}\}$, since otherwise E would have full 10-torsion over $\mathbb{Q}^{ab}$, contradicting Theorem 2.4. Thus, if $E(\mathbb{Q}^{ab})[5^\infty] \cong \mathbb{Z}/5\mathbb{Z} \times \mathbb{Z}/5\mathbb{Z}$, then $E(\mathbb{Q}^{ab})_{tors} = E(\mathbb{Q}^{ab})[5^\infty] \cong \mathbb{Z}/5\mathbb{Z} \times \mathbb{Z}/5\mathbb{Z}$. If E does not have full 5-torsion over $\mathbb{Q}^{ab}$, then $E(\mathbb{Q}^{ab})[5^\infty] \cong \mathbb{Z}/25\mathbb{Z}$ in order for $C_5(E) = 3$. Then $E(\mathbb{Q}^{ab})_{tors} \cong \mathbb{Z}/25\mathbb{Z}$ or $\mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/50\mathbb{Z}$.

Suppose $C_5(E) = 2$ and $C_3(E) \leq 2$ and $C_2(E) = 1$. Then $E(\mathbb{Q}^{ab})[5^\infty] \cong \mathbb{Z}/5\mathbb{Z}$ and $E(\mathbb{Q}^{ab})[3^\infty] \subseteq \mathbb{Z}/3\mathbb{Z}$ by Lemma 2.3. Again by Lemma 3.6 we have $E(\mathbb{Q}^{ab})[2^\infty] \cong \{\mathcal{O}\}$ or $\mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}$. Thus, $E(\mathbb{Q}^{ab})_{tors} \subseteq \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/30\mathbb{Z}$.

Suppose $C_5(E) = 2$ and $C_3(E) = 1$ and $C_2(E) \leq 2$. Then again $E(\mathbb{Q}^{ab})[5^\infty] \cong \mathbb{Z}/5\mathbb{Z}$. By Table 1, the largest $E(\mathbb{Q}^{ab})[2^\infty]$ can be so that $C_2(E) = 2$ is $\mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/4\mathbb{Z}$. Further, E does not have full torsion of any order prime to 2 by Corollary 2.5. Thus, $E(\mathbb{Q}^{ab})_{tors} \subseteq \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/20\mathbb{Z}$. □

Proposition 4.6. *Let $E/\mathbb{Q}$ be an elliptic curve. Suppose E has a 7-isogeny. Then either $E(\mathbb{Q}^{ab})_{tors} \subseteq \mathbb{Z}/21\mathbb{Z}$ or $\mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/28\mathbb{Z}$.*

Proof. By Theorem 2.2 we have $C_p(E) = 1$ for all primes $p \neq 2, 3, 7$ and either $C_3(E) \leq 2$ and $C_2(E) = 1$, or $C_3(E) = 1$ and $C_2(E) \leq 2$.

Suppose $C_3(E) = 2$ and $C_2(E) = 1$. Then E has a 7-isogeny and a 3-isogeny and so E has a 21-isogeny. Since there are only finitely many rational points on $X_0(21)$, there are only a finite number of j-invariants for elliptic curves over $\mathbb{Q}$ with a 21-isogeny. We can fix a model for each of these curves and explicitly check that none of these families have full m-torsion for any $2 \leq m \leq 8$. Thus, by Lemma 2.3, Lemma 2.7, and Theorem 2.4 we have $E(\mathbb{Q}^{\mathrm{ab}}) \cong \mathbb{Z}/21\mathbb{Z}$.

Suppose instead that $C_3(E) = 1$ and $C_2(E) = 2$. Since $C_3(E) = 1$, Corollary 2.5 tells us that E does not have full 3-torsion. Further, since $C_2(E) = 2$, by Proposition 3.5, it follows that $E(\mathbb{Q}^{\mathrm{ab}})[2^\infty] \subseteq \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/4\mathbb{Z}$. Therefore, by Lemma 2.7 we have that $E(\mathbb{Q}^{\mathrm{ab}})_{\mathrm{tors}} \subseteq \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/28\mathbb{Z}$.

Finally if $C_3(E) = C_2(E) = 1$, then by Lemma 2.7, Corollary 2.5, and Lemma 3.6 we have that $E(\mathbb{Q}^{\mathrm{ab}})_{\mathrm{tors}} \subseteq \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/14\mathbb{Z}$. □

Proposition 4.7. *Let $E/\mathbb{Q}$ be an elliptic curve, let $p = 11, 17, 19, 37, 43, 67,$ or 163, and suppose that E has a p-isogeny. Then $E(\mathbb{Q}^{\mathrm{ab}})_{\mathrm{tors}} \cong \mathbb{Z}/p\mathbb{Z}$.*

Proof. By Lemma 2.3 we have that $E(\mathbb{Q}^{\mathrm{ab}})_{\mathrm{tors}} \supseteq \mathbb{Z}/p\mathbb{Z}$. For these values of p, note that there are no rational isogenies of degree divisible by p besides isogenies of degree exactly p, and therefore, by Lemma 2.7 it follows that $E(\mathbb{Q}^{\mathrm{ab}})_{\mathrm{tors}} \subseteq \mathbb{Z}/m\mathbb{Z} \times \mathbb{Z}/m\mathbb{Z} \times \mathbb{Z}/p\mathbb{Z}$ for some m with $(m, p) = 1$. However, from Theorem 2.2 it follows that E has no other rational isogenies. Thus, Corollary 2.5 implies that m is a power of 2. Combining that with Lemma 3.6 shows that $m = 1$ or 2.

For any given p in this list there are only finitely many j-invariants of elliptic curves having a p-isogeny, as $X_0(p)$ has genus greater than 0. Given that these j-invariants are not 0 or 1728, by Lemma 3.1 it suffices to fix a representative E_j and compute (via Magma) that E_j does not have full 2-torsion defined over $\mathbb{Q}^{\mathrm{ab}}$. □

Proposition 4.8. *Let $E/\mathbb{Q}$ be an elliptic curve. Suppose E has a 13-isogeny. Then $E(\mathbb{Q}^{\mathrm{ab}})_{\mathrm{tors}} \cong \mathbb{Z}/13\mathbb{Z}$ or $\mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/26\mathbb{Z}$.*

Proof. Since there are no curves over $\mathbb{Q}$ with rational isogenies of degree properly divisible by 13, it follows from Lemma 2.7 that $E(\mathbb{Q}^{\mathrm{ab}})_{\mathrm{tors}} \cong \mathbb{Z}/m\mathbb{Z} \times \mathbb{Z}/m\mathbb{Z} \times \mathbb{Z}/13\mathbb{Z}$ for some $m \geq 1$. However, by Theorem 2.2 we have that $C_p(E) = 1$ for all primes $p \neq 13$. Thus, by Corollary 2.5 and Lemma 3.6 we have that $m = 1$ or 2. □

Note that from here a quick count of the possible sizes of the torsion subgroups along with Lemma 2.3 for the example of 26569a1 having a point of order 163 over $\mathbb{Q}^{\mathrm{ab}}$ is already enough to prove Corollary 1.3.

5. Eliminating possible torsion

We restate the classification theorem for convenience.

Theorem 5.1. *Let $E/\mathbb{Q}$ be an elliptic curve. Then $E(\mathbb{Q}^{ab})_{tors}$ is isomorphic to one of the following groups*:

$$\begin{array}{ll}
\mathbb{Z}/N_1\mathbb{Z}, & N_1 = 1,3,5,7,9,11,13,15,17,19,21,25,27,37,43,67,163,\\
\mathbb{Z}/2\mathbb{Z}\times\mathbb{Z}/2N_2\mathbb{Z}, & N_2 = 1,2,\dots,9,\\
\mathbb{Z}/3\mathbb{Z}\times\mathbb{Z}/3N_3\mathbb{Z}, & N_3 = 1,3,\\
\mathbb{Z}/4\mathbb{Z}\times\mathbb{Z}/4N_4\mathbb{Z}, & N_4 = 1,2,3,4,\\
\mathbb{Z}/5\mathbb{Z}\times\mathbb{Z}/5\mathbb{Z}, & \\
\mathbb{Z}/6\mathbb{Z}\times\mathbb{Z}/6\mathbb{Z}, & \\
\mathbb{Z}/8\mathbb{Z}\times\mathbb{Z}/8\mathbb{Z}. &
\end{array}$$

Each of these groups appear as $E(\mathbb{Q}^{ab})_{tors}$ for some elliptic curve over $\mathbb{Q}$.

We now eliminate the possibility of many of the groups appearing in the previous propositions as possible torsion subgroups over $\mathbb{Q}^{ab}$ for some elliptic curve $E/\mathbb{Q}$. We begin with a simple observation about 2-torsion over $\mathbb{Q}^{ab}$ from Proposition 3.5.

Lemma 5.2. *Let $E/\mathbb{Q}$ be an elliptic curve. If $E(\mathbb{Q}^{ab})[2] \neq \{\mathbb{O}\}$ then $E(\mathbb{Q}^{ab})[2] \cong \mathbb{Z}/2\mathbb{Z}\times\mathbb{Z}/2\mathbb{Z}$. Thus, $E(\mathbb{Q}^{ab})\mathrm{tors} \ncong \mathbb{Z}/2N\mathbb{Z}$ for any $N \geq 1$.*

This eliminates many possible torsion structures over $\mathbb{Q}^{ab}$. In particular, after we combine the possibilities for $E(\mathbb{Q}^{ab})_{tors}$ from Propositions 4.8, 4.6, 4.5, 4.4, 4.3, and 4.7, and eliminate those groups ruled out by Lemma 5.2, we can compare them to the classification in Theorem 1.2 to see that it remains to rule out the following groups as possibilities for $E(\mathbb{Q}^{ab})_{tors}$:

$$\begin{array}{ll}
\mathbb{Z}/2\mathbb{Z}\times\mathbb{Z}/2N_2\mathbb{Z}, & N_2 = 10,\ 12,\ 13,\ 14,\ 15,\ 18,\ 25,\\
\mathbb{Z}/3\mathbb{Z}\times\mathbb{Z}/27\mathbb{Z}, & \\
\mathbb{Z}/6\mathbb{Z}\times\mathbb{Z}/12\mathbb{Z}. &
\end{array}$$

Proposition 5.3. *Let $E/\mathbb{Q}$ be an elliptic curve. Then $E(\mathbb{Q}^{ab})_{tors}$ is not isomorphic to $\mathbb{Z}/2\mathbb{Z}\times\mathbb{Z}/28\mathbb{Z}$ or $\mathbb{Z}/2\mathbb{Z}\times\mathbb{Z}/30\mathbb{Z}$.*

Proof. In the case $\mathbb{Z}/2\mathbb{Z}\times\mathbb{Z}/28\mathbb{Z}$ the curve has a 14-isogeny by Lemma 2.7 of which there are only two possible isomorphism classes of curves given by the j-invariants $-3^3 5^3$ and $3^3 5^3 17^3$ (see for instance [Lozano-Robledo 2013, Table 4]). Using division polynomials we can check that in both cases there are no points of order 4 defined over an abelian extension of $\mathbb{Q}$.

In the case $\mathbb{Z}/2\mathbb{Z}\times\mathbb{Z}/30\mathbb{Z}$ the curve has a 15-isogeny by Lemma 2.7. Here there are four possible j-invariants, $-5^2/2$, $-5^2\cdot 241^3/2^3$, $-5\cdot 29^3/2^5$, and $5\cdot 211^3/2^{15}$. Again using division polynomials we can check that none of these curves have a point of order 2 defined over an abelian extension of $\mathbb{Q}$. □

Proposition 5.4. *Let $E/\mathbb{Q}$ be an elliptic curve. Then $E(\mathbb{Q}^{ab})_{tors} \ncong \mathbb{Z}/2\mathbb{Z}\times\mathbb{Z}/26\mathbb{Z}$.*

Proof. Suppose that $E(\mathbb{Q}^{ab})_{tors} \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/26\mathbb{Z}$. Then E has a 13-isogeny, and so by [Lozano-Robledo 2013, Table 3] the curve has a j-invariant of the form

$$j(E) = \frac{(h^2+5h+13)(h^4+7h^3+20h^2+19h+1)^3}{h}$$

for some $h \in \mathbb{Q}$ with $h \neq 0$. Thus, E must be a twist of the curve

$$E' : y^2 + xy = x^3 - \frac{36}{j(E)-1728}x - \frac{1}{j(E)-1728}.$$

Since $E(\mathbb{Q}^{ab})[2^\infty] \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}$ but E does not have any 2-isogenies by Theorem 2.2, we must have $\mathrm{Gal}(\mathbb{Q}(E[2])/\mathbb{Q}) \cong \mathbb{Z}/3\mathbb{Z}$ by Theorem 2.4, implying that the discriminant of E is a square. Since E is a twist of E', the discriminant of E differs from the discriminant of E' by at most a square. Thus, we obtain a formula $y^2 = \mathrm{Disc}(E')$, which we compute in terms of h. By absorbing squares into the y^2 term we obtain a curve

$$C : Y^2 = h(h^2+6h+13)$$

which is a modular curve describing precisely when E has a 13-isogeny and $\mathrm{Gal}(\mathbb{Q}(E[2])/\mathbb{Q}) \cong \mathbb{Z}/3\mathbb{Z}$. This curve is actually an elliptic curve with $C(\mathbb{Q}) = \{(0:0:1), (0:1:0)\} \cong \mathbb{Z}/2\mathbb{Z}$, both points being cusps. Therefore, there are no elliptic curves with $E(\mathbb{Q}^{ab}) \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/26\mathbb{Z}$. □

Proposition 5.5. *Let $E/\mathbb{Q}$ be an elliptic curve*; *then $E(\mathbb{Q}^{ab})_{tors} \ncong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/50\mathbb{Z}$.*

Proof. Suppose that $E(\mathbb{Q}^{ab})_{tors} \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/50\mathbb{Z}$. Then E has a 25-isogeny, and so by [Lozano-Robledo 2013, Table 3] the curve has a j-invariant of the form

$$j(E) = \frac{(h^{10}+10h^8+35h^6-12h^5+50h^4-60h^3+25h^2-60h+16)^3}{(h-1)(h^4+h^3+6h^2+6h+11)}$$

for some $h \in \mathbb{Q}$ with $h \neq 1$ By a similar argument made in Proposition 5.4 we have that the discriminant of E must be a square. We again obtain a formula $y^2 = \mathrm{Disc}(E)$, and by absorbing squares into the y^2 term we obtain a curve

$$C : Y^2 = h^7 + 9h^5 + 25h^3 - 11h^2 + 20h - 44$$

which is a modular curve describing precisely when E has a 25-isogeny and $\mathrm{Gal}(\mathbb{Q}(E[2])/\mathbb{Q}) \cong \mathbb{Z}/3\mathbb{Z}$. This is a genus-3 hyperelliptic curve. We write the curve in projective coordinates using $h = \frac{X}{Z}$.

We can construct a map π from C to an elliptic curve $\widetilde{C} : y^2 = x^3 + x^2 - x$ given by

$$(*) \qquad (X:Y:Z) \mapsto (x^3 - x^2z + 4xz^2 - 4z^3 : yz^2 : x^2z - 2xz^2 + z^3).$$

The curve $\widetilde{C}$ has Cremona label 20a2 and rank 0 with torsion isomorphic to $\mathbb{Z}/6\mathbb{Z}$. It has rational points

$$\widetilde{C}(\mathbb{Q}) = \{(0:1:0), (0:0:1), (-1:-1:1), (1:-1:1), (-1:1:1), (1:1:1)\}$$

and we can use $(*)$ to explicitly compute the preimage of each point under π to see that the only rational points on C are $(1:0:1)$ and $(0:1:0)$. Note that $h = \frac{X}{Z}$ for points $(X:Y:Z) \in C$. The first point corresponds to $h = 1$, which is a zero of the denominator of $j(E)$, and the second point is the point at infinity, which corresponds to $h = \infty$, which is not a value we can consider. Thus, both of these points are cusps, and therefore, there are no elliptic curves with $E(\mathbb{Q}^{\mathrm{ab}}) \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/50\mathbb{Z}$. □

Proposition 5.6. *Let $E/\mathbb{Q}$ be an elliptic curve; then $E(\mathbb{Q}^{\mathrm{ab}})_{\mathrm{tors}} \not\cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/20\mathbb{Z}$.*

Proof. Suppose for the sake of contradiction that E is an elliptic curve over $\mathbb{Q}$ such that $E(\mathbb{Q}^{\mathrm{ab}})_{\mathrm{tors}} \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/20\mathbb{Z}$. Then, E has a $\mathbb{Q}$-rational 10-isogeny, and so by [Lozano-Robledo 2013, Table 3] the curve has a

$$j(E) = \frac{(h^6 - 4h^5 + 16h + 16)^3}{(h+1)^2(h-4)h^5}$$

for some $h \in \mathbb{Q}$ with $h \neq -1, 0, 4$. Thus, E must be a twist of the curve

$$E' : y^2 + xy = x^3 - \frac{36}{j(E) - 1728}x - \frac{1}{j(E) - 1728}.$$

Moving the 2-torsion point to (0,0) yields a model of E' of the form

$$E' : y^2 = x^3 + b(h)x^2 + d(h)x$$

for the rational functions

$$\begin{aligned} b(h) &= \frac{-9h^{12} + 72h^9 - 144h^3 - 144}{h^{12} - 8h^9 - 8h^3 - 8}, \\ d(h) &= \big(1296h^{27} - 19440h^{24} + 62208h^{21} + 124416h^{18} - 248832h^{15} \\ &\qquad - 622080h^{12} + 995328h^6 + 995328h^3 + 331776\big) \\ &\quad \big/\big(h^{36} - 24h^{33} + 192h^{30} - 464h^{27} - 720h^{24} + 2304h^{21} + 2112h^{18} \\ &\qquad + 5760h^{15} + 14400h^{12} + 11776h^9 + 12288h^6 + 12288h^3 + 4096\big). \end{aligned}$$

Note that $j(E) \neq 0, 1728$ since E has a 10-isogeny, and thus, E is a quadratic twist of E'. By Lemma 3.1 we have that $E'(\mathbb{Q}^{\mathrm{ab}})_{\mathrm{tors}} \cong E(\mathbb{Q}^{\mathrm{ab}})_{\mathrm{tors}} \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/20\mathbb{Z}$. Now, since $E'(\mathbb{Q}^{\mathrm{ab}})[2^\infty] \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/4\mathbb{Z}$, Lemma 3.4 tells us that either $C_2(E) \geq 4$ or

$$d(h) \in (\mathbb{Q}^\times)^2 \quad \text{or} \quad (b(h)^2 - 4d(h))d(h) \in (\mathbb{Q}^\times)^2.$$

Note that since $C_5(E) \geq 2$, by Theorem 2.2 it is impossible for $C_2(E) \geq 4$. Denote the 4-torsion point over $\mathbb{Q}^{\mathrm{ab}}$ by Q.

Suppose $d(h) \in (\mathbb{Q}^\times)^2$. We obtain a formula $Y^2 = d(h)$, and by absorbing squares we obtain the curve

$$C : Y'^2 = h^3 + h^2 + 4h + 4$$

which is a modular curve describing precisely when E has a 10-isogeny and $\mathrm{Gal}(\mathbb{Q}(x(Q))/\mathbb{Q}) \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}$. This is the elliptic curve with Cremona label 20a1 and rational points

$$C(\mathbb{Q}) = \{(0:1:0), (0:-2:1), (0:2:1), (4:-10:1), (4:10:1), (-1:0:1)\} \cong \mathbb{Z}/6\mathbb{Z}.$$

However, all of these points are cusps as they correspond to $h = 0, -1, 4$, which are all zeros of the denominator of $j(E)$. Therefore, there are no such elliptic curves.

Suppose instead that $(b(h)^2 - 4d(h))d(h) \in (\mathbb{Q}^\times)^2$. Again we obtain a formula $Y^2 = (b(h)^2 - 4d(h))d(h)$, and by absorbing squares we obtain the curve

$$\widehat{C} : Y'^2 = h^3 - 3h^2 - 4h$$

which is a modular curve describing precisely when E has a 10-isogeny and $\mathrm{Gal}(\mathbb{Q}(x(Q))/\mathbb{Q}) \cong \mathbb{Z}/4\mathbb{Z}$. This is an elliptic curve with Cremona label 40a1 and rational points

$$\widehat{C}(\mathbb{Q}) = \{(0:0:1), (0:1:0), (-1:0:1), (4:0:1)\} \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}.$$

Again, all of these points are cusps as they correspond to $h = 0, -1, 4$. Therefore, there are no such elliptic curves. Thus, we can conclude that no such curve E exists. □

Proposition 5.7. *Let $E/\mathbb{Q}$ be an elliptic curve; then $E(\mathbb{Q}^{\mathrm{ab}})_{\mathrm{tors}} \not\cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/36\mathbb{Z}$.*

Proof. Suppose for the sake of contradiction that E is an elliptic curve over $\mathbb{Q}$ such that $E(\mathbb{Q}^{\mathrm{ab}})_{\mathrm{tors}} \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/36\mathbb{Z}$. Then, E has a $\mathbb{Q}$-rational 18-isogeny, and so by [Lozano-Robledo 2013, Table 3] the curve has a j-invariant of the form

$$j(E) = \frac{(h^3-2)^3(h^9-6h^6-12h^3-8)^3}{h^9(h^3-8)(h^3+1)^2}$$

for some $h \in \mathbb{Q}$ with $h \neq -1, 0, 2$. Thus, E must be a twist of the curve

$$E' : y^2 + xy = x^3 - \frac{36}{j(E)-1728}x - \frac{1}{j(E)-1728}.$$

Moving the 2-torsion point to (0,0) yields a model of E' of the form

$$E' : y^2 = x(x^2 + b(h)x + d(h))$$

for the rational functions

$$b(h) = \frac{(h^3-2)(h^9-6h^6-12h^3-8)}{h^{12}-8h^9-8h^3-8},$$
$$d(h) = \frac{(h+1)(h^2-h+1)(h^3-2)^2(h^9-6h^6-12h^3-8)^2}{(h^6-4h^3-8)^2(h^{12}-8h^9-8h^3-8)^2}.$$

Note that $j(E) \neq 0, 1728$ since E has an 18-isogeny, and thus, E is a quadratic twist of E'. By Lemma 3.1 we have that $E'(\mathbb{Q}^{\mathrm{ab}})_{\mathrm{tors}} \cong E(\mathbb{Q}^{\mathrm{ab}})_{\mathrm{tors}} \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/20\mathbb{Z}$. Now, since $E'(\mathbb{Q}^{\mathrm{ab}})[2^\infty] \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/4\mathbb{Z}$, Lemma 3.4 tells us that either $C_2(E) \geq 4$,

$$d(h) \in (\mathbb{Q}^\times)^2, \quad \text{or} \quad (b(h)^2 - 4d(h))d(h) \in (\mathbb{Q}^\times)^2.$$

Note that, since $C_3(E) \geq 3$, Theorem 2.2 implies that $C_2(E) < 4$. Denote the 4-torsion point over $\mathbb{Q}^{\mathrm{ab}}$ by Q.

Suppose $d(h) \in (\mathbb{Q}^\times)^2$. We obtain a formula $Y^2 = d(h)$, and by absorbing squares we obtain the curve

$$C : Y'^2 = h^3 + 1$$

which is a modular curve describing precisely when E has an 18-isogeny and $\mathrm{Gal}(\mathbb{Q}(x(Q))/\mathbb{Q}) \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}$. This is an elliptic curve with Cremona label 36a1 and rational points

$$C(\mathbb{Q}) = \{(0:1:0), (0:1:1), (0:-1:1), (2:3:1), (2:-3:1), (-1:0:1)\} \cong \mathbb{Z}/6\mathbb{Z}.$$

However, all of these points are cusps as they correspond to $h = -1, 0, 2$. Therefore, there are no such elliptic curves.

Suppose instead that $(b(h)^2 - 4d(h))d(h) \in (\mathbb{Q}^\times)^2$. Again we obtain a formula $Y^2 = (b(h)^2 - 4d(h))d(h)$, and by absorbing squares we obtain the curve

$$\widehat{C} : Y'^2 = h^7 - 7h^4 - 8h$$

which is a modular curve describing precisely when E has an 18-isogeny and $\mathrm{Gal}(\mathbb{Q}(x(Q))/\mathbb{Q}) \cong \mathbb{Z}/4\mathbb{Z}$. This is a genus-3 hyperelliptic curve with an automorphism φ defined by

$$(x:y:z)$$
$$\mapsto (2x^4-10x^3z+12x^2z^2+8xz^3-16z^4 : 36yz^3 : x^4-8x^3z+24x^2z^2-32xz^3+16z^4)$$

and taking the quotient of $\widehat{C}$ by φ gives a map π from $\widehat{C}$ to an elliptic curve $\widehat{C}_\varphi : y^2 = x^3 - x^2 + x$ given by

$$(**) \qquad (x:y:z) \mapsto (xz(x^2 - xz - 2z^2) : yz^3 : x^2(x+z)^2).$$

The curve $\widehat{C}_\varphi$ has Cremona label 24a4 and has rational points

$$\widehat{C}_\varphi(\mathbb{Q}) = \{(0:1:0), (0:0:1), (1:1:1), (1:-1:1)\}.$$

We can use (∗∗) to explicitly compute the preimage of each point under π to compute the rational points on $\widehat{C}$. We find that $\widehat{C}(\mathbb{Q}) = \{(-1:0:1), (0:0:1), (2:0:1), (0:1:0)\}$. These points correspond to $h = 0, -1, 2$, which are zeros of the denominator of $j(E)$ and so are cusps. Thus, we can conclude that no such curve E exists. □

Proposition 5.8. *Let $E/\mathbb{Q}$ be an elliptic curve; then $E(\mathbb{Q}^{\mathrm{ab}})_{\mathrm{tors}} \not\cong \mathbb{Z}/6\mathbb{Z} \times \mathbb{Z}/12\mathbb{Z}$.*

Proof. Suppose that $E(\mathbb{Q}^{\mathrm{ab}})_{\mathrm{tors}} \cong \mathbb{Z}/6\mathbb{Z} \times \mathbb{Z}/12\mathbb{Z}$. Since $E(\mathbb{Q}^{\mathrm{ab}})[3] \cong \mathbb{Z}/3\mathbb{Z} \times \mathbb{Z}/3\mathbb{Z}$, Corollary 2.5 gives that $C_3(E) \geq 3$. In particular, the comment after Corollary 2.5 shows that E has two independent 3-isogenies over $\mathbb{Q}$. Thus, Theorem 2.2 gives that $C_2(E) \leq 2$, and so $E(\mathbb{Q})[2^\infty] \subseteq \mathbb{Z}/2\mathbb{Z}$. By Lemma 4.2 we also have that $\mathrm{Gal}(\mathbb{Q}(E[2])/\mathbb{Q}) \cong \mathbb{Z}/2\mathbb{Z}$, and thus, E has a single nontrivial point P of order 2 over $\mathbb{Q}$. Therefore, E corresponds to a point on the modular curve $X_0(3, 6)$. We can find the j-map for $X_0(3, 6)$ as follows. Start with the j-map for $X_0(18)$ via [Lozano-Robledo 2013, Table 3] and create an elliptic curve over the function field $\mathbb{Q}(h)$ as done in previous propositions. This curve has a 9-isogeny. We can factor this 9-isogeny as the composition of two 3-isogenies and, using Velu's formulas, compute a model and the j-invariant for the intermediate elliptic curve, which has two independent 3-isogenies. The point of order 2 is preserved under the 3-isogeny, and so this is the j-map from $X_0(3, 6)$. Note that Magma has the functionality to do these computations.

We arrive at the following: an elliptic curve with two independent 3-isogenies has j-invariant of the form

$$j(E) = \frac{(h^3-2)^3(h^3+6h-2)^3(h^6-6h^4-4h^3+36h^2+12h+4)^3}{(h-2)^3h^3(h+1)^6(h^2-h+1)^6(h^2+2h+4)^3}$$

for some $h \in \mathbb{Q}$ with $h \neq 2, 0, -1$. Thus, E must be a twist of the curve

$$E' : y^2 + xy = x^3 - \frac{36}{j(E)-1728}x - \frac{1}{j(E)-1728}.$$

Moving the 2-torsion point to (0,0) yields a model of E' of the form

$$E' : y^2 = x(x^2 + b(h)x + d(h))$$

for the rational functions

$$b(h) = \frac{(h^3-2)(h^3+6h-2)(h^6-6h^4-4h^3+36h^2+12h+4)}{(h^4-2h^3-8h-2)(h^8+2h^7+4h^6-16h^5-14h^4+8h^3+64h^2-16h+4)},$$

$$\begin{aligned} d(h) = \big((h+1)^3&(h^2-h+1)^3(h^3-2)^2(h^3+6h-2)^2 \\ &\times (h^6-6h^4-4h^3+36h^2+12h+4)^2\big) \\ \big/\big(&(h^2+2h-2)^2(h^4-2h^3-8h-2)^2(h^4-2h^3+6h^2+4h+4)^2 \\ &\times (h^8+2h^7+4h^6-16h^5-14h^4+8h^3+64h^2-16h+4)^2\big). \end{aligned}$$

Note that $j(E) \neq 0, 1728$ since E is a quadratic twist of E'. By Lemma 3.1 we have that $E'(\mathbb{Q}^{\mathrm{ab}})_{\mathrm{tors}} \cong E(\mathbb{Q}^{\mathrm{ab}})_{\mathrm{tors}} \cong \mathbb{Z}/6\mathbb{Z} \times \mathbb{Z}/12\mathbb{Z}$. Now, since $E'(\mathbb{Q}^{\mathrm{ab}})[2^\infty] \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/4\mathbb{Z}$, Lemma 3.4 tells us that

$$d(h) \in (\mathbb{Q}^\times)^2, \quad \text{or} \quad (b(h)^2 - 4d(h))d(h) \in (\mathbb{Q}^\times)^2.$$

Suppose $d(h) \in (\mathbb{Q}^\times)^2$. We obtain a formula $Y^2 = d(h)$, and by absorbing squares we obtain the curve

$$C : Y'^2 = h^3 + 1.$$

If instead $(b(h)^2 - 4d(h))d(h) \in (\mathbb{Q}^\times)^2$, then we obtain $Y^2 = (b(h)^2 - 4d(h))d(h)$ and by absorbing squares we obtain the curve

$$\widehat{C} : Y'^2 = h^7 - 7h^4 - 8h.$$

Notice that both of these are the exact same hyperelliptic curves that appeared in the proof of Proposition 5.7. We have already found all rational points on these two curves, and again they all correspond to cusps. Thus, we can conclude that there do not exist any $E/\mathbb{Q}$ with $E(\mathbb{Q}^{\mathrm{ab}})_{\mathrm{tors}} \cong \mathbb{Z}/6\mathbb{Z} \times \mathbb{Z}/12\mathbb{Z}$. □

Note that it should not be too surprising that the same modular curves appear in the proof of Proposition 5.7 and Proposition 5.8. Indeed, elliptic curves with these torsion subgroups are linked via a 3-isogeny. One may attempt an alternative proof of Proposition 5.8 by making this connection rigorous and explicit.

Proposition 5.9. *Let $E/\mathbb{Q}$ be an elliptic curve; then $E(\mathbb{Q}^{\mathrm{ab}})_{\mathrm{tors}} \ncong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/24\mathbb{Z}$.*

Proof. Suppose for the sake of contradiction that E is an elliptic curve over $\mathbb{Q}$ such that $E(\mathbb{Q}^{\mathrm{ab}})_{\mathrm{tors}} \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/24\mathbb{Z}$. Since $E(\mathbb{Q}^{\mathrm{ab}})[2^\infty] \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/8\mathbb{Z}$, Table 1 shows that E has 2-powered isogenies of degrees 1, 2, 4, 4 or 1, 2, 4, 4, 8, 8. However, Lemma 2.7 implies that E has a 12-isogeny as well. Thus, Theorem 2.2 gives that the 2-powered isogenies of E must be restricted to ones of degree 1, 2, 4, and 4. Hence, $E(\mathbb{Q})[2^\infty] \subseteq \mathbb{Z}/4\mathbb{Z}$, and E has a point of order 2 over $\mathbb{Q}$. Moving the point of order 2 to $(0, 0)$ we obtain a model for E of the form

$$E : y^2 = x(x^2 + bx + d).$$

A similar argument to that made in the proof of Lemma 3.4 shows that any point $Q \in E(\mathbb{Q}^{\mathrm{ab}})$ of order 4 must lie over a $\mathbb{Q}$-rational point of order 2, otherwise $E[4] \subseteq E(\mathbb{Q}^{\mathrm{ab}})$. The argument is as follows: let α and $\bar{\alpha}$ be the two roots of $x^2 + bx + d$. By Lemma 3.2, a point that halves $(0, 0) \in E[2]$ is defined over $\mathbb{Q}^{\mathrm{ab}}$ if and only if $-\alpha$ and $-\bar{\alpha}$ are squares in $\mathbb{Q}^{\mathrm{ab}}$. Similarly, a point that halves $(\alpha, 0) \in E[2]$ is defined over $\mathbb{Q}^{\mathrm{ab}}$ if and only if α and $\alpha - \bar{\alpha}$ are squares in $\mathbb{Q}^{\mathrm{ab}}$. However, if α is a square in $\mathbb{Q}^{\mathrm{ab}}$, then since $\sqrt{-1} \in \mathbb{Q}^{\mathrm{ab}}$, it follows that $-\alpha$ and $-\bar{\alpha}$ are also squares in $\mathbb{Q}^{\mathrm{ab}}$. Thus, if a point of order 4 that halves $(\alpha, 0)$ exists in $\mathbb{Q}^{\mathrm{ab}}$, then so does a point of order 4 that halves (0, 0), implying that E has full 4-torsion over $\mathbb{Q}^{\mathrm{ab}}$.

Now, E has a $\mathbb{Q}$-rational 12-isogeny, and so by [Lozano-Robledo 2013, Table 3] the curve has a j-invariant of the form

$$j(E) = \frac{(h^2-3)^3(h^6-9h^4+3h^2-3)^3}{h^4(h^2-9)(h^2-1)^3}$$

for some $h \in \mathbb{Q}$ with $h \neq 0, \pm 1, \pm 3$. Thus, E must be a twist of the curve

$$E' : y^2 + xy = x^3 - \frac{36}{j(E)-1728}x - \frac{1}{j(E)-1728}.$$

Moving the 2-torsion point to (0,0) yields a model of E' of the form

$$E' : y^2 = x(x^2 + b(h)x + d(h))$$

for the rational functions

$$b(h) = \frac{(h^2-3)(h^6-9h^4+3h^2-3)}{h^8-12h^6+30h^4-36h^2+9},$$
$$d(h) = \frac{h^2(h^2-3)^2(h^6-9h^4+3h^2-3)^2}{(h^4-6h^2-3)^2(h^8-12h^6+30h^4-36h^2+9)^2}.$$

For ease of notation going forward, we will write $b = b(h)$ and $d = d(h)$, and it should be understood that many of the following variables are functions of h. Let α and $\bar{\alpha}$ be roots of $x^2 + bx + d$ (over $\mathbb{Q}[h]$) so that $E' : y^2 = x(x-\alpha)(x-\bar{\alpha})$.

From our argument above we may assume that any point Q of order 4 in $E'(\mathbb{Q}^{\mathrm{ab}})$ satisfies $2Q = (0, 0)$. Then, from Lemma 3.2 we have (without loss of generality) that Q has x-coordinate

$$(\sqrt{0-0})(\sqrt{0-\alpha}) \pm (\sqrt{0-0})(\sqrt{0-\bar{\alpha}}) \pm (\sqrt{0-\alpha})(\sqrt{0-\bar{\alpha}}) + 0 = \pm\sqrt{\alpha\bar{\alpha}} = \pm\sqrt{d}.$$

Suppose that the x-coordinate of Q is $\sqrt{d}$. Since there is a point of order 8 in $E(\mathbb{Q}^{\mathrm{ab}})$, there exists a point $R \in E(\mathbb{Q}^{\mathrm{ab}})$ such that $2R = Q$. Denote

$$\alpha = \frac{-b+\sqrt{b^2-4d}}{2} \quad \text{and} \quad \bar{\alpha} = \frac{-b-\sqrt{b^2-4d}}{2}$$

so that we have

$$E' : y^2 = x(x-\alpha)(x-\bar{\alpha}).$$

Since E does not have full 2-torsion over $\mathbb{Q}$, neither does E', and so in particular $\alpha \notin \mathbb{Q}$. For ease of notation we denote $\delta = \sqrt{d}$. We can apply Lemma 3.2 again to deduce that since such an R exists, we must have that δ, $\delta - \alpha$, and $\delta - \bar{\alpha}$ are all squares in $\mathbb{Q}^{\mathrm{ab}}$. Notice that through some simplification we have that $(\delta-\alpha)(\delta-\bar{\alpha}) = (b+2\delta)\delta$ and so it suffices to prove that δ, $(b+2\delta)\delta$, and $\delta - \alpha$ are squares in $\mathbb{Q}^{\mathrm{ab}}$.

For any $h \in \mathbb{Q}$ we have $\delta \in \mathbb{Q}$ and so clearly $\sqrt{\delta} \in \mathbb{Q}^{\text{ab}}$. Similarly, for all $h \in \mathbb{Q}$, we have that $(b+2\delta)\delta \in \mathbb{Q}$, and so $\sqrt{(b+2\delta)\delta} \in \mathbb{Q}^{\text{ab}}$.

To see when $\delta - \alpha$ is square in $\mathbb{Q}^{\text{ab}}$ we will find the minimal polynomial of $\sqrt{\delta-\alpha}$ over $\mathbb{Q}$, and find when this defines an abelian extension of $\mathbb{Q}$. Notice that $\delta - \alpha = \frac{1}{2}(b + 2\delta - \sqrt{b^2 - 4d})$. Let

$$\xi = \sqrt{\delta - \alpha} = \sqrt{\frac{b + 2\delta - \sqrt{b^2 - 4d}}{2}}.$$

We claim that $[\mathbb{Q}(\xi) : \mathbb{Q}(\alpha)] = 2$, which we will justify at the end of the proof, and $[\mathbb{Q}(\alpha) : \mathbb{Q}] = 2$, so $[\mathbb{Q}(\xi) : \mathbb{Q}] = 4$. Moreover, we find that ξ satisfies the polynomial

$$f(X) = X^4 - (b+2\delta)X^2 + (b+2\delta)\delta,$$

and so this is a minimal polynomial of ξ over $\mathbb{Q}$.

Now, we apply Proposition 3.3 and see that f defines an abelian extension of $\mathbb{Q}$ if and only if

$$(b+2\delta)\delta \in (\mathbb{Q}^\times)^2$$

or

$$((b+2\delta)^2 - 4(b+2\delta)\delta)(b+2\delta)\delta \in (\mathbb{Q}^\times)^2,$$

which by absorbing squares is equivalent to

$$(b - 2\delta)\delta \in (\mathbb{Q}^\times)^2.$$

These yield the curves

$$C_1 : y^2 = h^3 - 2h^2 - 3h \quad \text{and} \quad C_2 : y^2 = h^3 + 2h^2 - 3h,$$

respectively.

Now it remains to classify all rational points on C_1 and C_2. These are curves with Cremona labels 48a1 and 24a1, respectively, and have rank 0 with rational points

$$C_1(\mathbb{Q}) = \{(0:0:1), (0:1:0), (3:0:1), (-1:0:1)\}$$

and

$$C_2(\mathbb{Q}) = \big\{(0:0:1), (0:1:0), (-1:-2:1), (3:-6:1), (1:0:1), (3:6:1), (-1:2:1), (-3:0:1)\big\}.$$

Note that all of these points correspond to $h = 0, \pm 1, \pm 3$, which are zeros of the denominator of $j(E)$ and hence are cusps. Therefore, there are no curves over $\mathbb{Q}$ with $E(\mathbb{Q}^{\text{ab}})_{\text{tors}} \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/24\mathbb{Z}$.

To see that $[\mathbb{Q}(\xi):\mathbb{Q}(\alpha)]=2$, suppose otherwise, that $\delta-\alpha$ was a square in $\mathbb{Q}(\alpha)$. Then the norm of $\delta-\alpha$,

$$\mathrm{Nm}_{\mathbb{Q}(\alpha)/\mathbb{Q}}(\delta-\alpha)=(b+2\delta)\delta,$$

would be a square in $\mathbb{Q}$. This is precisely what we checked above, that this does not happen for any noncuspidal values of h. □

The following theorem applies broadly to any elliptic curve over $\overline{\mathbb{Q}}$ with complex multiplication, but we will use it to show specifically that the torsion subgroup $\mathbb{Z}/3\mathbb{Z}\times\mathbb{Z}/27\mathbb{Z}$ does not appear over $\mathbb{Q}^{\mathrm{ab}}$.

Theorem 5.10 [Bourdon and Clark 2016, Theorem 2.7]. *Let $\mathbb{O}_K$ denote the ring of integers of a quadratic imaginary number field K. Let $E/\mathbb{C}$ be an $\mathbb{O}_K$-CM elliptic curve, and let $M\subset E(\mathbb{C})$ be a finite $\mathbb{O}_K$-submodule. Then*:

(a) *We have $M=E[\operatorname{ann} M]$*; *hence*,

(b) $M\cong\mathbb{O}_K/(\operatorname{ann} M)$ *and*

(c) $\#M=|\operatorname{ann} M|$.

This gives us an understanding of $\mathbb{O}_K$-submodules of $E(\mathbb{C})$ for an elliptic curve with CM by the maximal order. We use these results to prove the following proposition.

Proposition 5.11. *Let $E/\mathbb{Q}$ be an elliptic curve*; *then $E(\mathbb{Q}^{\mathrm{ab}})_{\mathrm{tors}}\not\cong\mathbb{Z}/3\mathbb{Z}\times\mathbb{Z}/27\mathbb{Z}$.*

Proof. Suppose that $E(\mathbb{Q}^{\mathrm{ab}})_{\mathrm{tors}}\cong\mathbb{Z}/3\mathbb{Z}\times\mathbb{Z}/27\mathbb{Z}$. Then by Lemma 2.7 the curve E has a 9-isogeny over $\mathbb{Q}$. By the discussion in the paragraph following Corollary 2.5, E has an independent 3-isogeny as well. Thus, we have the isogeny graph

$$E'\xleftarrow{\;3\;}E\xrightarrow{\;9\;}E''.$$

Taking the dual isogeny also of degree 3 from E' to E and composing it with 9-isogeny from E to E'' shows that E' has a 27-isogeny. Note that this degree-27 isogeny is cyclic as the 9-isogeny and 3-isogeny are independent, i.e., their kernels have trivial intersection. The modular curve $X_0(27)$ has genus 1, and there is a unique 27-isogeny class of elliptic curves up to isomorphism. Examining the 27-isogeny class shows that E has CM by the maximal order of $K=\mathbb{Q}(\sqrt{-3})$.

Now, notice that $E(\mathbb{Q}^{\mathrm{ab}})_{\mathrm{tors}}$ is an $\mathbb{O}_K$-submodule of $E(\mathbb{C})$, since $K\subseteq\mathbb{Q}^{\mathrm{ab}}$. Since the prime $p=3$ ramifies in K, there is a unique prime ideal $\mathfrak{p}$ of $\mathbb{O}_K$ with $|\mathfrak{p}|=3$ and we have $(3)=\mathfrak{p}^2$. By Theorem 5.10(b) we have that $E[27]\cong\mathbb{O}_K/(3)^3\cong\mathbb{O}_K/\mathfrak{p}^6$. Suppose I is an ideal of $\mathbb{O}_K/\mathfrak{p}^6$. Then $\mathfrak{p}^6\subseteq I$ so $I\mid\mathfrak{p}^6$ and therefore $I=\mathfrak{p}^b$ for some $0\le b\le 6$ by the unique factorization of ideals into prime ideals. Thus, the $\mathbb{O}_K$-submodules of $E[27]$ are all of the form $\mathfrak{p}^b/\mathfrak{p}^6$ for some $0\le b\le 6$. Moreover, the exponent of $\mathbb{O}_K/\mathfrak{p}^b$ is the smallest power of 3 contained in $\mathfrak{p}^b$. Since $(3)^d=\mathfrak{p}^{2d}$, this smallest power is $3^{\lceil b/2 \rceil}$. Further, by Theorem 5.10(c) we have $\#\mathcal{O}_K/\mathfrak{p}^b = 3^b$, and we deduce that

$$\mathcal{O}_K/\mathfrak{p}^b \cong_{\mathbb{Z}} \mathbb{Z}/3^{\lfloor b/2 \rfloor}\mathbb{Z} \times \mathbb{Z}/3^{\lceil b/2 \rceil}\mathbb{Z}.$$

Notice that since $E(\mathbb{Q}^{\text{ab}})[27]$ is an $\mathcal{O}_K$-submodule of $E[27]$, we have that $\lfloor \frac{b}{2} \rfloor = 1$, implying $b = 2$ or $b = 3$, but also $\lceil \frac{b}{2} \rceil = 3$, implying $b = 5$ or $b = 6$, a contradiction. Thus, no such curve exists. □

6. Algorithm

We can combine our results to form an explicit algorithm to compute $E(\mathbb{Q}^{\text{ab}})_{\text{tors}}$ for any elliptic curve $E/\mathbb{Q}$. Note that this algorithm only relies on the information about subgroups excluded from appearing as $E(\mathbb{Q}^{\text{ab}})_{\text{tors}}$ by Sections 4 and 5. See https://sites.tufts.edu/michaelchou/research/ for the Magma code that implements this algorithm.

The algorithm uses Lemma 2.3 and Lemma 2.6 repeatedly, as well as Table 1. Moreover, the algorithm works for any elliptic curve $E/\mathbb{Q}$ because we exhaustively deal with all isogeny graphs possible by Theorem 2.2. We denote $T := E(\mathbb{Q}^{\text{ab}})_{\text{tors}}$.

- Compute the isogeny graph of E. Let I denote the degrees of the isogenies E has. Let N denote the largest value in I. Let I_2 and T_2 denote the 2-primary part of I and T, respectively.
- Lemmas 2.3 and 2.6 show that:
  - If $N = 11, 13, 15, 17, 19, 21, 25, 27, 37, 43, 67$, or 163, then $T \cong \mathbb{Z}/N\mathbb{Z}$.
  - If $N = 10, 14, 16$, or 18, then $T \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/N\mathbb{Z}$.
  - If $I = [1, 5, 5]$, then $T \cong \mathbb{Z}/5\mathbb{Z} \times \mathbb{Z}/5\mathbb{Z}$.
  - If $I = [1, 3, 3, 9]$, then $T \cong \mathbb{Z}/3\mathbb{Z} \times \mathbb{Z}/9\mathbb{Z}$.
  - If $I = [1, 3, 3]$, then $T \cong \mathbb{Z}/3\mathbb{Z} \times \mathbb{Z}/3\mathbb{Z}$. Note that we cannot have $T \cong \mathbb{Z}/6\mathbb{Z} \times \mathbb{Z}/6\mathbb{Z}$ because Lemma 4.2 would imply a 2-isogeny.
  - If $I = [1, 2, 3, 3, 6, 6]$, then $T \cong \mathbb{Z}/6\mathbb{Z} \times \mathbb{Z}/6\mathbb{Z}$.
- Table 1 shows that:
  - If $I = [1, 2, 2, 2, 4, 4, 4, 4]$, then $T \cong \mathbb{Z}/8\mathbb{Z} \times \mathbb{Z}/8\mathbb{Z}$.
  - If $I = [1, 2, 2, 2, 4, 4, 8, 8]$, then $T \cong \mathbb{Z}/4\mathbb{Z} \times \mathbb{Z}/16\mathbb{Z}$.
  - If $I = [1, 2, 4, 4, 8, 8, 8, 8]$ or $[1, 2, 2, 2, 4, 4]$, then $T \cong \mathbb{Z}/4\mathbb{Z} \times \mathbb{Z}/8\mathbb{Z}$.
  - If $I = [1, 2, 4, 4, 8, 8, 16, 16]$, then $T \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/16\mathbb{Z}$.
  - If $I = [1, 2, 4, 4, 8, 8]$, then $T \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/8\mathbb{Z}$.
  - If $I = [1, 2, 2, 2, 3, 6, 6, 6]$, then $T_2 \cong \mathbb{Z}/4\mathbb{Z} \times \mathbb{Z}/4\mathbb{Z}$ and $3 \in I$ shows that $T \cong \mathbb{Z}/4\mathbb{Z} \times \mathbb{Z}/12\mathbb{Z}$.
  - If $I = [1, 2, 2, 2]$, then $T_2 \cong \mathbb{Z}/4\mathbb{Z} \times \mathbb{Z}/4\mathbb{Z}$.

- The remaining cases require extra steps beyond simply computing I, as I does not uniquely determine T.
  - If $N = 1, 3, 5, 7$, or 9, then compute $E[2]$ to check whether $\mathbb{Q}(E[2])$ is abelian or not. If not, then $T \cong \mathbb{Z}/N\mathbb{Z}$. If so, then $T \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}2N\mathbb{Z}$.
  - If $I_2 = [1, 2, 4, 4]$, then compute $E[8]$ and $E[4]$ to determine whether E has a point of order 8 over $\mathbb{Q}^{\text{ab}}$ and whether $\mathbb{Q}(E[4])$ is abelian. This distinguishes between the following three cases:
    * $T_2 \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/4\mathbb{Z}$. If $3 \in I$, then $T \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/12\mathbb{Z}$. If $3 \notin I$, then $T \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/4\mathbb{Z}$.
    * $T_2 \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/8\mathbb{Z}$. This implies $T \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/8\mathbb{Z}$.
    * $T_2 \cong \mathbb{Z}/4\mathbb{Z} \times \mathbb{Z}/4\mathbb{Z}$. If $3 \in I$, then $T \cong \mathbb{Z}/4\mathbb{Z} \times \mathbb{Z}/12\mathbb{Z}$. If $3 \notin I$, then $T \cong \mathbb{Z}/4\mathbb{Z} \times \mathbb{Z}/4\mathbb{Z}$.
  - If $I_2 = [1, 2]$, then we compute $E[4]$ to determine whether E has a point of order 4 defined over $\mathbb{Q}^{\text{ab}}$. This distinguishes between the following two cases:
    * $T_2 \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}$. If $3 \in I$, then $T \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/6\mathbb{Z}$. If $5 \in I$, then $T \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/10\mathbb{Z}$. If $I = I_2 = 1, 2$ then $T \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/2\mathbb{Z}$.
    * $T_2 \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/4\mathbb{Z}$. If $3 \in I$, then $T \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/12\mathbb{Z}$. If $3 \notin I$, then $T \cong \mathbb{Z}/2\mathbb{Z} \times \mathbb{Z}/4\mathbb{Z}$.

7. Examples

We first examine all examples of curves with an n-isogeny where $X_0(n)$ has finitely many noncuspidal points over $\mathbb{Q}$ in Table 2. We refer to Table 4 of [Lozano-Robledo 2013] for the j-invariants. We give the torsion subgroup over $\mathbb{Q}^{\text{ab}}$, the j-invariant, the Cremona labels of the elliptic curves, and the Galois group of the field of definition of the abelian torsion. We then find examples for all the other torsion subgroups appearing in Theorem 1.2 in Table 3, computing the torsion subgroup over $\mathbb{Q}^{\text{ab}}$ using the method described in Section 6.

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$E(\mathbb{Q}^{ab})_{tors}$	$j(E)$	Cremona label	$\mathrm{Gal}(\mathbb{Q}(E(\mathbb{Q}^{ab})_{tors})/\mathbb{Q})$
$\mathbb{Z}/11\mathbb{Z}$	$-11\cdot 131^3$	121a1	$\mathbb{Z}/10\mathbb{Z}$
		121c2	$\mathbb{Z}/5\mathbb{Z}$
	-2^{15}	121b1	$\mathbb{Z}/5\mathbb{Z}$
		121b2	$\mathbb{Z}/10\mathbb{Z}$
	-11^2	121c1	$\mathbb{Z}/10\mathbb{Z}$
		121a2	$\mathbb{Z}/5\mathbb{Z}$
$\mathbb{Z}/15\mathbb{Z}$	$-5^2/2$	50a1	$\mathbb{Z}/4\mathbb{Z}$
		50b3	$\mathbb{Z}/4\mathbb{Z}$
	$-5^2\cdot 241^3/2^3$	50a2	$\mathbb{Z}/2\mathbb{Z}\times\mathbb{Z}/4\mathbb{Z}$
		50b4	$\mathbb{Z}/2\mathbb{Z}\times\mathbb{Z}/4\mathbb{Z}$
	$-5\cdot 29^3/2^5$	50a3	$\mathbb{Z}/2\mathbb{Z}$
		50b1	$\mathbb{Z}/2\mathbb{Z}$
	$5\cdot 211^3/2^{15}$	50a4	$\mathbb{Z}/2\mathbb{Z}\times\mathbb{Z}/2\mathbb{Z}$
		50b2	$\mathbb{Z}/2\mathbb{Z}$
$\mathbb{Z}/17\mathbb{Z}$	$-17^2\cdot 101^3/2$	14450p1	$\mathbb{Z}/16\mathbb{Z}$
	$-17\cdot 373^3/2^{17}$	14450p2	$\mathbb{Z}/8\mathbb{Z}$
$\mathbb{Z}/19\mathbb{Z}$	$-2^{15}\cdot 3^3$	361a1	$\mathbb{Z}/9\mathbb{Z}$
		361a2	$\mathbb{Z}/18\mathbb{Z}$
$\mathbb{Z}/21\mathbb{Z}$	$-3^2\cdot 5^6/2^3$	162b1	$\mathbb{Z}/3\mathbb{Z}$
		162c2	$\mathbb{Z}/6\mathbb{Z}$
	$3^3\cdot 5^3/2$	162b2	$\mathbb{Z}/6\mathbb{Z}$
		162c1	$\mathbb{Z}/6\mathbb{Z}$
	$-3^2\cdot 5^3\cdot 101^3/2^{21}$	162b3	$\mathbb{Z}/6\mathbb{Z}$
		162c4	$\mathbb{Z}/2\mathbb{Z}\times\mathbb{Z}/6\mathbb{Z}$
	$-3^3\cdot 5^3\cdot 383^3/2^7$	162b4	$\mathbb{Z}/2\mathbb{Z}\times\mathbb{Z}/6\mathbb{Z}$
		162c3	$\mathbb{Z}/6\mathbb{Z}$
$\mathbb{Z}/27\mathbb{Z}$	$-2^{15}\cdot 3\cdot 5^3$	27a2	$\mathbb{Z}/18\mathbb{Z}$
		27a4	$\mathbb{Z}/9\mathbb{Z}$
$\mathbb{Z}/37\mathbb{Z}$	$-7\cdot 11^3$	1225h1	$\mathbb{Z}/12\mathbb{Z}$
	$-7\cdot 137^3\cdot 2083^3$	1225h2	$\mathbb{Z}/36\mathbb{Z}$
$\mathbb{Z}/43\mathbb{Z}$	$-2^{18}\cdot 3^3\cdot 5^3$	1849a1	$\mathbb{Z}/21\mathbb{Z}$
		1849a2	$\mathbb{Z}/42\mathbb{Z}$
$\mathbb{Z}/67\mathbb{Z}$	$-2^{15}\cdot 3^3\cdot 5^3\cdot 11^3$	4489a1	$\mathbb{Z}/33\mathbb{Z}$
		4489a2	$\mathbb{Z}/66\mathbb{Z}$
$\mathbb{Z}/163\mathbb{Z}$	$-2^{18}\cdot 3^3\cdot 5^3\cdot 23^3\cdot 29^3$	26569a1	$\mathbb{Z}/81\mathbb{Z}$
		26569a2	$\mathbb{Z}/162\mathbb{Z}$
$\mathbb{Z}/2\mathbb{Z}\times\mathbb{Z}/14\mathbb{Z}$	$-3^3\cdot 5^3$	49a1	$\mathbb{Z}/6\mathbb{Z}$
		49a3	$\mathbb{Z}/6\mathbb{Z}$
	$-3^3\cdot 5^3\cdot 17^3$	49a2	$\mathbb{Z}/2\mathbb{Z}\times\mathbb{Z}/6\mathbb{Z}$
		49a4	$\mathbb{Z}/6\mathbb{Z}$
$\mathbb{Z}/3\mathbb{Z}\times\mathbb{Z}/9\mathbb{Z}$	0	27a1	$\mathbb{Z}/6\mathbb{Z}$
		27a3	$\mathbb{Z}/6\mathbb{Z}$

Table 2. Torsion from n-isogenies with $X_0(n)$ genus > 0.

$E(\mathbb{Q}^{ab})_{tors}$	$j(E)$	Cremona label	$\mathrm{Gal}(\mathbb{Q}(E(\mathbb{Q}^{ab})_{tors})/\mathbb{Q})$
$\{\mathbb{O}\}$	$2^{12}\cdot 3^3/37$	37a1	$\{1\}$
$\mathbb{Z}/3\mathbb{Z}$	$2^{13}/11$	44a1	$\{1\}$
$\mathbb{Z}/5\mathbb{Z}$	$-1/2^5\cdot 19$	38b1	$\{1\}$
$\mathbb{Z}/7\mathbb{Z}$	$3^3\cdot 4^3/2^7\cdot 13$	26b1	$\{1\}$
$\mathbb{Z}/9\mathbb{Z}$	$-3\cdot 73^3/2^9$	54b3	$\{1\}$
$\mathbb{Z}/13\mathbb{Z}$	$-2^{12}\cdot 7/3$	147b1	$\mathbb{Z}/3\mathbb{Z}$
$\mathbb{Z}/25\mathbb{Z}$	$-2^{12}/11$	11a3	$\mathbb{Z}/5\mathbb{Z}$
$\mathbb{Z}/2\mathbb{Z}\times\mathbb{Z}/2\mathbb{Z}$	$-5^6/3^2\cdot 23$	69a1	$\mathbb{Z}/2\mathbb{Z}$
$\mathbb{Z}/2\mathbb{Z}\times\mathbb{Z}/4\mathbb{Z}$	$11^6/3\cdot 5\cdot 7$	315b1	$\mathbb{Z}/2\mathbb{Z}\times\mathbb{Z}/2\mathbb{Z}$
$\mathbb{Z}/2\mathbb{Z}\times\mathbb{Z}/6\mathbb{Z}$	$2^8\cdot 7$	196a1	$\mathbb{Z}/6\mathbb{Z}$
$\mathbb{Z}/2\mathbb{Z}\times\mathbb{Z}/8\mathbb{Z}$	$12721^3/3\cdot 5\cdot 7\cdot 11^2$	3465e1	$(\mathbb{Z}/2\mathbb{Z})^3$
$\mathbb{Z}/2\mathbb{Z}\times\mathbb{Z}/10\mathbb{Z}$	$2161^3/2^{10}\cdot 3^5\cdot 11$	66c1	$\mathbb{Z}/2\mathbb{Z}$
$\mathbb{Z}/2\mathbb{Z}\times\mathbb{Z}/12\mathbb{Z}$	$71^3/2^4\cdot 3^3\cdot 5$	30a1	$\mathbb{Z}/2\mathbb{Z}\times\mathbb{Z}/2\mathbb{Z}$
$\mathbb{Z}/2\mathbb{Z}\times\mathbb{Z}/16\mathbb{Z}$	$103681^3/3^4\cdot 5$	15a5	$\mathbb{Z}/2\mathbb{Z}\times\mathbb{Z}/2\mathbb{Z}\times\mathbb{Z}/4$
$\mathbb{Z}/2\mathbb{Z}\times\mathbb{Z}/18\mathbb{Z}$	$-5^3\cdot 1637^3/2^{18}\cdot 7$	14a3	$\mathbb{Z}/2\mathbb{Z}\times\mathbb{Z}/6\mathbb{Z}$
$\mathbb{Z}/3\mathbb{Z}\times\mathbb{Z}/3\mathbb{Z}$	$-2^{18}\cdot 7^3/19^3$	19a1	$\mathbb{Z}/2\mathbb{Z}$
$\mathbb{Z}/4\mathbb{Z}\times\mathbb{Z}/4\mathbb{Z}$	$19^6/3^2\cdot 5^2\cdot 7^2$	315b2	$(\mathbb{Z}/2\mathbb{Z})^4$
$\mathbb{Z}/4\mathbb{Z}\times\mathbb{Z}/8\mathbb{Z}$	$37^3\cdot 109^3/2^4\cdot 3^4\cdot 7^2$	126b2	$(\mathbb{Z}/2\mathbb{Z})^4$
$\mathbb{Z}/4\mathbb{Z}\times\mathbb{Z}/12\mathbb{Z}$	$7^3\cdot 127^3/2^2\cdot 3^6\cdot 5^2$	30a2	$(\mathbb{Z}/2\mathbb{Z})^4$
$\mathbb{Z}/4\mathbb{Z}\times\mathbb{Z}/16\mathbb{Z}$	$241^3/3^2\cdot 5^2$	735e2	$(\mathbb{Z}/2\mathbb{Z})^3\times\mathbb{Z}/4\mathbb{Z}$
$\mathbb{Z}/5\mathbb{Z}\times\mathbb{Z}/5\mathbb{Z}$	$-2^{12}\cdot 31^3/11^5$	11a1	$\mathbb{Z}/4\mathbb{Z}$
$\mathbb{Z}/6\mathbb{Z}\times\mathbb{Z}/6\mathbb{Z}$	$5^3\cdot 43^4/2^6\cdot 7^3$	14a1	$\mathbb{Z}/2\mathbb{Z}\times\mathbb{Z}/2\mathbb{Z}$
$\mathbb{Z}/8\mathbb{Z}\times\mathbb{Z}/8\mathbb{Z}$	$13^3\cdot 17^3/3^4\cdot 5^4$	735e4	$(\mathbb{Z}/2\mathbb{Z})^5$

Table 3. Examples of remaining torsion subgroups

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LOCAL ESTIMATES FOR HÖRMANDER'S OPERATORS OF FIRST KIND WITH ANALYTIC GEVREY COEFFICIENTS AND APPLICATION TO THE REGULARITY OF THEIR GEVREY VECTORS

MAKHLOUF DERRIDJ

Following our preceding papers devoted to the case of general Hörmander's operators P with analytic-Gevrey coefficients on an open set Ω in $\mathbb{R}^n$, for which we established local relations of domination by powers of P and derived from it local s'-Gevrey regularity of local s-Gevrey vectors of P (with, furthermore, suitable relations between s, s' and the coefficient of the Sobolev estimate satisfied by P), this article deals with the case of Hörmander's operators of first kind (or of degenerate elliptic kind). We establish, in this case, precise local relations of domination by powers of P which give, when applied to the s'-Gevrey regularity of s-Gevrey vectors of P, in Ω_0, with $\overline{\Omega}_0 \subset \Omega$, an optimal relation between s, s' and the type of $\overline{\Omega}_0$ with respect to the system X of vector fields whose sum of squares is the leading part of P.

1. Introduction

Since the paper of T. Kotake and N. S. Narasimhan [1962] on the analytic regularity of analytic vectors of elliptic operators with analytic coefficients, many articles were published, trying to generalize their result in different directions such as nonelliptic operators, systems, s-Gevrey vectors (which generalize the notion of analytic vectors for $s > 1$, analytic corresponding to $s = 1$). The property proved by Kotake and Narasimhan for elliptic operators with analytic coefficients (also named "iteration property" or even "Kotake–Narasimhan property") was sought to be true for more general operators than elliptic ones and also for systems (see a survey on this subject in [Bolley et al. 1987] or in [Derridj 2017] for a more recent but short one). The "iteration property" is also true for s-Gevrey vectors of elliptic operators with s-Gevrey coefficients, $s \geq 1$, but it was proved by G. Métivier [1978] that it cannot be true for nonelliptic operators, meaning more precisely that if P

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is not elliptic, even with analytic coefficients, then an s-Gevrey vector of P is not necessarily in s-Gevrey class if $s > 1$.

For the value $s = 1$, M. S. Baouendi and Métivier [1982] proved that the iteration property is true for the class of hypoelliptic operators of principal type with analytic coefficients, showing a difference between the cases $s = 1$ and $s > 1$, in this question.

There are also many papers concerning systems of vector fields with analytic coefficients: M. Damlakhi and B. Helffer [1980] showed the "iteration property," in the case $s = 1$, for such real systems satisfying Hörmander's condition, followed by a more precise version of Helffer and C. Mattera [1980].

When the iteration property is not true one can ask for the s'-Gevrey regularity of s-Gevrey vectors of an operator or system, $s' \geq s$. There is a series of papers studying the case of systems of analytic complex vector fields, concerning analytic or Gevrey vectors [Barostichi et al. 2011; Castellanos et al. 2013], where the authors prove such s'-Gevrey regularity of analytic or s-Gevrey vectors with some relation between s, s' and the structure of the system under study.

A more recent paper by N. Braun Rodrigues, G. Chinni, P. Cordaro and M. Jahnke [Braun Rodrigues et al. 2016] was partly devoted to the global Gevrey regularity of global analytic Gevrey vectors of some subclass of Hörmander's operators on a product of tori. In that situation they showed global s'-Gevrey regularity of global analytic or s-Gevrey vectors of such operators, with an optimal result. A little later, we studied in [Derridj 2019b] the case of local Gevrey regularity of local k-Gevrey vectors ($k \in \mathbb{N}^*$) of Hörmander's operators of first kind obtaining also the same relation between s', k and the type of $\overline{\Omega}_0$, with Ω_0 open set in Ω on which we consider the k-Gevrey vectors. More recently, we studied the case of general Hörmander's operators P satisfying an a priori Sobolev estimate done by L. Hörmander [1967] for which we established local relations of domination by powers of P, when the coefficients of P are in $G^s(\Omega)$, $s \geq 1$. From such local relations we deduced the s'-Gevrey regularity of s-Gevrey vectors, with a suitable relation between s, s' and the coefficient σ of the Sobolev estimate, $\sigma = \frac{1}{p}$, $p \in \mathbb{N}^*$ [Derridj 2019a].

Here we study the same question for Hörmander's operators of first kind for which we give precise local relations of domination by powers of P, when the coefficients of P are in $G^s(\Omega)$. From these local relations we deduce an optimal relation between s', s and the type of $\overline{\Omega}_0$, with respect to the system X of the vector fields whose sum of squares is the leading part of P (see detailed theorems in the next sections).

In Section 2 are given some notation and definitions, with some preliminary facts. We recall in Section 3 the basic subelliptic estimate satisfied by Hörmander's operators, established by Hörmander [1967], J. J. Kohn [1978], and L. Rothschild and E. Stein [1976].

We use this basic estimate in order to give in Section 4 a finite family of localized estimates needed in the proof of our local relations of domination by powers of P, when the coefficients of P are in $G^s(\Omega_0)$. Then in Section 6, we prove a theorem (Theorem 6.1) which gives as a corollary the s'-Gevrey regularity in Ω_0, of s-Gevrey vectors of P ($s \geq 1$) on Ω_0 with s' optimal and a relation between s', s and the type of Ω_0 with respect to X (Theorem 6.3).

2. Some notations, definitions and preliminary facts

The differential operators we deal with in this paper are defined in an open set Ω of $\mathbb{R}^n$ and have the form:

$$P = \sum_{j=1}^{m} X_j^2 + Y + b, \tag{2-1}$$

where

$$\begin{aligned} &X = (X_1, \dots, X_m) \text{ is a system of real smooth vector fields in } \Omega,\\ &Y \text{ is a smooth vector field in } \Omega \text{ such that its imaginary part}\\ &\operatorname{Im} Y \text{ is a linear combination with smooth real coefficients in}\\ &\Omega \text{ of the vector fields } X_j,\ j = 1, \dots, m, \end{aligned} \tag{2-2}$$

and

$$\operatorname{Im} Y = \sum_{j=1}^{m} b_j X_j, \quad b_j \in C^\infty(\Omega, \mathbb{R}),\ b \in C^\infty(\Omega, \mathbb{C}). \tag{2-3}$$

In the case Y is real and P satisfies the following "Hörmander's condition for hypoellipticity:"

$$\begin{aligned} &\text{The Lie algebra, } \operatorname{Lie}(Y, X_1, \dots, X_m)\text{, generated by the smooth}\\ &\text{real vector fields } Y, X_1, \dots, X_m, \text{ is of maximal rank in } \Omega, \end{aligned} \tag{2-4}$$

P is hypoelliptic in Ω [Hörmander 1967].

We studied in [Derridj 2019a] the case where the coefficients of the vector fields $Y, X_1, \dots, X_m$ and b are in some Gevrey class, and established, under condition (2-4), local relations of domination by powers of P, with application to the Gevrey regularity of analytic-Gevrey vectors of P.

Here we prove precise local relations of domination by powers of P in the case of Hörmander's operators of first kind:

$$\begin{aligned} &\text{The Lie algebra, } \operatorname{Lie}(X_1, \dots, X_m), \text{ generated by the smooth}\\ &\text{real vector fields } X_1, \dots, X_m, \text{ is of maximal rank in } \Omega,\\ &P \text{ given by (2-1), satisfying (2-3).} \end{aligned} \tag{2-5}$$

More details are given in the next sections.

Let A be now a linear operator on $\mathcal{D}(\Omega)$, then

$$(2\text{-}6)\quad [P, A] = \sum_{j=1}^{m} (X_j[X_j, A] - [X_j, [X_j, A]]) + [Y + b, A] \qquad \text{with } [X, A] = XA - AX.$$

In the sequel, our operators will be ordinary derivatives ∂^α, with $\alpha \in \mathbb{N}^n$, or some elementary pseudodifferential operators T_σ or ψT_σ with $\psi \in \mathcal{D}(\Omega)$. Let us recall them and give some related facts.

Given $\sigma \in \mathbb{R}$, one defines T_σ, as operator acting on $\mathcal{S}(\mathbb{R}^n)$ (the Schwartz space on $\mathbb{R}^n$) by:

$$(2\text{-}7)\qquad \mathcal{S}(\mathbb{R}^n) \ni u \mapsto T_\sigma u \in \mathcal{S}(\mathbb{R}^n), \quad \text{with} \quad \widehat{T_\sigma u}(\xi) = (1 + |\xi|^2)^{\sigma/2} \hat{u}(\xi).$$

As we will work locally, generally in relatively compact open sets in Ω, we consider elementary pseudodifferential operators $\psi T_\sigma u$, with ψ in $\mathcal{D}(\Omega)$. Moreover when working on local regularity of a function u, knowing a property of Pu or of the sequence $P^k u$, $k \in \mathbb{N}$, we can assume by taking $\widetilde{X}_j = \psi X_j$, $\widetilde{Y} = \psi Y$, $\tilde{b} = \psi b$, and $\widetilde{P} = \sum_{j=1}^m \widetilde{X}_j^2 + \widetilde{Y} + \tilde{b}$, that the X_j's, Y and b have compact support, specifying the following:

$$(2\text{-}8)\qquad \begin{aligned} &\psi \in \mathcal{D}(\Omega), \psi = 1 \text{ on } V(\overline{\Omega}_1), \text{ with } \overline{\Omega}_1 \subset \Omega, \text{ then} \\ &Pu = \widetilde{P}u \quad \text{on } V(\overline{\Omega}_1) = \Omega_2, \ \overline{\Omega}_2 \subset \Omega. \end{aligned}$$

The Hörmander's hypothesis will be the same on Ω_1 and so, all the inequalities obtained when using such hypothesis. Coming back to our operator T_σ, we remark that, for $u \in \mathcal{D}(\mathbb{R}^n)$, $T_\sigma u$ is not necessarily in $\mathcal{D}(\mathbb{R}^n)$, but $\psi T_\sigma u$ is, when $\psi \in \mathcal{D}(\Omega) \subset \mathcal{D}(\mathbb{R}^n)$.

The following facts, which we will use along the proof, are, of course, common in the theory of pseudodifferential operators, but here can be proved easily as we work with the above defined simple operators. The Sobolev norms are:

$$(2\text{-}9)\qquad \|v\|_\sigma = \|T_\sigma v\|, \qquad \|\cdot\| \text{ being the } L^2-\text{norm}, \quad v \in \mathcal{S}(\mathbb{R}^n).$$

In particular, T_σ and so ψT_σ are linear continuous operators from $H^s(\mathbb{R}^n)$ to $H^{s-\sigma}(\mathbb{R}^n)$. The operator T_σ is of order σ. As we assumed the coefficients of the X_j's, Y and b with compact support (as we used the cut-off function, which has value 1 on Ω_1), we may consider the following:

$$(2\text{-}10)\qquad \begin{aligned} &[X_j, T_\sigma] \text{ and } [Y, T_\sigma] \text{ are of order } \sigma, \text{ satisfying} \\ &\quad \|[X_j, T_\sigma]v\|_\rho \le C_{\rho,\sigma} \|v\|_{\rho+\sigma} \quad \text{for all } v \in \mathcal{D}(\Omega), \\ &\qquad\qquad\qquad\qquad\qquad\qquad \text{same for } [Y + b, T_\sigma], \\ &\|[X_j, [X_j, T_\sigma]v\|_\rho \le C_{\rho,\sigma} \|v\|_{\rho+\sigma} \quad \text{for all } v \in \mathcal{D}(\Omega), \\ &\quad \|[\psi, T_\sigma]v\|_\rho \le C \|v\|_{\rho+\sigma-1}. \end{aligned}$$

The properties in (2-10) are the same replacing T_σ by ψT_σ.

We will use in the next sections the following facts:

(2-11) If Ω_1 is relatively compact in Ω_2 and $\psi \in \mathcal{D}(\Omega_2)$, $\psi|_{\Omega_1} = 1$, then
$$\|v\|_\sigma \le \|\psi T_\sigma v\| + C\|v\|_{\sigma-1}, \quad \text{for all } v \in \mathcal{D}(\Omega_1),\ C = C(\psi).$$

Equation (2-11) follows from: $\|T_\sigma v\| = \|T_\sigma \psi v\| \le \|\psi T_\sigma v\| + \|[T_\sigma, \psi]v\|$.

If $(\cdot,\cdot)$ denotes the scalar product in $L^2(\mathbb{R}^n)$ then

$$\text{(2-12)}\qquad \begin{aligned} &(T_\sigma v, w) = (v, T_\sigma w), && v, w \in \mathcal{S}(\mathbb{R}^n)\\ &|(v, w)| \le \text{s.c.}\|v\|_s + \text{l.c.}\|w\|_{-s}, && s \in \mathbb{R}, \end{aligned}$$

where s.c. stands for a small constant and l.c. for a corresponding large constant.

As we will need it in the next sections, we recall a relation between the scalar product (Pv, v), $v \in \mathcal{D}(\Omega)$ and the norms $\|X_j v\|$, $j = 1, \dots, m$, for $v \in \mathcal{D}(\Omega)$:

$$\text{(2-13)}\qquad (Pv, v) = -\sum_{j=1}^m \|X_j v\|^2 + O\Big(\sum_{j=1}^m \|X_j v\|\|v\| + \|v\|^2\Big) + (Yv, v).$$

Now from hypothesis (2-5), made on Y, we see that

$$\text{(2-14)}\qquad -\mathrm{Re}\,(Pv, v) = \sum_{j=1}^m \|X_j v\|^2 + O\Big(\sum_{j=1}^m \|X_j v\|\|v\| + \|v\|^2\Big).$$

Hence one gets, using that, if X_j is real, $\mathrm{Re}\,(X_j v, v) = O(\|v\|^2)$:

$$\text{(2-15)}\qquad \sum_{j=1}^m \|X_j v\|^2 \le C(|(Pv, v)| + \|v\|^2), \quad \text{for all } v \in \mathcal{D}(\Omega).$$

We finish this section recalling definitions of "analytic and Gevrey spaces" and "analytic and Gevrey vectors of an operator."

Definition 2.1. Given an open set Ω in $\mathbb{R}^n$, an analytic ($s = 1$) (respectively Gevrey, $s > 1$) function in Ω is a smooth function in Ω such that for every compact K in Ω, there exists $C_k > 0$ such that

$$\text{(2-16)}\qquad \|\partial^\alpha u\|_{L^2(K)} \le C_K^{|\alpha|+1}\alpha!^s, \quad \text{for all } \alpha \in \mathbb{N}^n,\ |\alpha| = \sum_{i=1}^n \alpha_i.$$

Definition 2.2. Given an operator P_m of order m in Ω, an analytic vector (case $s = 1$) and a Gevrey vector ($s > 1$) of P_m in Ω, is a function $u \in L^2_{\mathrm{loc}}(\Omega)$ such that, for every compact $K \subset \Omega$, there exists a constant $C_K > 0$ such that

$$\text{(2-17)}\qquad P_m^k u \in L^2(K) \quad\text{and}\quad \|P_m^k u\|_{L^2(K)} \le C_K^{k+1}(mk)!^s, \qquad \text{for all } k \in \mathbb{N}.$$

Remark 2.3. When Ω is compact, just take $K = \Omega$ in (2-16) or in (2-17).

In our case, in the sequel, $m = 2$, with P given by (2-4) and, as P is hypoelliptic [Hörmander 1967], or using directly the basic estimate, one can take $u \in C^\infty(\Omega)$, in Definition 2.2. We write $u \in G^s(\Omega)$ (Definition 2.1), $u \in G^s(P, \Omega)$ in Definition 2.2.

3. The Hörmander–Kohn–Rothschild–Stein basic estimate

In his paper on hypoellipticity, Hörmander [1967] introduced his condition, known as the bracket condition. in the case of operators P of first kind, it reads concretely as follows. Let, for any $i, j \in \{1, \dots, m\}$ and $I = (i_1, \dots, i_\ell)$

$$(3\text{-}1)\quad [X_i, X_j] = X_i \circ X_j - X_j \circ X_i, \qquad X_I = [X_{i_1}, \dots, [X_{i_{\ell-1}}, X_{i_\ell}]] \dots], \quad |I| = \text{length of } I = \ell.$$

For any open subset $\widetilde{\Omega} \subset \Omega$, we set

$$(3\text{-}2)\qquad (H_{\widetilde{\Omega}}):\ \text{For every } x \in \widetilde{\Omega},\ \operatorname{span}\{X_I(x),\ \forall I\} = T_x(\widetilde{\Omega}) \simeq \mathbb{R}^n.$$

Given any subset V contained in $\widetilde{\Omega}$, one can define its type relative to the system X as follows:

$$(3\text{-}3)\quad \operatorname{type}_X(V) = \sup\{\operatorname{type}_X(x) : x \in V\} \in \mathbb{R}_+ \cup \{+\infty\}, \qquad \text{where } \operatorname{type}_X(x) = \inf\bigl\{k \in \mathbb{N}^* : \operatorname{span}\{X_J(x), |J| \le k\} = \mathbb{R}^n\bigr\}.$$

Then, for the system $X = (X_1, \dots, X_m)$, one has the following basic subelliptic estimate:

Theorem 3.1. *Let* Ω_1 *open*, $\Omega_1 \Subset \Omega$, *such that* $\operatorname{type}_X(\overline{\Omega}_1) = p < +\infty$. *Then*, *if* $\sigma = \frac{1}{p}$, *one has*

$$(3\text{-}4)\qquad \|v\|_\sigma \le C\Bigl(\sum_j \|X_j v\| + \|v\|\Bigr), \quad C = C(\Omega_1, X),\ \textit{for all } v \in \mathcal{D}(\Omega_1).$$

The estimate (3-4), proved by Hörmander [1967] for $\sigma < \frac{1}{p}$, was improved by Rothschild and Stein [1976]. Kohn [1978] gave a subelliptic estimate with σ smaller, but with a simpler proof (in case $p = 2$, $\sigma = \frac{1}{2}$ also).

In the next sections, once Ω_1 with $\Omega_1 \Subset \Omega$ is fixed, one can assume that the X_j's, Y and b have compact support as we mentioned in (2-8) in the preceding section.

One may deduce from Theorem 3.1 an estimate involving P, which will be more useful to us, as we have information on the $Pu = f$, rather than on the $X_j u$'s. This estimate is

$$(3\text{-}5)\qquad \|v\|_\sigma^2 + \sum_{j=1}^m \|X_j v\|^2 \le C(|(Pv, v)| + \|v\|^2), \quad \text{for all } v \in \mathcal{D}(\Omega_1).$$

Now, given u such that Pu is known, $u \in C^\infty(\Omega_1)$, one way to use (3-5) with u playing some role, is to localize u by a cut-off function $\varphi \in \mathscr{D}(\Omega)$, with $\varphi|_{\Omega_2} = 1$ (so $\varphi u = u$ on Ω_2). So, taking $v = \varphi u$ in (3-5) we will have $(P\varphi u, \varphi u)$ in the second member.

In order to have information on $P\varphi u$, knowing Pu or φPu, if we look at it on Ω_2, is to write

$$P\varphi u = [P, \varphi]u + \varphi P u, \tag{3-6}$$

which gives, using (2-6),

$$P\varphi u = \textstyle\sum_j \big(2X_j \circ X_j(\varphi) - X_j^2(\varphi)u\big) + \varphi P u. \tag{3-7}$$

In the sequel, when we study estimates on derivatives of u, knowing locally derivatives of Pu, we will have to deal with the brackets of P with the operators ∂^α. So, from (2-6) we will face the brackets $[X_j, \partial^\alpha]$, $[Y, \partial^\alpha]$, $[X_j, [X_j, \partial^\alpha]]$. These are obviously differential operators of order α. As in our preceding paper [Derridj 2019a], we write them as:

$$\begin{gathered}
[X_j, \partial^\alpha] = \sum_{\substack{\beta<\alpha \\ \ell=1,\dots,n}} a_{j\alpha\beta\ell}\, \partial^{\beta+\ell}, \quad [Y, \partial^\alpha] = \sum_{\substack{\beta<\alpha \\ \ell=1,\dots,n}} b_{\alpha\beta\ell}\, \partial^{\beta+\ell}, \\
[X_j, [X_j, \partial^\alpha]] = \sum_{\substack{\beta<\alpha \\ k=1,\dots,n}} d_{jk\alpha\beta}\, \partial^{\beta+k} + \sum_{\substack{\beta<\alpha,\, |\beta|\le|\alpha|-2 \\ k,\ell=1,\dots,n}} c_{j\ell k\alpha\beta}\, \partial^{\beta+\ell+k}, \\
\text{where } \beta+\ell \text{ is the multiindex defined by} \\
(\beta+\ell)_i = \beta_i,\ i \neq \ell,\ (\beta+\ell)_\ell = \beta_\ell + 1, \\
[b, \partial^\alpha] = \textstyle\sum_{\beta<\alpha} b_{\alpha\beta}\, \partial^\beta.
\end{gathered} \tag{3-8}$$

We, often, delete the first subscript j in these coefficients, in the proofs of our estimates, writing for example X instead of X_j's. Let us now recall a proposition giving estimates for the coefficients in (3-8), when the coefficients of P are analytic ($s = 1$), or generally in the Gevrey class $G^s(\Omega_1)$ ($s \geq 1$), Ω_1 open set in Ω; we proved this proposition in [Derridj 2019a], see also [Derridj and Zuily 1973].

Proposition 3.2. *Assume the coefficients are in $G^s(\Omega_1)$, $\overline{\Omega}_1 \subset \Omega$. For every compact $K \subset \Omega_1$, there exists $B = B_K$ such that, if ∇ denotes the gradient operator,*

$$\begin{aligned}
|b_{\alpha\beta}|_K + |b_{\alpha\beta\ell}|_K + |a_{j\alpha\beta\ell}|_K &\leq B^{|\alpha-\beta|}\Big(\frac{\alpha!}{\beta!}\Big)^s, && \beta<\alpha,\ 1\leq\ell\leq n,\ 1\leq j\leq m, \\
|\nabla b_{\alpha\beta}|_K + |\nabla b_{\alpha\beta\ell}|_K + |\nabla a_{j\alpha\beta\ell}|_K &\leq B^{|\alpha-\beta|}\Big(\frac{\alpha!}{\beta!}\Big)^s, && \beta<\alpha,\ 1\leq\ell\leq n,\ 1\leq j\leq m, \\
|c_{j\ell\alpha\beta}|_K + |\nabla c_{j\ell\alpha\beta}|_K &\leq B^{|\alpha-\beta|}\Big(\frac{(\alpha+k)!}{(\beta+k)!}\Big)^s, && |\beta|\leq|\alpha|-2,\ 1\leq\ell\leq n, \\
|d_{jk\alpha\beta}|_K + |\nabla d_{jk\alpha\beta}|_K &\leq B^{|\alpha-\beta|}\Big((|\alpha|+1)\frac{\alpha!}{\beta!}\Big)^s.
\end{aligned} \tag{3-9}$$

Here we recall that $\alpha! = \prod_{i=1}^{n} \alpha_i!$,

$$\beta \le \alpha \Leftrightarrow \beta_i \le \alpha_i \quad \text{for } 1 \le i \le n; \qquad \beta < \alpha \Leftrightarrow \beta \le \alpha, \quad \beta \ne \alpha.$$

As a corollary of Proposition 3.2, we get:

Proposition 3.3. *Assume that the coefficients of the X_j's, Y and b are in $G^s(\overline{\Omega}_0)$, for some $s \ge 1$. Then there exists a constant $B > 0$ such that for $j = 1, \dots, m$ and $\beta < \alpha$, $1 \le \ell, k \le n$ and $0 \le \tau \le 1$:*

$$\|b_{\alpha\beta} v\|_\tau + \|b_{\alpha\beta\ell} v\|_\tau + \|a_{j\alpha\beta\ell} v\|_\tau \le B^{|\alpha-\beta|}\Big(\frac{\alpha!}{\beta!}\Big)^s \|v\|_\tau$$

$$\|c_{j\ell k\alpha\beta} v\|_\tau \le B^{|\alpha-\beta|}\Big(\frac{(\alpha+k)!}{(\beta+k)!}\Big)^s \|v\|_\tau \tag{3-10}$$

$$\|d_{jk\alpha\beta} v\|_\tau \le B^{|\alpha-\beta|}\Big(\frac{\alpha!(|\alpha|+1)}{\beta!}\Big)^s \|v\|_\tau, \quad \textit{for all } v \in \mathcal{D}(\Omega_0).$$

4. The basic localized estimates

We want to derive from the basic subelliptic estimate (3-5) with $\sigma = \frac{1}{p}$, $p \in \mathbb{N}$, a finite family of localized estimates, which we will use in order to prove our local relations of domination by powers of P. These localized estimates are expressed in the following result.

Proposition 4.1. *Let Ω_1, $\overline{\Omega}_1 \subset \Omega_0$, and assume that* (3-5) *is true on Ω_0. Then there exists a constant $C > 0$ such that for all $(u, \varphi) \in C^\infty(\Omega_1) \times \mathcal{D}(\Omega_1)$ and $\alpha \in \mathbb{N}^n$:*

$$\begin{aligned} &\|\varphi \partial^\alpha u\|_\sigma \\ &\le C\Bigg\{ (\|\varphi\partial^\alpha P u\| \|\varphi\partial^\alpha u\|)^{1/2} + \sum_{|\beta_1|+|\beta_2|\le 2} (\|\varphi^{(\beta_1)}\partial^\alpha u\| \|\varphi^{(\beta_2)}\partial^\alpha u\|)^{1/2} \\ &\quad + \Bigg(\sum_{\substack{|\beta|\le 1 \\ j=1,\dots,m}} \|\varphi^{(\beta)}[X_j, \partial^\alpha]u\|^{1/2} + \sum_{j=1}^{m} \|\varphi[X_j, [X_j, \partial^\alpha]]u\|^{1/2} \\ &\quad + \|\varphi[Y+b, \partial^\alpha]u\|^{1/2} \Bigg) \cdot \|\varphi\partial^\alpha u\|^{1/2} \Bigg\} \end{aligned} \tag{4-1}$$

and for $1 \le \ell \le p-1$,

$$\begin{aligned} &\|\varphi \partial^\alpha u\|_{(\ell+1)\sigma} \\ &\le C\Bigg\{ \|\varphi\partial^\alpha P u\|_{(\ell-1)\sigma} + \sum_{|\beta|\le 1} \|\varphi^{(\beta)}\partial^\alpha u\|_{\ell\sigma} + \sum_{|\beta|=2} \|\varphi^{(\beta)}\partial^\alpha u\|_{(\ell-1)\sigma} \\ &\quad + \sum_{\substack{|\beta|\le 1 \\ j=1,\dots,m}} \|\varphi^{(\beta)}[X_j, \partial^\alpha]u\|_{(\ell-1)\sigma} + \sum_{j=1}^{m} \|\varphi[X_j, [X_j, \partial^\alpha]u\|_{(\ell-1)\sigma} \\ &\quad + \|\varphi[Y+b, \partial^\alpha]u\|_{(\ell-1)\sigma} \Bigg\}. \end{aligned} \tag{4-2}$$

It is important to note the difference between the two cases (4-1) and (4-2). The first one has in the second member terms which are square roots of products of two factors and the second one has just norms, but in suitable Sobolev spaces which permit to obtain an optimal result.

Proof of Proposition 4.1. We begin with the proof of (4-1). We first mention that the constant $C > 0$, in the following, may vary from line to line, but as ℓ is in $\{0, \dots, p\}$, at the end we will have a constant $C > 0$, valid for all the estimates in (4-2). Moreover, in all the proof of our proposition, s.c. will denote a small constant and l.c. a large constant, which will be determined along the proof; in order to get a fixed constant $C > 0$, valid for all $\ell \in \{0, \dots, p\}$ and all $\alpha \in \mathbb{N}^n$, we use the basic estimate (3-5) for $v = \varphi\partial^\alpha u$. So

$$\|\varphi\partial^\alpha u\|_\sigma + \sum_{j=1}^{m} \|X_j\varphi\partial^\alpha u\| \le C_0\big(|(P\varphi\partial^\alpha u, \varphi\partial^\alpha u)|^{1/2} + \|\varphi\partial^\alpha u\|\big). \tag{4-3}$$

Then write

$$\begin{aligned}
&[P, \varphi\partial^\alpha]u \\
&= [P, \varphi]\partial^\alpha u + \varphi[P, \partial^\alpha]u \\
&= \sum_{j=1}^{m}\big(2X_j \circ X_j(\varphi) - X_j^2(\varphi)\big)\,\partial^\alpha u + \varphi \sum_j \big(2X_j[X_j, \partial^\alpha]u - [X_j, [X_j, \partial^\alpha]]u\big) \\
&\qquad + Y(\varphi)\,\partial^\alpha u + \varphi[Y + b, \partial^\alpha]u
\end{aligned} \tag{4-4}$$

Now the only terms which are not trivially bounded by the second member of (4-1) are

$$\big|(2X \cdot X(\varphi)\partial^\alpha u, \varphi\partial^\alpha u)\big|^{1/2} \quad \text{and} \quad \big|(2\varphi X[X, \partial^\alpha]u, \varphi\partial^\alpha u)\big|^{1/2}.$$

But

$$\begin{aligned}
|(X \circ X(\varphi)\partial^\alpha u, \varphi\partial^\alpha u)|^{1/2} &= |(X(\varphi)\partial^\alpha u, (-X + a)\varphi\partial^\alpha u)|^{1/2} \\
&\le \text{s.c.}\|X\varphi\partial^\alpha u\| + \text{l.c.}(\|\varphi\partial^\alpha u\| + \|X(\varphi)\partial^\alpha u\|)
\end{aligned} \tag{4-5}$$

$$\begin{aligned}
&|(\varphi X[X, \partial^\alpha]u, \varphi\partial^\alpha u)|^{1/2} \\
&\le |(X(\varphi)[X, \partial^\alpha]u, \varphi\partial^\alpha u)|^{1/2} + |(X \circ \varphi[X, \partial^\alpha]u, \varphi\partial^\alpha u)|^{1/2} \\
&\le \|X(\varphi)[X, \partial^\alpha]u\|^{1/2}\|\varphi\partial^\alpha u\|^{1/2} + |(\varphi[X, \partial^\alpha]u, (-X + a)\varphi\partial^\alpha u)|^{1/2} \\
&\le \text{s.c.}\|X \circ \varphi\partial^\alpha u\| + \text{l.c.}(\|\varphi[X, \partial^\alpha]u)\| + \|\varphi\partial^\alpha u\|) \\
&\qquad + \|X(\varphi)[X, \partial^\alpha]u\|^{1/2}\|\varphi\partial^\alpha u\|^{1/2}
\end{aligned} \tag{4-6}$$

Now taking the small constant s.c. less than $\frac{1}{2}C_0$, in view of (4-3), s.c.$\|X(\varphi)\partial^\alpha u\|$ will be absorbed by the left hand, which will be bounded by the right member of

(4-1). Once s.c. is so well chosen, the constant l.c. will be fixed and so get our constant C, needed in (4-1).

In order to prove (4-2), we need our hypothesis that the subelliptic estimate is valid in Ω_0: so in all the sequel we fix a test function $\psi \in \mathcal{D}(\Omega_0)$, $\psi|_{|\Omega_1} = 1$.

We will prove in fact the following estimate:

$$\|\varphi\partial^\alpha u\|_{(\ell+1)\sigma} + \sum_{j=1}^{m} \|X_j\varphi\partial^\alpha u\|_{\ell\sigma} \le C\big\{\text{second member in (4-2)}\big\}. \tag{4-7}$$

Now we set $v = \partial^\alpha u$, and then we get from (2-9)

$$\begin{aligned}\|\varphi v\|_{(\ell+1)\sigma} &+ \sum_{j=1}^{m} \|X_j\varphi v\|_{\ell\sigma} \\ &\le \|\psi\varphi v\|_{(\ell+1)\sigma} + \sum_{j=1}^{m} \|X_j\psi\varphi v\|_{\ell\sigma} \\ &\le \|T_{\ell\sigma}\psi\varphi v\|_\sigma + \sum_{j=1}^{m} \|T_{\ell\sigma}X_j\psi\varphi v\| \\ &\le \|[T_{\ell\sigma},\psi]\varphi v\|_\sigma + \|\psi T_{\ell\sigma}\varphi v\|_\sigma + \sum_{j=1}^{m}\big(\|[T_{\ell\sigma},X_j\psi]\varphi v\| + \|X_j\psi T_{\ell\sigma}\varphi v\|\big).\end{aligned} \tag{4-8}$$

Now, using that $[T_{\ell\sigma},\psi]$ is of order $\ell\sigma - 1 \le 0$, as $\ell \le p$ and $[T_{\ell\sigma}, X_j\psi]$ is of order $\ell\sigma$, we get:

$$\begin{aligned}\|\varphi v\|_{(\ell+1)\sigma} &+ \sum_{j=1}^{m} \|X_j\varphi v\|_{\ell\sigma} \\ &\le \text{s.c.}\|\varphi v\|_{(\ell+1)\sigma} + \text{l.c.}\|\varphi v\| + \|\psi T_{\ell\sigma}\varphi v\|_\sigma + \sum_{j=1}^{m} \|X_j\psi T_{\ell\sigma}\varphi v\|.\end{aligned} \tag{4-9}$$

Now we apply the basic estimate to the last two terms:

$$\begin{aligned}\|\psi T_{\ell\sigma}\varphi v\|_\sigma &+ \sum_j \|X_j\psi T_{\ell\sigma}\varphi v\| \\ &\le C_0\big(|(P\psi T_{\ell\sigma}\varphi v, \psi T_{\ell\sigma}\varphi v)|^{1/2} + \|\varphi v\|_{\ell\sigma}\big) \\ &\le C_0\big(|(P\psi T_{\ell\sigma}\varphi v, \psi T_{\ell\sigma}\varphi v)|^{1/2} + \text{s.c.}\|\varphi v\|_{(\ell+1)\sigma} + \text{l.c.}\|\varphi v\|\big).\end{aligned} \tag{4-10}$$

Gathering (4-8), (4-9) and (4-10), we obtain

$$\begin{aligned}\|\varphi v\|_{(\ell+1)\sigma} &+ \sum_{j=1}^{m} \|X_j\varphi v\| \\ &\le C_0|(P\psi T_{\ell\sigma}\varphi v, \psi T_{\ell\sigma}\varphi v)|^{1/2} + \text{s.c.}\|\varphi v\|_{(\ell+1)\sigma} + \text{l.c.}\|\varphi v\|, \quad \text{with } v = \partial^\alpha u.\end{aligned} \tag{4-11}$$

So we are reduced to study the term $|(P\psi T_{\ell\sigma}\varphi\partial^\alpha u,\, \psi T_{\ell\sigma}\varphi\partial^\alpha u)|^{1/2}$. We decompose $P\psi T_{\ell\sigma}\varphi\partial^\alpha u$ as follows:

$$P\psi T_{\ell\sigma}\varphi\partial^\alpha u = \psi T_{\ell\sigma}\varphi\partial^\alpha Pu + [P,\psi T_{\ell\sigma}]\varphi\partial^\alpha u + \psi T_{\ell\sigma}[P,\varphi]\partial^\alpha u + \psi T_{\ell\sigma}\varphi[P,\partial^\alpha]u. \tag{4-12}$$

So we are led to bound the following expressions:

(A) A bound to $|(\psi T_{\ell\sigma}\varphi\partial^\alpha Pu,\, \psi T_{\ell\sigma}\varphi\partial^\alpha u)|^{1/2} = E_1$.

The term E_1 can be bounded as follows, using (2-12):

$$E_1 \le \text{s.c.}\|\varphi\partial^\alpha u\|_{(\ell+1)\sigma} + \text{l.c.}\|\varphi\partial^\alpha Pu\|_{(\ell-1)\sigma}. \tag{4-13}$$

(B) A bound to $|([P,\psi T_{\ell\sigma}]\varphi\partial^\alpha u,\, \psi T_{\ell\sigma}\varphi\partial^\alpha u)|^{1/2} = E_2$.

Using the expression of the bracket given in (2-6), we have to bound the following three terms $E_{2,1}$, $E_{2,2}$, $E_{3,3}$.

(a) $$E_{2,1} \le \sum_{j=1}^m |(X_j[X_j,\psi T_{\ell\sigma}]\varphi\partial^\alpha u,\, \psi T_{\ell\sigma}\varphi\partial^\alpha u)|^{1/2}.$$

Using that $X_j^* = -X_j + a_j$ and $[X_j,\psi T_{\ell\sigma}]$ is of order $\ell\sigma$:

$$E_{2,1} \le \text{s.c.}\sum_{j=1}^m \|X_j\psi T_{\ell\sigma}\varphi\partial^\alpha u\| + \text{l.c.}\|\varphi\partial^\alpha u\|_{\ell\sigma}.$$

Similarly:

(b) $$E_{2,2} \le \sum_{j=1}^m |([X_j,[X_j,\psi T_{\ell\sigma}]]\varphi\partial^\alpha u,\, \psi T_{\ell\sigma}\varphi\partial^\alpha u)|^{1/2} \le \text{s.c.}\|\varphi\partial^\alpha u\|_{(\ell+1)\sigma} + \text{l.c.}\|\varphi\partial^\alpha u\|.$$

(c) $$E_{2,3} \le |([Y+b,\psi T_{\ell\sigma}]\varphi\partial^\alpha,\, \varphi\partial^\alpha u)|^{1/2} \le \text{s.c.}\|\varphi\partial^\alpha u\|_{(\ell+1)\sigma} + \text{l.c.}\|\varphi\partial^\alpha u\|.$$

Hence, as $E_2 = E_{2,1} + E_{2,2} + E_{2,3}$, we obtain

$$E_2 \le \text{s.c.}\|\varphi\partial^\alpha u\|_{(\ell+1)\sigma} + \text{l.c.}\|\varphi\partial^\alpha u\|. \tag{4-14}$$

(C) A bound to $|(\psi T_{\ell\sigma}[P,\varphi]\partial^\alpha u,\, \psi T_{\ell\sigma}\varphi\partial^\alpha u)|^{1/2} = E_3$.

Using the expression of the bracket $[P,\varphi]$ given in (2-6) we have to bound the following three terms.

(a) $$E_{3,1} \le 2\sum_{j=1}^m |(\psi T_{\ell\sigma}X_j \circ X_j(\varphi)\partial^\alpha u,\, \psi T_{\ell\sigma}\varphi\partial^\alpha u)|^{1/2}.$$

$$\begin{aligned} E_{3,1} &\le 2\sum_{j=1}^m \big|\big(\psi T_{\ell\sigma}X_j \circ X_j(\varphi)\partial^\alpha u,\, \psi T_{\ell\sigma}\varphi\partial^\alpha u\big)\big|^{1/2} \\ &\le \sum_{j=1}^m \big(\text{s.c.}\|X_j\psi T_{\ell\sigma}\varphi\partial^\alpha u\| + \text{l.c.}(\|X_j(\varphi)\partial^\alpha u\|_{\ell\sigma} + \|\varphi\partial^\alpha u\|_{\ell\sigma})\big), \end{aligned}$$

where we have used that $X_j^* = -X_j + a_j$.

(b)
$$E_{3,2} \le \sum_{j=1}^m |(\psi T_{\ell\sigma} X_j^2(\varphi)\partial^\alpha u, \psi T_{\ell\sigma}\varphi\partial^\alpha u)|^{1/2}.$$

and hence:

$$E_{3,2} \le \text{s.c.}\|\varphi\partial^\alpha u\|_{(\ell+1)\sigma} + \text{l.c.}\sum_{j=1}^m \|X_j^2(\varphi)\partial^\alpha u\|_{(\ell-1)\sigma}.$$

(c) $E_{3,3} \le |(\psi T_{\ell\sigma}[Y+b,\varphi]\partial^\alpha u, \psi T_{\ell\sigma}\varphi\partial^\alpha u)|^{1/2} \le \|Y(\varphi)\partial^\alpha u\|_{\ell\sigma} + \|\varphi\partial^\alpha u\|_{\ell\sigma}$.
Therefore, as $E_3 = E_{3,1}+E_{3,2}+E_{3,3}$, we get

$$\begin{aligned}(4\text{-}15)\quad E_3 &\le \text{s.c.}\Big(\|\varphi\partial^\alpha u\|_{(\ell+1)\sigma} + \sum_{j=1}^m \|X_j\varphi\partial^\alpha u\|_{\ell\sigma}\Big)\\ &\quad + \text{l.c.}\Big(\sum_{j=1}^m \|X_j(\varphi)\partial^\alpha u\|_{\ell\sigma} + \|Y(\varphi)\partial^\alpha u\|_{\ell\sigma} + \|\varphi\partial^\alpha u\|_{\ell\sigma} + \sum_{j=1}^m \|X_j^2(\varphi)\partial^\alpha u\|_{(\ell-1)\sigma}\Big).\end{aligned}$$

(D) A bound to $|(\psi T_{\ell\sigma}\varphi[P,\partial^\alpha]u, \psi T_{\ell\sigma}\varphi\partial^\alpha u)|^{1/2} = E_4$.
Using again the expression of $[P,\partial^\alpha]$, we get

$$\begin{aligned}E_4 &\le \sum_{j=1}^m \big(|(2\psi T_{\ell\sigma}\varphi X_j[X_j,\partial^\alpha]u, \psi T_{\ell\sigma}\varphi\partial^\alpha u)|^{1/2}\\ &\qquad + |(\psi T_{\ell\sigma}\varphi[X_j,[X_j,\partial^\alpha]]u, \psi T_{\ell\sigma}\varphi\partial^\alpha u)|^{1/2}\big),\\ &= E_{4,1}+E_{4,2},\end{aligned}$$

modulo a term trivially bounded by the second member of (4-2). Now,

$$\begin{aligned}&E_{4,1}\\ &\le 2\sum_{j=1}^m \Big\{|(\psi T_{\ell\sigma}X_j(\varphi)[X_j,\partial^\alpha]u, \psi T_{\ell\sigma}\varphi\partial^\alpha u)|^{1/2}\\ &\qquad + |([\psi T_{\ell\sigma}, X_j]\varphi[X_j,\partial^\alpha]u, \psi T_{\ell\sigma}\varphi\partial^\alpha u)|^{1/2}\\ &\qquad\qquad + |(X_j\psi T_{\ell\sigma}\varphi[X_j,\partial^\alpha]u, \psi T_{\ell\sigma}\varphi\partial^\alpha u)|^{1/2}\Big\}\\ &\le \text{s.c.}\Big(\|\varphi\partial^\alpha u\|_{(\ell+1)\sigma} + \sum_{j=1}^m \|X_j\varphi\partial^\alpha u\|_{\ell\sigma}\Big)\\ &\qquad + \text{l.c.}\Big(\sum_{j=1}^m \|X_j(\varphi)[X_j,\partial^\alpha]u\|_{(\ell-1)\sigma} + \sum_{j=1}^m \|\varphi[X_j,\partial^\alpha]u\|_{\ell\sigma}\Big),\end{aligned}$$

$$E_{4,2} \le \text{s.c.}\|\varphi\partial^\alpha u\|_{(\ell+1)\sigma} + \text{l.c.}\|\varphi[X_j[X_j,\partial^\alpha]]u\|_{(\ell-1)\sigma}.$$

Hence

$$(4\text{-}16)\quad E_4 \le \text{s.c.}\Big(\|\varphi\partial^\alpha u\|_{(\ell+1)\sigma} + \sum_{j=1}^m \|X_j\varphi\partial^\alpha u\|_{\ell\sigma}\Big) + \text{l.c.}\Big\{\|\varphi\partial^\alpha u\|_{\ell\sigma} + \sum_{j=1}^m\Big(\|X_j(\varphi)[X_j,\partial^\alpha]u\|_{(\ell-1)\sigma} + \|\varphi[X_j,\partial^\alpha]u\|_{\ell\sigma} + \|\varphi[X_j,[X_j,\partial^\alpha]]u\|_{(\ell-1)\sigma}\Big)\Big\},$$

modulo a term trivially bounded by the second member of (4-2).

Therefore from (4-13)–(4-16), we obtain

$$(4\text{-}17)\quad |(P\psi T_{\ell\sigma}\varphi\partial^\alpha u, \psi T_{\ell\sigma}\varphi\partial^\alpha u)|^{1/2} \le \text{s.c.}\Big(\|\varphi\partial^\alpha u\|_{(\ell+1)\sigma} + \sum_{j=1}^m \|X_j\varphi\partial^\alpha u\|_{\ell\sigma}\Big) + \text{l.c.}\Big\{\|\varphi\partial^\alpha u\|_{\ell\sigma} + \sum_{j=1}^m \|X_j(\varphi)\partial^\alpha u\|_{\ell\sigma} + \|Y(\varphi)\partial^\alpha u\|_{\ell\sigma} + \sum_{j=1}^m \|X_j^2(\varphi)\partial^\alpha u\|_{(\ell-1)\sigma} + \sum_{j=1}^m \|X_j(\varphi)[X_j,\partial^\alpha]u\|_{(\ell-1)\sigma} + \sum_{j=1}^m \|\varphi[X_j[X_j,\partial^\alpha]]u\|_{(\ell-1)\sigma}\Big\},$$

modulo a term trivially bounded by the second member of (4-2).

Now, coming back to (4-11), (4-17) and taking "s.c." small enough, say $\frac{1}{2}$, one gets with the corresponding "l.c." a constant $C > 0$ in the estimates (4-2) (as the coefficients of the X_j and their first derivatives are bounded on Ω_0). The proof of Proposition 4.1 is complete. □

5. Precise local relations of domination by powers of *P*

Before stating our main theorem, in case P has analytic ($s = 1$) or Gevrey coefficients ($s > 1$), giving suitable local bounds of ordinary derivatives of functions under study, let us give some further notations of expressions needed in its proof. As $s \ge 1$ will be fixed, in the statement of the theorem, we do not include it in the notation below, except when it is really needed. First we recall the expression $N^\epsilon_{j,\gamma}(u,\varphi)$ we introduced in [Derridj 2019a]:

(5-1) For $\epsilon > 0$, $\Omega_1 \Subset \Omega$, $j \in \mathbb{N}$, $\gamma \in \mathbb{N}^n$, and $(u,\varphi) \in C^\infty(\Omega_1) \times \mathcal{D}(\Omega_1)$,

$$N^\epsilon_{j,\gamma}(u,\varphi) = \epsilon^{|\gamma|+2j}|\gamma|!^{-s}(2j)!^{-s}\|\varphi^{(\gamma)}P^j u\|.$$

Now, in this work, we introduce new expressions:

Given $p \in \mathbb{N}$, for every k, we denote

$$\mathcal{I}_k = \Big\{ (j_1, \dots, j_{2^k}, \gamma_1, \dots, \gamma_{2^k}) = (j, \gamma) \in \mathbb{N}^{2^k} \times (\mathbb{N}^n)^{2^k} \quad \text{s.t.} \quad \text{if } |j| = \sum_{\rho=1}^{2^k} j_\rho,\ |\gamma| = \sum_{\rho=1}^{2^k} |\gamma_\rho|,\ |\gamma_\rho| \le (p+1)k,\ \forall \rho,\ |\gamma| + 2|j| \le 2^k pk \Big\} \tag{5-2}$$

Of course, p in (5-2) will be the type of our considered relatively compact set, as Ω_1, we spoke about.

Then we introduce

(5-3) For $\epsilon > 0$, p as above, $k \in \mathbb{N}$, $(u, \varphi) \in C^\infty(\Omega_1) \times \mathcal{D}(\Omega_1)$,

$$\mathcal{N}_k^{\epsilon,p}(u, \varphi) = \Big(\sum_{(j,\gamma)\in \mathcal{I}_k} \prod_{\rho=1}^{2^k} N_{j_\rho,\gamma_\rho}(u, \varphi) \Big)^{2^{-k}}.$$

(5-4) For $\epsilon > 0$, p as above, $k \in \mathbb{N}$, $\ell = 1, \dots, p$, $(u, \varphi) \in C^\infty(\Omega_1) \times \mathcal{D}(\Omega_1)$,

$$\mathcal{N}_{k,\ell}^{\epsilon,p}(u, \varphi) = \Big(\sum_{(j,\gamma)\in \mathcal{I}_{k,\ell}} \prod_{\rho=1}^{2^{k+1}} N_{j_\rho,\gamma_\rho}(u, \varphi) \Big)^{2^{-(k+1)}},$$

where $\mathcal{I}_{k,\ell} = \Big\{ (j_1, \dots, j_{2^{k+1}}, \gamma_1, \dots, \gamma_{2^{k+1}}) : |\gamma_\rho| \le (p+1)k + \ell + 1,\ \forall \rho,\ |\gamma| + 2|j| \le 2^{k+1}(pk + \ell) \Big\}$.

Remark 5.1. As p will be fixed with the relatively compact open set considered (say mostly Ω_1 but it may be $\Omega_2 \dots$), it will be deleted in the notation (5-3), (5-4).

Sometimes we denote also, when (u, φ) are specified,

$$\mathcal{N}_k^\epsilon = \mathcal{N}_k^{\epsilon,p} = \mathcal{N}_{k,0}^\epsilon. \tag{5-5}$$

When there is no ambiguity we delete ϵ. But looking at the $\mathcal{N}_{k,\ell}^\epsilon$, $\ell = 0, \dots, p$, there is a difference in the expressions, between the case $\ell = 0$ and $1 \le \ell \le p$. Of course, there are some relations between these expressions which we give in the following lemma.

Lemma 5.2. *We have the following inequalities*:

$$\mathcal{N}_k^\epsilon \le \mathcal{N}_{k,1}^\epsilon \le \cdots \le \mathcal{N}_{k,p}^\epsilon = \mathcal{N}_{k+1}^\epsilon \tag{5-6}$$

Proof. The inequalities $\mathcal{N}_{k,1} \le \cdots \le \mathcal{N}_{k,p}$ are trivial as $\mathcal{I}_{k,\ell} \subset \mathcal{I}_{k,\ell+1}$ for $\ell = 1, \dots, p-1$, and $\mathcal{N}_{k,p} = \mathcal{N}_{k+1}$ is clear. So what needs a proof is the first inequality.

In order to prove it, we compare $\mathcal{N}_k^{2^{k+1}}$ and $\mathcal{N}_{k,1}^{2^{k+1}}$, meaning establishing whether or not the following inequality is true:

$$\Big(\sum_{(j,\gamma)\in\mathcal{I}_k}\prod_{\rho=1}^{2^k} N_{j_\rho,\gamma_\rho}\Big)^2 \le \sum_{(j,\gamma)\in\mathcal{I}_{k,1}}\prod_{\rho=1}^{2^{k+1}} N_{j_\rho,\gamma_\rho}. \tag{5-7}$$

In the first member of (5-7), we have the following products:

$$\Big(\prod_{\rho=1}^{2^k} N_{j_\rho,\gamma_\rho}\Big)\Big(\prod_{\rho'=1}^{2^k} N_{i_{\rho'},\delta_{\rho'}}\Big), \quad \text{with } (j,\gamma)\in\mathcal{I}_k,\ (i,\delta)\in\mathcal{I}_k.$$

These products are contained in the products in the right member of (5-7), via the map

$$N_{j_\rho,\gamma_\rho}\cdot N_{i_{\rho'},\delta_{\rho'}} \to N_{q_{\rho''},\nu_{\rho''}}, \tag{5-8}$$
$$q=(j_1,\dots,j_{2^k},i_1,\dots,i_{2^k}),\ \nu=(\gamma_1,\dots,\gamma_{2^k},\delta_1,\dots,\delta_{2^k}),$$

after observing that $(q,\nu)\in\mathcal{I}_{k,1}$. □

Now, we will need, in the sequel, to compare the preceding expressions, when one has different couples (u,φ). More precisely, denoting $\mathcal{N}^\epsilon_{\alpha,\ell}=\mathcal{N}^\epsilon_{|\alpha|,\ell}$, we have:

Lemma 5.3. (1) *Let $(i,\beta)\in\mathbb{N}\times\mathbb{N}^n$ and $\mu\in\mathbb{N}$. Then, for $(j,\gamma)\in\mathbb{N}\times\mathbb{N}^n$,*

$$\mu!^s N^\epsilon_{j,\gamma}(P^i u,\varphi^{(\beta)}) \le \epsilon^{-(|\beta|+2i)}(\mu+|\beta|+2i)!^s N_{j+i,\gamma+\beta}(u,\varphi) \tag{5-9}$$
$$\textit{for } |\gamma|+2j\le\mu,\ (u,\varphi)\in C^\infty(\Omega_1)\times\mathcal{D}(\Omega_1).$$

(2) *For $(u,\varphi)\in C^\infty(\Omega_1)\times\mathcal{D}(\Omega_1)$,*

$$\begin{aligned}
(p|\alpha|)!^s\mathcal{N}^\epsilon_\alpha(Pu,\varphi) &\le \epsilon^{-2}(p|\alpha|+2)!^s\,\mathcal{N}^\epsilon_{\alpha,1}(u,\varphi),\\
(p|\alpha|+\ell)!^s\mathcal{N}^\epsilon_{\alpha,\ell}(Pu,\varphi) &\le \epsilon^{-2}(p|\alpha|+\ell+2)!^s\,\mathcal{N}^\epsilon_{\alpha,\ell+2}(u,\varphi), && \ell+2\le p,\\
(p|\alpha|)!^s\mathcal{N}^\epsilon_\alpha(u,\varphi^{(\beta)}) &\le \epsilon^{-|\beta|}(p|\alpha|+|\beta|)!^s\,\mathcal{N}^\epsilon_{\alpha,1}(u,\varphi), && |\beta|\le 2,\\
(p|\alpha|+\ell)!^s\mathcal{N}^\epsilon_{\alpha,\ell}(u,\varphi^{(\beta)}) &\le \epsilon^{-|\beta|}(p|\alpha|+\ell+|\beta|)!^s\mathcal{N}^\epsilon_{\alpha,\ell+|\beta|}(u,\varphi), && \ell+|\beta|\le p.
\end{aligned} \tag{5-10}$$

For the proof of Lemma 5.3, we need a simple lemma, for which, we give a proof, in order to be complete.

Lemma 5.4. *Let $q\in\mathbb{N}$ and $(a_1,\dots,a_q)\in(\mathbb{R}^n_+)^q$. Then*

$$\prod_{j=1}^q a_j \le \Big(\frac{\sum_{j=1}^q a_j}{q}\Big)^q. \tag{5-11}$$

Proof of Lemma 5.4. The inequality is trivial for $q=1$. Assume it is true for q. Considering the function $f:\mathbb{R}_+\to\mathbb{R}$ given by

$$f(\lambda)=\Big(\frac{\sum_1^q a_j}{q}\Big)^q\lambda-\Big(\frac{\sum_1^q a_j+\lambda}{q+1}\Big)^{q+1},$$

and computing its derivative, one can see that f takes its maximum value at $\lambda = \frac{q+1}{q}\sum_{j=1}^{q} a_j$, which is zero. Hence $f \le 0$ on $\mathbb{R}_+$. Then taking $\lambda = a_{q+1}$, one deduces (5-11) for $q+1$. □

Proof of Lemma 5.3. The proof of (5-9) is easy to see:

$$\text{(5-12)}\quad \begin{aligned} &N^{\epsilon}_{j,\gamma}(P^i u, \varphi^{|(\beta)})\\ &= \epsilon^{-(|\beta|+2i)}\big\{(|\gamma|+1)\cdots(|\gamma|+|\beta|)(2j+1)\cdots(2j+2i)\big\}^s N^{\epsilon}_{j+i,\gamma+\beta}(u,\varphi).\end{aligned}$$

Then, if $|\gamma| + 2j \le \mu$, (5-12) gives (5-9).

Now, looking at the expression of $\mathcal{N}^{\epsilon}_{\alpha}$, for any $\rho \in \{1, \dots, 2^{|\alpha|}\}$, we use (5-12) and consider the product $\prod_{\rho=1}^{2^{|\alpha|}} N^{\epsilon}_{j_\rho,\gamma_\rho}(Pu,\varphi)$:

$$\text{(5-13)}\qquad \prod_{\rho=1}^{2^{|\alpha|}} N^{\epsilon}_{j_\rho,\gamma_\rho}(Pu,\varphi) = \prod_{\rho=1}^{2^{|\alpha|}} \epsilon^{-2}\{(2j_\rho+1)(2j_\rho+2)\}^s N_{j_\rho+1,\gamma_\rho}(u,\varphi)$$

Then using Lemma 5.4, for $\lambda = 1, 2$,

$$\text{(5-14)}\qquad \prod_{\rho=1}^{2^{|\alpha|}} (2j_\rho+\lambda) \le \left(\frac{\sum_1^{2^{|\alpha|}}(2j_\rho+\lambda)}{2^{|\alpha|}}\right)^{2^{|\alpha|}} = \left(\frac{2|j| + \lambda 2^{|\alpha|}}{2^{|\alpha|}}\right)^{2^{|\alpha|}}, \quad \lambda = 1, 2.$$

Moreover, in the expression of $\mathcal{N}^{\epsilon}_{\alpha}$, we have $2|j| \le 2^{|\alpha|} p|\alpha|$ and $|\gamma_\rho| \le (p+1)|\alpha|$, $\rho \in \{1, \dots, 2^{|\alpha|}\}$. So, from (5-14), we get

$$\text{(5-15)}\qquad \prod_{\lambda=1}^{2}\prod_{\rho=1}^{2^{|\alpha|}} (2j_\rho+\lambda) \le \prod_{\lambda=1}^{2} (p|\alpha|+\lambda)^{2^{|\alpha|}}.$$

So

$$\text{(5-16)}\qquad \prod_{\rho=1}^{2^{|\alpha|}} N_{j_\rho,\gamma_\rho}(Pu,\varphi) \le \prod_{\lambda=1}^{2} (p|\alpha|+\lambda)^{s2^{|\alpha|}} \epsilon^{-2^{|\alpha|+1}} \prod_{\rho=1}^{2^{|\alpha|}} N_{j_\rho+1,\gamma_\rho}(u,\varphi)$$

So coming back to the expression of $\mathcal{N}^{\epsilon}_{\alpha}(Pu,\varphi)$:

$$\text{(5-17)}\qquad \mathcal{N}^{\epsilon}_{\alpha}(Pu,\varphi) \le \epsilon^{-2}\left(\prod_{\lambda=1}^{2}(p|\alpha|+\lambda)\right)^{s} \left\{\sum_{(j,\gamma)\in\mathcal{I}_{|\alpha|}} \prod_{\rho=1}^{2^{|\alpha|}} N_{j_\rho+1,\gamma_\rho}(u,\varphi)\right\}^{2^{|\alpha|}}.$$

Now we want to prove

$$\text{(5-18)}\qquad \left(\sum_{(j,\gamma)\in\mathcal{I}_{|\alpha|}} \prod_{\rho=1}^{2^{|\alpha|}} N_{j_\rho+1,\gamma_\rho}(u,\varphi)\right)^2 \le \sum_{(i,\delta)\in\mathcal{I}_{|\alpha|,1}} \prod_{\rho'=1}^{2^{|\alpha|+1}} N_{i_{\rho'},\delta_{\rho'}}(u,\varphi).$$

But this is like what we did in (5-7), after observing that $(j_\rho+1, k_{\rho''+1}, \gamma_\rho, \tilde{\gamma}_{\rho''}) \in \mathcal{I}_{|\alpha|,1}$ when $(j,\gamma) \in \mathcal{I}_{|\alpha|}$, $(k,\tilde{\gamma}) \in \mathcal{I}_{|\alpha|}$.

Taking the two members in (5-18) at a power $2^{-(|\alpha|+1)}$, we obtain the first inequality in (5-10), using

$$(p|\alpha|)!^s\Big(\prod_{\lambda=1}^{2}(p|\alpha|+\lambda)\Big)^s \le (p|\alpha|+2)!^s. \tag{5-19}$$

The proofs of the other inequalities are similar. Let us give that of the last line which seems the "worst." Using (5-9) or (5-12), we get

$$N^{\epsilon}_{j,\gamma}(u,\varphi^{(\beta)}) = \epsilon^{-|\beta|}\big((|\gamma|+1)\cdots(|\gamma|+|\beta|)\big)^s N^{\epsilon}_{j,\gamma+\beta}(u,\varphi). \tag{5-20}$$

So, looking at the expression of $\mathcal{N}^{\epsilon}_{\alpha,\ell}$, for any $\rho\in\{1,\dots,2^{|\alpha|+1}\}$,

$$\prod_{\rho=1}^{2^{|\alpha|+1}} N^{\epsilon}_{j_\rho,\gamma_\rho}(u,\varphi^{(\beta)}) = \prod_{\rho=1}^{2^{|\alpha|+1}} \epsilon^{-|\beta|}\big((|\gamma_\rho|+1)\cdots(|\gamma_\rho|+|\beta|)\big)^s N^{\epsilon}_{j_\rho,\gamma_\rho+\beta}(u,\varphi). \tag{5-21}$$

Using Lemma 5.4, we get, as in (5-14),

$$\prod_{\lambda=1}^{|\beta|}\prod_{\rho=1}^{2^{|\alpha|+1}}(|\gamma_\rho|+\lambda) \le \prod_{\lambda=1}^{|\beta|}\Big(\frac{|\gamma|+\lambda 2^{|\alpha|+1}}{2^{|\alpha|+1}}\Big)^{2^{|\alpha|+1}}. \tag{5-22}$$

Now, in the expression of $\mathcal{N}^{\epsilon}_{\alpha,\ell}$ one has

$$|\gamma|\le 2^{|\alpha|+1}(p|\alpha|+\ell) \quad\text{and}\quad |\gamma_\rho|\le (p+1)|\alpha|+\ell+1.$$

So, from (5-22), we obtain

$$\prod_{\lambda=1}^{|\beta|}\prod_{\rho=1}^{2^{|\alpha|+1}}(|\gamma_\rho|+\lambda) \le \prod_{\lambda=1}^{|\beta|}(p|\alpha|+\ell+\lambda)^{2^{|\alpha|+1}}. \tag{5-23}$$

So,

$$\prod_{\rho=1}^{2^{|\alpha|+1}} N_{j_\rho,\gamma_\rho}(u,\varphi^{(\beta)}) \le \prod_{\lambda=1}^{|\beta|}(p|\alpha|+\ell+\lambda)^{s\,2^{|\alpha|+1}}\epsilon^{-|\beta|2^{|\alpha|+1}}\prod_{\rho=1}^{2^{|\alpha|+1}} N_{j_\rho,\gamma_\rho+\beta}(u,\varphi). \tag{5-24}$$

So, coming back to the expression of $\mathcal{N}^{\epsilon}_{\alpha,\ell}(u,\varphi^{(\beta)})$:

$$\begin{aligned}\mathcal{N}^{\epsilon}_{\alpha,\ell}&(u,\varphi^{(\beta)})\\ &\le \epsilon^{-|\beta|}\prod_{\lambda=1}^{|\beta|}(p|\alpha|+\ell+\lambda)^s\Big\{\sum_{(j,\gamma)\in\mathcal{I}_{|\alpha|,\ell}}\prod_{\rho=1}^{2^{|\alpha|+1}} N_{j_\rho,\gamma_\rho+\beta}(u,\varphi)\Big\}^{2^{-(|\alpha|+1)}}\\ &\le \epsilon^{-|\beta|}\prod_{\lambda=1}^{|\beta|}(p|\alpha|+\ell+\lambda)^s\Big\{\sum_{(i,\delta)\in\mathcal{I}_{|\alpha|,\ell+|\beta|}}\prod_{\rho=1}^{2^{|\alpha|+1}} N_{i_\rho,\delta_\rho}(u,\varphi)\Big\}^{2^{-(|\alpha|+1)}}.\end{aligned} \tag{5-25}$$

Hence the proof is finished using

$$(p|\alpha|)!^s \prod_{\lambda=1}^{|\beta|}(p|\alpha|+\ell+\lambda)^s \le (p|\alpha|+\ell+|\beta|)!^s. \tag{5-26}$$ □

Let us now state our main theorem.

Theorem 5.5. *Let Ω_0 be a relatively compact open subset in Ω such that*

$$\mathrm{type}_X(\overline{\Omega}_0) = p$$

and set $\sigma = 1/p$. Assume that the coefficients of P are in $G^s(\overline{\Omega}_0)$ for some $s \ge 1$. For every $1 \ge \epsilon > 0$, there exists $M_\epsilon = M(\Omega_0, P, \epsilon)$ such that, for every $\alpha \in \mathbb{N}^n$, every couple $(u, \varphi) \in C^\infty(\Omega_0) \times \mathfrak{D}(\Omega_0)$,

$$\|\varphi \partial^\alpha u\| \le M_\epsilon^{2p|\alpha|+1}(p|\alpha|)!^s \mathcal{N}_\alpha^\epsilon(u, \varphi) \tag{5-27}$$

and

$$\|\varphi \partial^\alpha u\|_{\ell\sigma} \le M_\epsilon^{2p|\alpha|+\ell+1}(p|\alpha|+\ell)!^s \mathcal{N}_{\alpha,\ell}^\epsilon(u, \varphi), \quad \ell = 1, \dots, p. \tag{5-28}$$

Proof of Theorem 5.5. Our proof will be inductive on $|\alpha|$. In each step of the induction, we will find a condition or conditions on M_ϵ in order (5-27) and (5-28), $\ell = 1, \dots, p$, are valid. The key point is to show that these conditions do not depend on $|\alpha|$.

(A) Proof of (5-27) and (5-28), for $\alpha = 0$ and $\ell = 1, \dots, p$.

(1) Proof of (5-27) for $\alpha = 0$: We have just to observe that

$$\mathcal{N}_0^\epsilon(u, \varphi) = N_{0,0}^\epsilon(u, \varphi) = \|\varphi u\|.$$

So we just need

$$M_\epsilon \ge 1, \tag{5-29}$$

for the validity of (5-27).

(2) Proof of (5-28), $\alpha = 0$ and $\ell = 1, \dots, p$: In view of the above, $M_\epsilon \ge 1$ gives (5-27); so we have to show (5-28) for $\ell = 1$ and, by induction on ℓ (finite induction here), show that if (5-28) holds for $1 \le \ell \le i$, then (5-28) holds for $\ell = i+1$, under a condition or conditions on M_ϵ. In order to prove (5-28) for $\ell = 1$, we use the localized estimate (4-1), which is

$$\|\varphi u\|_\sigma \le C\Bigl(\|\varphi P u\|\|\varphi u\| + \sum_{|\beta_1|+|\beta_2|\le 2} \|\varphi^{(\beta_1)}\|\|\varphi^{(\beta_2)} u\|\Bigr)^{1/2}. \tag{5-30}$$

But since

$$\mathcal{N}^{\epsilon}_{0,1} = \Bigg(\sum_{(j,\gamma)\in\mathcal{I}_{0,1}} \epsilon^{|\gamma|+2|j|} \prod_{\rho=1}^{2} N_{j_\rho,\gamma_\rho} \Bigg)^{1/2}, \tag{5-31}$$

we see that

$$\|\varphi u\|_\sigma \le C\epsilon^{-1}\,\mathcal{N}^{\epsilon}_{0,1}(u,\varphi). \tag{5-32}$$

Hence we get (5-28) for $\ell = 1$ if

$$M_\epsilon \ge (C\epsilon^{-1})^{1/2}. \tag{5-33}$$

To continue the proof of A), we assume that (5-28) is true for $1 \le \ell \le i,\ 1 \le i \le p-1$; we want to prove (5-28) for $\ell = i+1$. For that, we use the localized estimate (4-2) for $\ell = i$:

$$\|\varphi u\|_{(i+1)\sigma} \le C\Bigg(\|\varphi Pu\|_{(i-1)\sigma} + \sum_{|\beta|\le 1} \|\varphi^{(\beta)}u\|_{i\sigma} + \sum_{|\beta|=2} \|\varphi^{(\beta)u}\|_{(i-1)\sigma} \Bigg). \tag{5-34}$$

Applying induction to the terms in the second member of (5-34):

$$\|\varphi Pu\|_{(i-1)\sigma} \le M^i_\epsilon (i-1)!^s \mathcal{N}^{\epsilon}_{0,i-1}(Pu,\varphi).$$

Then, using properties in (5-10), we get

$$\begin{aligned} \|\varphi Pu\|_{(i-1)\sigma} &\le \epsilon^{-2} M^i_\epsilon (i+1)!^s \mathcal{N}^{\epsilon}_{0,i+1}(u,\varphi), \quad \text{and similarly have} \\ \|\varphi^{(\beta)}u\|_{i\sigma} &\le M^{i+1}_\epsilon\, \epsilon^{-1}(i+1)!^s \mathcal{N}^{\epsilon}_{0,i+1}(u,\varphi), \quad |\beta| \le 1, \\ \|\varphi^{(\beta)}u\|_{(i-1)\sigma} &\le \epsilon^{-2}\, M^i_\epsilon (i+1)!^s \mathcal{N}^{\epsilon}_{0,i+1}(u,\varphi), \qquad |\beta| = 2. \end{aligned} \tag{5-35}$$

So, coming back to (5-34), we obtain

$$\begin{aligned} \|\varphi u\|_{(i+1)\sigma} &\le C((1+n^2)\epsilon^{-2}M^i_\epsilon + (1+n)\epsilon^{-1}M^{i+1}_\epsilon)(i+1)!^s \mathcal{N}^{\epsilon}_{0,i+1}(u,\varphi) \\ &\le M^{(i+1)+1}_\epsilon (i+1)!^s \mathcal{N}^{\epsilon}_{0,i+1}(u,\varphi), \end{aligned} \tag{5-36}$$

if the following condition is satisfied, as $1+n \le 1+n^2$:

$$C(1+n^2)(\epsilon M_\epsilon)^{-i}((\epsilon M_\epsilon)^{-1}+1) \le 1. \tag{5-37}$$

So, summarizing the conditions needed in order to prove (A), namely (5-27) and (5-28), $\ell = 1, \dots, p$, these are given in (5-29), (5-33) and (5-37). It is easy to see that (5-37) is deduced from

$$C(\epsilon M_\epsilon)^{-i} \le \frac{1}{2(1+n^2)}, \quad i \in \{1, \dots, p-1\}. \tag{5-38}$$

So, the simple condition (5-38) imply (5-27) and (5-28).

(B) Proof of (5-27) and (5-28) for $|\alpha| \ge 1$.

As we saw above, (5-27) and (5-28) are true for $\alpha = 0$. So we will use induction on $|\alpha| = \mu$; more precisely, assuming that (5-27) and (5-28), $\ell = 1, \dots, p$, are true for $|\alpha| \le \mu$, we will prove them for $|\alpha| = \mu + 1$.

(1) Proof of (5-27) for $\alpha = \beta + k$ for $|\beta| = \mu$ and $k \in \{1, \dots, n\}$: We have

$$\partial^\alpha = \partial^{\beta+k} = \partial_k \partial^\beta, \quad \text{where } \partial_k = \frac{\partial}{\partial x_k}.$$

So

$$\|\varphi \partial^{\beta+k} u\| = \|\varphi \partial_k \partial^\beta u\| \le \|\partial_k(\varphi)\partial^\beta u\| + \|\partial_k \varphi \partial^\beta u\|. \tag{5-39}$$

So,

$$\|\varphi \partial^{\beta+k} u\| \le \|\varphi^{(k)} \partial^\beta u\| + \|\varphi \partial^\beta u\|_{p\sigma}, \quad \text{with } \varphi^{(k)} = \partial_k \varphi. \tag{5-40}$$

We see that is suffices to apply (5-27) (with α replaced by β) for the couple $(u, \varphi^{(k)})$ and (5-28) with $\ell = p$ for the couple (u, φ). Hence,

$$\|\varphi^{(k)} \partial^\beta u\| \le M_\epsilon^{2p|\beta|+1} (p|\beta|)!^s \mathcal{N}_\beta^\epsilon(u, \varphi^{(k)}). \tag{5-41}$$

So from (5-10), we get:

$$\|\varphi^{(k)} \partial^\beta u\| \le M_\epsilon^{2p|\beta|+1} \epsilon^{-1} (p|\beta| + 1)!^s \mathcal{N}_{\beta,1}^\epsilon(u, \varphi). \tag{5-42}$$

Now,

$$\begin{aligned} \|\varphi \partial^\beta u\|_{p\sigma} &\le M_\epsilon^{2p|\beta|+p+1} (p|\beta| + p)!^s N_{\beta,p}^\epsilon(u, \varphi) \\ &\le M_\epsilon^{2p(|\beta|+1)+1} M_\epsilon^{-p} (p(|\beta| + 1))!^s N_{\beta+k}^\epsilon(u, \varphi) \end{aligned} \tag{5-43}$$

The last line in (5-43) is true using $\mathcal{N}_{\beta,p}^\epsilon = \mathcal{N}_{\beta+k}^\epsilon$ (see (5-6)).

Then gathering (5-42) and (5-43), we get, using (5-6),

$$\|\varphi \partial^{\beta+k} u\| \le M_\epsilon^{2p(|\beta|+1)+1} (\epsilon^{-1} M_\epsilon^{-2p} + M_\epsilon^{-p}) (p(|\beta| + 1))!^s \mathcal{N}_{\beta+k}^\epsilon(u, \varphi). \tag{5-44}$$

Hence, finally, we obtain (5-27) for $\alpha = \beta + k$ if

$$(\epsilon^{-1} M_\epsilon^{-p} + 1) M_\epsilon^{-p} \le 1. \tag{5-45}$$

For that, it suffices to take the simple condition

$$(\epsilon M_\epsilon^p)^{-1} \le \tfrac{1}{2}, \tag{5-46}$$

as it is easy to see that $(\epsilon M_\epsilon^p)^{-1} \le \frac{1}{2}$ and $M_\epsilon^{-p} \le \frac{1}{2}$ $(\epsilon \le 1)$. So under the condition (5-46), the inequality (5-27) holds true for $|\alpha| = \mu + 1$.

(2) Proof of (5-28) for $|\alpha| = \mu + 1$: It will be the longest proof of our theorem. Let us stay a moment, saying that we proved (5-27) and (5-28) for $|\alpha| \le \mu$, $\ell = 1 = 1, \dots, p$ and also (5-27) for $|\alpha| = \mu + 1$, properties that we will use in the sequel.

As there is a difference between the localized estimate (4-1) and the localized estimate (4-2) for $\ell = 1, \dots, p-1$, we first prove (5-28) with $\ell = 1$, for all α satisfying $|\alpha| = \mu+1$. For that, we apply (4-1) in order to bound $\|\varphi\partial^\alpha u\|_\sigma$. Looking at the second member, we need:

(i) *A bound on* $E_1 = (\|\varphi\partial^\alpha Pu\|\|\varphi\partial^\alpha u\|)^{1/2}$. We have to bound two terms, using (5-27) with $|\alpha| = \mu+1$ respectively to the couple (Pu, φ) and (φ, u). So, using (5-10), we obtain

$$\begin{aligned}\|\varphi\partial^\alpha Pu\| &\le M_\epsilon^{2p|\alpha|+1}(p|\alpha|)!^s \mathcal{N}_\alpha^\epsilon(Pu,\varphi)\\ &\le \epsilon^{-2} M_\epsilon^{2p|\alpha|+1}(p|\alpha|+2)!^s \mathcal{N}_{\alpha,1}^\epsilon(u,\varphi).\end{aligned} \tag{5-47}$$

So we deduce

$$\|\varphi\partial^\alpha Pu\|\|\varphi\partial^\alpha u\| \le (M_\epsilon^{2p|\alpha|+1})^2\epsilon^{-2}(p|\alpha|+2)!^s(p|\alpha|)!^s\mathcal{N}_\alpha^\epsilon(u,\varphi)\mathcal{N}_{\alpha,1}^\epsilon(u,\varphi). \tag{5-48}$$

Then, using (5-6), we obtain

$$\begin{aligned}(\|\varphi\partial^\alpha Pu\|\|\varphi\partial^\alpha u\|)^{1/2} &\le \epsilon^{-1} M_\epsilon^{2p|\alpha|+1}((p|\alpha|+2)!(p|\alpha|)!)!^{s/2}\mathcal{N}_{\alpha,1}^\epsilon(u,\varphi)\\ &\le 2^{s/2}\epsilon^{-1}M_\epsilon^{2p|\alpha|+1}((p|\alpha|+1)!)!^s\mathcal{N}_{\alpha,1}^\epsilon(u,\varphi)\\ &\le 2^{s/2}\epsilon^{-1}M_\epsilon^{-1}\big(M_\epsilon^{2p|\alpha|+1+1}((p|\alpha|+1)!)!^s\mathcal{N}_{\alpha,1}^\epsilon(u,\varphi)\big)\end{aligned} \tag{5-49}$$

(ii) *A bound on* $E_2 = \sum_{|\beta_1|+|\beta_2|\le 2}(\|\varphi^{(\beta_1)}u\|\|\varphi^{(\beta_2)}u\|)^{1/2}$. Similarly, we get, using (5-10),

$$\begin{aligned}&(\|\varphi^{(\beta_1)}u\|\|\varphi^{(\beta_2)}u\|)^{1/2}\\ &\qquad\le \epsilon^{-1}M_\epsilon^{2p|\alpha|+1}((p|\alpha|+|\beta_1|)!(p|\alpha|+|\beta_2|)!)!^{s/2}\mathcal{N}_{\alpha,1}^\epsilon(u,\varphi)\\ &\qquad\le 2^{s/2}\,\epsilon^{-1}M_\epsilon^{-1}\big(M_\epsilon^{2p|\alpha|+1+1}((p|\alpha|+1)!)!^s\mathcal{N}_{\alpha,1}^\epsilon(u,\varphi)\big)\end{aligned} \tag{5-50}$$

(iii) *A bound on* $E_3 = \sum_{|\beta|\le 1}(\|\varphi^{(\beta)}[X,\partial^\alpha]u\|\|\varphi\partial^\alpha u\|)^{1/2}$. There are $m(n+1)$ terms in (iii) as X represents the vector fields $X_1, \dots, X_m$. So, let us bound any one of them. Moreover in (3-8), we delete the subscript "j" in the expression of $[X, \partial^\alpha]$: $\sum_{\gamma<\alpha,\,\ell=1,\dots,n} a_{\alpha\gamma\ell}\,\partial^{\gamma+\ell}$ and the estimates (3-9) and (3-10). So we have

$$\|\varphi^{(\beta)}[X,\partial^\alpha]u\| \le \sum_{\substack{\gamma<\alpha\\ \ell=1,\dots,n}} \|a_{\alpha\gamma\ell}\varphi^{(\beta)}\partial^{\gamma+\ell}u\|. \tag{5-51}$$

Hence, using the estimates in Proposition 3.3, we get, with $v = \varphi^{(\beta)}\partial^{\gamma+\ell}u$,

$$\|\varphi^{(\beta)}[X,\partial^\alpha]u\| \le \sum_{\substack{\gamma<\alpha\\ \ell=1,\dots,n}} B^{|\alpha-\gamma|}\Big(\frac{\alpha!}{\beta!}\Big)^s\|\varphi^{(\beta)}\partial^{\gamma+\ell}u\|,\quad |\beta|\le 1.$$

As $\gamma < \alpha$, $|\gamma + \ell| = |\gamma| + 1 \le |\alpha|$. So we have, using (5-27) for the multiindex $\gamma + \ell$,

$$\|\varphi^{(\beta)}[X, \partial^\alpha]u\| \le n \sum_{\gamma<\alpha} B^{|\alpha-\gamma|}\Big(\frac{\alpha!}{\gamma!}\Big)^s M_\epsilon^{2p(|\gamma|+1)+1}(p(|\gamma|+1))!^s \mathcal{N}^\epsilon_{|\gamma|+1}(u, \varphi^{(\beta)}). \tag{5-52}$$

Now, one has, easily,

$$\frac{\alpha!}{\gamma!}(p(|\gamma|+1))! \le (p|\alpha|+1)! \tag{5-53}$$

Hence (5-52) and (5-53) yield

$$\begin{aligned}\|\varphi^{(\beta)}[X, \partial^\alpha]u\| &\le n \sum_{\gamma<\alpha} B^{|\alpha-\gamma|} M_\epsilon^{2p(|\gamma|+1)+1}(p|\alpha|+1)!^s \mathcal{N}^\epsilon_{|\gamma|+1}(u, \varphi^{(\beta)}) \\ &\le n \sum_{\gamma<\alpha} B^{|\alpha\gamma|}\epsilon^{-1} M_\epsilon^{2p(|\gamma|+1)+1}\,(p|\alpha|+2)!^s \mathcal{N}^\epsilon_{\alpha,1}(u, \varphi).\end{aligned} \tag{5-54}$$

The last line is derived from (5-10) and the fact $|\gamma| + 1 \le |\alpha|$. Now we use the following

$$\sum_{\gamma<\alpha} B^{|\alpha-\gamma|} M_\epsilon^{2p(|\gamma|+1)+1} = B \sum_{\gamma<\alpha}\Big(\frac{B}{M_\epsilon^{2p}}\Big)^{|\alpha-\gamma|-1} M_\epsilon^{2p|\alpha|+1} \tag{5-55}$$

Let us recall now the following lemma we proved in [Derridj 2019a, Lemma 4.3].

Lemma 5.6. *There exists $\theta_0 > 0$, independent of α, such that*

$$\sum_{\gamma<\alpha} \lambda^{|\alpha-\gamma|-1} \le n+1, \quad \textit{if } 0 \le \lambda < \theta_0. \tag{5-56}$$

So, taking $B < \theta_0 M_\epsilon^{2p}$, we get from (5-54)–(5-56)

$$\|\varphi^{(\beta)}[X, \partial^\alpha]u\| \le n\epsilon^{-1} B(n+1) M_\epsilon^{2p|\alpha|+1}(p|\alpha|+2)!^s \mathcal{N}^\epsilon_{\alpha,1}(u, \varphi). \tag{5-57}$$

We rewrite the above condition we used to get (5-57) as follows:

$$M_\epsilon^{2p} > B\theta_0^{-1}. \tag{5-58}$$

Now we deduce from (5-57),

$$\begin{aligned}\sum_{|\beta|\le 1} (\|\varphi^{(\beta)}[X, \partial^\alpha]u\|\,\|\varphi\partial^\alpha u\|)^{1/2} \\ \le (n+1)\big\{n\epsilon^{-1} B(n+1) M_\epsilon^{2p|\alpha|+1}(p|\alpha|+2)!^s \mathcal{N}^\epsilon_{\alpha,1}(u, \varphi)\big\}^{1/2} \\ \cdot \big\{M_\epsilon^{2p|\alpha|+1}(p|\alpha|)!^s \mathcal{N}^\epsilon_{\alpha}(u, \varphi)\big\}^{1/2}.\end{aligned} \tag{5-59}$$

Using again properties in (5-6) and (5-10) we get

$$\begin{aligned} E_3 &\le (n+1)(n(n+1)\epsilon^{-1}B)^{1/2} M^{2p|\alpha|+1} (p|\alpha|)!^s\, (p|\alpha|+2)!^s \mathcal{N}^{\epsilon}_{\alpha,1}(u,\varphi) \\ &\le (n+1)(n(n+1)\epsilon^{-1}B)^{1/2} 2^{s/2} M^{2p|\alpha|+1} (p|\alpha|+1)!^s \mathcal{N}^{\epsilon}_{\alpha,1}(u,\varphi). \end{aligned}$$

Now taking into account that X stands for all X_j's, $j=1,\dots,m$ and Y, we finally get

$$\sum_{j=1}^{m} \sum_{|\beta|\le 1} \big(\|\varphi^{(\beta)}[X_j,\partial^\alpha]u\|\,\|\varphi\partial^\alpha u\|\big)^{1/2} \le (*), \tag{5-60}$$

where $(*) = m(n+1)(2^s n(n+1)\epsilon^{-1}B)^{1/2} M_\epsilon^{-1} \cdot M^{2p|\alpha|+1+1}(p|\alpha|+1)!^s \mathcal{N}^{\epsilon}_{\alpha,1}(u,\varphi),$

and $\|\varphi[Y+b,\partial^\alpha]u\|\,\|\varphi\partial^\alpha u\|^{1/2} \le (*)$.

(iv) *A bound on* $E_4 = (\|\varphi[X[X,\partial^\alpha]]u\|\,\|\varphi\partial^\alpha u\|)^{1/2}$. It will be done as for (iii), the only difference being in the expression

$$[X,[X,\partial^\alpha]] = \sum_{\substack{\gamma<\alpha \\ k=1,\dots,n}} d_{k\alpha\gamma}\partial^{\gamma+k} + \sum_{\substack{\gamma<\alpha \\ \ell,k=1,\dots,n}} c_{\ell k\alpha\gamma}\partial^{\gamma+\ell+k}, \tag{5-61}$$

with estimates given in Proposition 3.3.

As in (iii) we have

$$\begin{aligned} &\|\varphi[X,[X,\partial^\alpha]]u\| \\ &\le \sum_{\gamma<\alpha} nB^{|\alpha-\gamma|}\Big((|\alpha|+1)\frac{\alpha!}{\gamma!}\Big)^s M_\epsilon^{2p(|\gamma|+1)+1}(p(|\gamma|+1))!^s \mathcal{N}^{\epsilon}_{|\gamma|+1}(u,\varphi) \\ &\quad + n\sum_{\substack{\gamma<\alpha,\ |\gamma|\le|\alpha|-2 \\ k=1,\dots,n}} B^{|\alpha-\gamma|}\Big(\frac{(\alpha+k)!}{(\gamma+k)!}\Big)^s M_\epsilon^{2p(|\gamma|+2)+1}(p(|\gamma|+2))!^s \mathcal{N}^{\epsilon}_{|\gamma|+2}(u,\varphi). \end{aligned} \tag{5-62}$$

All we have now to use are the following ingredients:

$$\begin{aligned} &(|\alpha|+1)\frac{\alpha!}{\gamma!}(p(|\gamma|+1))! \le (p(|\alpha|+2))!, \quad \text{when } |\gamma|+1\le|\alpha|. \\ &\frac{(\alpha+k)!}{(\gamma+k)!}(p(|\gamma|+2))! \le (p(|\alpha|+2))!, \quad \text{when } |\gamma|+2\le|\alpha|. \end{aligned} \tag{5-63}$$

and under condition (5-58)

$$\begin{aligned} &\sum_{\gamma<\alpha} B^{|\alpha-\gamma|} M_\epsilon^{2p(|\gamma|+1)+1} = B\sum_{\gamma<\alpha}\Big(\frac{B}{M_\epsilon^{2p}}\Big)^{|\alpha-\gamma|-1} M_\epsilon^{2p|\alpha|+1} \le (n+1)BM_\epsilon^{2p|\alpha|+1}, \\ &\sum_{\substack{\gamma<\alpha \\ |\gamma|\le|\alpha|-2}} B^{|\alpha-\gamma|} M^{2p(|\gamma|+2)+1} \le B^2\Big(\frac{B}{M^{2p}}\Big)^{|\alpha-\gamma|-2} M_\epsilon^{2p|\alpha|+1} \le (n^2+1)B^2 M_\epsilon^{2p|\alpha|+1}. \end{aligned} \tag{5-64}$$

The second line (5-64) follows from Lemma 5.6 with

$$\sum_{\substack{\gamma<\alpha\\|\gamma|\le|\alpha|-2}} \lambda^{|\alpha-\gamma|} \le n^2+1.$$

So from (5-62)-(5-64), we obtain

$$(5\text{-}65)\quad (\|\varphi[X,[X,\partial^\alpha]]u\|\|\varphi\partial^\alpha u\|)^{1/2} \le \big((n(n+1)B+n^2(n^2+1)B^2)(p|\alpha|+2)!^s\big)^{1/2} \cdot (M_\epsilon^{2p|\alpha|+1})^{1/2}(M_\epsilon^{2p|\alpha|+1}(p|\alpha|)!^s)^{1/2}\mathcal{N}_\alpha^\epsilon(u,\varphi).$$

as $\mathcal{N}^\epsilon_{|\gamma|+1}(u,\varphi)\le\mathcal{N}^\epsilon_\alpha(u,\varphi)$, $|\gamma|+1\le|\alpha|$, $\mathcal{N}^\epsilon_{|\gamma|+2}(u,\varphi)\le\mathcal{N}^\epsilon_\alpha(u,\varphi)$, $|\gamma|+2\le|\alpha|$.
Then finally we get

$$(\|\varphi[X,[X,\partial^\alpha]]u\|\|\varphi\partial^\alpha u\|)^{1/2}\le 2^s n(n+1)BM_\epsilon^{-1}\cdot M_\epsilon^{2p|\alpha|+1+1}(p|\alpha|+1)!^s\mathcal{N}_\alpha^\epsilon(u,\varphi).$$

Now, collecting the bounds obtained in (i)–(iv), we obtain

$$(5\text{-}66)\quad \|\varphi\partial^\alpha u\|_\sigma \le \big\{2^{s/2+1}\epsilon^{-1}+2^{s/2}mn(n+1)^2(\epsilon^{-1}B)^{1/2}+2^s n(n+1)B\big\} \cdot CM_\epsilon^{-1}\cdot M_\epsilon^{2p|\alpha|+1+1}(p|\alpha|+1)!^s\mathcal{N}^\epsilon_{\alpha,1}(u,\varphi),$$

under the condition (5-58), and C given in (4-1). Now we rewrite in a simpler manner

$$(5\text{-}67)\quad \|\varphi\partial^\alpha u\|_\sigma \le A(s,\epsilon,\Omega_0,P)CM_\epsilon^{-1}\cdot M_\epsilon^{2p|\alpha|+1+1}(p|\alpha|+1)!^s\mathcal{N}^\epsilon_{\alpha,1}(u,\varphi).$$

So we see that (5-28) for $\ell=1$ is true under the condition

$$(5\text{-}68)\qquad M_\epsilon\ge\sup\big\{CA(s,\epsilon,\Omega_0,P),(B\theta_0^{-1})^{1/(2p)}\big\},$$

in view of (5-58), (5-67).

So, our work now will be the proof of (5-28) for $|\alpha|=\mu+1$, $\ell=1,\dots,p$. For that, we assume that (5-28) is true for $|\alpha|=\mu+1$, $1\le\ell\le i$, $i\in\{1,\dots,p-1\}$; we want to prove (5-28) for $\ell=i+1$. Here the proof will be simpler than the preceding, as when using the localized estimate (4-2) with $\ell\in\{1,\dots,p-1\}$, one has no square root of products of norms. Moreover, some estimates are quite done in the preceding proof of (5-28) for $\ell=1$. We first use (4-2) for $\ell=i$ then looking at the second member of (4-2) with $\ell=i$, we have, as in the preceding, to bound terms, which are, here, simpler as they are norms of some functions in some Sobolev spaces, in place of square roots of products. Let us list them.

(i) *A bound on* $\|\varphi\partial^\alpha Pu\|_{(i-1)\sigma}$. The bound is, simply, given by applying (5-28) with $\ell=i-1$ to the couple (Pu,φ). So

$$(5\text{-}69)\qquad \|\varphi\partial^\alpha Pu\|_{(i-1)\sigma}\le M_\epsilon^{2p|\alpha|+i}(p|\alpha|+i-1)!^s\mathcal{N}^\epsilon_{\alpha,i-1}(Pu,\varphi).$$

Then using (5-10), we get, as $i-1+2=i+1\le p$,

$$\begin{aligned}(5\text{-}70)\quad \|\varphi\partial^\alpha Pu\|_{(i-1)\sigma} &\le \epsilon^{-2}M^{2p|\alpha|+i}(p|\alpha|+i+1)!^s\mathcal{N}^\epsilon_{\alpha,i+1}(u,\varphi)\\ &\le \epsilon^{-2}M_\epsilon^{-2}M_\epsilon^{2p|\alpha|+i+1+1}(p|\alpha|+i+1)!^s\mathcal{N}^\epsilon_{\alpha,i+1}(u,\varphi).\end{aligned}$$

(ii) *A bound on* $\sum_{|\beta|\le 1}\|\varphi^{(\beta)}\partial^\alpha u\|_{i\sigma}$. Similarly, we have by applying (5-28) for $\ell=i$ to $(u,\varphi^{(\beta)})$,

$$(5\text{-}71)\qquad \|\varphi^{(\beta)}\partial^\alpha u\|_{i\sigma}\le M_\epsilon^{2p|\alpha|+i+1}\,(p|\alpha|+i)!^s\mathcal{N}^\epsilon_{\alpha,i}(u,\varphi^{(\beta)}).$$

Then using (5-10), one has, as $i+|\beta|\le i+1\le p$,

$$(5\text{-}72)\quad \sum_{|\beta|\le 1}\|\varphi^{(\beta)}\partial^\alpha u\|_{i\sigma}\le (n+1)\epsilon^{-1}M_\epsilon^{-1}M_\epsilon^{2p|\alpha|+i+1+1}(p|\alpha|+i+1)!^s\mathcal{N}^\epsilon_{\alpha,i+1}(u,\varphi).$$

(iii) *A bound on* $\sum_{|\beta|=2}\|\varphi^{(\beta)}\partial^\alpha u\|_{(i-1)\sigma}$. We use exactly the same way, getting successively:

$$(5\text{-}73)\quad \|\varphi^{(\beta)}\partial^\alpha u\|_{(i-1)\sigma}\le M_\epsilon^{2p|\alpha|+i}(p|\alpha|+i-1)!^s\mathcal{N}^\epsilon_{\alpha,i-1}(u,\varphi^{(\beta)}),\qquad \text{as } i-1+|\beta|\le i+1,$$

$$(5\text{-}74)\quad \sum_{|\beta|=2}\|\varphi^{(\beta)}\partial^\alpha u\|_{(i-1)\sigma}\le n^2\epsilon^{-2}M_\epsilon^{-2}M_\epsilon^{2p|\alpha|+i+1+1}(p|\alpha|+i+1)!^s\mathcal{N}^\epsilon_{\alpha,i+1}(u,\varphi).$$

(iv) *A bound on*

$$\sum_{\substack{|\beta|\le 1\\ j=1,\dots,m}}\|\varphi^{(\beta)}[X_j,\partial^\alpha]u\|_{(i-1)\sigma}\quad\text{and}\quad \|\varphi[Y+b,\partial^\alpha]u\|_{(i-1)\sigma}.$$

We have just to consider $\|\varphi^{(\beta)}[X,\partial^\alpha]u\|_{(i-1)\sigma}$, $|\beta|\le 1$. So:

$$(5\text{-}75)\quad \|\varphi^{(\beta)}[X,\partial^\alpha]u\|_{(i-1)\sigma}\le \sum_{\substack{\gamma<\alpha\\ \ell=1,\dots,m}}B^{|\alpha-\gamma|}\Big(\frac{\alpha!}{\gamma!}\Big)^s\|\varphi^{(\beta)}\partial^{\gamma+\ell}u\|_{(i-1)\sigma}\quad\text{(see (3-8)).}$$

So applying (5-28) with $\ell=i-1$ and $\alpha=\gamma+\ell$ ((5-27) with $\alpha=\gamma+\ell$ when $i=1$) to $(u,\varphi^{(\beta)})$:

$$(5\text{-}76)\quad \|\varphi^{(\beta)}[X,\partial^\alpha]u\|_{(i-1)\sigma}\le \sum_{\substack{\gamma<\alpha\\ \ell=1,\dots,n}}B^{|\alpha-\gamma|}\Big(\frac{\alpha!}{\gamma!}\Big)^s M_\epsilon^{2p(|\gamma|+1)+i}\cdot(p(|\gamma|+1)+i-1)!^s\mathcal{N}^\epsilon_{\gamma+\ell,i-1}(u,\varphi^{(\beta)}),\qquad |\beta|\le 1.$$

Then using

$$(5\text{-}77)\qquad \frac{\alpha!}{\gamma!}(p(|\gamma|+1)+i-1)!\le (p|\alpha|+i)!,$$

(5-76) gives, with $|\beta|\le 1$,

$$\begin{aligned}
(5\text{-}78)\quad & \|\varphi^{(\beta)}[X,\partial^\alpha]u\|_{(i-1)\sigma}\\
&\le n\sum_{\gamma<\alpha} B^{|\alpha-\gamma|}M_\epsilon^{2p(|\gamma|+1)+i}(p|\alpha|+i)!^s\mathcal{N}^\epsilon_{\gamma+\ell,i-1}(u,\varphi^{(\beta)})\\
&\le n\sum_{\gamma<\alpha}\epsilon^{-1}B^{|\alpha-\gamma|}M_\epsilon^{2p(|\gamma|+1)+i}(p|\alpha|+i+1)!^s\mathcal{N}^\epsilon_{\gamma+\ell,i}(u,\varphi), && (5\text{-}10)\\
&\le n\sum_{\gamma<\alpha} B\Big(\frac{B}{M_\epsilon^{2p}}\Big)^{|\alpha-\gamma|-1}\epsilon^{-1}M_\epsilon^{2p|\alpha|+i}(p|\alpha|+i+1)!^s\mathcal{N}^\epsilon_{\alpha,i}(u,\varphi) && (5\text{-}6)\\
&\le n(n+1)\epsilon^{-1}BM_\epsilon^{-2}M_\epsilon^{2p|\alpha|+i+1+1}(p|\alpha|+i+1)!^s\mathcal{N}^\epsilon_{\alpha,i+1}(u,\varphi) && (5\text{-}6)
\end{aligned}$$

Hence

$$\begin{aligned}
(5\text{-}79)\quad & \sum_{|\beta|=1}\|\varphi^{(\beta)}[X,\partial^\alpha]u\|_{(i-1)\sigma}\\
&\qquad\le (n+1)^3\epsilon^{-1}BM_\epsilon^{-2}M_\epsilon^{2p|\alpha|+i+1+1}(p|\alpha|+i+1)!^s\mathcal{N}^\epsilon_{\alpha,i+1}(u,\varphi)
\end{aligned}$$

Of course the term $\|\varphi[Y+b,\partial^\alpha]u\|$ is easier to handle.

(v) *A bound on* $\sum_{j=1}^m\|\varphi[X_j,[X_j,\partial^\alpha]]u\|_{(i-1)\sigma}$. As in (5-62) where i corresponds to 1, we get

$$\begin{aligned}
(5\text{-}80)\quad & \|\varphi[X,[X,\partial^\alpha]]u\|_{(i-1)\sigma}\\
&\le\sum_{\gamma<\alpha} nB^{|\alpha-\beta|}\Big((|\alpha|+1)\frac{\alpha!}{\beta!}\Big)^s M_\epsilon^{2p(|\gamma|+1)+i}(p(|\gamma|+1)+i-1)!^s\mathcal{N}^\epsilon_{|\gamma|+1,i-1}(u,\varphi)\\
&\qquad+n\sum_{\substack{\gamma<\alpha,\,|\gamma|\le|\alpha|-2\\ k=1,\dots,n}} B^{|\alpha-\gamma|}\Big(\frac{(\alpha+k)!}{(\gamma+k)!}\Big)^s M_\epsilon^{2p(|\gamma|+2)+i}(p(|\gamma|+2)+i-1)!^s\\
&\hspace{10cm}\cdot\mathcal{N}^\epsilon_{|\gamma|+2,i-1}(u,\varphi).
\end{aligned}$$

Here, ingredients replacing (5-63) and (5-64) are

$$(5\text{-}81)\quad \begin{aligned}
&(|\alpha|+1)\frac{\alpha!}{\gamma!}(p(|\gamma|+1)+i-1)!\le(p|\alpha|+i-1)!, &&|\gamma|+1\le|\alpha|,\\
&\frac{(\alpha+k)!}{(\gamma+k)!}(p(|\gamma|+2)+i-1)!\le(p|\alpha|+i-1)!, &&|\gamma|+2\le|\alpha|.
\end{aligned}$$

Hence, under condition (5-58), we get

$$\begin{aligned}
(5\text{-}82)\quad \sum_{\gamma<\alpha}B^{|\alpha-\gamma|}M_\epsilon^{2p(|\gamma|+1)+i} &= B\sum_{\gamma<\alpha}\Big(\frac{B}{M_\epsilon^{2p}}\Big)^{|\alpha-\gamma|-1}M_\epsilon^{2p|\alpha|+i}\\
&\le(n+1)BM_\epsilon^{2p|\alpha|+i}.
\end{aligned}$$

And, again under condition (5-58), we have

$$\text{(5-83)}\qquad \sum_{\substack{\gamma<\alpha\\ |\gamma|\le|\alpha|-2}} B^{|\alpha-\gamma|} M_\epsilon^{2p(|\gamma|+2)+i} = B^2 \sum_{\substack{\gamma<\alpha\\ |\gamma|\le|\alpha|-2}} \left(\frac{B}{M_\epsilon^{2p}}\right)^{|\alpha-\beta|-2} M_\epsilon^{2p|\alpha|+i} \le (n^2+1) B^2 M_\epsilon^{2p|\alpha|+i}.$$

From (5-80)–(5-83), we deduce

$$\text{(5-84)}\qquad \|\varphi[X,[X,\partial^\alpha]]u\|_{(i-1)\sigma} \le \bigl(n(n+1)BM_\epsilon^{-2} + n(n^2+1)B^2M_\epsilon^{-2}\bigr) \cdot M_\epsilon^{2p|\alpha|+i+1+1}(p|\alpha|+i+1)!^s \mathcal{N}^\epsilon_{\alpha,i+1}(u,\varphi),$$

under condition (5-58). Now we collect all bounds in (i)–(v) to obtain

$$\text{(5-85)}\qquad \begin{aligned} &\|\varphi\partial^\alpha u\|_{(i+1)\sigma} \\ &\le C\Bigl\{\epsilon^{-2}M_\epsilon^{-2} + (n+1)\epsilon^{-1}M_\epsilon^{-1} + n^2\epsilon^{-2}M_\epsilon^{-2} + (n+1)^3\epsilon^{-1} \\ &\qquad BM_\epsilon^{-2}(m+1) + (m+1)(n+1)^3B^2M_\epsilon^{-2}\Bigr\} \\ &\qquad \cdot M_\epsilon^{2p|\alpha|+i+1+1}(p|\alpha|+i+1)!^s\mathcal{N}^\epsilon_{\alpha,i+1}(u,\varphi) \end{aligned}$$

So we see that in order to have (5-28) for $\ell = i+1$, we need that the factor of $M^{2p|\alpha|+i+2}(p|\alpha|+i+1)!^s\mathcal{N}^\epsilon_{\alpha,i+1}(u,\varphi)$ in (5-85) be less than 1. As $M_\epsilon \ge 1$, $\epsilon \le 1$, so $M_\epsilon^{-2} \le M_\epsilon^{-1}$, it suffices that

$$\text{(5-86)}\qquad CM_\epsilon^{-1}\cdot\bigl\{\epsilon^{-2}(n+2+(m+1)(n+1)^3B) + n^2 + (m+1)(n+1)^3B^2\bigr\} \le 1.$$

So, denoting by $D(\epsilon, B)$ the factor of M_ϵ^{-1} in (5-86):

$$\text{(5-87)}\qquad \begin{aligned} M_\epsilon &\ge D(\epsilon,B), \quad D(\epsilon,B) = D(\epsilon,\Omega_0,P), \\ M_\epsilon &\ge (B\theta_0^{-1})^{1/(2p)} \quad \text{(which is condition (5-58)).} \end{aligned}$$

Now summarizing all conditions needed along our proof of the theorem, we have:

$$\text{(5-88)}\qquad \begin{aligned} &M_\epsilon \ge 1, \quad \text{for validity of (5-27),} \\ &M_\epsilon \ge (C\epsilon^{-1})^{1/2}, \quad \text{for validity of (5-28), } \ell = 1, \\ &M_\epsilon \ge (2(1+n^2)\epsilon^{-1})^{p-1}, \quad \text{giving condition (5-38), } i = 1,\dots,p-1, \\ &M_\epsilon \ge (2\epsilon^{-1})^{1/p}, \quad \text{which is condition (5-46),} \\ &M_\epsilon \ge (B\theta_0^{-1})^{1/(2p)}, \quad \text{which is condition (5-58),} \\ &M_\epsilon \ge \sup\{CA(s,\epsilon,\Omega_0,P), (B\theta_0^{-1})^{1/(2p)}\}, \quad \text{which is (5-68),} \\ &M_\epsilon \ge D(\epsilon,\Omega_0,P), \quad \text{given in (5-87).} \end{aligned}$$

Then, denoting by $M(\epsilon, s, \Omega_0, P)$ the maximum of all numbers in the list above, any $M_\epsilon \geq M(\epsilon, s, \Omega_0, P)$ satisfies the estimates (5-27) and (5-28) for $\alpha \in \mathbb{N}^n$ and $\ell = 1, \dots, p$ and $(u, \varphi) \in C^\infty(\Omega) \times \mathcal{D}(\Omega)$; so our theorem is completely proved. □

6. Application to Gevrey regularity of analytic (Gevrey) vectors

Before applying Theorem 5.5 to Hörmander's operators of first kind, we want to state a theorem for more general operators of order m satisfying localized estimates that are similar to (5-5) but with a modified definition of $\mathcal{N}^\epsilon_\alpha$, due to the order m of the differential operator still denoted by P, on the open set Ω. The modifications are done in the following, where $(u, \varphi) \in C^\infty(\Omega_0) \times \mathcal{D}(\Omega_0)$:

$$\text{For } j \in \mathbb{N},\ \gamma \in \mathbb{N}^n,\ \epsilon \in [0, 1], \quad N^\epsilon_{j,\gamma}(u, \varphi) = \epsilon^{|\gamma|+mj} |\gamma|!^{-s} (mj)!^{-s} \|\varphi^\gamma P^j u\|,$$

$$\text{For } \alpha \in \mathbb{N}^n, \quad \mathcal{N}^\epsilon_\alpha(u, \varphi) = \left\{ \sum_{(j,\gamma)\in \mathcal{I}_{|\alpha|}} \prod_{\rho=1}^{2^{|\alpha|}} N^\epsilon_{j_\rho,\gamma_\rho}(u, \varphi) \right\}^{2^{-|\alpha|}}, \tag{6-1}$$

where $\mathcal{I}_{|\alpha|} = (j, \gamma),\ j = (j_1, \dots, j_{2^{|\alpha|}}),\ \gamma = (\gamma, \dots, \gamma_{2^{|\alpha|}})$ satisfying

$$|\gamma| + mj \leq 2^{|\alpha|} p|\alpha|,\ |\gamma_\rho| \leq q|\alpha|,\ \text{for } (p, q) \text{ given in } \mathbb{N}^2.$$

So we define property $(\mathcal{P}_s)$ for the operator P by:

$$\begin{gathered}\text{For every } \epsilon \in [0, 1],\ \text{there exists } M_\epsilon, \text{ such that,}\\ \text{for } \alpha \in \mathbb{N}^n,\ (u, \varphi) \in C^\infty(\Omega_0) \times \mathcal{D}(\Omega_0),\\ \|\varphi \partial^\alpha u\| \leq M_\epsilon^{|\alpha|+1} (p|\alpha|)!^s \mathcal{N}^\epsilon_\alpha(u, \varphi).\end{gathered} \tag{$\mathcal{P}_s$}$$

Theorem 6.1. *Assume that P satisfies $(\mathcal{P}_s)$, for some $s \geq 1$. Then every analytic* (case $s = 1$) *or s-Gevrey vector of P in Ω_0, is in $G^{ps}(\Omega_0)$.*

Proof. We distinguish between the cases $s > 1$ and $s = 1$. The case $s > 1$ is simpler as there exist elements in $G^s(\Omega_0)$ with compact support. More precisely, let u be a s-Gevrey vector.

(1) Case $s > 1$. In order to prove that u is in $G^{ps}(\Omega_0)$, we take any relatively compact open set Ω_1 in Ω_0 (i.e., $\Omega_1 \Subset \Omega_0$) and want to find a constant $D = D(\Omega_1)$ (depending on Ω_1) such that, for every $\alpha \in \mathbb{N}^n$,

$$\|\partial^\alpha u\|_{L^2(\Omega_1)} \leq D^{|\alpha|+1} (p|\alpha|)!^s. \tag{6-2}$$

For that, we pick a function $\varphi \in G^s(\Omega_0) \cap \mathcal{D}(\Omega_0),\ \Omega_0 \Subset \Omega_1,\ \varphi = 1$ on Ω_1. So, there exists $B > 0$ such that

$$|\varphi^{(\beta)}| \leq B^{|\beta|+1} |\beta|!^s, \quad \beta \in \mathbb{N}^n. \tag{6-3}$$

Moreover as u is an s-Gevrey vector of P in Ω_0 ($u \in G^s(P, \Omega_0)$), we have, enlarging B if necessary,

$$\|P^j u\|_{L^2(\Omega_1)} \le B^{mj+1}(mj)!^s, \quad j \in \mathbb{N}. \tag{6-4}$$

So

$$\|\varphi^{(\beta)} P^j u\| \le B^2 B^{|\beta|+mj} |\beta|!^s (mj)!^s, \quad \beta \in \mathbb{N}^n, \ j \in \mathbb{N}. \tag{6-5}$$

Hence

$$N^{\epsilon}_{j,\gamma}(u,\varphi) \le \widetilde{B}(\epsilon\widetilde{B})^{|\gamma|+m|j|}, \quad \widetilde{B} = B^2. \tag{6-6}$$

Therefore

$$\begin{aligned} \mathcal{N}^{\epsilon}_{\alpha}(u,\varphi) &\le \Bigg[\sum_{(j,\gamma)\in\mathcal{I}_{|\alpha|}} \prod_{\rho=1}^{2^{|\alpha|}} \widetilde{B}(\epsilon\widetilde{B})^{|\gamma_\rho|+mj_\rho}\Bigg]^{2^{-|\alpha|}} \\ &\le \widetilde{B}\Bigg[\sum_{|\gamma|+m|j|\le 2^{|\alpha|}p|\alpha|} (\epsilon\widetilde{B})^{|\gamma|+m|j|}\Bigg]^{2^{-|\alpha|}}. \end{aligned} \tag{6-7}$$

Now choose ϵ_0 such that

$$\epsilon_0\widetilde{B} = \tfrac{1}{2} \Leftrightarrow \epsilon_0 = (2\widetilde{B})^{-1}, \tag{6-8}$$

we get

$$\begin{aligned} \mathcal{N}^{\epsilon_0}_{\alpha}(u,\varphi) &\le \widetilde{B}\Bigg\{\sum_{\substack{|\gamma|\le 2^{|\alpha|}p|\alpha| \\ m|j|\le 2^{|\alpha|}p|\alpha|}} \big(\tfrac{1}{2}\big)^{|\gamma|}\big(\tfrac{1}{2}\big)^{m|j|}\Bigg\}^{2^{-|\alpha|}} \\ &\le \widetilde{B}\Bigg\{\sum_{|\gamma|\le 2^{|\alpha|}p|\alpha|} \big(\tfrac{1}{2}\big)^{|\gamma|} \sum_{m|j|\le 2^{|\alpha|}p|\alpha|} \big(\tfrac{1}{2}\big)^{m|j|}\Bigg\}^{2^{-|\alpha|}}. \end{aligned} \tag{6-9}$$

Now in the two sums, $\gamma \in \mathbb{N}^{n2^{|\alpha|}}$ and $j \in \mathbb{N}^{2^{|\alpha|}}$. So

$$\begin{aligned} \sum_{|\gamma|\le 2^{|\alpha|}p|\alpha|} \big(\tfrac{1}{2}\big)^{|\gamma|} = \sum_{k=0}^{2^{|\alpha|}p|\alpha|}\Big(\sum_{|\gamma|=k} 1\Big)\big(\tfrac{1}{2}\big)^k &\le \sum_{k=0}^{2^{|\alpha|}p|\alpha|} (k+1)^{n2^{|\alpha|}}\big(\tfrac{1}{2}\big)^k \\ &\le (2^{|\alpha}|p|\alpha|+1)^{n2^{|\alpha|}} \sum_{k=0}^{\infty}\big(\tfrac{1}{2}\big)^k \\ &\le 2(2^{|\alpha|}p|\alpha|+1)^{n2^{|\alpha|}}, \end{aligned} \tag{6-10}$$

$$\sum_{m|j|\le 2^{|\alpha|}p|\alpha|} \big(\tfrac{1}{2}\big)^{m|j|} \le (2^{|\alpha|}p|\alpha|+1)^{2^{|\alpha|}} \sum_{k=0}^{\infty}\big(\tfrac{1}{2}\big)^k \le 2(2^{|\alpha|}p|\alpha|+1)^{2^{|\alpha|}}.$$

Hence (6-9) and (6-10) imply

$$\text{(6-11)}\quad \mathcal{N}_\alpha^{\epsilon_0}(u,\varphi) \le \widetilde{B}2(2^{|\alpha|}p|\alpha|+1)^n\cdot 2(2^{|\alpha|}p|\alpha|+1) \le 4\widetilde{B}(2^{|\alpha|}p|\alpha|+1)^{n+1} \le A^{|\alpha|+1},$$

for some A. Now using property $(\mathcal{P}_s)$, we get

$$\text{(6-12)}\quad \|\partial^\alpha u\|_{L^2(\Omega_1)} \le \|\varphi\partial^\alpha u\| \le A^{|\alpha|+1}M_{\epsilon_0}^{|\alpha|+1}(p|\alpha|)!^s = (AM_{\epsilon_0})^{|\alpha|+1}(p|\alpha|)!^s.$$

This ends the proof in case $s>1$, as Ω_1 is any relatively compact open set in Ω_0.

(2) Case $s=1$. Now, let u be an analytic vector of P in Ω_0, and let Ω_1, Ω_2 with $\Omega_1 \Subset \Omega_2 \subset \overline{\Omega}_2 \subset \Omega_0$. As, now, we can not consider an analytic function with compact support, we supply by an Ehrenpreis sequence associated to the couple (Ω_1,Ω_2) (we used such a sequence in our preceding work concerning general Hörmander's operators, but with a less precise result [Derridj 2019a, Proposition 5.1]). Let us recall the proposition of L. Ehrenpreis [1960], giving the precise details regarding this sequence:

Proposition 6.2. *Let* (Ω_1,Ω_2) *be as above. Then there exists a constant* $\widetilde{C}>0$ *such that*

$$\text{(6-13)}\quad \textit{for all } N\in\mathbb{N},\ \textit{there exists } \varphi_N\in\mathcal{D}(\Omega_2),\ \varphi_N|_{\Omega_1}=1,\ \textit{such that}\quad |\varphi_N^{(\beta)}| \le \widetilde{C}^{|\beta|+1}N^{|\beta|},\quad \textit{for } |\beta|\le N.$$

In our proof below, in order to bound $\|\partial^\alpha u\|_{L^2(\Omega_1)}$, we use, in place of φ used in case (1), the function $\varphi_{q|\alpha|}$, where q is given in the definition of $\mathcal{I}_{|\alpha|}$ in (6-1) :

$$\text{(6-14)}\qquad \|\partial^\alpha u\|_{L^2(\Omega_1)} \le \|\varphi_{q|\alpha|}\partial^\alpha u\| \le M_\epsilon^{|\alpha|+1}(p|\alpha|)!^s\ \mathcal{N}_\alpha^\epsilon(u,\varphi_{q|\alpha|}).$$

In view of the definition of $\mathcal{N}_\alpha^\epsilon(u,\varphi_{q|\alpha|})$, we have

$$\text{(6-15)}\quad (\mathcal{N}_\alpha^\epsilon(u,\varphi_{q|\alpha|}))^{2^{|\alpha|}} \le \sum_{m|j|\le 2^{|\alpha|}p|\alpha|} \widetilde{B}^{2^{|\alpha|}}(\epsilon\widetilde{B})^{m|j|} \sum_{\substack{|\gamma_\rho|\le q|\alpha| \\ |\gamma|\le 2^{|\alpha|}p|\alpha|}} \prod_{\rho=1}^{2^{|\alpha|}} \widetilde{C}(\epsilon\widetilde{C})^{|\gamma_\rho|}(q|\alpha|)^{|\gamma_\rho|}\,|\gamma_\rho|!^{-1}$$
$$\le (\widetilde{B}\widetilde{C})^{2^{|\alpha|}} \sum_{m|j|\le 2^{|\alpha|}p|\alpha|} (2\widetilde{B})^{m|j|} \sum_{\substack{|\gamma|\le 2^{|\alpha|}p|\alpha| \\ |\gamma_\rho|\le q|\alpha|}} \prod_{\rho=1}^{2^{|\alpha|}} (\epsilon\widetilde{C}q|\alpha|)^{|\gamma_\rho|}|\gamma_\rho|!^{-1},$$

where $\widetilde{B}$ is given by (6-6). Choosing ϵ_0 such that

$$\text{(6-16)}\qquad \epsilon_0\widetilde{B} \le \tfrac{1}{2},$$

we have

(6-17)
$$(\mathcal{N}_\alpha^{\epsilon_0}(u,\varphi_{q|\alpha|}))^{2^{|\alpha|}} \le (\widetilde{B}\widetilde{C})^{2^{|\alpha|}} 2(2^{|\alpha|}p|\alpha|+1)^{2^{|\alpha|}} \cdot \sum_{|\gamma|\le 2^{|\alpha|}p|\alpha|} \prod_{\rho=1}^{2^{|\alpha|}} (\epsilon_0\widetilde{C}q|\alpha|)^{|\gamma_\rho|}|\gamma_\rho|!^{-1}.$$

So from Lemma 5.4 with $\widetilde{D}=2\widetilde{B}\widetilde{C}$,

(6-18)
$$\begin{aligned}(\mathcal{N}_\alpha^{\epsilon_0}(u,\varphi_{q|\alpha|}))^{2^{|\alpha|}} &\le \widetilde{D}^{2^{|\alpha|}}(2^{\alpha|}p|\alpha|+1)^{2^{|\alpha|}} \cdot \sum_{|\gamma|\le 2^{|\alpha|}p|\alpha|} \Big(\frac{1}{2^{|\alpha|}}\sum_{\rho=1}^{2^{|\alpha|}}(\epsilon_0\widetilde{C}q|\alpha|)^{|\gamma_\rho|}|\gamma_\rho|!^{-1}\Big)^{2^{|\alpha|}} \\ &\le \widetilde{D}^{2^{|\alpha|}}(2^{|\alpha|}p|\alpha|+1)^{2^{|\alpha|}} \cdot \sum_{|\gamma|\le 2^{|\alpha|}p|\alpha|} \Big(\frac{1}{2^{|\alpha|}}\exp(\epsilon_0\widetilde{C}q|\alpha|)\Big)^{2^{|\alpha|}}.\end{aligned}$$

Hence with $\epsilon_0\widetilde{C}q|\alpha| \le (2\widetilde{B})^{-1}\widetilde{C}q|\alpha| = \widetilde{A}|\alpha|$, we get

(6-19)
$$\begin{aligned}\mathcal{N}_\alpha^{\epsilon_0}(u,\varphi) &\le \widetilde{D}(2^{\alpha|}p|\alpha|+1)\cdot\Big\{\sum_{|\gamma|\le 2^{|\alpha|}p|\alpha|}\Big(\frac{1}{2^{|\alpha|}}\exp(\widetilde{A}|\alpha|)\Big)^{2^{|\alpha|}}\Big\}^{2^{-|\alpha|}} \\ &\le \widetilde{D}(2^{\alpha|}p|\alpha|+1)\frac{e^{\widetilde{A}|\alpha|}}{2^{|\alpha|}}\Big\{\sum_{|\gamma|\le 2^{|\alpha|}p|\alpha|}1\Big\}^{2^{-|\alpha|}}.\end{aligned}$$

But

(6-20)
$$\begin{aligned}\sum_{|\gamma|\le 2^{|\alpha|}p|\alpha|} 1 \le \sum_{k=0}^{2^{|\alpha|}p|\alpha|}\Big(\sum_{|\gamma|=k}1\Big) &\le \sum_{k=0}^{2^{|\alpha|}p|\alpha|}(k+1)^{n2^{|\alpha|}} \\ &\le (2^{|\alpha|}p|\alpha|+1)(2^{|\alpha|}p|\alpha|+1)^{n2^{|\alpha|}}.\end{aligned}$$

Hence

(6-21)
$$\Big[\sum_{|\gamma|\le 2^{|\alpha|}p|\alpha|}1\Big]^{2^{-|\alpha|}} \le (2^{|\alpha|}p|\alpha|+1)^{n+2^{-|\alpha|}},$$

so

$$\mathcal{N}_\alpha^{\epsilon_0}(u,\varphi_{q|\alpha|}) \le \widetilde{D}(2^{|\alpha|}p|\alpha|+1)^{n+2}\Big(\frac{e^{\widetilde{A}}}{2}\Big)^{|\alpha|} < A^{|\alpha|+1}, \quad \text{for some } A>0.$$

Then in view of (6-14),

(6-22)
$$\|\partial^\alpha u\|_{L^2(\Omega_1)} \le (AM_{\epsilon_0})^{|\alpha|+1}(p|\alpha|)!^s, \quad \alpha\in\mathbb{N}^n.$$

This finishes the proof of Theorem 6.1 in the remaining case $s=1$. □

As a corollary of Theorems 5.5 and 6.1, we have:

Theorem 6.3. *Let P be given by* (2-1) *satisfying* (2-2) *and* (2-3) *in an open set $\Omega \subset \mathbb{R}^n$. Let Ω_0 be a relatively compact open subset of Ω and $s \geq 1$. Assume that the coefficients of Y, X_j's and b are in $G^s(\overline{\Omega}_0)$ and* $\text{type}_X(\overline{\Omega}_0) = p$. *Then any s-Gevrey vector of P in Ω_0* (analytic vector when $s = 1$) *belongs to the Gevrey class $G^{ps}(\Omega_0)$.*

Remark 6.4. In [Braun Rodrigues et al. 2016], the authors showed for a particular class of Hörmander's operators in a product of two tori, a global version of Theorem 6.3, also proving its optimality. This implies that Theorem 6.3 is optimal.

Remark 6.5. We proved Theorem 6.3, in case $s \in \mathbb{N}^*$ (in particular for analytic vectors of P in Ω_0) using the method of addition of one variable in [Derridj 2019b]. Let us mention that D. Tartakoff [2018] suggests a different way to attack this question (without a complete proof).

Remark 6.6. Theorem 6.1 shows that estimates (5-27) imply the ps-Gevrey regularity in Ω_0 of any s-Gevrey vector of P in Ω_0. As the ps-Gevrey regularity in Ω_0 is optimal (Remark 6.4), we deduce that the integer p is optimal in the estimates (5-27), so giving optimal (5-27) estimates in that sense.

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BOUNDEDNESS OF SINGULAR INTEGRALS WITH FLAG KERNELS ON WEIGHTED FLAG HARDY SPACES

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We establish a weighted Hardy space theory associated with flag structures. This theory differs from those in the classical one-parameter and the product settings, and includes weighted Hardy spaces $H^p_{\mathcal{F},w}$, weighted Carleson measure spaces $CMO^p_{\mathcal{F},w}$ (the dual spaces of $H^p_{\mathcal{F},w}$), and the boundedness of singular integrals with flag kernels on these spaces. We also derive a Calderón–Zygmund decomposition and provide interpolation of operators acting on $H^p_{\mathcal{F},w}$. Examples and counterexamples are constructed to clarify the relations between classes of one-parameter, product and flag A_p weights. The main tool for our approach is the weighted Littlewood–Paley–Stein theory associated with the flag structure.

1. Introduction

The classical singular integral operators are extensions of the Hilbert transform, which have singularity at the origin only. The nature of this singularity leads to the invariance of these singular integral operators under the classical dilations on $\mathbb{R}^n$ given by $\delta x = (\delta x_1, \dots, \delta x_n)$ for $\delta > 0$. On the other hand, the Calderón–Zygmund

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product theory of singular integral operators on $\mathbb{R}^n$ is concerned with those singular integral operators which are invariant under the n-fold dilations:

$$\delta x = (\delta_1 x_1, \delta_2 x_2, \dots, \delta_n x_n),$$

$\delta_j > 0$ for $1 \le j \le n$. The product theory of $\mathbb{R}^n$ began with the strong maximal function studied by Zygmund, then continued with the Marcinkiewicz multiplier theorem and has been studied in a variety of directions; for example, product singular integrals and Hardy and BMO spaces studied in [Chang 1979; Chang and Fefferman 1980; 1982; 1985; Fefferman 1986; 1987; 1988; Fefferman and Stein 1982; Gundy and Stein 1979; Journé 1985; 1988; Pipher 1986]. Multiparameter analysis appeared implicitly in [Phong and Stein 1982] and has come to light with the proof by Müller, Ricci and Stein [1995] for the L^p boundedness, $1 < p < \infty$, of Marcinkiewicz multipliers on the Heisenberg group $\mathbb{H}^n$. This is surprising since Marcinkiewicz multipliers, which are invariant under a two-parameter group of dilations on $\mathbb{C}^n \times \mathbb{R}$, are bounded on $L^p(\mathbb{H}^n)$, despite the absence of a two-parameter automorphic group of dilation on $\mathbb{H}^n$. Moreover, Müller, Ricci and Stein showed that Marcinkiewicz multipliers can be characterized by a convolution operator of the form $f * K$, where, however, K is a flag kernel. Sharp L^p estimates for Marcinkiewicz multipliers on H-type groups were established in [Müller et al. 1996]. Nagel, Ricci and Stein [2001] proved that product kernels can be written as finite sums of flag kernels and that flag kernels have good regularity, restriction and composition properties. Applying the theory of singular integrals with flag kernels to the study of the $\square_b$-complex on certain quadratic CR submanifolds of $\mathbb{C}^n$, they obtained L^p regularity for certain derivatives of the relative fundamental solution of $\square_b$ and for the corresponding Szegő projections onto the null space of $\square_b$ by showing that the distribution kernels of these operator are finite sums of flag kernels. Applying a type of singular integral operators whose novel features are related to singular integrals with flag kernels, Nagel and Stein [2006] provided the optimal estimates for solutions of the Kohn–Laplacian for certain classes of model domains in several complex variables. These operators differ essentially from the standard Calderón–Zygmund operators that have been used in these problems hitherto. More recently, Nagel et al. [2012; 2018] further generalized the theory of singular integrals with flag kernels to a more general setting, namely, homogeneous group. They proved that on a homogeneous group, singular integral operators with flag kernels are bounded on L^p, $1 < p < \infty$, and form an algebra. See also [Głowacki 2007] and [Głowacki 2010] and the correction to the latter. Weighted norm inequalities for flag singular integrals on homogeneous groups were established in [Wu 2014a].

As mentioned in [Nagel et al. 2001], on the Euclidean space a singular integral with a flag kernel is a special case of product singular integrals. As a consequence, the L^p, $1 < p < \infty$, boundedness of singular integrals with flag kernels follows automatically from the same result for product singular integrals (see [Fefferman and Stein 1982]). Note that the product theory is not available on the Heisenberg groups; it is interesting to ask: Can one provide the Hardy space boundedness for the Marcinkiewicz multiplier on the Heisenberg groups [Müller et al. 1995]? To answer this, the multiparameter Hardy spaces associated with the flag structure on the Heisenberg groups were developed in [Han et al. 2014]. A kind of atomic decomposition for flag Hardy spaces was provided in [Wu 2014b]. For related function spaces on Euclidean spaces, we refer to [Ding et al. 2010; Han and Lu 2010; Yang 2009].

Another interesting class of operators are flag paraproducts. Such operators were studied in [Muscalu 2007; 2010; Muscalu and Schlag 2013], and are closely related to the lacunary version of bilinear Hilbert transform. Miyachi and Tomita [2016] investigated L^∞ and H^p estimates for trilinear flag paraproducts. Flag paraproducts also appear naturally and play an important role in the study of nonlinear dispersive PDEs; see the work of Germain, Masmoudi and Shatah [2012a; 2012b] and Muscalu and Schlag [2013].

The purpose of this paper is to establish a weighted Hardy space theory associated with flag structures. This theory differs from those in the classical one parameter and the product settings, and includes weighted Hardy spaces $H^p_{\mathcal{F},w}$ and weighted Carleson measure spaces $CMO^p_{\mathcal{F},w}$ (the dual spaces of $H^p_{\mathcal{F},w}$), and the boundedness of singular integrals with flag kernels on these spaces. We will also derive a Calderón–Zygmund decomposition and provide interpolation of operators acting on $H^p_{\mathcal{F},w}$. To achieve this goal, we will employ the following approaches.

(1) Introduce a test function space and distributions: It is well known that in the classical case, the test function space and distributions are important for the development of the Hardy space theory. As in the remarkable work of C. Fefferman and Stein [1972], these are just the Schwartz test functions and tempered distributions. To introduce the Hardy spaces associated with flag kernels, in the current paper, we shall use the *partial* cancellation conditions to define a new test function space, which is different from that used in [Han et al. 2014]. Roughly speaking, any test function satisfies the cancellation conditions in one subvariable only. Such cancellation conditions are fulfilled by flag atoms (see [Wu 2014b]) and were also used by Nagel, Ricci, Stein and Wainger in [Nagel et al. 2012].

(2) Establish discrete Calderón's reproducing formulae: The classical Calderón reproducing formula was first introduced in [Calderón 1964]. Various forms of Calderón reproducing formulae proved to be very powerful tools in both harmonic analysis and wavelet analysis; see, for instance, [David et al. 1985; Frazier and Jawerth 1990; Han 2000; Meyer 1992]. To show the L^p $(1 < p < \infty)$ estimates of flag singular integrals, Nagel, Ricci, Stein and Wainger [Nagel et al. 2012] established a continuous Calderón reproducing formula on homogeneous groups.

In this paper, we shall build two kinds of discrete Calderón's reproducing formulae associated with the flag structure. The first one is expressed in terms of Schwartz functions whose Fourier transforms are compactly supported, and it converges in the above-mentioned test function space and distributions. The second one involves bump functions and converges in L^2 norm. Both formulae will be the main tools for developing the whole theory.

(3) Provide a Plancherel–Pólya type inequality and develop a Littlewood–Paley–Stein theory: The classical Plancherel–Pólya inequality says that the L^p norm of f whose Fourier transform has compact support is equivalent to the ℓ^p norm of the restriction of f at appropriate lattices (see [Plancherel and Pólya 1936]). It is well known that the classical and product Plancherel–Pólya inequalities play a crucial role for developing the Littlewood–Paley–Stein theory (see [Han 1998; Ding et al. 2012]). In this paper, we will provide the Plancherel–Pólya inequality associated with the flag structure and develop the Littlewood–Paley–Stein theory. As a consequence, the weighted flag Hardy spaces are well defined.

(4) Introduce generalized Carleson measure spaces: In the classical one parameter case, it is well known that BMO, the dual of H^1, can be characterized by the Carleson measures. Moreover, applying atomic decompositions of product Hardy spaces, Chang and R. Fefferman [1980] proved that the dual of the product H^1 can be characterized by the product Carleson measure. In this paper, we will characterize the dual of the weighted flag Hardy spaces via generalized Carleson measures. Our approach involves applying techniques of weighted sequence spaces, which enables us to avoid using the atomic decompositions.

(5) Prove a Calderón–Zygmund decomposition for $H^p_{\mathcal{F},w}$: The Calderón–Zygmund decomposition plays a crucial role in developing the Calderón–Zygmund operator theory and has many applications in harmonic analysis and PDEs. Such a decomposition in the product Euclidean spaces was first provided by Chang and R. Fefferman [1982] via atomic decompositions. In this paper, Calderón–Zygmund decomposition is achieved by applying the discrete Calderón's reproducing formula and the weighted flag version of Fefferman–Stein vector-valued maximal inequality. As an application, we derive interpolation results for sublinear operators on $H^p_{\mathcal{F},w}$.

We would like to remark that R. Fefferman [1987] established a criterion for the product H^p to L^p boundedness of product singular integral operators in Journé's class by considering their actions only on rectangle atoms via Journé's lemma. However, R. Fefferman's criterion cannot be extended to three or more parameters without further assumptions on the nature of the operators as shown in Journé [1988]. In fact, Journé provided a counter-example of singular integral operators in the three-parameter setting such that R. Fefferman's criterion breaks down. This means that in the classical product theory, there are substantial differences between the two-parameter case and the setting for three or more parameters. However, our approach works for any parameter case, and hence we shall focus on the case of three parameters and from the proofs given in this paper it is straightforward to extend the theory to the case of k ($k = 2$ and $k > 3$) parameters.

To describe the main results in this paper, we first recall some definitions and notation. A rectangle R in $\mathbb{R}^{n_1} \times \mathbb{R}^{n_2} \times \mathbb{R}^{n_3} := \mathbb{R}^N$ is called an *acceptable rectangle* (or a *flag rectangle*) if $R = Q_1 \times Q_2 \times Q_3$, where Q_i's are cubes in $\mathbb{R}^{n_i}$ with side-length satisfying

$$\ell(Q_1) \le \ell(Q_2) \le \ell(Q_3).$$

Denote by $\mathcal{R}_{\mathcal{F}}$ the set of all flag rectangles associated with $\mathcal{F}$ and by $\mathcal{R}^d_{\mathcal{F}}$ the set of all *dyadic* flag rectangles associated with $\mathcal{F}$. For $J = (j_1, j_2, j_3)$, the set $\mathcal{R}^J_{\mathcal{F}}$ consists of all dyadic flag rectangles $R = Q_1 \times Q_2 \times Q_3$ of side-length $\ell(Q_1) = 2^{j_1}$, $\ell(Q_2) = 2^{j_1 \vee j_2}$, $\ell(Q_3) = 2^{j_1 \vee j_2 \vee j_3}$, where $a \vee b$ denotes $\max\{a, b\}$.

The following *flag maximal function* was introduced in [Nagel et al. 2012]:

$$\mathcal{M}_{\mathcal{F}}(f)(x) = \sup_{\substack{R \ni x,\\ R \in \mathcal{R}_{\mathcal{F}}}} \frac{1}{|R|} \int_R |f(y)|\, dy.$$

The Muckenhoupt weight class associated with $\mathcal{F}$ can be defined as follows.

Definition 1.1. Let $1 < p < \infty$ and w be a weight function on $\mathbb{R}^N$; that is, a nonnegative locally integrable function on $\mathbb{R}^N$ that take values in $(0, \infty)$ almost everywhere. We say that w is a *flag A_p weight*, denoted by $w \in A^{\mathcal{F}}_p(\mathbb{R}^N)$, if

$$[w]_{A^{\mathcal{F}}_p} := \sup_{R \in \mathcal{R}_{\mathcal{F}}} \left(\frac{1}{|R|} \int_R w(x)\, dx\right)\left(\frac{1}{|R|} \int_R w(x)^{-1/(p-1)}\, dx\right)^{p-1} < \infty.$$

We say that w is in $A^{\mathcal{F}}_1(\mathbb{R}^N)$ if there is a constant C such that

$$\mathcal{M}_{\mathcal{F}}(w)(x) \le C w(x) \qquad \text{a.e. } x \in \mathbb{R}^N.$$

Let $A^{\mathcal{F}}_\infty(\mathbb{R}^N) := \bigcup_{1 \le p < \infty} A^{\mathcal{F}}_p(\mathbb{R}^N)$. If $w \in A^{\mathcal{F}}_\infty$, the *critical index of* w is defined by

$$q_w := \inf\{q : w \in A^{\mathcal{F}}_q(\mathbb{R}^N)\}.$$

We remark that this class of Muckenhoupt weights is different from the classical weight class $A_p(\mathbb{R}^N)$ and the product weight class $A^{\text{pro}}_p(\mathbb{R}^N)$. More precisely, their relations are as follows (see Section 5 for more details):

$$A^{\text{pro}}_p(\mathbb{R}^N) \subsetneq A^{\mathcal{F}}_p(\mathbb{R}^N) \subsetneq A_p(\mathbb{R}^N) \quad \text{for } 1 < p < \infty.$$

To develop the weighted Hardy space theory associated with flag singular integrals, as in the classical case, appropriate test functions and distributions are needed. For this purpose, we define *flag test functions* as follows.

Definition 1.2. A Schwartz function f on $\mathbb{R}^N$ is said to be a *flag test function* in $\mathcal{S}_{\mathcal{F}}(\mathbb{R}^N)$ if it satisfies the partial cancellation conditions

$$\int_{\mathbb{R}^{n_3}} f(x_1, x_2, x_3)x_3^\alpha \, dx_3 = 0 \quad \text{for all multi-indices } \alpha \text{ and every } (x_1, x_2) \in \mathbb{R}^{n_1+n_2}.$$

The seminorms on $\mathcal{S}_{\mathcal{F}}(\mathbb{R}^N)$ are the same as the ones on $\mathcal{S}(\mathbb{R}^N)$ and these seminorms make $\mathcal{S}_{\mathcal{F}}$ a topological vector space. Let $\mathcal{S}'_{\mathcal{F}}(\mathbb{R}^N)$ denote the topological dual space of $\mathcal{S}_{\mathcal{F}}(\mathbb{R}^N)$.

Recall that a Schwartz function f is called a classical test function, denoted by $f \in \mathcal{S}_\infty(\mathbb{R}^N)$, if

$$\int_{\mathbb{R}^{n_1+n_2+n_3}} f(x_1, x_2, x_3)\, x_1^\alpha\, x_2^\beta\, x_3^\gamma \, dx_1\, dx_2\, dx_3 = 0 \quad \text{for all multi-indices } \alpha, \beta, \gamma.$$

We say that a Schwartz function f is a product test function, denoted by $f \in \mathcal{S}_\infty(\mathbb{R}^{n_1} \times \mathbb{R}^{n_2} \times \mathbb{R}^{n_3})$, if

$$\int_{\mathbb{R}^{n_1}} f(x_1, x_2, x_3)x_1^\alpha \, dx_1 = 0 \quad \text{for all multi-indices } \alpha \text{ and all } x_2 \in \mathbb{R}^{n_2}, x_3 \in \mathbb{R}^{n_3},$$

$$\int_{\mathbb{R}^{n_2}} f(x_1, x_2, x_3)x_2^\beta \, dx_2 = 0 \quad \text{for all multi-indices } \beta \text{ and all } x_1 \in \mathbb{R}^{n_1}, x_3 \in \mathbb{R}^{n_3},$$

and

$$\int_{\mathbb{R}^{n_3}} f(x_1, x_2, x_3)x_3^\gamma \, dx_3 = 0 \quad \text{for all multi-indices } \gamma \text{ and all } x_1 \in \mathbb{R}^{n_1}, x_2 \in \mathbb{R}^{n_2}.$$

Clearly, $\mathcal{S}_\infty(\mathbb{R}^{n_1} \times \mathbb{R}^{n_2} \times \mathbb{R}^{n_3}) \subsetneq \mathcal{S}_{\mathcal{F}}(\mathbb{R}^N) \subsetneq \mathcal{S}_\infty(\mathbb{R}^N)$.

Let $N_1 = n_1+n_2+n_3$, $N_2 = n_2+n_3$ and $N_3 = n_3$. For $i = 1, 2, 3$, let $\psi^{(i)} \in \mathcal{S}(\mathbb{R}^{N_i})$ satisfy

$$\text{(1-1)} \qquad \operatorname{supp} \widehat{\psi^{(i)}} \subset \{\xi^i \in \mathbb{R}^{N_i} : 1/2 < |\xi^i| \le 2\}$$

and

$$\text{(1-2)} \qquad \sum_{j_i \in \mathbb{Z}} \widehat{\psi^{(i)}}(2^{j_i}\xi^i)^2 = 1 \quad \text{for all } \xi^i \in \mathbb{R}^{N_i} \backslash \{0\}.$$

Define $\psi_{j_i}^{(i)}(x^i) = 2^{-j_i N_i}\psi^{(i)}(2^{-j_i}x^i)$, $x^i \in \mathbb{R}^{N_i}$ and $\widetilde{\psi}_{j_i}^{(i)} = \delta_{\mathbb{R}^{N-N_i}} \otimes \psi_{j_i}^{(i)}$, $i = 1, 2, 3$. For $J = (j_1, j_2, j_3) \in \mathbb{Z}^3$, set $\psi_J = \widetilde{\psi}_{j_1}^{(1)} * \widetilde{\psi}_{j_2}^{(2)} * \widetilde{\psi}_{j_3}^{(3)}$. The departure of our approach is the Calderón reproducing formula (see Theorem 2.1 below)

$$f(x) = \sum_{J \in \mathbb{Z}^3} \sum_{R \in \mathcal{R}_{\mathcal{F}}^J} |R|\psi_J(x - x_R)\psi_J * f(x_R),$$

where x_R denotes the “lower left corner” of R (i.e., the corner of R with the least value of each coordinate component), and the series converges in $L^2(\mathbb{R}^N)$, $\mathcal{S}_{\mathcal{F}}(\mathbb{R}^N)$ and $\mathcal{S}'_{\mathcal{F}}(\mathbb{R}^N)$ whenever f is in the corresponding space.

Based on the above reproducing formula, the *Littlewood–Paley–Stein square function* of $f \in \mathcal{S}'_{\mathcal{F}}(\mathbb{R}^N)$ is defined by

$$g_{\mathcal{F}}(f)(x) = \bigg(\sum_{J\in\mathbb{Z}^3}\sum_{R\in\mathcal{R}^J_{\mathcal{F}}} |\psi_J * f(x_R)|^2\chi_R(x)\bigg)^{\frac{1}{2}},$$

where χ_R is the indicator function of R.

Definition 1.3. Let $0 < p < \infty$ and $w \in A^{\mathcal{F}}_\infty(\mathbb{R}^N)$. The *weighted flag Hardy space* $H^p_{\mathcal{F},w}(\mathbb{R}^N)$ is defined by

$$H^p_{\mathcal{F},w}(\mathbb{R}^N) = \{f \in \mathcal{S}'_{\mathcal{F}}(\mathbb{R}^N) : g_{\mathcal{F}}(f) \in L^p_w(\mathbb{R}^N)\}$$

with quasinorm $\|f\|_{H^p_{\mathcal{F},w}(\mathbb{R}^N)} := \|g_{\mathcal{F}}(f)\|_{L^p_w(\mathbb{R}^N)}$.

To see that the definition of $H^p_{\mathcal{F},w}$ is independent of the choice of $\{\psi_J\}$, we will prove the following theorem:

Theorem 1.4. *Let* $0 < p < \infty$ *and* $w \in A^{\mathcal{F}}_\infty(\mathbb{R}^N)$. *Suppose that both* $\{\psi_J\}$ *and* $\{\varphi_J\}$ *satisfy conditions* (1-1) *and* (1-2). *Then for* $f \in \mathcal{S}'_{\mathcal{F}}(\mathbb{R}^N)$,

$$\bigg\|\bigg\{\sum_{J\in\mathbb{Z}^3}\sum_{R\in\mathcal{R}^J_{\mathcal{F}}} |\psi_J*f(x_R)|^2\chi_R\bigg\}^{\frac{1}{2}}\bigg\|_{L^p_w(\mathbb{R}^N)} \approx \bigg\|\bigg\{\sum_{J\in\mathbb{Z}^3}\sum_{R\in\mathcal{R}^J_{\mathcal{F}}} |\varphi_J*f(x_R)|^2\chi_R\bigg\}^{\frac{1}{2}}\bigg\|_{L^p_w(\mathbb{R}^N)}.$$

Remark. Note that $\mathcal{S}'_{\mathcal{F}}(\mathbb{R}^N)$ can be identified as the space of tempered distributions on $\mathbb{R}^N$ modulo the tensor product of tempered distributions on $\mathbb{R}^{n_1+n_2}$ and polynomials on $\mathbb{R}^{n_3}$, and thus each element in $H^p_{\mathcal{F},w}$ is given by an equivalent class. As in the classical case, using the equivalent classes rather than distributions ensures that $\|\cdot\|_{H^p_{\mathcal{F},w}}$ is a quasinorm (a norm if $1 \le p < \infty$) and that $H^p_{\mathcal{F},w}$ is a quasi-Banach space (a Banach space if $1 \le p < \infty$). We shall prove in Corollary 2.6 below that $L^2 \cap H^p_{\mathcal{F},w}$ is dense in $H^p_{\mathcal{F},w}$, so that each element $f \in H^p_{\mathcal{F},w}$ can be identified as the limit in $H^p_{\mathcal{F},w}$ of some sequence $\{f_n\} \subset L^2 \cap H^p_{\mathcal{F},w}$. See [Frazier and Jawerth 1990] for similar results in the classical case.

Remark. As mentioned before, it was shown in [Nagel et al. 2001] that flag kernels form a subclass of product kernels. Therefore, singular integrals with flag kernels are bounded automatically on the weighted product Hardy spaces $H^p_w(\mathbb{R}^{n_1} \times \mathbb{R}^{n_2} \times \mathbb{R}^{n_3})$, when w is a *product* A_∞ *weight* (see [Ding et al. 2012]). However, by Proposition 5.1, a flag weight is not necessarily a product weight, so our theory of weighted flag Hardy spaces does not fall under the scope of the product theory. Moreover, all functions $f \in L^2(\mathbb{R}^N) \cap H^p_{\mathcal{F}}(\mathbb{R}^N)$ (the unweighted flag Hardy space) fulfill the partial cancellation condition

$$\int_{\mathbb{R}^{n_3}} f(x_1, x_2, x_3)\, dx_3 = 0 \quad \text{for almost every } (x_1, x_2) \in \mathbb{R}^{n_1} \times \mathbb{R}^{n_2},$$

which is different from the cancellation properties for product Hardy spaces; for more details, see the remark after the proof of Theorem 1.10 on page 585. This is an indication that weighted flag Hardy spaces are strictly larger than product ones. Nevertheless, we will prove, in Theorem 1.9 below, that singular integrals with flag kernels are bounded on these larger spaces $H^p_{\mathcal{F},w}(\mathbb{R}^N)$. This, indeed, was the main motivation to develop the weighted Hardy space theory.

Remark. If $1 < p < \infty$ and $w \in A^{\mathcal{F}}_p(\mathbb{R}^N)$, then, by a result in [Wu 2014a] and an argument similar to the proof of Theorem 1.4, the two spaces $H^p_{\mathcal{F},w}(\mathbb{R}^N)$ and $L^p_w(\mathbb{R}^N)$ coincide with comparable norms. However, if $p > 1$ there is a $w \notin A_p$ such that $H^p_{\mathcal{F},w} \neq L^p_w$. To see this, refer to the work of Strömberg and Wheeden [1982]. Indeed, if $u(x) = |q(x)|^p w(x)$, where $q(x)$ is a polynomial and $w(x)$ satisfies the Muckenhoupt A_p condition, they proved that H^p_u and L^p_u can be identified when all the zeros of $q(x)$ are real and that otherwise H^p_u can be identified with a certain proper subspace of L^p_u. Similar results in product spaces were obtained in [Strömberg and Wheeden 1989].

To study the dual of $H^p_{\mathcal{F},w}(\mathbb{R}^N)$, we introduce the following weighted Carleson measure spaces $CMO^p_{\mathcal{F},w}(\mathbb{R}^N)$.

Definition 1.5. Let $0 < p \le 1$, $w \in A^{\mathcal{F}}_\infty(\mathbb{R}^N)$. Suppose that $\{\psi_J\}$ satisfies (1-1) and (1-2). We say that $f \in \mathcal{S}'_{\mathcal{F}}(\mathbb{R}^N)$ belongs to $CMO^p_{\mathcal{F},w}(\mathbb{R}^N)$ if

$$\|f\|_{CMO^p_{\mathcal{F},w}(\mathbb{R}^N)} := \sup_{\Omega \subset \mathbb{R}^N} \left\{ \frac{1}{[w(\Omega)]^{2/p-1}} \sum_{J \in \mathbb{Z}^3} \sum_{\substack{R \in \mathcal{R}^J_{\mathcal{F}},\\ R \subset \Omega}} \frac{|R|^2}{w(R)} |\psi_J * f(x_R)|^2 \right\}^{\frac{1}{2}} < \infty,$$

where the supremum is taken over all open sets Ω with $w(\Omega) < \infty$.

Note that the flag structure is involved in the definition of $CMO^p_{\mathcal{F},w}$. To see that the weighted Carleson measure spaces $CMO^p_{\mathcal{F},w}$ are well defined, we need the following theorem:

Theorem 1.6. *Let $w \in A^{\mathcal{F}}_\infty(\mathbb{R}^N)$. Suppose that both $\{\psi_J\}$ and $\{\varphi_J\}$ satisfy* (1-1) *and* (1-2). *Then, for $f \in \mathcal{S}'_{\mathcal{F}}(\mathbb{R}^N)$,*

$$\sup_{\Omega \subset \mathbb{R}^N} \left\{ \frac{1}{[w(\Omega)]^{2/p-1}} \sum_{J \in \mathbb{Z}^3} \sum_{\substack{R \in \mathcal{R}^J_{\mathcal{F}},\\ R \subset \Omega}} \frac{|R|^2}{w(R)} |\psi_J * f(x_R)|^2 \right\}^{\frac{1}{2}}$$

$$\approx \sup_{\Omega\subset\mathbb{R}^N} \left\{ \frac{1}{[w(\Omega)]^{2/p-1}} \sum_{J\in\mathbb{Z}^3} \sum_{\substack{R\in\mathcal{R}^J_{\mathcal{F}},\\ R\subset\Omega}} \frac{|R|^2}{w(R)} |\varphi_J * f(x_R)|^2 \right\}^{\frac{1}{2}},$$

where the suprema run over all open sets Ω *with* $w(\Omega) < \infty$.

The duality between $H^p_{\mathcal{F},w}$ and $CMO^p_{\mathcal{F},w}$ can be stated as follows.

Theorem 1.7. *Let* $0 < p \le 1$. *Then* $(H^p_{\mathcal{F},w}(\mathbb{R}^N))^* = CMO^p_{\mathcal{F},w}(\mathbb{R}^N)$. *More precisely, if* $g \in CMO^p_{\mathcal{F},w}(\mathbb{R}^N)$, *the mapping* ℓ_g *given by* $\ell_g(f) = \langle f, g\rangle$, *defined initially for* $f \in \mathcal{S}_{\mathcal{F}}(\mathbb{R}^N)$, *extends to a unique continuous linear functional on* $H^p_{\mathcal{F},w}(\mathbb{R}^N)$ *with* $\|\ell_g\| \lesssim \|g\|_{CMO^p_{\mathcal{F},w}(\mathbb{R}^N)}$.

Conversely, for every $\ell \in (H^p_{\mathcal{F},w}(\mathbb{R}^N))^*$, *there exists a unique* $g \in CMO^p_{\mathcal{F},w}(\mathbb{R}^N)$ *such that* $\ell = \ell_g$ *with* $\|g\|_{CMO^p_{\mathcal{F},w}} \lesssim \|\ell\|$.

In order to state the boundedness results for singular integrals with flag kernels on $H^p_{\mathcal{F},w}(\mathbb{R}^N)$, we need to recall some definitions from [Nagel et al. 2001]. A k-normalized bump function on $\mathbb{R}^N$ is a C^k function supported on the unit ball with norm bounded by 1. As pointed out in [Nagel et al. 2001], the definitions given below are independent of the choices of k, and thus we will simply refer to "normalized bump function" without specifying k.

In this paper, we will consider the singular integrals with the following flag kernels. See [Nagel et al. 2012] for this definition on homogeneous groups.

Definition 1.8. A flag kernel is a distribution $\mathcal{K}$ on $\mathbb{R}^N$ which coincides with a C^∞ function away from the coordinate subspace $x_1 = 0$ and satisfies the following:

(i) (differential inequalities) For each $\alpha = (\alpha_1, \alpha_2, \alpha_3) \in \mathbb{Z}^3$,

$$|\partial^{\alpha_1}_{x_1}\partial^{\alpha_2}_{x_2}\partial^{\alpha_3}_{x_3}\mathcal{K}(x)| \lesssim |x_1|^{-n_1-|\alpha_1|}(|x_1|+|x_2|)^{-n_2-|\alpha_2|}(|x_1|+|x_2|+|x_3|)^{-n_3-|\alpha_3|}$$

for $x_1 \ne 0$.

(ii) (cancellation conditions)

(a) Given normalized bump functions ψ_i, $i = 1, 2, 3$, on $\mathbb{R}^{n_i}$ and any scaling parameter $r > 0$, define a distribution $\mathcal{K}_{\psi_i,r}$ by setting

$$\langle \mathcal{K}_{\psi_i,r}, \varphi\rangle = \langle \mathcal{K}, (\psi_i)_r \otimes \varphi\rangle \tag{1-3}$$

for any test function $\varphi \in \mathcal{S}(\mathbb{R}^{N-n_i})$. Then the distributions $\mathcal{K}_{\psi_i,r}$ satisfy the differential inequalities

$$|\partial^{\alpha_2}_{x_2}\partial^{\alpha_3}_{x_3}\mathcal{K}_{\psi_1,r}(x_2,x_3)| \lesssim |x_2|^{-n_2-|\alpha_2|}(|x_2|+|x_3|)^{-n_3-|\alpha_3|},$$
$$|\partial^{\alpha_1}_{x_1}\partial^{\alpha_3}_{x_3}\mathcal{K}_{\psi_2,r}(x_1,x_3)| \lesssim |x_1|^{-n_1-|\alpha_1|}(|x_1|+|x_3|)^{-n_3-|\alpha_3|},$$
$$|\partial^{\alpha_1}_{x_1}\partial^{\alpha_2}_{x_2}\mathcal{K}_{\psi_3,r}(x_1,x_2)| \lesssim |x_1|^{-n_1-|\alpha_1|}(|x_1|+|x_2|)^{-n_2-|\alpha_2|}.$$

(b) For any bump functions $\overline{\psi}_i$ on $\mathbb{R}^{N-n_i}$ and any parameters $r = (r_1, r_2)$, we define the distributions $\mathcal{K}_{\overline{\psi}_i,r}$ by (1-3). Then the distributions $\mathcal{K}_{\overline{\psi}_i,r}$, $i = 1, 2, 3$, are one-parameter kernels and satisfy

$$|\partial_{x_i}^{\alpha_i} \mathcal{K}_{\overline{\psi}_i,r}(x_i)| \lesssim |x_i|^{-n_i-|\alpha_i|}.$$

(c) For any bump function ψ on $\mathbb{R}^N$ and $r_1, r_2, r_3 > 0$, we have

$$|\langle \mathcal{K}, \psi(r_1\cdot, r_2\cdot, r_3\cdot)\rangle| \lesssim 1.$$

Moreover, the corresponding constants that appear in these differential inequalities are independent of r, r_1, r_2.

A *flag singular integral* $T_{\mathcal{F}}$ is of the form $T_{\mathcal{F}}(f) = \mathcal{K} * f$, where $\mathcal{K}$ is a flag kernel on $\mathbb{R}^N$ defined as above.

A typical example of flag kernel adapted to the flag $\mathcal{F}$,

$$\{(0, 0, 0)\} \subset \{(0, 0, z)\} \subset \{(0, y, z)\} \subset \mathbb{R}^3,$$

is

$$\frac{\operatorname{sgn}(y)\operatorname{sgn}(z)}{x\sqrt{x^2+y^2}\sqrt{x^2+y^2+z^2}}$$

(see [Nagel et al. 2001]).

The following result establishes the boundedness of flag singular integrals on the weighted flag Hardy spaces.

Theorem 1.9. *Let $0 < p < \infty$ and $w \in A_\infty^{\mathcal{F}}(\mathbb{R}^N)$. Then the flag singular integral operator $T_{\mathcal{F}}$ is bounded on $H^p_{\mathcal{F},w}(\mathbb{R}^N)$. Moreover, for $f \in H^p_{\mathcal{F},w}(\mathbb{R}^N)$ there exists a constant C_p such that*

$$\|T_{\mathcal{F}}(f)\|_{H^p_{\mathcal{F},w}(\mathbb{R}^N)} \le C_p \|f\|_{H^p_{\mathcal{F},w}(\mathbb{R}^N)}.$$

Remark. As a consequence of Theorem 1.9 and the remark on page 552, we can obtain the boundedness of flag singular integrals on the weighted Lebesgue spaces; that is,

$$\|T_{\mathcal{F}}(f)\|_{L^p_w(\mathbb{R}^N)} \le C_p \|f\|_{L^p_w(\mathbb{R}^N)}, \quad 1 < p < \infty,$$

provided that $w \in A_p^{\mathcal{F}}(\mathbb{R}^N)$ and $f \in L^p_w(\mathbb{R}^N)$.

The following result gives a general principle on the $H^p_{\mathcal{F},w}(\mathbb{R}^N) \to L^p_w(\mathbb{R}^N)$ boundedness of operators.

Theorem 1.10. *Suppose $w \in A_\infty^{\mathcal{F}}(\mathbb{R}^N)$ and $0 < p \le 1$. For any linear operator T which is bounded on both $L^2(\mathbb{R}^N)$ and $H^p_{\mathcal{F},w}(\mathbb{R}^N)$, T is bounded from $H^p_{\mathcal{F},w}(\mathbb{R}^N)$ to $L^p_w(\mathbb{R}^N)$. As a consequence, the flag singular integral operator $T_{\mathcal{F}}$ is bounded from $H^p_{\mathcal{F},w}(\mathbb{R}^N)$ to $L^p_w(\mathbb{R}^N)$.*

Theorem 1.11 gives the $CMO^p_{\mathcal{F},w}(\mathbb{R}^N)$ boundedness of flag singular integrals.

Theorem 1.11. *Let $T_{\mathcal{F}}$ be a singular integral with flag kernel. For $0 < p \le 1$ and $w \in A_\infty^{\mathcal{F}}(\mathbb{R}^N)$, $T_{\mathcal{F}}$ extends uniquely to a bounded operator on $CMO_{\mathcal{F},w}^p(\mathbb{R}^N)$. Moreover, for any $f \in CMO_{\mathcal{F},w}^p(\mathbb{R}^N)$ there exists a constant C_p such that*

$$\|T_{\mathcal{F}}(f)\|_{CMO_{\mathcal{F},w}^p(\mathbb{R}^N)} \le C_p \|f\|_{CMO_{\mathcal{F},w}^p(\mathbb{R}^N)}.$$

Note that $CMO_{\mathcal{F},w}^1(\mathbb{R}^N) = BMO_{\mathcal{F},w}(\mathbb{R}^N)$, the dual of $H_{\mathcal{F},w}^1(\mathbb{R}^N)$. Therefore, Theorem 1.11 provides the endpoint estimate for singular integrals with flag kernels on $BMO_{\mathcal{F},w}(\mathbb{R}^N)$.

Our last main results are the Calderón–Zygmund decomposition and interpolation for $H_{\mathcal{F},w}^p$.

Theorem 1.12. *Let $w \in A_\infty^{\mathcal{F}}(\mathbb{R}^N)$, $p_1 \in (0, 1]$ and $p_1 < p < p_2 < \infty$. Given $f \in H_{\mathcal{F},w}^p(\mathbb{R}^N)$ and $\alpha > 0$, we have the decomposition $f = g + b$, where $g \in H_{\mathcal{F},w}^{p_2}(\mathbb{R}^N)$ and $b \in H_{\mathcal{F},w}^{p_1}(\mathbb{R}^N)$ with*

$$\|g\|_{H_{\mathcal{F},w}^{p_2}(\mathbb{R}^N)}^{p_2} \lesssim \alpha^{p_2-p} \|f\|_{H_{\mathcal{F},w}^p(\mathbb{R}^N)}^p \quad \text{and} \quad \|b\|_{H_{\mathcal{F},w}^{p_1}(\mathbb{R}^N)}^{p_1} \lesssim \alpha^{p_1-p} \|f\|_{H_{\mathcal{F},w}^p(\mathbb{R}^N)}^p.$$

We would like to point out that the above result was first proved by Chang and Fefferman [1982] for the product Hardy spaces on the product of upper half space.

As an application of Theorem 1.12, we immediately have the following interpolation of operators.

Theorem 1.13. *Let $w \in A_\infty^{\mathcal{F}}(\mathbb{R}^N)$ and $0 < p_1 < p_2 < \infty$. If T is a sublinear operator bounded from $H_{\mathcal{F},w}^{p_1}(\mathbb{R}^N)$ to $L_w^{p_1}(\mathbb{R}^N)$ and bounded from $H_{\mathcal{F},w}^{p_2}(\mathbb{R}^N)$ to $L_w^{p_2}(\mathbb{R}^N)$, then T is bounded from $H_{\mathcal{F},w}^p(\mathbb{R}^N)$ to $L_w^p(\mathbb{R}^N)$ for all $p \in (p_1, p_2)$. Similarly, if T is bounded both on $H_{\mathcal{F},w}^{p_1}(\mathbb{R}^N)$ and $H_{\mathcal{F},w}^{p_2}(\mathbb{R}^N)$, then T is bounded on $H_{\mathcal{F},w}^p(\mathbb{R}^N)$ for all $p \in (p_1, p_2)$.*

Finally, we make the following remark. In contrast with the product case and the unweighted flag case (see [Ding et al. 2012; Han et al. 2014]), the whole theory of weighted flag Hardy spaces is built on the acceptable rectangles. A typical example is the strong maximal operator, which is bounded on the L^p, $1 < p < \infty$, but is not bounded on L_w^p if $w \in A_p^{\mathcal{F}} \backslash A_p^{\text{pro}}(\mathbb{R}^N)$ (see Section 5 for examples of weight functions in $A_p^{\mathcal{F}} \backslash A_p^{\text{pro}}(\mathbb{R}^N)$). In the current paper, we shall use the intrinsic maximal operator $\mathcal{M}_{\mathcal{F}}$, which reflects the geometry of the flag multiparameter structure.

This paper is organized as follows. In Section 2, we establish the weighted theory of flag Hardy and Carleson measure spaces. The boundedness of flag singular integrals on these spaces are proved in Section 3. Section 4 is devoted to the Calderón–Zygmund decomposition and interpolation in these spaces. Finally, in Section 5, we give some examples and counterexamples to clarify the relationships among the classes of flag weights, classical weights and product weights.

2. Weighted Hardy spaces, Carleson measure spaces and the dual theorem

The main purpose of this section is to prove Theorems 1.4, 1.6 and 1.7. To this end, we need the following *discrete Calderón reproducing formula.*

Theorem 2.1. *Suppose that* $\{\psi_J\}$ *satisfy* (1-1) *and* (1-2). *Then*

$$(2\text{-}1)\quad f(x)=\sum_{J\in\mathbb{Z}^3}\sum_{\ell\in\mathbb{Z}^N}2^{J\cdot n}\psi_J(x-2^J\ell)\psi_J*f(2^J\ell)=\sum_{J\in\mathbb{Z}^3}\sum_{R\in\mathcal{R}^J_{\mathcal{F}}}|R|\psi_J(x-x_R)\psi_J*f(x_R),$$

where $2^J\ell=(2^{j_1}\ell_1,2^{j_1\vee j_2}\ell_2,2^{j_1\vee j_2\vee j_3}\ell_3)=x_R$ *denotes the lower left corner of* R, $2^{J\cdot n}=2^{j_1n_1+(j_1\vee j_2)n_2+(j_1\vee j_2\vee j_3)n_3}$ *is the measure of* $R\in\mathcal{R}^J_{\mathcal{F}}$, *and the series converges in* $L^2(\mathbb{R}^N)$, $\mathcal{S}_{\mathcal{F}}(\mathbb{R}^N)$ *and* $\mathcal{S}'_{\mathcal{F}}(\mathbb{R}^N)$ (*whenever* f *is in the corresponding space*).

Proof. The proof of the convergence of the series in L^2 is similar to the classical case. Assume $f\in L^2(\mathbb{R}^N)$. By Fourier transform, $f=\sum_{J\in\mathbb{Z}^3}\psi_J*\psi_J*f$ with the series convergent in $L^2(\mathbb{R}^N)$. Similar to the method used in [Frazier et al. 1991], set $g=\psi_J*f$ and $h=\psi_J$. For $\xi\in\mathbb{R}^N$, the Fourier transforms of g and h are, respectively, given by

$$\hat g(\xi_1,\xi_2,\xi_3)=\widehat{\psi^{(1)}}(2^{j_1}\xi_1,2^{j_1}\xi_2,2^{j_1}\xi_3)\widehat{\psi^{(2)}}(2^{j_2}\xi_2,2^{j_2}\xi_3)\widehat{\psi^{(3)}}(2^{j_3}\xi_3)\hat f(\xi_1,\xi_2,\xi_3),$$
$$\hat h(\xi_1,\xi_2,\xi_3)=\widehat{\psi^{(1)}}(2^{j_1}\xi_1,2^{j_1}\xi_2,2^{j_1}\xi_3)\widehat{\psi^{(2)}}(2^{j_2}\xi_2,2^{j_2}\xi_3)\widehat{\psi^{(3)}}(2^{j_3}\xi_3).$$

Note that the Fourier transforms of g and h are both compactly supported in

$$R_j:=\{\xi\in\mathbb{R}^N:\ |\xi_1|\le 2^{-j_1}\pi,\ |\xi_2|\le 2^{-j_1\vee j_2}\pi,\ |\xi_3|\le 2^{-j_1\vee j_2\vee j_3}\pi\}.$$

By first expanding $\hat g$ in a Fourier series on the rectangle R_j,

$$\hat g(\xi)=\sum_{\ell\in\mathbb{Z}^N}2^{J\cdot n}(2\pi)^{-N}\biggl(\int_{R_j}\hat g(\xi')e^{i[(2^J\ell)\cdot\xi']}d\xi'\biggr)e^{-i[(2^J\ell)\cdot\xi]},$$

and then replacing the domain R_J by $\mathbb{R}^N$ as $\hat g$ is supported in R_J, we get

$$\hat g(\xi)=\sum_{\ell\in\mathbb{Z}^N}2^{J\cdot n}g(2^J\ell)e^{-i[(2^J\ell)\cdot\xi]}.$$

Multiplying both sides by $\hat h(\xi)$ and noticing $\hat h(\xi)e^{-i[(2^J\ell)\cdot\xi]}=[h(\cdot-2^J\ell)]\hat{}(\xi)$ yields

$$(g*h)(x)=\sum_{\ell\in\mathbb{Z}^N}2^{J\cdot n}g(2^J\ell)h(x-2^J\ell).$$

Substituting g by ψ_J*f and h by ψ_J into the above identity gives the discrete Calderón reproducing formula (2-1) and the convergence in $L^2(\mathbb{R}^N)$.

To finish the proof, we only need to show that the series in (2-1) converges in $\mathcal{S}_{\mathcal{F}}(\mathbb{R}^N)$ if $f \in \mathcal{S}_{\mathcal{F}}(\mathbb{R}^N)$; the convergence in $\mathcal{S}'_{\mathcal{F}}(\mathbb{R}^N)$ then follows from a standard duality argument. The key to doing this are the following almost-orthogonality estimates: for any $L, M > 0$ and $f \in \mathcal{S}_{\mathcal{F}}(\mathbb{R}^N)$,

$$|f * \psi_J(x)| \lesssim 2^{-(|j_1|+|j_2|+|j_3|)L} \frac{1}{(1+|x|)^M}. \tag{2-2}$$

Assume that (2-2) holds for the moment. Then for any multi-index $\alpha \in \mathbb{N}^N$,

$$\begin{aligned}
&\Big|\sum_{\ell\in\mathbb{Z}^N} 2^{J\cdot n}(\partial^\alpha\psi_J)(x-2^J\ell)\psi_J * f(2^J\ell)\Big| \\
&\qquad \lesssim 2^{-(|j_1|+|j_2|+|j_3|)L'} \sum_{\ell\in\mathbb{Z}^N} 2^{J\cdot n} \frac{1}{(1+|2^{j_1}\ell_1|+|2^{j_1\vee j_2}\ell_2|+|2^{j_1\vee j_2\vee j_3}\ell_3|)^M} \\
&\qquad\qquad \times \frac{1}{(1+|x_1-2^{j_1}\ell_1|+|x_2-2^{j_1\vee j_2}\ell_2|+|x_3-2^{j_1\vee j_2\vee j_3}\ell_3|)^M} \\
&\qquad \lesssim 2^{-(|j_1|+|j_2|+|j_3|)L'}(1+|x|)^{-M} \quad \text{for some } L' > 0,
\end{aligned}$$

which would further imply that

$$\sum_{|j_1|,|j_2|,|j_3|>k} \sum_{\ell\in\mathbb{Z}^N} 2^{J\cdot n}\psi_J(x-2^J\ell)\psi_J * f(2^J\ell) \to 0 \quad \text{in } \mathcal{S}_{\mathcal{F}}(\mathbb{R}^N)$$

as $k \to +\infty$.

It remains to verify (2-2) under the assumption $f \in \mathcal{S}_{\mathcal{F}}(\mathbb{R}^N)$. We note that for any $(x_1, x_2) \in \mathbb{R}^{n_1+n_2}$, $f(x_1, x_2, \cdot) \in \mathcal{S}_\infty(\mathbb{R}^{n_3})$, the space of Schwartz functions with all vanishing moments. It follows from the classical almost-orthogonality estimate on $\mathbb{R}^{n_3}$ (see [Han et al. 2010, p. 2840]) that

$$|\widetilde{\psi}^{(3)}_{j_3} * f(x)| \lesssim 2^{-|j_3|L}(1+|x|)^{-M},$$

which implies

$$|\widetilde{\psi}_J * f(x)| \lesssim 2^{-|j_3|L} 2^{(|j_2|+|j_3|)M}(1+|x|)^{-M}. \tag{2-3}$$

Likewise, using the fact $f(x_1, \cdot, \cdot) \in \mathcal{S}_\infty(\mathbb{R}^{n_2+n_3})$ for any $x_1 \in \mathbb{R}^{n_1}$, we can derive

$$|\widetilde{\psi}_J * f(x)| \lesssim 2^{-|j_2|L} 2^{(|j_1|+|j_3|)M}(1+|x|)^{-M}. \tag{2-4}$$

We finally use $f \in \mathcal{S}_\infty(\mathbb{R}^N)$ to get

$$|\widetilde{\psi}_J * f(x)| \lesssim 2^{-|j_1|L} 2^{(|j_2|+|j_3|)M}(1+|x|)^{-M}. \tag{2-5}$$

Choosing $L > 100M$ in (2-3)–(2-5) and taking the geometric mean, (2-2) follows. □

The following almost orthogonality estimate will be frequently used in the subsequent part of this section. The proof follows directly from the one-parameter orthogonality estimate (see [Han et al. 2010]); see also [Nagel et al. 2012] for similar estimates on homogeneous groups.

Lemma 2.2. *Given positive integers L and M, there exists some constant $C = C(L, M) > 0$ such that*

$$|\psi_J * \varphi_{J'}(x)| \le C2^{-(|j_1-j_1'|+|j_2-j_2'|+|j_3-j_3'|)L} \prod_{i=1}^{3} \frac{\max_{1\le k\le i} 2^{(j_k\vee j_k')M}}{(\max_{1\le k\le i} 2^{j_k\vee j_k'} + |x_i|)^{n_i+M}},$$

where $\{\psi_J\}$ and $\{\varphi_{J'}\}$ are Schwartz functions satisfying (1-1).

Remark. The conclusion of Lemma 2.2 remains valid if the Schwartz functions $\{\psi^{(i)}\}$ and $\{\varphi^{(i)}\}$, where $i = 1, 2, 3$, have vanishing moments up to order M_0 (see Theorem 3.3 for choosing such an M_0). In such a case, the above inequality holds for any $M > 0$ and $L \le M_0 + 1$.

The following maximal function estimate is also frequently needed.

Lemma 2.3. *Let $J, J' \in \mathbb{Z}^3$, $R = Q_1 \times Q_2 \times Q_3 \in \mathcal{R}_{\mathcal{F}}^J$ and $M > 2N$. Then, for any $x, \bar{x} \in R$ and $\delta \in \big(\frac{N}{M}, 1\big]$, we have*

$$\sum_{R'\in\mathcal{R}_{\mathcal{F}}^{J'}} |R'| \Bigg[\prod_{i=1}^{3} \frac{\max_{1\le k\le i} 2^{(j_k\vee j_k')M}}{(\max_{1\le k\le i} 2^{(j_k\vee j_k')} + |\bar{x}_i - x_i'|)^{n_i+M}}\Bigg] |g(x')| \tag{2-6}$$
$$\le C\Bigg\{\prod_{i=1}^{3} [2^{3n_i(j_i-j_i')} \vee 1]\Bigg\}^{\frac{1}{\delta}-1} \Bigg\{\mathcal{M}_{\mathcal{F}}\Bigg[\Bigg(\sum_{R'\in\mathcal{R}_{\mathcal{F}}^{J'}} |g(x')|^2 \chi_{R'}\Bigg)^{\frac{\delta}{2}}\Bigg](x)\Bigg\}^{\frac{1}{\delta}}, \quad \forall\, x'\in R',$$

where C is a constant depending only on N and M.

Proof. The proof of this lemma is similar to the classical case. We fix an $x' \in R'$ for each $R' \in \mathcal{R}_{\mathcal{F}}^{J'}$. For $i = 1, 2, 3$, set

$$A_0^i = \{Q_i' : |\bar{x}_i - x_i'| \le \max_{1\le k\le i} 2^{(j_k\vee j_k')}\}$$

and

$$A_{r_i}^i = \Bigg\{Q_i' : 2^{r_i-1} < \frac{|\bar{x}_i - x_i'|}{\max_{1\le k\le i} 2^{(j_k\vee j_k')}} \le 2^{r_i}\Bigg\}, \quad \forall\, r_i \in \mathbb{Z}_+.$$

For any fixed $r = (r_1, r_2, r_3) \in \mathbb{N}^3$, for $i = 1, 2, 3$, we set

$$E_r = \big\{(w_1, w_2, w_3) \in \mathbb{R}^{n_1} \times \mathbb{R}^{n_2} \times \mathbb{R}^{n_3} : |w_i - \bar{x}_i| \le 2^{r_1\vee r_2\vee r_3} \max_{1\le k\le i} \{2^{(j_k\vee j_k')+1}\}\big\}.$$

Then for each $R' \in \mathcal{R}_{\mathcal{F}}^{J'}$, $R' \subset E_r$ for some triple $r = (r_1, r_2, r_3)$. Also, if $R' \in \mathscr{A}_r := A_{r_1}^1 \times A_{r_2}^2 \times A_{r_3}^3$, then $R' \subset E_r$. Obviously, $E_r \in \mathcal{R}_{\mathcal{F}}$ and $|E_r| \le C2^{(r_1\vee r_2\vee r_3)N} \prod_{i=1}^{3} \max_{1\le k\le i} 2^{n_i(j_k\vee j_k')}$. Hence, for any $\delta \in \big(\frac{N}{M}, 1\big]$, the left-hand side of (2-6) is dominated by

$$\sum_{R'\in\mathcal{R}^{J'}_{\mathcal{F}}}|R'|\biggl[\prod_{i=1}^{3}\frac{\max_{1\le k\le i}2^{(j_k\vee j_k')M}}{(\max_{1\le k\le i}2^{(j_k\vee j_k')}+|\bar{x}_i-x_i'|)^{n_i+M}}\biggr]|g(x')| \tag{2-7}$$

$$\le C\sum_{r\in\mathbb{N}^3}\biggl[\prod_{i=1}^{3}2^{-r_i(M+n_i)}(\max_{1\le k\le i}2^{-n_i(j_k\vee j_k')})\biggr]|R'|\biggl(\sum_{R'\in\mathscr{A}_r}|g(x')|^{\delta}\biggr)^{\frac{1}{\delta}}$$

$$= C\sum_{r\in\mathbb{N}^3}\biggl[\prod_{i=1}^{3}2^{-r_i(M+n_i)}(\max_{1\le k\le i}2^{-n_i(j_k\vee j_k')})\biggr]|R'|^{1-\frac{1}{\delta}}|E_r|^{\frac{1}{\delta}}$$

$$\times\biggl(\frac{1}{|E_r|}\int_{E_r}\sum_{R'\in\mathscr{A}_r}|g(x')|^{\delta}\chi_{R'}(y)\,dy\biggr)^{\frac{1}{\delta}},$$

where $C=2^{3M+N}$. For any $x\in R$, since $\bar{x}$ is also in R, we see that $|x_i-\bar{x}_i|\le 2^{j_i}$ for $i=1,2,3$; hence $x\in E_r$ for any $r\in\mathbb{N}^3$, by the definition of E_r. The expression in the last parentheses above is the average of the function $y\mapsto\sum_{R'\in\mathscr{A}_r}|g(x')|^{\delta}\chi_{R'}(y)$ over a flag rectangle E_r containing x, therefore being bounded by the flag maximal function $\mathcal{M}_{\mathcal{F}}\bigl(\sum_{R'\in\mathcal{R}^{J'}_{\mathcal{F}}}|g(x')|^{\delta}\chi_{R'}\bigr)(x)$. Hence we can continue the estimate in (2-7) as

$$\le C\biggl(\sum_{r\in\mathbb{N}^3}\prod_{i=1}^{3}2^{-r_i(M+n_i-\frac{N}{\delta})}\biggr)\biggl(\prod_{i=1}^{3}[2^{3n_i(j_i-j_i')}\vee 1]\biggr)^{\frac{1}{\delta}-1}\biggl(\mathcal{M}_{\mathcal{F}}\biggl(\sum_{R'\in\mathcal{R}^{J'}_{\mathcal{F}}}|g(x')|^{\delta}\chi_{R'}\biggr)(x)\biggr)^{\frac{1}{\delta}}$$

$$\le C'\biggl(\prod_{i=1}^{3}[2^{3n_i(j_i-j_i')}\vee 1]\biggr)^{\frac{1}{\delta}-1}\biggl(\mathcal{M}_{\mathcal{F}}\biggl(\sum_{R'\in\mathcal{R}^{J'}_{\mathcal{F}}}|g(x')|^{\delta}\chi_{R'}\biggr)(x)\biggr)^{\frac{1}{\delta}},$$

where C' depends only on M and N. This completes the proof of Lemma 2.3. □

For $x=(x_1,x_2,x_3)\in\mathbb{R}^{n_1}\times\mathbb{R}^{n_2}\times\mathbb{R}^{n_3}$, we denote $x^1=x\in\mathbb{R}^{N_1}$, $x^2=(x_2,x_3)\in\mathbb{R}^{N_2}$ and $x^3=x_3\in\mathbb{R}^{N_3}$. For $i=1,2,3$, write $x=(\bar{x}^i,x^i)\in\mathbb{R}^{N-N_i}\times\mathbb{R}^{N_i}$. We say that $w\in A_p^{(i)}(\mathbb{R}^N)$ if $w(\bar{x}^i,\cdot)$ is a classical $A_p(\mathbb{R}^{N_i})$ uniformly in $\bar{x}^i$; that is,

$$\operatorname*{ess\,sup}_{\bar{x}^i\in\mathbb{R}^{N-N_i}}\ \sup_{Q\subset R^{N_i}}\biggl(\frac{1}{|Q|}\int_Q w(\bar{x}^i,x^i)dx^i\biggr)\biggl(\frac{1}{|Q|}\int_Q w(\bar{x}^i,x^i)^{-1/(p-1)}dx^i\biggr)^{p-1}<\infty.$$

Let $\mathcal{M}_i$ denote the Hardy–Littlewood maximal operator on $\mathbb{R}^{N_i}$. The *lifted maximal operator* $\widetilde{\mathcal{M}}_i$ on $\mathbb{R}^N$ was introduced in [Nagel et al. 2012] by

$$\widetilde{\mathcal{M}}_i:=\delta_{\mathbb{R}^{N-N_i}}\otimes\mathcal{M}_i,$$

where $\delta_{\mathbb{R}^{N-N_i}}$ is the Dirac mass at $0\in\mathbb{R}^{N-N_i}$.

The following result was proved in [Wu 2014a].

Lemma 2.4. *Let* $1 < p < \infty$ *and* w *be a weight function. Then the following statements are equivalent*:

(i) $w \in A_p^{\mathcal{F}}(\mathbb{R}^N)$.

(ii) $w \in A_p^{(1)} \cap A_p^{(2)} \cap A_p^{(3)}(\mathbb{R}^N)$.

(iii) $\widetilde{\mathcal{M}}_3 \circ \widetilde{\mathcal{M}}_2 \circ \widetilde{\mathcal{M}}_1$ *is bounded on* $L_w^p(\mathbb{R}^N)$.

(iv) $\mathcal{M}_{\mathcal{F}}$ *is bounded on* $L_w^p(\mathbb{R}^N)$.

Using Lemma 2.4 and applying Rubio de Francia's extrapolation (see [García-Cuerva and Rubio de Francia 1985]), one can easily obtain the following weighted Fefferman–Stein vector-valued inequality.

Corollary 2.5. *Let* $w \in A_p^{\mathcal{F}}(\mathbb{R}^N)$ *and* $\{f_j\}_{j\in\mathbb{Z}} \in L_w^p(\ell^q)$. *Then, for all* $1 < p, q < \infty$,

$$\int_{\mathbb{R}^N} |\{\mathcal{M}_{\mathcal{F}}(\{f_j\})(x)\}|_{\ell^q}^p w(x)dx \le C \int_{\mathbb{R}^N} |\{f_j(x)\}|_{\ell^q}^p w(x)dx,$$

where $|\cdot|_{\ell^q}$ *means the classical* ℓ^q*-norm.*

We now are ready to prove Theorem 1.4.

Proof of Theorem 1.4. Let $f \in \mathcal{S}'_{\mathcal{F}}(\mathbb{R}^N)$ and $w \in A_\infty^{\mathcal{F}}(\mathbb{R}^N)$. In what follows, we use $a \wedge b$ to represent $\min\{a, b\}$. Denote $x_R = 2^J \ell$ and $x_{R'} = 2^{J'}\ell'$. Applying Theorem 2.1, Lemma 2.2 with

$$M > N[((q_w/p) + 1) \vee 2]$$

and $L = 10M$ and Lemma 2.3, we obtain that, for $\frac{N}{M} < \delta < \big(\frac{p}{q_w} \wedge 1\big)$ and for any $x \in R$,

$$\begin{aligned}
&|(\psi_J * f)(x_R)| \\
&\quad\approx \Big|\sum_{J'\in\mathbb{Z}^3}\sum_{R'\in\mathcal{R}_{\mathcal{F}}^{J'}} |R'|\psi_J * \varphi_{J'}(x_R - x_{R'})\varphi_J * f(x_{R'})\Big| \\
&\quad\lesssim \sum_{J'\in\mathbb{Z}^3} 2^{-(|j_1-j_1'|+|j_2-j_2'|+|j_3-j_3'|)L} \\
&\qquad\times \sum_{R'\in\mathcal{R}_{\mathcal{F}}^{J'}} |R'|\Bigg[\prod_{i=1}^{3} \frac{\max_{1\le k\le i} 2^{(j_k\vee j_k')M}}{(\max_{1\le k\le i} 2^{(j_k\vee j_k')} + |x_{Q_i} - x_{Q_i'}|)^{n_i+M}}\Bigg]|\varphi_{J'} * f(x_{R'})| \\
&\quad\lesssim \sum_{J'\in\mathbb{Z}^3} 2^{-(|j_1-j_1'|+|j_2-j_2'|+|j_3-j_3'|)L'}\Bigg\{\mathcal{M}_{\mathcal{F}}\Bigg[\Bigg(\sum_{R'\in\mathcal{R}_{\mathcal{F}}^{J'}} |\varphi_{J'} * f(x_{R'})|^2\chi_{R'}\Bigg)^{\frac{\delta}{2}}\Bigg](x)\Bigg\}^{\frac{1}{\delta}},
\end{aligned}$$

where $L' = L - 3N(1/\delta - 1) > 7M > 0$.

Squaring both sides, then multiplying χ_R, summing over all $J \in \mathbb{Z}^3$ and $R \in \mathcal{R}_{\mathcal{F}}^J$, and finally applying Hölder's inequality, for all $x \in \mathbb{R}^N$ and $\frac{N}{M} < \delta < \left(\frac{p}{q_w} \wedge 1\right)$,

$$\begin{aligned}
&\sum_{J\in\mathbb{Z}^3}\sum_{R\in\mathcal{R}_{\mathcal{F}}^J} |\psi_J * f(x_R)|^2\chi_R \\
&\quad\lesssim \sum_{J\in\mathbb{Z}^3}\Big\{\sum_{J'\in\mathbb{Z}^3} 2^{-(|j_1-j_1'|+|j_2-j_2'|+|j_3-j_3'|)L'}\Big\} \\
&\qquad\times\Big\{\sum_{J'\in\mathbb{Z}^3} 2^{-(|j_1-j_1'|+|j_2-j_2'|+|j_3-j_3'|)L'}\Big\{\mathcal{M}_{\mathcal{F}}\Big[\Big(\sum_{R'\in\mathcal{R}_{\mathcal{F}}^{J'}} |\varphi_{J'} * f(x_{R'})|^2\chi_{R'}\Big)^{\frac{\delta}{2}}\Big](x)\Big\}^{\frac{2}{\delta}}\Big\} \\
&\quad\lesssim \sum_{J'\in\mathbb{Z}^3}\Big\{\mathcal{M}_{\mathcal{F}}\Big[\Big(\sum_{R'\in\mathcal{R}_{\mathcal{F}}^{J'}} |\varphi_{J'} * f(x_{R'})|^2\chi_{R'}\Big)^{\frac{\delta}{2}}\Big](x)\Big\}^{\frac{2}{\delta}},
\end{aligned}$$

where we used the estimates

$$\sum_{J'\in\mathbb{Z}^3} 2^{-(|j_1-j_1'|+|j_2-j_2'|+|j_3-j_3'|)L'} \le C \quad\text{and}\quad \sum_{J\in\mathbb{Z}^3} 2^{-(|j_1-j_1'|+|j_2-j_2'|+|j_3-j_3'|)L'} \le C$$

in the last inequality. Note that $(2 \wedge p)/\delta > q_w$ implies $w \in A^{\mathcal{F}}_{p/\delta}(\mathbb{R}^N)$. Applying Corollary 2.5 with $L_w^{p/\delta}(\ell^{2/\delta})$ yields

$$\Big\|\Big\{\sum_{J\in\mathbb{Z}^3}\sum_{R\in\mathcal{R}_{\mathcal{F}}^J} |\psi_J * f(x_R)|^2\chi_R\Big\}^{\frac{1}{2}}\Big\|_{L_w^p(\mathbb{R}^N)} \lesssim \Big\|\Big\{\sum_{J\in\mathbb{Z}^3}\sum_{R\in\mathcal{R}_{\mathcal{F}}^J} |\varphi_J * f(x_R)|^2\chi_R\Big\}^{\frac{1}{2}}\Big\|_{L_w^p(\mathbb{R}^N)}.$$

The converse inequality follows by symmetry. □

As a consequence of Theorem 1.4, we obtain a density result of $H^p_{\mathcal{F},w}$ which will be useful to show the $H^p_{\mathcal{F},w} \to L^p_w$ boundedness of operators, the weak density of $CMO^p_{\mathcal{F},w}$ and the Calderón–Zygmund decomposition for $H^p_{\mathcal{F},w}$.

Corollary 2.6. *Let $0 < p < \infty$ and $w \in A^{\mathcal{F}}_\infty(\mathbb{R}^N)$. Then $\mathcal{S}_{\mathcal{F}}(\mathbb{R}^N)$ is dense in $H^p_{\mathcal{F},w}(\mathbb{R}^N)$ and, in consequence, $L^2(\mathbb{R}^N) \cap H^p_{\mathcal{F},w}(\mathbb{R}^N)$ is dense in $H^p_{\mathcal{F},w}(\mathbb{R}^N)$.*

Proof. Let $f \in H^p_{\mathcal{F},w}(\mathbb{R}^N)$. For any fixed $L > 0$, denote

$$\mathscr{E}_L = \{(J, R) : |j_1|, |j_2|, |j_3| \le L,\ R \in \mathcal{R}^J_{\mathcal{F}},\ R \subset B(0, L)\}$$

and

$$f_L(x) = \sum_{(J,R)\in\mathscr{E}_L} |R|\psi_J(x - x_R)\psi_J * f(x_R).$$

Since f_L is a finite linear combination of $\psi_J(\cdot - x_R) \in \mathcal{S}_{\mathcal{F}}(\mathbb{R}^N)$, it is obvious that $f_L \in \mathcal{S}_{\mathcal{F}}(\mathbb{R}^N)$. Repeating the proof of Theorem 1.4, we conclude that $\|f_L\|_{H^p_{\mathcal{F},w}(\mathbb{R}^N)} \lesssim \|f\|_{H^p_{\mathcal{F},w}(\mathbb{R}^N)}$.

To see that f_L tends to f in $H^p_{\mathcal{F},w}(\mathbb{R}^N)$, we use the discrete Calderón reproducing formula to write

$$[g_{\mathcal{F}}(f-f_L)(x)]^2 = \sum_{J'\in\mathbb{Z}^3}\sum_{R'\in\mathcal{R}^{J'}_{\mathcal{F}}}\Big|\sum_{(J,R)\in\mathscr{E}^c_L}|R|(\psi_{J'}*\psi_J)(x_{R'}-x_R)(\psi_J*f)(x_R)\Big|^2\chi_{R'}(x).$$

Now repeating the same argument as in the proof of Theorem 1.4, we get

$$\|g_{\mathcal{F}}(f-f_L)\|_{L^p_w(\mathbb{R}^N)} \lesssim \bigg\|\bigg\{\sum_{(J,R)\in\mathscr{E}^c_L}|(\psi_J*f)(x_R)|^2\chi_R\bigg\}^{\frac{1}{2}}\bigg\|_{L^p_w(\mathbb{R}^N)},$$

where the last term tends to 0 as L goes to infinity. This implies that f_L tends to f in $H^p_{\mathcal{F},w}(\mathbb{R}^N)$ and hence the proof is finished. □

We follow the classical case (see [Stein 1993; García-Cuerva and Rubio de Francia 1985]) to get the following lemma.

Lemma 2.7. *Suppose $w\in A^{\mathcal{F}}_\infty(\mathbb{R}^n)$ and $q>q_w$. There exist $0<\delta<1<q<\infty$ such that, for all flag rectangles R and all measurable subsets A of R,*

$$\left(\frac{|A|}{|R|}\right)^q \lesssim \frac{w(A)}{w(R)} \lesssim \left(\frac{|A|}{|R|}\right)^\delta.$$

In particular, the measure $w(x)dx$ is doubling with respect to flag rectangles.

Lemma 2.8. *Let $w\in A^{\mathcal{F}}_\infty(\mathbb{R}^N)$. Then, for all flag rectangles R and R' and for $q>q_w$,*

$$\frac{w(R')}{w(R)} \lesssim \prod_{i=1}^3\left(\frac{|Q_i|}{|Q'_i|}\vee\frac{|Q'_i|}{|Q_i|}\right)^q\left(1+\frac{|x_{Q_i}-x_{Q'_i}|}{\ell(Q_i)\vee\ell(Q'_i)}\right)^{n_iq}.$$

Proof. Observe that $Q'_i\subset A_iQ_i$, $i=1,2,3$, where

$$A_i = C[\ell(Q_i)\vee\ell(Q'_i)+|x_{Q_i}-x_{Q'_i}|]/\ell(Q_i).$$

This implies $R'\subset\bar{R}$, where $\bar{R}=C[(A_1Q_1)\times(A_2Q_2)\times(A_3Q_3)]$. By Lemma 2.7, for any $q>q_w$,

$$\begin{aligned}\frac{w(R')}{w(R)} \le \frac{w(\bar{R})}{w(R)} \lesssim \left[\frac{|\bar{R}|}{|R|}\right]^q &\lesssim \prod_{i=1}^3\left[\frac{\ell(Q_i)\vee\ell(Q'_i)+|x_{Q_i}-x_{Q'_i}|}{\ell(Q_i)}\right]^{n_iq}\\ &\lesssim \prod_{i=1}^3\left[\frac{|Q_i|}{|Q'_i|}\vee\frac{|Q'_i|}{|Q_i|}\right]^q\left[1+\frac{|x_{Q_i}-x_{Q'_i}|}{\ell(Q_i)\vee\ell(Q'_i)}\right]^{n_iq}.\end{aligned}$$

Hence the proof is concluded. □

We now prove Theorem 1.6.

Proof of Theorem 1.6. For $R \in \mathcal{R}_{\mathcal{F}}^{J}$ and $R' \in \mathcal{R}_{\mathcal{F}}^{J'}$, set

$$S_R = |\psi_J * f(x_R)|^2 \quad \text{and} \quad T_{R'} = |\varphi_{J'} * f(x_{R'})|^2.$$

Theorem 2.1 and Lemma 2.2 yield

$$\begin{aligned}
S_R^{\frac{1}{2}} &= \Bigg| \sum_{J' \in \mathbb{Z}^3} \sum_{R' \in \mathcal{R}_{\mathcal{F}}^{J'}} |R'| \varphi_{J'} * f(x_{R'}) \psi_J * \varphi_{J'}(x_R - x_{R'}) \Bigg| \\
&\lesssim \sum_{J' \in \mathbb{Z}^3} \sum_{R' \in \mathcal{R}_{\mathcal{F}}^{J'}} 2^{-(|j_1-j_1'|+|j_2-j_2'|+|j_3-j_3'|)NL} |R'| \\
&\qquad \times \Bigg[\prod_{i=1}^{3} \frac{\max_{1\le k\le i} 2^{(j_k \vee j_k')M}}{(\max_{1\le k\le i} 2^{(j_k \vee j_k')} + |x_{Q_i} - x_{Q_i'}|)^{n_i+M}} \Bigg] |\varphi_{J'} * f(x_{R'})| \\
&\lesssim \sum_{J' \in \mathbb{Z}^3} \sum_{R' \in \mathcal{R}_{\mathcal{F}}^{J'}} r(R, R') P(R, R') T_{R'}^{\frac{1}{2}},
\end{aligned}$$

where

$$r(R, R') := \prod_{i=1}^{3} \Bigg[\frac{|Q_i|}{|Q_i'|} \wedge \frac{|Q_i'|}{|Q_i|} \Bigg]^L$$

and

$$P(R, R') := \prod_{i=1}^{3} \Bigg(1 + \frac{|x_{Q_i} - x_{Q_i'}|}{\max_{1\le k\le i}[\ell(Q_k) \vee \ell(Q_k')]} \Bigg)^{-n_i-M}.$$

Squaring both sides, multiplying by $|R|^2/w(R)$, adding up all the terms over $J \in \mathbb{Z}^3$, $R \in \mathcal{R}_{\mathcal{F}}^{J}$, $R \subset \Omega$ and applying Hölder's inequality, we obtain

$$\begin{aligned}
&\sup_{\Omega} \Bigg\{ \frac{1}{[w(\Omega)]^{2/p-1}} \sum_{\substack{R \in \mathcal{R}_{\mathcal{F}}^{d},\\ R \subset \Omega}} |R|^2 w(R)^{-1} S_R \Bigg\} \\
&\quad \lesssim \sup_{\Omega} \Bigg\{ \frac{1}{[w(\Omega)]^{2/p-1}} \sum_{\substack{R \in \mathcal{R}_{\mathcal{F}}^{d},\\ R \subset \Omega}} |R|^2 w(R)^{-1} \Bigg[\sum_{R' \in \mathcal{R}_{\mathcal{F}}^{d}} r(R, R') P(R, R') \Bigg] \\
&\qquad \times \Bigg[\sum_{R' \in \mathcal{R}_{\mathcal{F}}^{d}} r(R, R') P(R, R') T_{R'} \Bigg] \Bigg\} \\
&\quad \lesssim \sup_{\Omega} \Bigg\{ \frac{1}{[w(\Omega)]^{2/p-1}} \sum_{\substack{R \in \mathcal{R}_{\mathcal{F}}^{d},\\ R \subset \Omega}} \sum_{R' \in \mathcal{R}_{\mathcal{F}}^{d}} |R|^2 w(R)^{-1} r(R, R') P(R, R')) T_{R'} \Bigg\}.
\end{aligned}$$

Here and hereafter, we use $\sum_{R\in\mathcal{R}^d_{\mathcal{F}}}$ to denote $\sum_{J\in\mathbb{Z}^3}\sum_{R\in\mathcal{R}^J_{\mathcal{F}}}$ and similarly for $\sum_{R'\in\mathcal{R}^d_{\mathcal{F}}}$. Applying Lemma 2.8, we get

$$\sup_{\Omega}\left\{\frac{1}{[w(\Omega)]^{2/p-1}}\sum_{\substack{R\in\mathcal{R}^d_{\mathcal{F}},\\ R\subset\Omega}}|R|^2w(R)^{-1}S_R\right\} \lesssim \sup_{\Omega}\left\{\frac{1}{[w(\Omega)]^{2/p-1}}\sum_{\substack{R\in\mathcal{R}^d_{\mathcal{F}},\\ R\subset\Omega}}\sum_{R'\in\mathcal{R}^d_{\mathcal{F}}}|R'|^2w(R')^{-1}\tilde{r}(R,R')\widetilde{P}(R,R'))T_{R'}\right\}. \tag{2-8}$$

Here the definition of $\tilde{r}(R,R')$ and $\widetilde{P}(R,R')$ are defined as $r(R,R')$ and $P(R,R')$ with smaller L and M. Since L and M can be chosen arbitrarily large, in what follows, we still use $r(R,R')$ and $P(R,R')$ to denote $\tilde{r}(R,R')$ and $\widetilde{P}(R,R')$, respectively.

To finish the proof, it suffices to show the right-hand side of (2-8) is bounded by

$$C\sup_{\bar{\Omega}}\left\{\frac{1}{[w(\bar{\Omega})]^{2/p-1}}\sum_{\substack{R'\in\mathcal{R}^d_{\mathcal{F}},\\ R'\subset\bar{\Omega}}}|R'|^2w(R')^{-1}T_{R'}\right\}.$$

We point out that $r(R,R')$ and $P(R,R')$ characterize the geometrical properties between two flag rectangles R and R'. Namely, when the difference of the sizes of R and R' grows bigger, $r(R,R')$ becomes smaller; when the distance between R and R' gets larger, $P(R,R')$ becomes smaller. The following argument is quite geometric. More precisely, we shall first decompose the set of dyadic flag rectangles $\{R'\}$ into annuli according to the distance of R and R'. Next, in each annulus, precise estimates are given by considering the difference of the sizes of R and R'. Finally, add up all the estimates in each annulus to finish the proof.

We now turn to details. For $J=(j_1,j_2,j_3)\in\mathbb{N}^3$ and $R\in\mathcal{R}^d_{\mathcal{F}}$, denote

$$R_J=R_{j_1,j_2,j_3}=(2^{j_1}Q_1)\times(2^{j_1\vee j_2}Q_2)\times(2^{j_1\vee j_2\vee j_3}Q_3),\quad \Omega^J=\Omega^{j_1,j_2,j_3}=\bigcup_{R\subset\Omega}3R_J.$$

For any flag rectangle $R\subset\Omega$ and $J=(j_1,j_2,j_3)\in\mathbb{Z}^3_+$, let

$$\mathscr{A}_{0,0,0}(R)=\{R':3R'_{0,0,0}\cap 3R\neq\varnothing\},$$

$$\mathscr{A}_{j_1,0,0}(R)=\{R':3R'_{j_1,0,0}\cap 3R\neq\varnothing \text{ and } 3R'_{j_1-1,0,0}\cap 3R=\varnothing\},$$

$$\mathscr{A}_{0,j_2,0}(R)=\{R':3R'_{0,j_2,0}\cap 3R\neq\varnothing \text{ and } 3R'_{0,j_2-1,0}\cap 3R=\varnothing\},$$

$$\mathscr{A}_{0,0,j_3}(R)=\{R':3R'_{0,0,j_3}\cap 3R\neq\varnothing \text{ and } R'_{0,0,j_3-1}\cap 3R=\varnothing\},$$

$$\mathscr{A}_{j_1,j_2,0}(R)=\{R':3R'_{j_1,j_2,0}\cap 3R\neq\varnothing,\ 3R'_{j_1-1,j_2,0}\cap 3R=\varnothing \text{ and } 3R'_{j_1,j_2-1,0}\cap 3R=\varnothing\},$$

$$\mathscr{A}_{j_1,0,j_3}(R)=\{R':3R'_{j_1,0,j_3}\cap 3R\neq\varnothing,\ 3R'_{j_1-1,0,j_3}\cap 3R=\varnothing \text{ and } 3R'_{j_1,0,j_3-1}\cap 3R=\varnothing\},$$

$$\mathscr{A}_{0,j_2,j_3}(R) = \{R' : 3R'_{0,j_2,j_3} \cap 3R \neq \varnothing,\ 3R'_{0,j_2-1,j_3} \cap 3R = \varnothing \text{ and } 3R'_{0,j_2,j_3-1} \cap 3R = \varnothing\},$$

$$\mathscr{A}_{j_1,j_2,j_3}(R) = \{R' : 3R'_{j_1,j_2,j_3} \cap 3R \neq \varnothing,\ 3R'_{j_1-1,j_2,j_3} \cap 3R = \varnothing, 3R'_{j_1,j_2-1,j_3} \cap 3R = \varnothing \text{ and } 3R'_{j_1,j_2,j_3-1} \cap 3R = \varnothing\},$$

where all R' are dyadic flag rectangles.

Let $R \subset \Omega$ be any fixed dyadic flag rectangle. For any flag rectangle R', there exists a $J \in \mathbb{N}^3$ such that $R' \in \mathscr{A}_J(R)$, where $\mathscr{A}_J(R)$ represents one of the sets defined above; therefore $\mathcal{R}^d_{\mathcal{F}} = \bigcup_{J \in \mathbb{N}^3} \mathscr{A}_J(R)$. Hence,

$$\begin{aligned}
&\frac{1}{[w(\Omega)]^{\frac{2}{p}-1}} \sum_{\substack{R \in \mathcal{R}^d_{\mathcal{F}},\\ R \subset \Omega}} \sum_{R' \in \mathcal{R}^d_{\mathcal{F}}} |R'|^2 w(R')^{-1} r(R,R') P(R,R') T_{R'} \\
&\leq \frac{1}{[w(\Omega)]^{\frac{2}{p}-1}} \sum_{\substack{R \in \mathcal{R}^d_{\mathcal{F}},\\ R \subset \Omega}} \sum_{R' \in \mathscr{A}_{0,0,0}(R)} |R'|^2 w(R')^{-1} r(R,R') P(R,R') T_{R'} \\
&\quad + \sum_{j_1 \in \mathbb{Z}_+} \frac{1}{[w(\Omega)]^{\frac{2}{p}-1}} \sum_{\substack{R \in \mathcal{R}^d_{\mathcal{F}},\\ R \subset \Omega}} \sum_{R' \in \mathscr{A}_{j_1,0,0}(R)} |R'|^2 w(R')^{-1} r(R,R') P(R,R') T_{R'} \\
&\quad + \sum_{j_2 \in \mathbb{Z}_+} \frac{1}{[w(\Omega)]^{\frac{2}{p}-1}} \sum_{\substack{R \in \mathcal{R}^d_{\mathcal{F}},\\ R \subset \Omega}} \sum_{R' \in \mathscr{A}_{0,j_2,0}(R)} |R'|^2 w(R')^{-1} r(R,R') P(R,R') T_{R'} \\
&\quad + \sum_{j_3 \in \mathbb{Z}_+} \frac{1}{[w(\Omega)]^{\frac{2}{p}-1}} \sum_{\substack{R \in \mathcal{R}^d_{\mathcal{F}},\\ R \subset \Omega}} \sum_{R' \in \mathscr{A}_{0,0,j_3}(R)} |R'|^2 w(R')^{-1} r(R,R') P(R,R') T_{R'} \\
&\quad + \sum_{j_1,j_2 \in \mathbb{Z}_+} \frac{1}{[w(\Omega)]^{\frac{2}{p}-1}} \sum_{\substack{R \in \mathcal{R}^d_{\mathcal{F}},\\ R \subset \Omega}} \sum_{R' \in \mathscr{A}_{j_1,j_2,0}(R)} |R'|^2 w(R')^{-1} r(R,R') P(R,R') T_{R'} \\
&\quad + \sum_{j_1,j_3 \in \mathbb{Z}_+} \frac{1}{[w(\Omega)]^{\frac{2}{p}-1}} \sum_{\substack{R \in \mathcal{R}^d_{\mathcal{F}},\\ R \subset \Omega}} \sum_{R' \in \mathscr{A}_{j_1,0,j_3}(R)} |R'|^2 w(R')^{-1} r(R,R') P(R,R') T_{R'} \\
&\quad + \sum_{j_2,j_3 \in \mathbb{Z}_+} \frac{1}{[w(\Omega)]^{\frac{2}{p}-1}} \sum_{\substack{R \in \mathcal{R}^d_{\mathcal{F}},\\ R \subset \Omega}} \sum_{R' \in \mathscr{A}_{0,j_2,j_3}(R)} |R'|^2 w(R')^{-1} r(R,R') P(R,R') T_{R'} \\
&\quad + \sum_{j_1,j_2,j_3 \in \mathbb{Z}_+} \frac{1}{[w(\Omega)]^{\frac{2}{p}-1}} \sum_{\substack{R \in \mathcal{R}^d_{\mathcal{F}},\\ R \subset \Omega}} \sum_{R' \in \mathscr{A}_{j_1,j_2,j_3}(R)} |R'|^2 w(R')^{-1} r(R,R') P(R,R') T_{R'} \\
&:= I + II + III + IV + V + VI + VII + VIII.
\end{aligned}$$

In the sequel, we always assume $R, R' \in \mathcal{R}^d_{\mathcal{F}}$. To estimate I, we denote $\mathscr{B}_{0,0,0} = \{R' : 3R' \cap \Omega^{0,0,0} \neq \varnothing\}$. For any $R' \notin \mathscr{B}_{0,0,0}$, we have $3R' \cap \Omega^{0,0,0} = \varnothing$. This implies that $3R' \cap 3R = \varnothing$ for every $R \subset \Omega$ and thus $R' \notin \mathscr{A}_{0,0,0}(R)$. This shows that $\bigcup_{R\subset\Omega} \mathscr{A}_{0,0,0}(R) \subset \mathscr{B}_{0,0,0}$. Hence

$$I \leq \frac{1}{[w(\Omega)]^{\frac{2}{p}-1}} \sum_{R' \in \mathscr{B}_{0,0,0}} \sum_{\substack{R: R\subset\Omega \\ R' \in \mathscr{A}_{0,0,0}(R)}} |R'|^2 w(R')^{-1} r(R, R') P(R, R') T_{R'}.$$

For each integer $h \geq 1$, let $\mathscr{F}_h^{0,0,0} = \{R' \in \mathscr{B}_{0,0,0}, |3R' \cap \Omega^{0,0,0}| \geq 1/2^h |3R'|\}$, $\mathscr{D}_h^{0,0,0} = \mathscr{F}_h^{0,0,0} \backslash \mathscr{F}_{h-1}^{0,0,0}$ and $\Omega_h^{0,0,0} = \bigcup_{R' \in \mathscr{D}_h^{0,0,0}} R'$. Note that $\mathscr{B}_{0,0,0} = \bigcup_{h \geq 1} \mathscr{D}_h^{0,0,0}$ and that $P(R, R') \leq 1$ for any R, R'. Thus

$$I \leq \frac{1}{[w(\Omega)]^{\frac{2}{p}-1}} \sum_{h\geq 1} \sum_{R' \subset \Omega_h^{0,0,0}} |R'|^2 w(R')^{-1} T_{R'} \sum_{\substack{R: R\subset\Omega, \\ R' \in \mathscr{A}_{0,0,0}(R)}} r(R, R').$$

Note that for $x \in \Omega_h^{0,0,0}$, there exists a dyadic flag rectangle $R \subset \Omega_h^{0,0,0}$ such that $x \in R$. Therefore $\mathcal{M}_{\mathcal{F}}(\chi_{\Omega^{0,0,0}})(x) \geq |3R' \cap \Omega^{0,0,0}|/|3R'| \geq 2^{-h}$. For $q \in (q_w, pL/(2-p))$, we apply the $L^q_w(\mathbb{R}^N)$ boundedness of $\mathcal{M}_{\mathcal{F}}$ and Lemma 2.7 to obtain

$$w(\Omega_h^{0,0,0}) \leq w(\{x : \mathcal{M}_{\mathcal{F}}(\chi_{\Omega^{0,0,0}})(x) \geq 2^{-h}\}) \lesssim 2^{hq} w(\Omega^{0,0,0}) \lesssim 2^{hq} w(\Omega).$$

We claim that if L is sufficiently large, there is a sequence $\{\sigma_1(h)\}_{h\geq 1}$ such that

$$\sum_{\substack{R: R\subset\Omega, \\ R' \in \mathscr{A}_{0,0,0}(R)}} r(R, R') \lesssim \sigma_1(h) \quad \text{and} \quad \sum_{h\geq 1} \sigma_1(h) 2^{hq\left(\frac{2}{p}-1\right)} \lesssim 1. \tag{2-9}$$

Assume this claim holds for the moment, we can conclude the proof for I as follows.

$$\begin{aligned}
I &\lesssim \frac{1}{[w(\Omega)]^{\frac{2}{p}-1}} \sum_{h\geq 1} \sum_{R' \subset \Omega_h^{0,0,0}} \sigma_1(h) \frac{|R'|^2}{w(R')} T_{R'} \\
&\lesssim \frac{1}{[w(\Omega)]^{\frac{2}{p}-1}} \sum_{h\geq 1} \sigma_1(h) [w(\Omega_h^{0,0,0})]^{\frac{2}{p}-1} \frac{1}{[w(\Omega_h^{0,0,0})]^{\frac{2}{p}-1}} \sum_{R' \subset \Omega_h^{0,0,0}} \frac{|R'|^2}{w(R')} T_{R'} \\
&\lesssim \frac{1}{[w(\Omega)]^{\frac{2}{p}-1}} \sum_{h\geq 1} \sigma_1(h) (2^{hq})^{\frac{2}{p}-1} [w(\Omega)]^{\frac{2}{p}-1} \left(\sup_{\bar{\Omega}} \frac{1}{[w(\bar{\Omega})]^{\frac{2}{p}-1}} \sum_{R' \subset \bar{\Omega}} \frac{|R'|^2}{w(R')} T_{R'} \right) \\
&\lesssim \sup_{\bar{\Omega}} \frac{1}{[w(\bar{\Omega})]^{\frac{2}{p}-1}} \sum_{R' \subset \bar{\Omega}} \frac{|R'|^2}{w(R')} T_{R'}.
\end{aligned}$$

It is sufficient to show claim (2-9). Note that $R' \in \mathscr{A}_{0,0,0}(R)$ implies $3R \cap 3R' \neq \varnothing$. Using an idea of Chang and R. Fefferman [1980], for each R, we consider the following eight cases:

Case 1: $|Q_1'| \geq |Q_1|,\ |Q_2'| \geq |Q_2|,\ |Q_3'| \geq |Q_3|$.

Case 2: $|Q_1'| \geq |Q_1|,\ |Q_2'| \geq |Q_2|,\ |Q_3'| < |Q_3|$.

Case 3: $|Q_1'| \geq |Q_1|,\ |Q_2'| < |Q_2|,\ |Q_3'| \geq |Q_3|$.

Case 4: $|Q_1'| < |Q_1|,\ |Q_2'| \geq |Q_2|,\ |Q_3'| \geq |Q_3|$.

Case 5: $|Q_1'| \geq |Q_1|,\ |Q_2'| < |Q_2|,\ |Q_3'| < |Q_3|$.

Case 6: $|Q_1'| < |Q_1|,\ |Q_2'| \geq |Q_2|,\ |Q_3'| < |Q_3|$.

Case 7: $|Q_1'| < |Q_1|,\ |Q_2'| < |Q_2|,\ |Q_3'| \geq |Q_3|$.

Case 8: $|Q_1'| < |Q_1|,\ |Q_2'| < |Q_2|,\ |Q_3'| < |Q_3|$.

It suffices to verify (2-9) in each case.

We first consider Case 1. In this case,

$$|R| \leq |3R \cap 3R'| \leq |3R' \cap \Omega^{0,0,0}| \leq 2^{1-h}|3R'| \leq 2^{2N+1-h}|R'|,$$

which implies that $|R'| = 2^{h-1-2N+\theta}|R|$ for some integer $\theta \geq 0$. For each fixed θ, the number of such R's must be less than $C(\theta+h)^N 2^{\theta+h}$. Consequently,

$$\sum_{R \in \text{Case 1}} r(R, R') \leq C \sum_{\theta \geq 0} \left(\frac{1}{2^{\theta+h}}\right)^L (\theta+h)^N 2^{\theta+h} \leq C 2^{-hL'},$$

where $L' = L - (N+1) > 0$. This gives (2-9) with $\sigma_1(h) = 2^{-hL'}$.

We next deal with Case 2. We have

$$|3R'||Q_1 \times Q_2|/(2^{2N}|Q_1' \times Q_2'|) \leq |3R \cap 3R'| \leq 2^{1-h}|3R'|,$$

which implies that $|Q_1' \times Q_2'| = 2^{h+\theta-1-2N}|Q_1 \times Q_2|$ for some integer $\theta \geq 0$. For each fixed θ, the number of such $Q_1 \times Q_2$'s must be less than $C(\theta+h)^N \cdot 2^{\theta+h}$. Similarly, $|Q_3| = 2^{\lambda}|Q_3'|$ for some $\lambda \geq 0$. For each λ, $3Q_3 \cap 3Q_3' \neq \varnothing$ implies that the number of such Q_3's is less than 5^N. It follows that

$$\sum_{R \in \text{Case 2}} r(R, R') \lesssim \sum_{\theta \geq 0} \sum_{\lambda \geq 0} \left(\frac{1}{2^{\theta+h+\lambda}}\right)^L (\theta+h)^N 2^{\theta+h} \lesssim 2^{-hL'},$$

which verifies (2-9) with $\sigma_1(h) = 2^{-hL'}$. Cases 3 and 4 can be handled by symmetry.

For Case 5, by the same argument as in Case 2, we get $|Q_1'| = 2^{h+\theta'-1-2N}|Q_1|$ and $|Q_2 \times Q_3| = 2^{\lambda'}|Q_2' \times Q_3'|$ for some $\theta',\ \lambda' \geq 0$. Moreover, for each θ' and λ', the number of Q_1's is less than $C(\theta+h)^N \cdot 2^{\theta+h}$, and the number of $Q_2 \times Q_3$ less than C. Then (2-9) follows in the same way as in Case 2. Cases 6 and 7 can be treated similarly.

For Case 8, we have

$$|R'| \le |3R\cap 3R'| \le |3R'\cap \Omega^{0,0,0}| \le 2^{1-h}|3R'| \le 2^{1-h+2N}|R'|,$$

which implies $h \le 2N+1$. Since in this case $|R'|\le |R|$, we have $|R| = 2^\theta |R'|$ for some integer $\theta \ge 0$. For each fixed θ, the number of such R's must be less than 5^N. Therefore,

$$\sum_{R\in \text{Case } 8} r(R,R') \lesssim \chi_{\mathbb{Z}\cap(0,2N+1]}(h)\sum_{\theta\ge 0}\left(\frac{1}{2^\theta}\right)^L \lesssim \chi_{\mathbb{Z}\cap(0,2N+1]}(h),$$

which verifies (2-9) with $\sigma_1(h) = \chi_{\mathbb{Z}\cap(0,2N+1]}(h)$. This concludes all estimates for I.

We next deal with $VIII$. For $J=(j_1,j_2,j_3)$ with $j_1, j_2, j_3 \ge 1$, set

$$a_J = a_{j_1,j_2,j_3} := \frac{1}{[w(\Omega)]^{\frac{2}{p}-1}} \sum_{R\subset\Omega}\sum_{R'\in\mathscr{A}_J(R)} |R'|^2 w(R')^{-1} r(R,R')P(R,R')T_{R'}$$

and $\mathscr{B}_J := \{R' : R'_J \cap \Omega^{0,0,0} \ne \varnothing\}$. For any $R'\notin \mathscr{B}_J$, we have $R'_J\cap\Omega^{0,0,0}=\varnothing$. Thus for every $R\subset\Omega$, we have $R'_J \cap 3R = \varnothing$, which implies $R'\notin \mathscr{A}_J(R)$ and therefore $\bigcup_{R\subset\Omega}\mathscr{A}_J(R)\subset\mathscr{B}_J$. Hence,

$$a_J \le \frac{1}{[w(\Omega)]^{\frac{2}{p}-1}} \sum_{R'\in\mathscr{B}_J}\sum_{\substack{R:R\subset\Omega,\\ R'\in\mathscr{A}_J(R)}} |R'|^2 w(R')^{-1} r(R,R')P(R,R')T_{R'}.$$

Let $\mathscr{F}_h^J = \{R'\in\mathscr{B}_J : |R'_J\cap\Omega^{0,0,0}| \ge 1/2^h |R'_J|\}$ for $h\ge 0$, $\mathscr{D}_h^J = \mathscr{F}_h^J \setminus \mathscr{F}_{h-1}^J$ for $h\ge 1$, and $\mathscr{D}_0^J = \varnothing$. Note that $\mathscr{B}_J = \bigcup_{h\ge 1}\mathscr{D}_h^J$. Thus,

$$a_J \le \frac{1}{[w(\Omega)]^{\frac{2}{p}-1}} \sum_{h\ge 1}\sum_{R'\in\mathscr{D}_h^J} |R'|^2 w(R')^{-1} T_{R'}\Bigg(\sum_{\substack{R:R\subset\Omega,\\ R'\in\mathscr{A}_J(R)}} r(R,R')P(R,R')\Bigg).$$

Define $\Omega_h^J = \bigcup_{R'\in\mathscr{D}_h^J} R'$ for $h\ge 1$. If $x\in\Omega_h^J$, then $x\in\widetilde{R}'$ for some dyadic flag rectangle $\widetilde{R}'\in\mathscr{D}_h^J$; therefore

$$\mathcal{M}_{\mathcal{F}}(\chi_{\Omega^{0,0,0}})(x) \ge |\widetilde{R}'_J\cap\Omega^{0,0,0}|/|\widetilde{R}'_J| \ge 2^{-h}.$$

Taking $L > n_1 q_w\big(\frac{2}{p}-1\big)+2N$, $q\in\big(q_w, \frac{p(L-2N)}{n_1(2-p)}\big)$ and applying the L^q_w boundedness of $\mathcal{M}_{\mathcal{F}}$ and Lemma 2.7, we get

$$w(\Omega_h^J) \le w(\{x : \mathcal{M}_{\mathcal{F}}(\chi_{\Omega^{0,0,0}})(x)\ge 2^{-h}\}) \lesssim 2^{hq} w(\Omega^{0,0,0}) \lesssim 2^{hq} w(\Omega).$$

We claim that for L large enough, $M > NL$, and any $R'\in\mathscr{D}_h^J$, there exists some sequence $\{\sigma_8(h, j_1, j_2, j_3)\}_{h, j_1, j_2, j_3 \ge 1}$ such that

$$\begin{cases} \displaystyle\sum_{h, j_1, j_2, j_3 \ge 1} 2^{qh\left(\frac{2}{p}-1\right)} \sigma_8(h, j_1, j_2, j_3) \lesssim 1, \\ \displaystyle\sum_{\substack{R: R\subset\Omega,\\ R' \in \mathscr{A}_J(R)}} r(R, R') P(R, R') \lesssim \sigma_8(h, j_1, j_2, j_3), \qquad \forall\, j_1, j_2, j_3 \ge 1. \end{cases} \tag{2-10}$$

Assuming (2-10) holds for the moment, we can conclude the proof for *VIII* as follows.

$$\begin{aligned} &\sum_{j_1, j_2, j_3 \ge 1} a_J \\ &\quad \lesssim \sum_{j_1, j_2, j_3, h \ge 1} \sigma(h, j_1, j_2, j_3) \left(\frac{w(\Omega_h^J)}{w(\Omega)}\right)^{\frac{2}{p}-1} \frac{1}{[w(\Omega_h^J)]^{\frac{2}{p}-1}} \sum_{R' \subset \Omega_h^J} |R'|^2 w(R')^{-1} T_{R'} \\ &\quad \lesssim \sum_{j_1, j_2, j_3, h \ge 1} \sigma(h, j_1, j_2, j_3) 2^{qh\left(\frac{2}{p}-1\right)} \left(\sup_{\bar\Omega} \frac{1}{[w(\bar\Omega)]^{\frac{2}{p}-1}} \sum_{R' \subset \bar\Omega} |R'|^2 w(R')^{-1} T_{R'}\right) \\ &\quad \lesssim \sup_{\bar\Omega} \frac{1}{[w(\bar\Omega)]^{\frac{2}{p}-1}} \sum_{R' \subset \bar\Omega} |R'|^2 w(R')^{-1} T_{R'}. \end{aligned}$$

To finish the estimate of *VIII*, it suffices to show (2-10). For any $j_1, j_2, j_3 \ge 1$, $R' \in \mathscr{A}_J(R)$ implies

$$|x_{Q_i} - x_{Q_i'}| > [2^{\max_{1\le k\le i} j_k} \ell(Q_i')] \vee \ell(Q_i) \quad \text{for } i = 1, 2, 3. \tag{2-11}$$

Similar to the proof for I, we consider the following eight cases:

Case 1: $|2^{j_1} Q_1'| \ge |Q_1|$, $|2^{j_1\vee j_2} Q_2'| \ge |Q_2|$, $|2^{j_1\vee j_2\vee j_3} Q_3'| \ge |Q_3|$.

Case 2: $|2^{j_1} Q_1'| \ge |Q_1|$, $|2^{j_1\vee j_2} Q_2'| \ge |Q_2|$, $|2^{j_1\vee j_2\vee j_3} Q_3'| < |Q_3|$.

Case 3: $|2^{j_1} Q_1'| \ge |Q_1|$, $|2^{j_1\vee j_2} Q_2'| < |Q_2|$, $|2^{j_1\vee j_2\vee j_3} Q_3'| \ge |Q_3|$.

Case 4: $|2^{j_1} Q_1'| < |Q_1|$, $|2^{j_1\vee j_2} Q_2'| \ge |Q_2|$, $|2^{j_1\vee j_2\vee j_3} Q_3'| \ge |Q_3|$.

Case 5: $|2^{j_1} Q_1'| \ge |Q_1|$, $|2^{j_1\vee j_2} Q_2'| < |Q_2|$, $|2^{j_1\vee j_2\vee j_3} Q_3'| < |Q_3|$.

Case 6: $|2^{j_1} Q_1'| < |Q_1|$, $|2^{j_1\vee j_2} Q_2'| \ge |Q_2|$, $|2^{j_1\vee j_2\vee j_3} Q_3'| < |Q_3|$.

Case 7: $|2^{j_1} Q_1'| < |Q_1|$, $|2^{j_1\vee j_2} Q_2'| < |Q_2|$, $|2^{j_1\vee j_2\vee j_3} Q_3'| \ge |Q_3|$.

Case 8: $|2^{j_1} Q_1'| < |Q_1|$, $|2^{j_1\vee j_2} Q_2'| < |Q_2|$, $|2^{j_1\vee j_2\vee j_3} Q_3'| < |Q_3|$.

We shall handle Case 5 first. Since $|(2^{j_1\vee j_2} Q_2') \times (2^{j_1\vee j_2\vee j_3} Q_3')| \le |Q_2 \times Q_3|$, there exists some $\kappa \ge 0$ such that $2^{(j_1\vee j_2)n_2 + (j_1\vee j_2\vee j_3)n_3 + \kappa} |Q_2' \times Q_3'| = |Q_2 \times Q_3|$. And for each κ, the number of such $Q_2 \times Q_3$'s must be $\lesssim 1$.

For each $h \geq 1$ and $R' \in \mathscr{D}_h^J$, since $|Q_1 \times [2^{j_1 \vee j_2} Q_2'] \times [2^{j_1 \vee j_2 \vee j_3} Q_3']| \leq |3R_J' \cap 3R|$, we get

$$\frac{|Q_1|}{|3 \cdot 2^{j_1} Q_1'|}|3R_J'| \leq |3R_J' \cap 3R| \leq |3R_J' \cap \Omega^{0,0,0}| \leq \frac{1}{2^{h-1}}|3R_J'|,$$

which yields $2^{h-1}|Q_1| \leq 3^{n_1} 2^{j_1 n_1}|Q_1'| \leq 2^{(j_1+2)n_1}|Q_1'|$. We consider two subcases.

Subcase 5.1: $|Q_1'| \geq |Q_1|$. In this subcase, since $2^{h-1-j_1 n_1}|Q_1| \lesssim |Q_1'|$, we have $|Q_1'| \approx 2^{h-1-j_1 n_1+k}|Q_1|$ for some integer $k \geq 0$. And for each fixed k, the number of such Q_1's must be $\lesssim (k+h)^N 2^{k+h}$. By (2-11), $|x_{Q_1} - x_{Q_1'}| \geq 2^{j_1}\ell(Q')$.

Subcase 5.2: $|Q_1'| < |Q_1|$. In this subcase, $|Q_1'| < |Q_1| \leq |2^{j_1} Q_1'|$. So $2^l \ell(Q_1') = \ell(Q_1)$ for some integer l satisfying $1 \leq l \leq j_1$. For each l, the number of Q_1's must be $\lesssim 1$. Moreover, $2^{h-1}2^{ln_1}|Q_1'| = 2^{h-1}|Q_1| \leq 2^{(j_1+2)n_1}|Q_1'|$, which implies $h \leq 3n_1 j_1$. By (2-11),

$$\frac{|x_{Q_1} - x_{Q_1'}|}{\ell(Q_1)} = \frac{|x_{Q_1} - x_{Q_1'}|}{\ell(Q_1')}\frac{\ell(Q_1')}{\ell(Q_1)} \gtrsim 2^{j_1 - l}.$$

These considerations imply that, for $M > n_1 L$,

$$\begin{aligned}
&\sum_{\text{Subcase 5.1}} r(R, R')P(R, R') \\
&\quad \leq \sum_{\text{Subcase 5.1}} \left(\frac{|Q_1|}{|Q_1'|}\right)^L \left(\frac{|Q_2' \times Q_3'|}{|Q_2 \times Q_3|}\right)^L \left(1 + \frac{|x_{Q_1} - x_{Q_1'}|}{\ell(Q_1')}\right)^{-(n_1+M)} \\
&\quad \lesssim \sum_{k,\kappa \geq 0} (k+h)^N 2^{k+h} 2^{-[h+k-j_1 n_1]L} 2^{-[(j_1 \vee j_2)n_2 + (j_1 \vee j_2 \vee j_3)n_3 + \kappa]L} 2^{-(n_1+M)j_1} \\
&\quad \lesssim 2^{-h(L-N-1)} 2^{-j_1(M-n_1 L)} 2^{-[(j_1 \vee j_2)n_2 + (j_1 \vee j_2 \vee j_3)n_3]L}
\end{aligned}$$

and

$$\begin{aligned}
&\sum_{\text{Subcase 5.2}} r(R, R')P(R, R') \\
&\quad \leq \sum_{\text{Subcase 5.2}} \left(\frac{|Q_1'|}{|Q_1|}\right)^L \left(\frac{|Q_2' \times Q_3'|}{|Q_2 \times Q_3|}\right)^L \left(1 + \frac{|x_{Q_1} - x_{Q_1'}|}{\ell(Q_1)}\right)^{-(n_1+M)} \\
&\quad \lesssim \chi_{\mathbb{Z} \cap (0, 3Nj_1)}(h) \sum_{l=1}^{j_1} \sum_{\kappa \geq 0} 2^{-n_1 l L} 2^{-[(j_1 \vee j_2)n_2 + (j_1 \vee j_2 \vee j_3)n_3 + \kappa]L} 2^{-M(j_1 - l)} \\
&\quad \lesssim \chi_{\mathbb{Z} \cap (0, 3Nj_1)}(h) 2^{-j_1 n_1 L} 2^{-[(j_1 \vee j_2)n_2 + (j_1 \vee j_2 \vee j_3)n_3]L},
\end{aligned}$$

both of which satisfy the required estimates for σ_8 in (2-10). Cases 6 and 7 can be treated similarly by symmetry.

We next deal with Case 2. Since $|2^{j_1\vee j_2\vee j_3}Q_3'|<|Q_3|$, there exists some $\kappa\geq 0$ such that $|Q_3|=2^{(j_1\vee j_2\vee j_3)n_3+\kappa}|Q_3'|$. From

$$|Q_1\times Q_2\times(2^{j_1\vee j_2\vee j_3}Q_3')|\leq|3R_J'\cap 3R|\leq|3R_J'\cap\Omega^{0,0,0}|\leq\frac{1}{2^{h-1}}|3R_J'|,$$

it follows that

$$2^{h-1}|Q_1\times Q_2|\lesssim 2^{j_1n_1+(j_1\vee j_2)n_2}|Q_1'\times Q_2'|. \tag{2-12}$$

We consider four subcases by comparing $|Q_1|$ with $|Q_1'|$, and $|Q_2|$ with $|Q_2'|$.

Subcase 2.1: $|Q_1'|\geq|Q_1|$ and $|Q_2'|\geq|Q_2|$. By arguments similar to those used in Subcase 5.1, we get $|Q_1'|\approx 2^{h-1-j_1n_1+k_1}|Q_1|$ and $|Q_2'|\approx 2^{h-1-(j_1\vee j_2)n_2+k_2}|Q_2|$ for some $k_1,k_2\geq 0$. For each k_i, $i=1,2$, the number of Q_i's is smaller than $C(k_i+h)2^{k_i+h}$. Hence

$$\begin{aligned}\sum_{\text{Subcase 2.1}} & r(R,R')P(R,R')\\ &\lesssim\sum_{k_1,k_2,\kappa\geq 0}(k_1+h)^N(k_2+h)^N2^{k_1+h}2^{k_2+h}2^{-(h+k_1-j_1n_1)L}2^{-(h+k_2-(j_1\vee j_2)n_2)L}\\ &\qquad\qquad\times 2^{-[(j_1\vee j_2\vee j_3)n_3+\kappa]L}2^{-j_1(n_1+M)-(j_1\vee j_2)(n_2+M)}\\ &\lesssim 2^{-h(L-N-1)}2^{-j_1(M-n_1L)}2^{-(j_1\vee j_2)(M-n_2L)}2^{-(j_1\vee j_2\vee j_3)n_3L}.\end{aligned}$$

Subcase 2.2: $|Q_1'|\geq|Q_1|$ and $|Q_2'|<|Q_2|$. By (2-12),

$$2^{h-1}|Q_1|\lesssim 2^{j_1n_1+(j_1\vee j_2)n_2}|Q_1'|,$$

and therefore $2^{h-1+k}|Q_1|\approx 2^{j_1n_1+(j_1\vee j_2)n_2}|Q_1'|$ for some $k\geq 0$. Moreover, for each $k\geq 0$, the number of Q_1's is less than $C(h+k)^N2^{h+k}$. On the other hand, since $|Q_2'|<|Q_2|\leq|2^{j_1\vee j_2}Q_2'|$, we see that $\ell(Q_2)=2^l\ell(Q_2')$ for some $1\leq l\leq j_1\vee j_2$. For each l, the number of Q_2's must be $\lesssim 1$. Moreover, by (2-11),

$$\frac{|x_{Q_2}-x_{Q_2'}|}{\ell(Q_2)}=\frac{|x_{Q_2}-x_{Q_2'}|}{\ell(Q_2')}\frac{\ell(Q_2')}{\ell(Q_2)}\gtrsim 2^{j_1\vee j_2-l}.$$

By the above considerations, we can deduce that

$$\begin{aligned}\sum_{\text{Subcase 2.2}} & r(R,R')P(R,R')\\ &\leq\sum_{\text{Subcase 2.2}}\left(\frac{|Q_1|}{|Q_1'|}\frac{|Q_2'|}{|Q_2|}\frac{|Q_3'|}{|Q_3|}\right)^L\left(\frac{|x_{Q_1}-x_{Q_1'}|}{\ell(Q_1')}\right)^{-(n_1+M)}\left(\frac{|x_{Q_2}-x_{Q_2'}|}{\ell(Q_2)}\right)^{-(n_2+M)}\\ &\lesssim\sum_{k,\kappa\geq 0}\sum_{l=1}^{j_1\vee j_2}(k+h)^N2^{k+h}2^{-[h+k-j_1n_1-(j_1\vee j_2)n_2]L}2^{-ln_2L}\\ &\qquad\qquad\times 2^{-[(j_1\vee j_2\vee j_3)n_3+\kappa]L}2^{-(n_1+M)j_1}2^{-M(j_1\vee j_2-l)}\\ &\lesssim 2^{-h(L-N-1)}2^{-j_1(M-n_1L)}2^{-[(j_1\vee j_2)n_2+(j_1\vee j_2\vee j_3)n_3]L}.\end{aligned}$$

Subcase 2.3: $|Q_1'| < |Q_1|$ and $|Q_2'| \geq |Q_2|$. This is symmetric to Subcase 2.2, and similar arguments yield

$$\sum_{\text{Subcase 2.3}} r(R, R')P(R, R') \lesssim 2^{-h(L-N-1)} 2^{-(j_1 \vee j_2)(M-n_2 L)} 2^{-[j_1 n_1 + (j_1 \vee j_2 \vee j_3) n_3]L}.$$

Subcase 2.4: $|Q_1'| < |Q_1|$ and $|Q_2'| < |Q_2|$. Since $|Q_1'| < |Q_1| \leq |2^{j_1} Q_1'|$ and $|Q_2'| < |Q_2| \leq |2^{j_1 \vee j_2} Q_2'|$, we see that $\ell(Q_1) = 2^{l_1} \ell(Q_1')$ for some $1 \leq l_1 \leq j_1$ and that $\ell(Q_2) = 2^{l_2} \ell(Q_2')$ for some $1 \leq l_2 \leq j_1 \vee j_2$. For each l_1 and l_2, the numbers of Q_1's and Q_2's are both $\lesssim 1$. Moreover, by (2-11),

$$\frac{|x_{Q_1} - x_{Q_1'}|}{\ell(Q_1)} \gtrsim 2^{j_1 - l_1}, \qquad \frac{|x_{Q_2} - x_{Q_2'}|}{\ell(Q_2)} \gtrsim 2^{j_1 \vee j_2 - l_2}.$$

By (2-12), $2^{h-1} 2^{l_1 n_1 + l_2 n_2} |Q_1' \times Q_2'| = 2^{h-1} |Q_1 \times Q_2| \lesssim 2^{j_1 n_1 + (j_1 \vee j_2) n_2} |Q_1' \times Q_2'|$, and thus $2^h \lesssim 2^{j_1 n_1 + (j_1 \vee j_2) n_2}$. Hence

$$\begin{aligned}
&\sum_{\text{Subcase 2.4}} r(R, R')P(R, R') \\
&\leq \sum_{\text{Subcase 2.4}} \left(\frac{|Q_1' \times Q_2'|}{|Q_1 \times Q_2|}\right)^L \left(\frac{|Q_3'|}{|Q_3|}\right)^L \left(1 + \frac{|x_{Q_1} - x_{Q_1'}|}{\ell(Q_1)}\right)^{-(n_1+M)} \\
&\qquad\qquad \times \left(1 + \frac{|x_{Q_2} - x_{Q_2'}|}{\ell(Q_2)}\right)^{-(n_2+M)} \\
&\lesssim \sum_{l_1=1}^{j_1} \sum_{l_2=1}^{j_1 \vee j_2} \sum_{\kappa \geq 0} 2^{-(n_1 l_1 + n_2 l_2)L} 2^{-[(j_1 \vee j_2 \vee j_3) n_3 + \kappa]L} 2^{-M(j_1 - l_1)} \\
&\qquad\qquad \times 2^{-M(j_1 \vee j_2 - l_2)} \chi_{\mathbb{Z} \cap (0, C[j_1 \vee j_2])}(h) \\
&\lesssim 2^{-j_1 n_1 L} 2^{-(j_1 \vee j_2) n_2 L} 2^{-(j_1 \vee j_2 \vee j_3) n_3 L} \chi_{\mathbb{Z} \cap (0, C[j_1 \vee j_2])}(h).
\end{aligned}$$

Cases 3 and 4 can be treated by symmetry. Case 8 is easier, and can be handled similarly. For Case 1, we consider eight subcases by comparing $|Q_i|$ with $|Q_i'|$ for $i = 1, 2, 3$; in each subcase the desired estimate can be proved by using arguments given in Subcases 2.1–2.4. This concludes all estimates for *VIII*.

Finally, the remaining terms *II–VII* can be handled similarly. We only consider *VII* and indicate the necessary modifications. As before we consider eight cases by comparing $|Q_1'|$ with $|Q_1|$, $|2^{j_2} Q_2'|$ with $|Q_2|$, and $|2^{j_2 \vee j_3} Q_3'|$ with $|Q_3|$, and matters are reduced to showing certain decay estimates for

$$\sum_{\substack{R: R \subset \Omega, \\ R' \in \mathscr{A}_{0, j_1, j_2}(R)}} r(R, R')P(R, R')$$

in each case. Recall that, in dealing with *VIII*, we used (2-11) to derive certain decay factors in j_1, in order to sum over $j_1 \in \mathbb{Z}_+$. But for *VII*, the decay factors in j_1 are no longer needed, and we use the trivial inequality instead

$$P_1(Q_1, Q_1') := \left(1 + \frac{|x_{Q_1} - x_{Q_1'}|}{\ell(Q_1') \vee \ell(Q_1)}\right)^{-(n_1+M)} \leq 1.$$

The rest of the proof is similar to that for *VIII*, and we omit the details.

This completes the proof of Theorem 1.6. □

To show that $CMO^p_{\mathcal{F},w}(\mathbb{R}^N)$ is the dual space of $H^p_{\mathcal{F},w}(\mathbb{R}^N)$, we introduce the multiparameter flag weighted sequence spaces.

Definition 2.9. Let $0 < p \leq 1$ and $w \in A^{\mathcal{F}}_\infty(\mathbb{R}^N)$. We use $s^p_w(\mathbb{R}^N)$ to express the collection of all sequences $\{s_R\}$ satisfying

$$\|\{s_R\}\|_{s^p_w(\mathbb{R}^N)} := \left\| \left\{ \sum_{J\in\mathbb{Z}^3} \sum_{R\in\mathcal{R}^J_{\mathcal{F}}} \frac{|s_R|^2}{|R|} \chi_R \right\}^{\frac{1}{2}} \right\|_{L^p_w(\mathbb{R}^N)} < \infty.$$

We also use $c^p_w(\mathbb{R}^N)$ to denote the collection of all sequences $\{t_R\}$ such that

$$\|\{t_R\}\|_{c^p_w(\mathbb{R}^N)} := \sup_{\Omega\subset\mathbb{R}^N} \left\{ \frac{1}{[w(\Omega)]^{2/p-1}} \sum_{J\in\mathbb{Z}^3} \sum_{\substack{R\in\mathcal{R}^J_{\mathcal{F}},\\ R\subset\Omega}} |t_R|^2 \frac{|R|}{w(R)} \right\}^{\frac{1}{2}} < \infty,$$

where the supremum runs over all open sets Ω with $w(\Omega) < \infty$.

We will show the duality relationship between s^p_w and c^p_w.

Theorem 2.10. *Let* $0 < p \leq 1$. *Then* $(s^p_w(\mathbb{R}^N))^* = c^p_w(\mathbb{R}^N)$. *More precisely, for every* $\{t_R\} \in c^p_w(\mathbb{R}^N)$, *the mapping* $\ell_s : \{s_R\} \mapsto \sum_R s_R \bar{t}_R$ *defines a continuous linear functional on* $s^p_w(\mathbb{R}^N)$ *with operator norm* $\|\ell_s\| \lesssim \|t\|_{c^p_w(\mathbb{R}^N)}$. *Conversely, for every* $\ell \in (s^p_w(\mathbb{R}^N))^*$, *there is a unique* $\{t_R\} \in c^p_w(\mathbb{R}^N)$ *such that* $\ell(s_R) = \sum_R s_R \bar{t}_R$ *and* $\|\{t\}_R\|_{c^p_w} \lesssim \|\ell\|$.

Proof. We first prove $c^p_w(\mathbb{R}^N) \subset (s^p_w(\mathbb{R}^N))^*$. Suppose that $\{t_R\} \in c^p_w(\mathbb{R}^N)$. For $\{s_R\} \in s^p_w(\mathbb{R}^N)$, let

$$\mathcal{G}(\{s_R\})(x) = \left\{ \sum_{J\in\mathbb{Z}^3} \sum_{R\in\mathcal{R}^J_{\mathcal{F}}} |s_R|^2 |R|^{-1} \chi_R(x) \right\}^{\frac{1}{2}}.$$

For $i \in \mathbb{Z}$, set $\Omega_i = \{x \in \mathbb{R}^N : \mathcal{G}(\{s_R\})(x) > 2^i\}$, $\widetilde{\Omega}_i = \{x \in \mathbb{R}^N : \mathcal{M}_{\mathcal{F}}(\chi_{\Omega_i})(x) > 1/2\}$, and $\mathscr{B}_i = \{R \in \mathcal{R}_{\mathcal{F}} : |R \cap \Omega_i| > 1/2|R|,\ |R \cap \Omega_{i+1}| \leq 1/2|R|\}$. If $x \in R \in \mathscr{B}_i$, then $\mathcal{M}_{\mathcal{F}}(\chi_{\Omega_i})(x) \geq \frac{1}{|R|} \int_R \chi_{\Omega_i}(y)dy = |R \cap \Omega_i|/|R| > 1/2$, which implies

$$\bigcup_{R\in\mathscr{B}_i} R \subset \widetilde{\Omega}_i. \tag{2-13}$$

Moreover, for $q > q_w$, by the $L^q_w(\mathbb{R}^N)$ boundedness of $\mathcal{M}_{\mathcal{F}}$,

$$w(\widetilde{\Omega}_i) \lesssim w(\Omega_i), \tag{2-14}$$

and by Lemma 2.7,

$$\frac{w(R \cap (\Omega_i \setminus \Omega_{i+1}))}{w(R)} = \frac{w(R \setminus \Omega_{i+1})}{w(R)} \gtrsim \left(\frac{|R \setminus \Omega_{i+1}|}{|R|}\right)^q \geq \frac{1}{2^q}. \tag{2-15}$$

Suppose $\{t_R\} \in c^p_w(\mathbb{R}^N)$. By (2-13)–(2-15) and Schwarz's inequality,

$$\begin{aligned}
\Bigl|\sum_{J\in\mathbb{Z}^3}\sum_{R\in\mathcal{R}^J_{\mathcal{F}}} s_R\bar{t}_R\Bigr| &\lesssim \Bigl|\sum_{i\in\mathbb{Z}}\int_{\widetilde{\Omega}_i\setminus\Omega_{i+1}}\sum_{R\in\mathscr{B}_i}|\bar{t}_R|\frac{|R|^{\frac12}}{w(R)}|s_R|\,|R|^{-\frac12}\chi_R(x)w(x)dx\Bigr| \\
&\leq \sum_{i\in\mathbb{Z}}\Bigl\{\sum_{R\subset\widetilde{\Omega}_i}|t_R|^2\frac{|R|}{w(R)}\Bigr\}^{\frac12}\Bigl\{\int_{\widetilde{\Omega}_i\setminus\Omega_{i+1}}\sum_{R\in\mathscr{B}_i}\frac{|s_R|^2}{|R|}\chi_R(x)w(x)dx\Bigr\}^{\frac12} \\
&\lesssim \|\{t_R\}\|_{c^p_w}\sum_{i\in\mathbb{Z}}[w(\widetilde{\Omega}_i)]^{\left(\frac2p-1\right)\frac12}\Bigl\{\int_{\widetilde{\Omega}_i\setminus\Omega_{i+1}}[\mathcal{G}(\{s_R\})(x)]^2w(x)dx\Bigr\}^{\frac12} \\
&\lesssim \|\{t_R\}\|_{c^p_w}\sum_{i\in\mathbb{Z}}2^i[w(\Omega_i)]^{\frac1p} \\
&\lesssim \|\{t_R\}\|_{c^p_w}\|\mathcal{G}(\{s_R\})\|_{L^p_w} = \|\{t_R\}\|_{c^p_w}\|\{s_R\}\|_{s^p_w},
\end{aligned}$$

which implies the inclusion $c^p_w(\mathbb{R}^N) \subset (s^p_w(\mathbb{R}^N))^*$.

For the converse, we assume that $\ell \in (s^p_w(\mathbb{R}^N))^*$. Then it is clear that $\ell(\{s_R\}) = \sum_R s_R\bar{t}_R$ for some $\{t_R\}$. Now fix an open set $\Omega \subset \mathbb{R}^N$ with $w(\Omega) < \infty$. Let μ be a measure of $\mathcal{R}_{\mathcal{F}}$ such that $\mu(R) = [w(\Omega)]^{1-2/p}|R|[w(R)]^{-1}$ if $R \subset \Omega$ and otherwise $\mu(R) = 0$. Set

$$\|\{s_R\}\|_{\ell^2(\Omega,\mu)} = \Bigl\{\sum_{J\in\mathbb{Z}^3}\sum_{\substack{R\in\mathcal{R}^J_{\mathcal{F}},\\ R\subset\Omega}}|s_R|^2[w(\Omega)]^{1-\frac2p}\frac{|R|}{w(R)}\Bigr\}^{\frac12}.$$

Then

$$\begin{aligned}
&\Bigl\{\frac{1}{[w(\Omega)]^{2/p-1}}\sum_{J\in\mathbb{Z}^3}\sum_{\substack{R\in\mathcal{R}^J_{\mathcal{F}},\\ R\subset\Omega}}|t_R|^2\frac{|R|}{w(R)}\Bigr\}^{\frac12} \\
&\qquad= \|\{t_R\}\|_{\ell^2(\Omega,\mu)} = \sup_{\|\{s_R\}\|_{\ell^2(\Omega,\mu)}\leq 1}\Bigl|\sum_{J\in\mathbb{Z}^3}\sum_{\substack{R\in\mathcal{R}^J_{\mathcal{F}},\\ R\subset\Omega}}s_R\bar{t}_R[w(\Omega)]^{1-2/p}\frac{|R|}{w(R)}\Bigr| \\
&\qquad\leq \|\ell\|\sup_{\|\{s_R\}\|_{\ell^2(\Omega,\mu)}\leq 1}\Bigl\|s_R[w(\Omega)]^{1-2/p}\frac{|R|}{w(R)}\Bigr\|_{s^p_w},
\end{aligned}$$

where $\{s_R\}$ satisfies $s_R = 0$ if R is not contained in Ω. However, for such $\{s_R\}$, Hölder's inequality yields

$$\left\| s_R [w(\Omega)]^{1-2/p} \frac{|R|}{w(R)} \right\|_{s_w^p(\mathbb{R}^N)}$$

$$= \left\{ \int_\Omega \left[\sum_{J\in\mathbb{Z}^3} \sum_{\substack{R\in\mathcal{R}_{\mathcal{F}}^J \\ R\subset\Omega}} |s_R|^2 [w(\Omega)]^{2-4/p} \frac{|R|}{w(R)^2} \chi_R(x) \right]^{\frac{p}{2}} w(x)dx \right\}^{\frac{1}{p}}$$

$$\leq [w(\Omega)]^{\frac{1}{p}-\frac{1}{2}} \left\{ \int_\Omega \sum_{J\in\mathbb{Z}^3} \sum_{\substack{R\in\mathcal{R}_{\mathcal{F}}^J, \\ R\subset\Omega}} |s_R|^2 [w(\Omega)]^{2-4/p} \frac{|R|}{w(R)^2} \chi_R(x) w(x)dx \right\}^{\frac{1}{2}}$$

$$= \|\{s_R\}\|_{\ell^2(\Omega,\mu)} \leq 1.$$

Combining the above estimates yields

$$\|\{t_R\}\|_{c_w^p(\mathbb{R}^N)} \leq \|\ell\|,$$

and hence $\{t_R\} \in c_w^p(\mathbb{R}^N)$. □

Now we define a *lifting operator* $\mathcal{L}$ on $\mathcal{S}'_{\mathcal{F}}(\mathbb{R}^N)$ and a *projection operator* $\mathcal{T}$ on sequence spaces by

$$\mathcal{L}(f) := \{|R|^{\frac{1}{2}} \psi_J * f(x_R)\} \quad \text{for } f \in \mathcal{S}'_{\mathcal{F}}(\mathbb{R}^N)$$

and

$$\mathcal{T}(\{t_R\})(x) := \sum_{J\in\mathbb{Z}^3} \sum_{\mathcal{R}\in\mathcal{R}_{\mathcal{F}}^J} |R|^{\frac{1}{2}} \psi_J(x-x_R) t_R,$$

where $\{\psi_J\}$ satisfies (1-1) and (1-2).

To prove Theorem 1.7, we need the following:

Theorem 2.11. *The lifting operator $\mathcal{L}$ is bounded from $H^p_{\mathcal{F},w}(\mathbb{R}^N)$ to $s^p_w(\mathbb{R}^N)$ and bounded from $CMO^p_{\mathcal{F},w}(\mathbb{R}^N)$ to $c^p_w(\mathbb{R}^N)$. The projection operator $\mathcal{T}$ is bounded from $s^p_w(\mathbb{R}^N)$ to $H^p_{\mathcal{F},w}(\mathbb{R}^N)$ and bounded from $c^p_w(\mathbb{R}^N)$ to $CMO^p_{\mathcal{F},w}(\mathbb{R}^N)$. Moreover, $\mathcal{T}\circ\mathcal{L}$ is the identity both on $H^p_{\mathcal{F},w}(\mathbb{R}^N)$ and $CMO^p_{\mathcal{F},w}(\mathbb{R}^N)$.*

Proof. The boundedness of $\mathcal{L}$ from $H^p_{\mathcal{F},w}(\mathbb{R}^N)$ to $s^p_w(\mathbb{R}^N)$ and from $CMO^p_{\mathcal{F},w}(\mathbb{R}^N)$ to $c^p_w(\mathbb{R}^N)$ follows directly from the definition of $\mathcal{L}$.

We now show that $\mathcal{T}$ is bounded from $s^p_w(\mathbb{R}^N)$ to $H^p_{\mathcal{F},w}(\mathbb{R}^N)$. By definition,

$$\|\mathcal{T}(\{t_R\})\|_{H^p_{\mathcal{F},w}(\mathbb{R}^N)} = \left\| \left\{ \sum_{J\in\mathbb{Z}^3} \sum_{R\in\mathcal{R}_{\mathcal{F}}^J} |\psi_J * \mathcal{T}(\{t_R\})(x_R)|^2 \chi_R \right\}^{\frac{1}{2}} \right\|_{L^p_w(\mathbb{R}^N)}.$$

A similar argument to the proof of Theorem 1.4 yields

$$\|\mathcal{T}(\{t_R\})\|_{H^p_{\mathcal{F},w}} \lesssim \left\| \left\{ \sum_{J'\in\mathbb{Z}^3} \left\{ \mathcal{M}_{\mathcal{F}} \left[\sum_{R'\in\mathcal{R}^{J'}_{\mathcal{F}}} t^2_{R'} |R'|^{-1} \chi_{R'} \right]^{\frac{\delta}{2}} \right\}^{\frac{2}{\delta}} \right\}^{\frac{1}{2}} \right\|_{L^p_w}$$

$$\lesssim \left\| \left\{ \sum_{J'\in\mathbb{Z}^3} \sum_{R'\in\mathcal{R}^{J'}_{\mathcal{F}}} t^2_{R'} |R'|^{-1} \chi_{R'} \right\}^{\frac{1}{2}} \right\|_{L^p_w} = \|t\|_{s^p_w}.$$

Next, we prove that the operator $\mathcal{T}$ is bounded from $c^p_w(\mathbb{R}^N)$ to $CMO^p_{\mathcal{F},w}(\mathbb{R}^N)$. Suppose $\{t_R\} \in c^p_w(\mathbb{R}^N)$. Then, for any open set $\Omega \subset \mathbb{R}^N$ with $w(\Omega) < \infty$,

$$\sum_{J\in\mathbb{Z}^3} \sum_{\substack{R\in\mathcal{R}^J_{\mathcal{F}},\\ R\subset\Omega}} |t_R|^2 \frac{|R|}{w(R)} \le C[w(\Omega)]^{\frac{2}{p}-1}.$$

Therefore,

$$\sum_{J\in\mathbb{Z}^3} \sum_{\substack{R\in\mathcal{R}^J_{\mathcal{F}},\\ R\subset\Omega}} |\psi_J * \mathcal{T}(\{t_R\})(x_R)|^2 \frac{|R|^2}{w(R)}$$
$$= \sum_{J\in\mathbb{Z}^3} \sum_{\substack{R\in\mathcal{R}^J_{\mathcal{F}},\\ R\subset\Omega}} \left(\sum_{J'\in\mathbb{Z}^3} \sum_{R\in\mathcal{R}^{J'}_{\mathcal{F}}} |\psi_J * \psi_{J'}(x_R - x_{R'})| \cdot t_{R'} \cdot |R'|^{\frac{1}{2}} \right)^2 \frac{|R|^2}{w(R)}.$$

Repeating the same argument as in Theorem 1.6, we obtain

$$\|\mathcal{T}(\{t_R\})\|_{CMO^p_{\mathcal{F},w}(\mathbb{R}^N)} \lesssim \sup_{\bar{\Omega}} \left\{ \frac{1}{[w(\bar{\Omega})]^{2/p-1}} \sum_{R'\subset\bar{\Omega}} |t_{R'}|^2 \frac{|R'|^2}{w(R')} \right\}^{\frac{1}{2}} \approx \|\{t_R\}\|_{c^p_w(\mathbb{R}^N)}.$$

Finally, the fact that $\mathcal{T} \circ \mathcal{L}$ is the identity both on $H^p_{\mathcal{F},w}(\mathbb{R}^N)$ and $CMO^p_{\mathcal{F},w}(\mathbb{R}^N)$ follows directly from the discrete Calderón identity in Theorem 2.1. □

Proof of Theorem 1.7. We first prove the inclusion $CMO^p_{\mathcal{F},w}(\mathbb{R}^N) \subset (H^p_{\mathcal{F},w}(\mathbb{R}^N))^*$. Let $g \in CMO^p_{\mathcal{F},w}(\mathbb{R}^N)$. For $f \in \mathcal{S}_\infty(\mathbb{R}^N)$, define the mapping $\ell_g(f) := \langle f, g\rangle$. Applying Theorems 2.1, 2.10 and 2.11, we obtain

$$|\ell_g(f)| = |\langle f, g\rangle| = \left| \left\langle \sum_{J\in\mathbb{Z}^3} \sum_{R\subset\mathcal{R}^J_{\mathcal{F}}} |R| \psi_J(\cdot - x_R) \psi_J * f(x_R), g \right\rangle \right|$$
$$= \left| \sum_{J\in\mathbb{Z}^3} \sum_{R\subset\mathcal{R}^J_{\mathcal{F}}} |R|^{\frac{1}{2}} \psi_J * f(x_R) |R|^{\frac{1}{2}} \psi_J * g(x_R) \right|$$
$$= |\langle \mathcal{L}(f), \mathcal{L}(g)\rangle| \lesssim \|\mathcal{L}(f)\|_{s^p_w(\mathbb{R}^N)} \|\mathcal{L}(g)\|_{c^p_w(\mathbb{R}^N)}$$
$$\lesssim \|f\|_{H^p_{\mathcal{F},w}(\mathbb{R}^N)} \|g\|_{CMO^p_{\mathcal{F},w}(\mathbb{R}^N)},$$

where we have chosen $\psi^{(1)}(-x) = \psi^{(1)}(x)$ and $\psi^{(2)}(-x) = \psi^{(2)}(x)$. Since $\mathcal{S}_\infty(\mathbb{R}^N)$

is dense in $H^p_{\mathcal{F},w}(\mathbb{R}^N)$ (by Corollary 2.6), it follows that the mapping $\ell_g(f) = \langle f, g\rangle$ can be extended to a continuous linear functional on $H^p_{\mathcal{F},w}(\mathbb{R}^N)$ and $\|\ell_g\| \lesssim \|g\|_{CMO^p_{\mathcal{F},w}(\mathbb{R}^N)}$.

Conversely, let $\ell \in (H^p_{\mathcal{F},w}(\mathbb{R}^N))^*$ and $\ell_1 = \ell\circ\mathcal{T}$. For $\{s_R\}\in s^p_w(\mathbb{R}^N)$, Theorem 2.11 gives

$$|\ell_1(\{s_R\})| = |\ell(\mathcal{T}(\{s_R\}))| \le \|\ell\|\cdot\|\mathcal{T}(\{s_R\})\|_{H^p_{\mathcal{F},w}(\mathbb{R}^N)} \lesssim \|\ell\|\cdot\|\{s_R\}\|_{s^p_w(\mathbb{R}^N)},$$

which implies that $\ell_1 \in (s^p_w(\mathbb{R}^N))^*$. Then by Theorem 2.10, there exists $\{t_R\} \in c^p_w(\mathbb{R}^N)$ such that $\ell_1(\{s_R\}) = \sum_R s_R\bar{t}_R$ for all $\{s_R\} \in s^p_w(\mathbb{R}^N)$ and $\|\{t_R\}\|_{c^p_w(\mathbb{R}^N)} \lesssim \|\ell_1\| \lesssim \|\ell\|$. By Theorem 2.10 again, $\ell = \ell\circ\mathcal{T}\circ\mathcal{L} = \ell_1\circ\mathcal{L}$. Hence,

$$\ell(f) = \ell_1(\mathcal{L}(f)) = \langle\mathcal{L}(f), t\rangle = \langle f, g\rangle,$$

where $g = \sum_{J\in\mathbb{Z}^3}\sum_{R\in\mathcal{R}^J_{\mathcal{F}}} |R|^{\frac12}\, t_R\, \psi_J(x_R - x)$. This implies that $\ell = \ell_g$, and, by Theorem 2.10,

$$\|g\|_{CMO^p_{\mathcal{F},w}(\mathbb{R}^N)} \lesssim \|\{t_R\}\|_{c^p_w(\mathbb{R}^N)} \lesssim \|\ell_g\|.$$

This concludes the proof of Theorem 1.7. □

3. Weighted boundedness of singular integrals with flag kernels

This section is devoted to proving the boundedness results given in Theorems 1.9, 1.10 and 1.11 for flag singular integrals. To prove Theorem 1.9, we need the following orthogonality estimates.

Lemma 3.1. *Let $\varphi \in \mathcal{S}(\mathbb{R}^N)$ satisfy*

(3-1)
$$\begin{cases} \displaystyle\int_{\mathbb{R}^{n_1}} \varphi(x_1,x_2,x_3)\,dx_1 = 0 & \text{for almost every } (x_2,x_3)\in\mathbb{R}^{n_2+n_3},\\ \displaystyle\int_{\mathbb{R}^{n_2}} \varphi(x_1,x_2,x_3)\,dx_2 = 0 & \text{for almost every } (x_1,x_3)\in\mathbb{R}^{n_1+n_3},\\ \displaystyle\int_{\mathbb{R}^{n_3}} \varphi(x_1,x_2,x_3)\,dx_3 = 0 & \text{for almost every } (x_1,x_2)\in\mathbb{R}^{n_1+n_2},\end{cases}$$

and define φ_J by $\varphi_J(x) := 2^{-j_1n_1+j_2n_2+j_3n_3}\varphi(2^{-j_1}x_1, 2^{-j_2}x_2, 2^{-j_3}x_3)$. Also let $\psi_{J'} \in \mathcal{S}(\mathbb{R}^n)$ be defined as in Section 1. Then there exists $\epsilon > 0$ such that, for any $M > 0$,

(3-2)
$$|\varphi_J * \psi_{J'}(x)| \lesssim 2^{-\epsilon(|j_1-j_1'|+|j_2-j_2'|+|j_3-j_3'|)}\left[\prod_{i=1}^{3}\frac{\max_{1\le k\le i} 2^{j_k'M}}{(\max_{1\le k\le i} 2^{j_k'} + |x_i|)^{n_i+M}}\right].$$

Proof. We consider eight cases separately.

Case 1: $j_1 \le j_1'$, $j_2 \le j_2'$, $j_3 \le j_3'$. By (3-1),

$$|\varphi_J * \psi^{(1)}_{j_1}(x)| = \left| \int_{\mathbb{R}^N} \varphi_J(u)[\psi^{(1)}_{j_1}(x-u) - \psi^{(1)}_{j_1}(x)]\, dy \right| \lesssim 2^{-|j_1 - j_1'|} \frac{2^{(j_1 \vee j_1')M}}{(2^{j_1 \vee j_1'} + |x_1|)^{M+n_1}} \frac{2^{(j_2 \vee j_1')M}}{(2^{j_2 \vee j_1'} + |x_2|)^{M+n_2}} \frac{2^{(j_3 \vee j_1')M}}{(2^{j_3 \vee j_1'} + |x_3|)^{M+n_3}}.$$

This together with

$$|\psi^{(2)}_{j_2'} *_2 \psi^{(3)}_{j_3'}(x_2, x_3)| \lesssim \frac{2^{j_2' M}}{(2^{j_2'} + |x_2|)^{M+n_2}} \frac{2^{(j_2' \vee j_3')M}}{(2^{j_2' \vee j_3'} + |x_3|)^{M+n_3}}$$

yields

$$\begin{aligned} |\varphi_J * \psi_{J'}(x)| &= |[\varphi_J * \psi^{(1)}_{j_1}] *_2 [\psi^{(2)}_{j_2'} *_2 \psi^{(3)}_{j_3'}](x)| \\ &\lesssim 2^{-|j_1 - j_1'|} \left[\prod_{i=1}^{3} \frac{\max_{1 \le k \le i} 2^{(j_k \vee j_k')M}}{(\max_{1 \le k \le i} 2^{j_k \vee j_k'} + |x_i|)^{n_i + M}} \right] \\ &= 2^{-|j_1 - j_1'|} \left[\prod_{i=1}^{3} \frac{\max_{1 \le k \le i} 2^{j_k' M}}{(\max_{1 \le k \le i} 2^{j_k'} + |x_i|)^{n_i + M}} \right]. \end{aligned} \tag{3-3}$$

The same techniques yield

$$\begin{aligned} |\varphi_J * \psi_{J'}(x)| &= |[\varphi_J *_{2,3} \psi^{(2)}_{j_2}] * [\psi^{(1)}_{j_1'} *_3 \psi^{(3)}_{j_3'}](x)| \\ &\lesssim 2^{-|j_2 - j_2'|} \left[\prod_{i=1}^{3} \frac{\max_{1 \le k \le i} 2^{j_k' M}}{(\max_{1 \le k \le i} 2^{j_k'} + |x_i|)^{n_i + M}} \right] \end{aligned} \tag{3-4}$$

and

$$\begin{aligned} |\varphi_J * \psi_{J'}(x)| &= |[\varphi_J *_3 \psi^{(3)}_{j_3}] * [\psi^{(1)}_{j_1'} *_{2,3} \psi^{(2)}_{j_2'}](x)| \\ &\lesssim 2^{-|j_3 - j_3'|} \left[\prod_{i=1}^{3} \frac{\max_{1 \le k \le i} 2^{j_k' M}}{(\max_{1 \le k \le i} 2^{j_k'} + |x_i|)^{n_i + M}} \right]. \end{aligned} \tag{3-5}$$

Taking the geometric mean of (3-3)–(3-5), we obtain (3-2) with $\epsilon = 1/3$.

Case 2: $j_1 > j_1'$, $j_2 \le j_2'$, $j_3 \le j_3'$. We use the moment condition of $\psi^{(1)}$ and Taylor's remainder theorem to get

$$\begin{aligned} &|\varphi_J * \psi^{(1)}_{j_1}(x)| \\ &\qquad = \left| \int_{\mathbb{R}^N} [\varphi_J(x-y) - P_{L-1}[\psi_J](x)] \psi^{(1)}_{j_1}(y)\, dy \right| \end{aligned}$$

$$\lesssim \Big(\sum_{L_1+L_2=L} 2^{-|j_1-j_1'|L_1}2^{-|j_2-j_1'|L_2}\Big)$$
$$\times \frac{2^{(j_1\vee j_1')M}}{(2^{j_1\vee j_1'}+|x_1|)^{M+n_1}}\frac{2^{(j_2\vee j_1')M}}{(2^{j_2\vee j_1'}+|x_2|)^{M+n_2}}\frac{2^{(j_3\vee j_1')M}}{(2^{j_3\vee j_1'}+|x_3|)^{M+n_3}}$$
$$\lesssim 2^{-|j_1-j_1'|L}\frac{2^{(j_1\vee j_1')M}}{(2^{j_1\vee j_1'}+|x_1|)^{M+n_1}}\frac{2^{(j_2\vee j_1')M}}{(2^{j_2\vee j_1'}+|x_2|)^{M+n_2}}\frac{2^{(j_3\vee j_1')M}}{(2^{j_3\vee j_1'}+|x_3|)^{M+n_3}},$$

where in the last inequality we have used the fact that $|j_1-j_1'|\geq|j_2-j_1'|$ and $P_{L-1}[f]$ is the $(L-1)$-th order Taylor's polynomial of f. It follows that

$$|\varphi_J*\psi_{J'}(x)|=|[\varphi_J*\psi^{(1)}_{j_1}]*_2[\psi^{(2)}_{j_2'}*_2\psi^{(3)}_{j_3'}](x)|$$
$$\lesssim 2^{-L|j_1-j_1'|}\frac{2^{j_1M}}{(2^{j_1}+|x_1|)^{M+n_1}}\frac{2^{(j_1'\vee j_2')M}}{(2^{j_1'\vee j_2'}+|x_2|)^{M+n_2}}\frac{2^{(j_1'\vee j_2'\vee j_3')M}}{(2^{j_1'\vee j_2'\vee j_3'}+|x_3|)^{M+n_3}}$$
$$\lesssim 2^{-(L-M)|j_1-j_1'|}\Bigg[\prod_{i=1}^{3}\frac{\max_{1\leq k\leq i}2^{j_k'M}}{(\max_{1\leq k\leq i}2^{j_k'}+|x_i|)^{n_i+M}}\Bigg].$$

The other cases, $\{j_1\leq j_1',\ j_2>j_2',\ j_3\leq j_3'\}$, $\{j_1>j_1',\ j_2>j_2',\ j_3\leq j_3'\}$, $\{j_1\leq j_1',\ j_2\leq j_2',\ j_3<j_3'\}$, $\{j_1>j_1',\ j_2\leq j_2',\ j_3<j_3'\}$, $\{j_1\leq j_1',\ j_2>j_2',\ j_3<j_3'\}$, and $\{j_1>j_1',\ j_2>j_2',\ j_3<j_3'\}$, can be handled in the same manner and details are left to the reader. □

Lemma 3.2. *Let $\mathcal{K}$ be a flag kernel. We have*

$$|\psi_J*\mathcal{K}*\psi_{J'}(x)|\lesssim 2^{-10M(|j_1-j_1'|+|j_2-j_2'|+|j_3-j_3'|)}\prod_{i=1}^{3}\frac{\max_{1\leq k\leq i}2^{j_k'M}}{(\max_{1\leq k\leq i}2^{j_k'}+|x_i|)^{1+M}}. \tag{3-6}$$

Proof. It is well known that $\psi^{(i)}_{j_i}*\psi^{(i)}_{j_i'}$ and $2^{-L|j_i-j_i'|}\psi^{(i)}_{j_i\vee j_i'}$ satisfy the same differential inequalities and moment conditions on $\mathbb{R}^{N_i}$. Thus,

$$\psi_J*\psi_{J'}=[\psi^{(1)}_{j_1}*\psi^{(1)}_{j_1'}]*_{2,3}[\psi^{(2)}_{j_2}*\psi^{(2)}_{j_2'}]*_3[\psi^{(3)}_{j_3}*\psi^{(3)}_{j_3'}]$$

satisfies the same properties as $2^{-L(|j_1-j_1'|+|j_2-j_2'|+|j_3\vee j_3'|)}\psi_{J\vee J'}$, where

$$\psi_{J\vee J'}:=\psi^{(1)}_{j_1\vee j_1'}*_{2,3}\psi^{(2)}_{j_2\vee j_2'}*_3\psi^{(3)}_{j_3\vee j_3'}.$$

By [Nagel et al. 2001, Corollary 2.4.4],

$$\mathcal{K}=\sum_{j_1\leq j_2\leq j_3}\varphi^{(J)}_J,$$

where $\{\varphi^{(J)}\}$ is a bounded collection of C^∞ functions, each of which is supported on $\{|x_i|\leq c,\ i=1,2,3\}$ with (3-1), and the series converges in the sense of distributions.

Lemma 3.1 yields

$$
\begin{aligned}
|\psi_J*\mathcal{K}*\psi_{J'}(x)| &\le \sum_{j_1''\le j_2''\le j_3''} \left|\varphi_{J''}^{(J'')}*[\psi_J*\psi_{J'}](x)\right| \\
&\lesssim \sum_{j_1''\le j_2''\le j_3''} 2^{-L(|j_1''-(j_1\vee j_1')|+|j_2''-(j_2\vee j_2')|+|j_3''-(j_3\vee j_3')|)} \\
&\qquad \times 2^{-L(|j_1-j_1'|+|j_2-j_2'|+|j_3-j_3'|)} \prod_{i=1}^{3} \frac{\max_{1\le k\le i} 2^{(j_k\vee j_k')M}}{(\max_{1\le k\le i} 2^{j_k\vee j_k'}+|x_i|)^{1+M}} \\
&\lesssim 2^{-(|j_1-j_1'|+|j_2-j_2'|+|j_3-j_3'|)L} \left[\prod_{i=1}^{3} \frac{\max_{1\le k\le i} 2^{(j_k\vee j_k')M}}{(\max_{1\le k\le i} 2^{(j_k\vee j_k')}+|x_i|)^{n_i+M}}\right].
\end{aligned}
$$

This finishes the proof of (3-6). □

Proof of Theorem 1.9. By the discrete Calderón reproducing formula,

$$
\begin{aligned}
&\|T_{\mathcal{F}}(f)\|_{H^p_{\mathcal{F},w}} \\
&= \left\| \left\{ \sum_{J\in\mathbb{Z}^3} \sum_{R\in\mathcal{R}^J_{\mathcal{F}}} |\psi_J*\mathcal{K}*f(x_R)|^2\chi_R \right\}^{\frac12} \right\|_{L^p_w} \\
&= \left\| \left\{ \sum_{J\in\mathbb{Z}^3} \sum_{R\in\mathcal{R}^J_{\mathcal{F}}} \left| \sum_{J'\in\mathbb{Z}^3} \sum_{R'\in\mathcal{R}^J_{\mathcal{F}}} |R'|\psi_{J'}*f(x_{R'})\psi_J*\mathcal{K}*\psi_{J'}(x_R-x_{R'}) \right|^2 \chi_R \right\}^{\frac12} \right\|_{L^p_w}.
\end{aligned}
$$

Equation (3-6) says that, for each $J, J'\in\mathbb{Z}^3$, $\psi_J*\mathcal{K}*\psi_{J'}$ satisfies the same orthogonality estimate as $\psi_J*\psi_{J'}$. Thus, repeating the same argument as in the proof of Theorem 1.4, we obtain

$$
\begin{aligned}
&\|Tf\|_{H^p_{\mathcal{F},w}(\mathbb{R}^N)} \\
&\qquad \lesssim \left\| \left\{ \sum_{J'\in\mathbb{Z}^3} \left[\mathcal{M}_{\mathcal{F}} \left(\sum_{R'\in\mathcal{R}^J_{\mathcal{F}}} |\psi_{J'}*f(x_{R'})|^2\chi_{R'} \right)^{\frac{\delta}{2}} \right]^{\frac{2}{\delta}} \right\}^{\frac12} \right\|_{L^p_w(\mathbb{R}^N)} \lesssim \|f\|_{H^p_{\mathcal{F},w}(\mathbb{R}^N)}.
\end{aligned}
$$

This concludes the proof of Theorem 1.9. □

To prove Theorem 1.10, we need a new Calderón type identity in terms of bump functions. For $i=1,2,3$, let $\phi^{(i)}, \phi'^{(i)}\in\mathcal{S}(\mathbb{R}^{N_i})$ be such that $\operatorname{supp}\widehat{\phi^{(i)}}$ is compact and bounded away from origin, $\phi'^{(i)}$ is supported on $B(0,2)$, and they satisfy

$$
\int_{\mathbb{R}^{N_i}} \phi'^{(i)}(x^i)(x^i)^{\alpha_i}\,dx^i = 0 \quad \text{for } 0\le|\alpha|\le M_0,
$$

where M_0 is a large positive integer given in Theorem 3.3 below, and

$$\sum_{j_i\in\mathbb{Z}} \widehat{\phi^{(i)}}(2^{j_i}\xi^i)\widehat{\phi'^{(i)}}(2^{j_i}\xi^i) = 1 \quad \text{for } \xi^i \in \mathbb{R}^{N_i}\backslash\{0\};$$

see [Frazier and Jawerth 1990, Theorem 4.2]. For $J = (j_1, j_2, j_3) \in \mathbb{Z}^3$, set $\phi_J = (\widetilde{\phi}^{(1)}_{j_1} * \widetilde{\phi}^{(2)}_{j_2} * \widetilde{\phi}^{(3)}_{j_3})$, where $\widetilde{\phi}^{(i)}_{j_i} = \delta_{\mathbb{R}^{N-N_i}} \otimes \phi^{(i)}_{j_i}$, and $\widetilde{\phi}_J$ is defined similarly in terms of $\phi'^{(i)}_{j_i}$.

Theorem 3.3. *Let $0 < p \le 1$ and $w \in A^{\mathcal{F}}_\infty(\mathbb{R}^N)$. Let $M_0 \ge 10(N\{[q_w/p-1]\vee 2\}+1)$ (here $[\,\cdot\,]$ means the greatest integer function). For a fixed sufficiently large integer K, let $\mathcal{R}^{J,K}_{\mathcal{F}} = \mathcal{R}^{j_1-K,j_2-K,j_3-K}_{\mathcal{F}}$ and let x_R denote the lower left corner of R. Then, for every $f \in L^2(\mathbb{R}^N) \cap H^p_{\mathcal{F},w}(\mathbb{R}^N)$ there exists some function*

$$h = h_f \in L^2(\mathbb{R}^N) \cap H^p_{\mathcal{F},w}(\mathbb{R}^N)$$

depending only on f such that

$$f(x) \overset{L^2}{=} \sum_{J\in\mathbb{Z}^3} \sum_{R\in\mathcal{R}^{J,K}_{\mathcal{F}}} |R|\widetilde{\phi}_J(x-x_R)\phi_J * h(x_R).$$

Moreover,

$$\|f\|_{H^p_{\mathcal{F},w}} \approx \|h\|_{H^p_{\mathcal{F},w}}. \tag{3-7}$$

Proof. For $f \in L^2(\mathbb{R}^N) \cap H^p_{\mathcal{F},w}(\mathbb{R}^N)$, applying the Fourier transform gives $f = \sum_{J\in\mathbb{Z}^3} \widetilde{\phi}_J * \phi_J * f$, where the series converges in $L^2(\mathbb{R}^N)$ norm. Using Coifman's idea of the decomposition of the identity operator, we have

$$\begin{aligned} f(x) &= \sum_{J\in\mathbb{Z}^3} \sum_{R\in\mathcal{R}^{J,K}_{\mathcal{F}}} |R|\widetilde{\phi}_J(x-x_R)\phi_J * f(x_R) \\ &\quad + \sum_{J\in\mathbb{Z}^3} \sum_{R\in\mathcal{R}^{J,K}_{\mathcal{F}}} \int_R [\widetilde{\phi}_J(x-x')(\phi_J * f)(x') - \widetilde{\phi}_J(x-x_R)(\phi_J * f)(x_R)]\,dx' \\ &=: T_K(f)(x) + R_K(f)(x), \end{aligned}$$

where K is a fixed large integer to be determined later.

We can decompose $R_K(f)$ further as

$$\begin{aligned} R_K(f)(x) &= \sum_{J\in\mathbb{Z}^3} \sum_{R\in\mathcal{R}^{J,K}_{\mathcal{F}}} \int_R [\widetilde{\phi}_J(x-x') - \widetilde{\phi}_J(x-x_R)](\phi_J * f)(x')\,dx' \\ &\quad + \sum_{J\in\mathbb{Z}^3} \sum_{R\in\mathcal{R}^{J,K}_{\mathcal{F}}} \int_R \widetilde{\phi}_J(x-x_R)[(\phi_J * f)(x') - (\phi_J * f)(x_R)]\,dx' \\ &=: R^1_K(f)(x) + R^2_K(f)(x). \end{aligned}$$

We claim that for $k = 1, 2$,

$$\|R_K^k(f)\|_{H^p_{\mathcal{F},w}} \le C2^{-K}\|f\|_{H^p_{\mathcal{F},w}}, \tag{3-8}$$

where C is a constant independent of f, K and x_R.

Assume the claim for the moment. Then choosing sufficiently large K such that $C2^{-K} < 1$ implies that both T_K and $T_K^{-1} = \sum_{n=0}^{\infty}(R_K)^n$ are bounded on $L^2(\mathbb{R}^N)$ and on $H^p_{\mathcal{F},w}(\mathbb{R}^N)$. Setting $h = R_K^{-1}(f)$ gives (3-7). Moreover,

$$f = T_K(T_K^{-1}(f)) = \sum_{J\in\mathbb{Z}^3}\sum_{R\in\mathcal{R}_{\mathcal{F}}^{J,K}} |R|\widetilde{\phi}_J(\cdot - x_R)(\phi_J * h)(x_R),$$

where the series converges in $L^2(\mathbb{R}^N)$.

To finish the proof of Theorem 1.10, it suffices to verify the claim. Since the proofs for R_K^1 and R_K^2 are similar, we only treat R_K^1. The discrete Calderón reproducing formula in Theorem 2.1 yields

$$\begin{aligned}
&\psi_{J'} * R_K^1(f)(x)\\
&= \sum_{J\in\mathbb{Z}^3}\sum_{R\in\mathcal{R}_{\mathcal{F}}^{J,K}} \int_R \psi_{J'} * [\widetilde{\phi}_J(\cdot - x') - \widetilde{\phi}_J(\cdot - x_R)](x)(\phi_J * f)(x')\,dx'\\
&= \sum_{J\in\mathbb{Z}^3}\sum_{R\in\mathcal{R}_{\mathcal{F}}^{J,K}} \int_R \psi_{J'} * [\widetilde{\phi}_J(\cdot - x') - \widetilde{\phi}_J(\cdot - x_R)](x)\\
&\qquad \times\Bigg(\sum_{J''\in\mathbb{Z}^3}\sum_{R''\in\mathcal{R}_{\mathcal{F}}^{J''}} |R''|\cdot\psi_{J''} * f(x_{R''})\phi_J * \psi_{J''}(x' - x_{R''})\Bigg)\,dx',
\end{aligned} \tag{3-9}$$

where $x_{R''} = (x_{Q_1''}, x_{Q_2''}, x_{Q_3''})$ denotes the lower left corner of R''. Set

$$\widetilde{\widetilde{\phi}}_J(u) = \widetilde{\phi}_J(u - x') - \widetilde{\phi}_J(u - x_R).$$

Applying Lemma 2.2 with M sufficiently large (which will be determined later) and $L = 10M$, we obtain that for some constant C (depending only on M, ψ and ϕ, but independent of K),

$$\begin{aligned}
&|\psi_{J'} * \widetilde{\widetilde{\phi}}_J(x)|\\
&\qquad \le C2^{-K}2^{-10M(|j_1-j_1'|+|j_2-j_2'|+|j_3-j_3'|)}\prod_{i=1}^{3}\frac{\max_{1\le k\le i} 2^{j_k'M}}{(\max_{1\le k\le i} 2^{j_k'} + |x_i - x_i'|)^{1+M}},
\end{aligned}$$

and, similarly,

$$\begin{aligned}
&|\phi_J * \psi_{J''}(x' - x_{R''})|\\
&\qquad \le C2^{-10M(|j_1-j_1''|+|j_2-j_2''|+|j_3-j_3''|)}\prod_{i=1}^{3}\frac{\max_{1\le k\le i} 2^{j_k''M}}{(\max_{1\le k\le i} 2^{j_k''} + |x_i' - x_{Q_i''}|)^{1+M}}.
\end{aligned}$$

Substituting both estimates into the last term of (3-9) yields

$$
\begin{aligned}
&|\psi_{J'} * R_K^1(f)(x)| \\
&\qquad \lesssim \sum_{J''\in\mathbb{Z}^3} \sum_{R''\in\mathcal{R}_{\mathcal{F}}^{J''}} |R''|\,|\psi_{J''} * f(x_{R''})| \\
&\qquad\quad \times \sum_{J\in\mathbb{Z}^3} \sum_{R\in\mathcal{R}_{\mathcal{F}}^{J,K}} \int_R 2^{-K} \prod_{i=1}^{3} 2^{-|j_i-j_i'|3M} \frac{\max_{1\le k\le i} 2^{j_k' M}}{(\max_{1\le k\le i} 2^{j_k'} + |x_i - x_i'|)^{1+M}} \\
&\qquad\quad \times 2^{-|j_i-j_i''|3M} \frac{\max_{1\le k\le i} 2^{j_k'' M}}{(\max_{1\le k\le i} 2^{j_k''} + |x_i' - x_{Q_i''}|)^{1+M}} dx' \\
&\qquad \lesssim 2^{-K} \sum_{J''\in\mathbb{Z}^3} \sum_{R''\in\mathcal{R}_{\mathcal{F}}^{J''}} 2^{-(|j_1'-j_1''|+|j_2'-j_2''|+|j_3'-j_3''|)M} |R''| \\
&\qquad\quad \times \left(\prod_{i=1}^{3} \frac{\max_{1\le k\le i} 2^{(j_k'\vee j_k'')M}}{(\max_{1\le k\le i} 2^{j_k'\vee j_k''} + |x_i - x_{Q_i''}|)^{1+M}} \right) |\psi_{J''} * f(x_{R''})|.
\end{aligned}
$$

Now we may choose $M = N\{[q_w/p+1]\vee 2\}+1$, $L = 10M$ and $N/M < \delta < 1$. Then $p/\delta > q_w$ so that $w \in A_{p/\delta}^{\mathcal{F}}(\mathbb{R}^N)$. Arguing as in the proof of Theorem 1.4, we obtain

$$
\begin{aligned}
&\|R_K^1(f)\|_{H_{\mathcal{F},w}^p} \\
&\quad \lesssim 2^{-K} \left\| \left\{ \sum_{J''\in\mathbb{Z}^3} \left\{ \mathcal{M}_{\mathcal{F}} \Bigg(\sum_{R''\in\mathcal{R}_{\mathcal{F}}^{J''}} |\psi_{J''} * f(x_{R''})| \chi_{R''} \Bigg)^{\delta} \right\}^{\frac{2}{\delta}} \right\}^{\frac{1}{2}} \right\|_{L_w^p} \lesssim 2^{-K} \|f\|_{H_{\mathcal{F},w}^p}.
\end{aligned}
$$

This verifies claim (3-8) and hence Theorem 3.3 follows. □

Using a similar argument to the one in the proof of Theorem 1.4, one can prove the following:

Corollary 3.4. *Suppose $w \in A_\infty^{\mathcal{F}}(\mathbb{R}^N)$. Then, for $f \in H_{\mathcal{F},w}^p(\mathbb{R}^N) \cap L^2(\mathbb{R}^N)$ and $0 < p \le 1$, we have*

$$
\|f\|_{H_{\mathcal{F},w}^p(\mathbb{R}^N)} \approx \|\tilde{g}_{\mathcal{F}}(f)\|_{L_w^p(\mathbb{R}^N)} := \left\| \left\{ \sum_{J\in\mathbb{Z}^3} \sum_{R\in\mathcal{R}_{\mathcal{F}}^{J,K}} |\phi_J * h(x_R)|^2 \chi_R \right\}^{\frac{1}{2}} \right\|_{L_w^p(\mathbb{R}^N)},
$$

where $h = h_f$ and K are the same as in Theorem 3.3.

The key to the proof of Theorem 1.10 is the following.

Lemma 3.5. *Suppose $0 < p \le 1$ and $w \in A_\infty^{\mathcal{F}}(\mathbb{R}^N)$. If $f \in H_{\mathcal{F},w}^p(\mathbb{R}^N) \cap L^2(\mathbb{R}^N)$, then $f \in L_w^p(\mathbb{R}^N)$ and there is a constant $C_p > 0$ independent of the $L^2(\mathbb{R}^N)$ norm of f such that*

$$
\|f\|_{L_w^p(\mathbb{R}^N)} \le C_p \|f\|_{H_{\mathcal{F},w}^p(\mathbb{R}^N)}.
$$

Proof. Without loss of generality, we may assume $w \in A_q^{\mathcal{F}}(\mathbb{R}^N)$ for some $q \in [2, \infty)$. Given $f \in L^2(\mathbb{R}^N) \cap H^p_{\mathcal{F},w}(\mathbb{R}^N)$, set $\Omega_i = \{x \in \mathbb{R}^N : \tilde{g}_{\mathcal{F}}(h)(x) > 2^i\}$ where $h = h_f$ is given by Theorem 3.3, and

$$\mathscr{U}_i = \{(J, R) : J \in \mathbb{Z}^3,\ R \in \mathcal{R}_{\mathcal{F}}^{J,K},\ |R \cap \Omega_i| > (1/2)|R|,\ |R \cap \Omega_{i+1}| \le (1/2)|R|\}.$$

By the discrete Calderón reproducing formula in Theorem 3.3,

$$f = \sum_{i\in\mathbb{Z}} \sum_{(J,R)\in\mathscr{U}_i} |R|\widetilde{\phi}_J(\cdot - x_R)\phi_J * h(x_R).$$

We claim that

$$\Big\| \sum_{(J,R)\in\mathscr{U}_i} |R|\widetilde{\phi}_J(\cdot - x_R)\phi_J * h(x_R)\Big\|^p_{L^p_w(\mathbb{R}^N)} \lesssim 2^{pi} w(\Omega_i). \tag{3-10}$$

Since $0 < p \le 1$, the above claim together with Theorem 3.3 yields

$$\begin{aligned}\|f\|^p_{L^p_w(\mathbb{R}^N)} &\le \sum_{i\in\mathbb{Z}} \Big\| \sum_{(J,R)\in\mathscr{U}_i} |R|\widetilde{\phi}_J(\cdot - x_R)\phi_J * h(x_R)\Big\|^p_{L^p_w(\mathbb{R}^N)}\\ &\lesssim \sum_{i\in\mathbb{Z}} 2^{pi} w(\Omega_i) \lesssim \|\tilde{g}(h)\|^p_{L^p_w(\mathbb{R}^N)} \approx \|h\|^p_{H^p_{\mathcal{F},w}(\mathbb{R}^N)} \approx \|f\|^p_{H^p_{\mathcal{F},w}(\mathbb{R}^N)}\end{aligned}$$

and Lemma 3.5 follows.

To show claim (3-10), we note that if $(J, R) \in \mathscr{U}_i$, the function $x \mapsto \widetilde{\phi}_J(x - x_R)$ is supported in $\widetilde{\Omega}_i := \{x : \mathcal{M}_{\mathcal{F}}(\chi_{\Omega_i})(x) > 1/100\}$. By Hölder's inequality,

$$\begin{aligned}&\Big\| \sum_{(J,R)\in\mathscr{U}_i} |R|\widetilde{\phi}_J(\cdot - x_R)\phi_J * h(x_R)\Big\|^p_{L^p_w(\mathbb{R}^N)}\\ &\qquad \lesssim w(\widetilde{\Omega}_i)^{1-(p/q)} \Big\| \sum_{(J,R)\in\mathscr{U}_i} |R|\widetilde{\phi}_J(\cdot - x_R)\phi_J * h(x_R)\Big\|^p_{L^q_w(\mathbb{R}^N)}.\end{aligned} \tag{3-11}$$

We now estimate the last L^q_w-norm by a duality argument. For $\zeta \in L^{q'}_{w^{1-q'}}(\mathbb{R}^N)$ with $\|\zeta\|_{L^{q'}_{w^{1-q'}}(\mathbb{R}^N)} \le 1$,

$$\begin{aligned}&\Big|\Big\langle \sum_{(J,R)\in\mathscr{U}_i} |R|\widetilde{\phi}_J(\cdot - x_R)\phi_J * h(x_R), \zeta\Big\rangle\Big| = \Big| \sum_{(J,R)\in\mathscr{U}_i} \int \overline{\phi}_J * \zeta(x_R)\phi_J * h(x_R)\chi_R(x)\,dx\Big|\\ &\le \Big\|\Big\{ \sum_{(J,R)\in\mathscr{U}_i} |\phi_J * h(x_R)|^2\chi_R\Big\}^{\frac12}\Big\|_{L^q_w(\mathbb{R}^N)} \Big\|\Big\{ \sum_{(J,R)\in\mathscr{U}_i} |\overline{\phi}_J * \zeta(x_R)|^2\chi_R\Big\}^{\frac12}\Big\|_{L^{q'}_{w^{1-q'}}(\mathbb{R}^N)}\\ &:= I_1 \times I_2,\end{aligned}$$

where $\overline{\phi}_J(x) = \widetilde{\phi}_J(-x)$.

We first estimate I_2. Since $w \in A_q^{\mathcal{F}}(\mathbb{R}^N)$ implies $w^{1-q'} \in A_{q'}^{\mathcal{F}}(\mathbb{R}^N)$, Corollary 3.4 and the remark on page 552 yield

$$I_2 \lesssim \left\| \left\{ \sum_{J\in\mathbb{Z}^3} \sum_{R\in\mathcal{R}_{\mathcal{F}}^{J,K}} |\overline{\phi}_J * \zeta(x_R)|^2 \chi_R \right\}^{\frac{1}{2}} \right\|_{L^{q'}_{w^{1-q'}}(\mathbb{R}^N)} \approx \|\zeta\|_{L^{q'}_{w^{1-q'}}(\mathbb{R}^N)} \le 1. \tag{3-12}$$

As for I_1, note that $\Omega_i \subset \widetilde{\Omega}_i$ and $w(\widetilde{\Omega}_i) \lesssim w(\Omega_i)$ due to the $L^q_w(\mathbb{R}^N)$ boundedness of $\mathcal{M}_{\mathcal{F}}$. For any $(J, R) \in \mathscr{U}_i$ and $x \in R$, $\mathcal{M}_{\mathcal{F}}(\chi_{R\cap\widetilde{\Omega}_i\setminus\Omega_{i+1}})(x) > \frac{1}{2}$. Applying Corollary 2.5 again, we have

$$\begin{aligned} I_1^q &= \int_{\mathbb{R}^N} \left\{ \sum_{(J,R)\in\mathscr{U}_i} |\phi_J * h(x_R)|^2 \chi_R(x) \right\}^{\frac{q}{2}} w(x)\,dx \\ &\lesssim \int_{\mathbb{R}^N} \left\{ \sum_{(J,R)\in\mathscr{U}_i} |\phi_J * h(x_R) \mathcal{M}_{\mathcal{F}}(\chi_{R\cap\widetilde{\Omega}_i\setminus\Omega_{i+1}})(x)|^2 \right\}^{\frac{q}{2}} w(x)\,dx \\ &\lesssim \int_{\widetilde{\Omega}_i\setminus\Omega_{i+1}} \left\{ \sum_{(J,R)\in\mathscr{U}_i} |\phi_J * h(x_R)|^2 \chi_R(x) \right\}^{\frac{q}{2}} w(x)\,dx \\ &\lesssim 2^{iq} w(\widetilde{\Omega}_i) \lesssim 2^{iq} w(\Omega_i). \end{aligned} \tag{3-13}$$

Combining both estimates (3-12) and (3-13), we obtain

$$\left\| \sum_{(J,R)\in\mathscr{U}_i} |R| \widetilde{\phi}_J(\cdot - x_R) \phi_J * h(x_R) \right\|_{L^q_w(\mathbb{R}^N)} \lesssim 2^{iq} w(\Omega_i).$$

Plugging this estimate into (3-11) yields claim (3-10), and so Lemma 3.5 follows. □

Proof of Theorem 1.10. For $f \in L^2(\mathbb{R}^N) \cap H^p_{\mathcal{F},w}(\mathbb{R}^N)$, by Theorem 1.9 and Lemma 3.5,

$$\|T(f)\|_{L^p_w(\mathbb{R}^N)} \le C\|T(f)\|_{H^p_{\mathcal{F},w}(\mathbb{R}^N)} \le C\|f\|_{H^p_{\mathcal{F},w}(\mathbb{R}^N)}.$$

Corollary 2.6 together with a limiting argument yields Theorem 1.10. □

We remark that, as mentioned before, the flag Hardy space $H^p_{\mathcal{F}}(\mathbb{R}^N)$ (where $w \equiv 1$) differs from those of the classical one parameter and the product Hardy space. To see this, by Lemma 3.5, if $f \in L^2(\mathbb{R}^N) \cap H^p_{\mathcal{F}}(\mathbb{R}^N)$, then $f \in L^1(\mathbb{R}^N)$ and

$$\int f(x_1, x_2, x_3)\,dx_3 = 0 \quad \text{for almost every } (x_1, x_2) \in \mathbb{R}^{n_1} \times \mathbb{R}^{n_2}. \tag{3-14}$$

Indeed, for $f \in L^2(\mathbb{R}^N) \cap H^p_{\mathcal{F}}(\mathbb{R}^N)$, Lemma 3.5 gives that $f \in L^p(\mathbb{R}^N) \cap L^2(\mathbb{R}^N)$, and hence $f \in L^1(\mathbb{R}^N)$ by interpolation. To see $\int f(x_1, x_2, x_3)\,dx_3 = 0$, applying the Calderón reproducing formula in Theorem 2.1,

$$f(x)=\sum_{J\in\mathbb{Z}^3}\sum_{R\in\mathcal{R}^J_{\mathcal{F}}}|R|\psi_J(x-x_R)\psi_J*f(x_R)$$

where the series converges in both $L^2(\mathbb{R}^N)$ and $H^p_{\mathcal{F}}(\mathbb{R}^N)$. Let $\mathscr{E}_L$ and f_L be defined as in the proof of Corollary 2.6. Therefore,

$$f-f_L=\sum_{\mathscr{E}^c_L}|R|\psi_J(x-x_R)\psi_J*f(x_R)$$

converges to zero in both $L^2(\mathbb{R}^N)$ and $H^p_{\mathcal{F}}(\mathbb{R}^N)$ as L tends to infinity. Applying Lemma 3.5 and interpolation, we obtain

$$\begin{aligned}\Big\|\sum_{\mathscr{E}^c_L}|R|\psi_J(x-x_R)\psi_J*f(x_R)\Big\|_{L^1}&\\ \lesssim\Big\|\sum_{\mathscr{E}^c_L}|R|\psi_J(x-x_R)\psi_J*f(x_R)\Big\|_{L^2}&+\Big\|\sum_{\mathscr{E}^c_L}|R|\psi_J(x-x_R)\psi_J*f(x_R)\Big\|_{H^p_{\mathcal{F}}},\end{aligned}$$

which implies that $\|f-f_L\|_{L^1}$ tends to zero as L tends to infinity. Therefore, for almost every $(x_1,x_2)\in\mathbb{R}^{n_1}\times\mathbb{R}^{n_2}$,

$$\int_{\mathbb{R}^{n_3}}f(x_1,x_2,x_3)\,dx_3=\lim_{L\to\infty}\int_{\mathbb{R}^{n_3}}\sum_{\mathscr{E}_L}|R|\psi_J(x-x_R)\psi_J*f(x_R)\,dx_3=0,$$

where the last equality follows from the cancellation property of $\psi_J(x-x_R)$. This indicates that all L^2 elements in $H^p_{\mathcal{F}}$ satisfy only "partial" cancellation property (3-14), which is different from cancellation conditions for classical one parameter and the product Hardy spaces.

Finally, we prove Theorem 1.11. It is known that $L^2(\mathbb{R}^N)\cap H^p_{\mathcal{F},w}(\mathbb{R}^N)$ is dense in $H^p_{\mathcal{F},w}(\mathbb{R}^N)$. This allows us to use the discrete Calderón reproducing formula in Theorem 3.3, which plays a crucial role in the proof of the boundedness of flag singular integral operators on $H^p_{\mathcal{F},w}(\mathbb{R}^N)$. For $CMO^p_{\mathcal{F},w}$, we prove the following so-called *weak density* result which will offer the same service as the above density does in $H^p_{\mathcal{F},w}$.

Lemma 3.6. *Let $0<p\le 1$ and $w\in A^{\mathcal{F}}_\infty(\mathbb{R}^N)$. Then $L^2(\mathbb{R}^N)\cap CMO^p_{\mathcal{F},w}(\mathbb{R}^N)$ is dense in $CMO^p_{\mathcal{F},w}(\mathbb{R}^N)$ in the weak topology $\langle H^p_{\mathcal{F},w}(\mathbb{R}^N), CMO^p_{\mathcal{F},w}(\mathbb{R}^N)\rangle$. More precisely, for any $f\in CMO^p_{\mathcal{F},w}(\mathbb{R}^N)$, there exists a sequence*

$$\{f_n\}\subset L^2(\mathbb{R}^N)\cap CMO^p_{\mathcal{F},w}(\mathbb{R}^N)$$

satisfying $\|f_n\|_{CMO^p_{\mathcal{F},w}(\mathbb{R}^N)}\lesssim\|f\|_{CMO^p_{\mathcal{F},w}(\mathbb{R}^N)}$ and

$$\lim_{n\to\infty}\langle f_n,g\rangle=\langle f,g\rangle\quad\text{for any } g\in H^p_{\mathcal{F},w}(\mathbb{R}^N).$$

Proof. Suppose $f \in CMO^p_{\mathcal{F},w}(\mathbb{R}^N)$. Set

$$f_n(x) = \sum_{|j|\le n, |k|\le n} \sum_{R\subset B(0,n)} |R|\psi_J * f(x_R)\psi_J(x-x_R),$$

where $\{\psi_J\}$ satisfy (1-1) and (1-2). It is easy to see that $f_n \in L^2(\mathbb{R}^N)$. Repeating the same proof as the one in Theorem 1.6, we have $\|f_n\|_{CMO^p_{\mathcal{F},w}(\mathbb{R}^N)} \le C\|f\|_{CMO^p_{\mathcal{F},w}(\mathbb{R}^N)}$ and hence $f_n \in L^2(\mathbb{R}^N) \cap CMO^p_{\mathcal{F},w}(\mathbb{R}^N)$. For any $g \in \mathcal{S}_\infty(\mathbb{R}^N)$, the discrete Calderón reproducing formula given in Theorem 2.1 yields

$$\begin{aligned}\langle f - f_n, g\rangle &= \Big\langle \sum_{|j|>n, \text{ or } |k|>n, \text{ or } R\subsetneq B(0,n)} |R|\psi_J * f(x_R)\psi_J(\cdot - x_R), g\Big\rangle \\ &= \Big\langle f, \sum_{|j|>n, \text{ or } |k|>n, \text{ or } R\subsetneq B(0,n)} |R|\psi_J * g(x_R)\psi_J(\cdot - x_R)\Big\rangle.\end{aligned}$$

By Corollary 2.6, the function

$$\sum_{|j|>n, \text{ or } |k|>n, \text{ or } R\subsetneq B(0,n)} |R|\psi_J * g(x_R)\psi_J(x - x_R)$$

belongs to $H^p_{\mathcal{F},w}(\mathbb{R}^N)$ and its $H^p_{\mathcal{F},w}(\mathbb{R}^N)$ norm tends to 0 as $n \to \infty$. Hence, Theorem 1.7 implies that $\langle f - f_n, g\rangle$ tends to zero as $n \to \infty$. Since $\mathcal{S}_\infty(\mathbb{R}^N)$ is dense in $H^p_{\mathcal{F},w}(\mathbb{R}^N)$, a standard limiting argument finishes the proof of Lemma 3.6. □

Now let us show how a flag singular integral operator $T_{\mathcal{F}}$ acts on $CMO^p_{\mathcal{F},w}(\mathbb{R}^N)$. Given $f \in CMO^p_{\mathcal{F},w}(\mathbb{R}^N)$, by Lemma 3.6, there is a sequence

$$\{f_n\} \subset L^2(\mathbb{R}^N) \cap CMO^p_{\mathcal{F},w}(\mathbb{R}^N)$$

such that

$$\begin{cases} \|f_n\|_{CMO^p_{\mathcal{F},w}(\mathbb{R}^N)} \le C\|f\|_{CMO^p_{\mathcal{F},w}(\mathbb{R}^N)}, \\ \lim_{n\to\infty} \langle f_n, g\rangle = \langle f, g\rangle \quad \text{for any } g \in L^2(\mathbb{R}^N) \cap H^p_{\mathcal{F},w}(\mathbb{R}^N). \end{cases} \tag{3-15}$$

We thus define

$$\langle T_{\mathcal{F}}(f), g\rangle = \lim_{n\to\infty} \langle T_{\mathcal{F}}(f_n), g\rangle \quad \text{for any } g \in L^2(\mathbb{R}^N) \cap H^p_{\mathcal{F},w}(\mathbb{R}^N).$$

To see that the limit exists, write $\langle (T_{\mathcal{F}})(f_j - f_k), g\rangle = \langle f_j - f_k, (T_{\mathcal{F}})^*(g)\rangle$ since both $f_j - f_k$ and g belong to $L^2(\mathbb{R}^N)$, and $T_{\mathcal{F}}$ is bounded on $L^2(\mathbb{R}^N)$. By Theorem 1.9, $(T_{\mathcal{F}})^*$ is bounded on $H^p_{\mathcal{F},w}(\mathbb{R}^N)$, and therefore $(T_{\mathcal{F}})^*(g) \in L^2(\mathbb{R}^N) \cap H^p_{\mathcal{F},w}(\mathbb{R}^N)$. Thus, by Lemma 3.6, $\langle f_j - f_k, (T_{\mathcal{F}})^*(g)\rangle$ tends to zero as $j, k \to \infty$. It is also easy to verify that the definition of $T_{\mathcal{F}}(f)$ is independent of the choice of the sequence f_n satisfying the conditions in Lemma 3.6.

We are now ready to prove Theorem 1.11.

Proof of Theorem 1.11. We first show that for $f \in L^2(\mathbb{R}^N) \cap CMO^p_{\mathcal{F},w}(\mathbb{R}^N)$ and any open set Ω with $w(\Omega) < \infty$,

$$\left\{ \frac{1}{[w(\Omega)]^{2/p-1}} \sum_{J \in \mathbb{Z}^3} \sum_{\substack{R \in \mathcal{R}^J_{\mathcal{F}},\\ R \subset \Omega}} |\psi_J * K_{\mathcal{F}} * f(x_R)|^2 \frac{|R|^2}{w(R)} \right\}^{\frac{1}{2}} \lesssim \|f\|_{CMO^p_{\mathcal{F},w}(\mathbb{R}^N)}. \tag{3-16}$$

Using the discrete Calderón reproducing formula given in Theorem 2.1, we write

$$\begin{aligned} &\sum_{J \in \mathbb{Z}^3} \sum_{\substack{R \in \mathcal{R}^J_{\mathcal{F}},\\ R \subset \Omega}} |\psi_J * K_{\mathcal{F}} * f(x_R)|^2 \frac{|R|^2}{w(R)} \\ &\qquad = \sum_{J \in \mathbb{Z}^3} \sum_{\substack{R \in \mathcal{R}^J_{\mathcal{F}},\\ R \subset \Omega}} \left| \sum_{J' \in \mathbb{Z}^3} \sum_{R' \in \mathcal{R}^{J'}_{\mathcal{F}}} t_{R'} |R'|^{\frac{1}{2}} \psi_J * \mathcal{K} * \psi_{J'}(x_R - x_{R'}) \right|^2 \frac{|R|^2}{w(R)}, \end{aligned}$$

where $t_{R'} = \psi_{J'} * f(x_{R'})|R'|^{\frac{1}{2}}$. By (3-6), $\psi_J * \mathcal{K} * \psi_{J'}$ satisfies the same almost-orthogonality estimate as $\psi_J * \psi_{J'}$. Repeating the same argument as in Theorem 1.6 yields (3-16).

For $f \in CMO^p_{\mathcal{F},w}(\mathbb{R}^N)$, there is a sequence

$$\{f_n\} \subset L^2(\mathbb{R}^N) \cap CMO^p_{\mathcal{F},w}(\mathbb{R}^N)$$

satisfying (3-15). By the definition of $T_{\mathcal{F}}(f)$ and the boundedness of $T_{\mathcal{F}}$ on $L^2(\mathbb{R}^N) \cap CMO^p_{\mathcal{F},w}(\mathbb{R}^N)$,

$$\begin{aligned} \|T_{\mathcal{F}}(f)\|_{CMO^p_{\mathcal{F},w}(\mathbb{R}^N)} &\le \liminf_{n\to\infty} \|T_{\mathcal{F}}(f_n)\|_{CMO^p_{\mathcal{F},w}(\mathbb{R}^N)} \\ &\lesssim \liminf_{n\to\infty} \|f_n\|_{CMO^p_{\mathcal{F},w}(\mathbb{R}^N)} \lesssim \|f\|_{CMO^p_{\mathcal{F},w}(\mathbb{R}^N)}, \end{aligned}$$

which concludes the proof of Theorem 1.11. □

4. Calderón–Zygmund decomposition and interpolation

We first prove the Calderón–Zygmund decomposition for $H^p_{\mathcal{F},w}$.

Proof of Theorem 1.12. According to Corollary 2.6, $L^2(\mathbb{R}^N) \cap H^p_{\mathcal{F},w}(\mathbb{R}^N)$ is dense in $H^p_{\mathcal{F},w}(\mathbb{R}^N)$. Thus it suffices to prove Theorem 1.12 for $f \in L^2(\mathbb{R}^N) \cap H^p_{\mathcal{F},w}(\mathbb{R}^N)$. Given any fixed $\alpha > 0$, let $\Omega_l = \{x \in \mathbb{R}^N : \tilde{g}_{\mathcal{F}}(f)(x) > \alpha 2^l\}$, $l \in \mathbb{N}$, where $\tilde{g}_{\mathcal{F}}(f)$ and K are the same as in Corollary 3.4. For $J \in \mathbb{Z}^3$, set

$$\begin{aligned} \mathcal{R}^{J,K}_0 &= \left\{ R \in \mathcal{R}^{J,K}_{\mathcal{F}} : |R \cap \Omega_0| < \tfrac{1}{2}|R| \right\}, \quad \text{and} \\ \mathcal{R}^{J,K}_l &= \left\{ R \in \mathcal{R}^{J,K}_{\mathcal{F}} : |R \cap \Omega_{l-1}| \ge \tfrac{1}{2}|R|,\ |R \cap \Omega_l| < \tfrac{1}{2}|R| \right\} \quad \text{for } l \ge 1. \end{aligned}$$

It follows from Theorem 3.3 that there exists some $h \in L^2 \cap H^p_{\mathcal{F},w}$ such that

$$f(x) = \sum_{J\in\mathbb{Z}^3} \sum_{R\in\mathcal{R}_0^{J,K}} |R|\phi_J * h(x_R)\widetilde{\phi}_J(x-x_R) \\ + \sum_{J\in\mathbb{Z}^3} \sum_{l\geq 1} \sum_{R\in\mathcal{R}_l^{J,K}} |R|\phi_J * h(x_R)\widetilde{\phi}_J(x-x_R) =: g(x)+b(x).$$

We first estimate $\|g\|_{H^{p_2}_{\mathcal{F},w}}$. Repeating the same argument as in the proof of Theorem 1.4, we deduce that for $N/M < \delta < \min\{(p_2/q_w), 1\}$,

$$\sum_{J\in\mathbb{Z}^3} \sum_{R\in\mathcal{R}^J_{\mathcal{F}}} |\psi_J * g(x_R)|^2 \chi_R(x) \lesssim \sum_{J'\in\mathbb{Z}^3} \left\{ \mathcal{M}_{\mathcal{F}}\left[\left(\sum_{R'\in\mathcal{R}_0^{J',K}} |\phi_{J'} * g(x_{R'})|^2 \chi_{R'}\right)^{\frac{\delta}{2}}\right](x)\right\}^{\frac{2}{\delta}}.$$

Take the square root on both sides and apply Corollary 2.5 on $L^{p_2/\delta}_w(\ell^{2/\delta})$ (note that $w \in A^{\mathcal{F}}_{p_2/\delta}$) to derive

$$\|g\|_{H^{p_2}_{\mathcal{F},w}(\mathbb{R}^N)} \lesssim \left\| \left\{ \sum_{J'\in\mathbb{Z}^3} \sum_{R'\in\mathcal{R}_0^{J',K}} |\phi_{J'} * h(x_{R'})|^2 \chi_{R'} \right\}^{\frac{1}{2}} \right\|_{L^{p_2}_w(\mathbb{R}^N)}.$$

We claim

$$\text{(4-1)} \quad \int_{\{\tilde{g}_{\mathcal{F}}(f)(x)\leq\alpha\}} [\tilde{g}_{\mathcal{F}}(f)(x)]^{p_2} w(x)\,dx \\ \gtrsim \left\| \left\{ \sum_{J'\in\mathbb{Z}^3} \sum_{R\in\mathcal{R}_0^{J',K}} |\phi_{J'} * h(x_{R'})|^2 \chi_{R'} \right\}^{\frac{1}{2}} \right\|^{p_2}_{L^{p_2}_w(\mathbb{R}^N)},$$

which implies

$$\|g\|^{p_2}_{H^{p_2}_{\mathcal{F},w}(\mathbb{R}^N)} \lesssim \int_{\{\tilde{g}_{\mathcal{F}}(f)(x)\leq\alpha\}} [\tilde{g}_{\mathcal{F}}(f)(x)]^{p_2} w(x)\,dx \\ \leq \alpha^{p_2-p} \int_{\{\tilde{g}_{\mathcal{F}}(f)(x)\leq\alpha\}} [\tilde{g}_{\mathcal{F}}(f)(x)]^{p} w(x)\,dx \lesssim \alpha^{p_2-p} \|f\|^p_{H^p_{\mathcal{F},w}(\mathbb{R}^N)}$$

as desired. It suffices to verify claim (4-1). Choose $\delta < \min\{p_2/q_w, 1\}$ and get

$$\int_{\{\tilde{g}_{\mathcal{F}}(f)(x)\leq\alpha\}} [\tilde{g}_{\mathcal{F}}(f)(x)]^{p_2} w(x)\,dx \\ = \int_{\mathbb{R}^N} \left\{ \sum_{J\in\mathbb{Z}^3} \sum_{R\in\mathcal{R}^{J,K}_{\mathcal{F}}} |\phi_J * h(x_R)|^2 \chi_{R\cap \complement\Omega_0}(x) \right\}^{\frac{p_2}{2}} w(x)\,dx$$

$$\gtrsim \int_{\mathbb{R}^N} \Big\{ \sum_{J\in\mathbb{Z}^3} \sum_{R\in\mathcal{R}_{\mathcal{F}}^{J,K}} (|\phi_J * h(x_R)|^\delta \mathcal{M}_{\mathcal{F}}(\chi_{R\cap\complement\Omega_0})(x))^{\frac{2}{\delta}} \Big\}^{\frac{p_2}{2}} w(x)\,dx$$

$$\gtrsim \Big\| \Big\{ \sum_{J\in\mathbb{Z}^3} \sum_{R\in\mathcal{R}_{\mathcal{F}}^{J,K}} |\phi_J * h(x_R)|^2 \chi_R \Big\}^{\frac{1}{2}} \Big\|_{L_w^{p_2}(\mathbb{R}^N)}^{p_2},$$

where in the last inequality we used the estimate $\chi_R(x) \le 2^{1/\delta}\mathcal{M}_{\mathcal{F}}(\chi_{R\cap\complement\Omega_0})^{1/\delta}(x)$ for $R\in\mathcal{R}_{\mathcal{F}}^{J,K}$, and the first inequality follows from Corollary 2.5 with $q = 2/\delta$ and $p = p_2/\delta$.

Now, we turn to the estimate for the $H^{p_1}_{\mathcal{F},w}(\mathbb{R}^N)$ norm of b. Set $\widetilde{\Omega}_l = \{x\in\mathbb{R}^N : \mathcal{M}_{\mathcal{F}}(\chi_{\Omega_l}) > \frac{1}{2}\},\ l\in\mathbb{Z}$. Then the desired estimate follows from

$$\Big\| \sum_{J\in\mathbb{Z}^3} \sum_{R\in\mathcal{R}_l^{J,K}} |R|\phi_J * h(x_R)\widetilde{\phi}_J(\cdot - x_R) \Big\|_{H^{p_1}_{\mathcal{F},w}}^{p_1} \lesssim (2^l\alpha)^{p_1} w(\widetilde{\Omega}_{l-1}), \tag{4-2}$$

for any $0 < p_1 \le 1$ and $l \ge 1$. Indeed, by the $L^q_w(\mathbb{R}^N)$ $(q > q_w)$ boundedness of $\mathcal{M}_{\mathcal{F}}$,

$$w(\widetilde{\Omega}_{l-1}) \lesssim \int_{\mathbb{R}^N} [\mathcal{M}_{\mathcal{F}}(\chi_{\Omega_{l-1}})(x)]^q w(x)\,dx \lesssim w(\Omega_{l-1}).$$

This fact together with (4-2) yields

$$\begin{aligned}\|b\|^{p_1}_{H^{p_1}_{\mathcal{F},w}(\mathbb{R}^N)} &\lesssim \sum_{l\ge1} (2^l\alpha)^{p_1} w(\widetilde{\Omega}_{l-1}) \lesssim \sum_{l\ge1} (2^l\alpha)^{p_1} w(\Omega_{l-1}) \\ &\lesssim \int_{\{\tilde{g}_{\mathcal{F}}(f)(x)>\alpha\}} [\tilde{g}_{\mathcal{F}}(f)(x)]^{p_1} w(x)\,dx \\ &\lesssim \alpha^{p_1-p} \int_{\{\tilde{g}_{\mathcal{F}}(f)(x)>\alpha\}} [\tilde{g}_{\mathcal{F}}(f)(x)]^{p} w(x)\,dx \lesssim \alpha^{p_1-p}\|f\|^p_{H^p_{\mathcal{F},w}(\mathbb{R}^N)}.\end{aligned}$$

Thus to finish the proof, it remains to establish (4-2). Following the same argument as in the estimation of $\|g\|_{H^{p_2}_{\mathcal{F},w}}$, we get that for any $l \ge 1$,

$$\Big\| \sum_{J\in\mathbb{Z}^3} \sum_{R\in\mathcal{R}_l^{J,K}} |R|\phi_J * h(x_R)\widetilde{\phi}_J(\cdot - x_R) \Big\|_{H^{p_1}_{\mathcal{F},w}} \lesssim \Big\| \Big\{ \sum_{J\in\mathbb{Z}^3} \sum_{R\in\mathcal{R}_l^{J,K}} |\phi_J * h(x_R)|^2 \chi_R \Big\}^{\frac{1}{2}} \Big\|_{L^{p_1}_w}. \tag{4-3}$$

Note that $R \subset \widetilde{\Omega}_{l-1}$ for $R\in\mathcal{R}_l^{J,K}$. Thus, $|R\cap(\widetilde{\Omega}_{l-1}\setminus\Omega_l)| > \frac{1}{2}|R|$, which implies

$$\chi_R(x) \le 2^{\frac{1}{\delta}} \mathcal{M}_{\mathcal{F}}(\chi_{R\cap(\widetilde{\Omega}_{l-1}\setminus\Omega_l)})^{\frac{1}{\delta}}(x).$$

As in the proof of claim (4-1), picking $\delta < \min\{2, p_1/q_w\}$ and applying Corollary 2.5, we have

$$
\begin{aligned}
(2^l\alpha)^{p_1} w(\widetilde{\Omega}_{l-1}) &\geq \int_{\mathbb{R}^N} \Big\{ \sum_{J\in\mathbb{Z}^3} \sum_{R\in\mathcal{R}_{\mathcal{F}}^{J,K}} |\phi_J * h(x_R)|^2 \chi_{R\cap(\widetilde{\Omega}_{l-1}\setminus\Omega_l)}(x) \Big\}^{\frac{p_1}{2}} w(x)\,dx \\
&\gtrsim \int_{\mathbb{R}^N} \Big\{ \sum_{J\in\mathbb{Z}^3} \sum_{R\in\mathcal{R}_l^{J,K}} |\phi_J * h(x_R)|^2 \mathcal{M}_{\mathcal{F}}(\chi_{R\cap(\widetilde{\Omega}_{l-1}\setminus\Omega_l)})^{\frac{2}{\delta}}(x) \Big\}^{\frac{p_1}{2}} w(x)\,dx \\
&\gtrsim \Big\| \Big\{ \sum_{J\in\mathbb{Z}^3} \sum_{R\in\mathcal{R}_l^{J,K}} |\phi_J * h(x_R)|^2 \chi_R \Big\}^{\frac{1}{2}} \Big\|_{L_w^{p_1}(\mathbb{R}^N)}^{p_1}.
\end{aligned}
$$

Combining this with (4-3) yields (4-2), and hence Theorem 1.12 follows. □

Proof of Theorem 1.13. Suppose that T is bounded from $H^{p_1}_{\mathcal{F},w}(\mathbb{R}^N)$ to $L^{p_1}_w(\mathbb{R}^N)$ and bounded from $H^{p_2}_{\mathcal{F},w}(\mathbb{R}^N)$ to $L^{p_2}_w(\mathbb{R}^N)$. Given $f \in H^{p}_{\mathcal{F},w}(\mathbb{R}^N)$, $p_1 < p < p_2$, the Calderón–Zygmund decomposition shows that $f = g + b$ with

$$
\|g\|^{p_2}_{H^{p_2}_{\mathcal{F},w}(\mathbb{R}^N)} \lesssim \alpha^{p_2-p} \|f\|^{p}_{H^{p}_{\mathcal{F},w}(\mathbb{R}^N)} \quad \text{and} \quad \|b\|^{p_1}_{H^{p_1}_{\mathcal{F},w}(\mathbb{R}^N)} \lesssim \alpha^{p_1-p} \|f\|^{p}_{H^{p}_{\mathcal{F},w}(\mathbb{R}^N)}.
$$

Moreover, in the proof of Theorem 1.12, we have shown that

$$
\|g\|^{p_2}_{H^{p_2}_{\mathcal{F},w}(\mathbb{R}^N)} \lesssim \int_{\{\tilde{g}_{\mathcal{F}}(f)(x)\leq\alpha\}} [\tilde{g}_{\mathcal{F}}(f)(x)]^{p_2} w(x)\,dx
$$

and

$$
\|b\|^{p_1}_{H^{p_1}_{\mathcal{F},w}(\mathbb{R}^N)} \lesssim \int_{\{\tilde{g}_{\mathcal{F}}(f)(x)>\alpha\}} [\tilde{g}_{\mathcal{F}}(f)(x)]^{p_1} w(x)\,dx.
$$

Therefore,

$$
\begin{aligned}
\|Tf\|^{p}_{L^{p}_w(\mathbb{R}^N)} &\leq p\int_0^\infty \alpha^{p-1} w\Big(\Big\{x : |T(g)(x)| > \frac{\alpha}{2}\Big\}\Big)\,d\alpha \\
&\qquad + p\int_0^\infty \alpha^{p-1} w\Big(\Big\{x : |T(b)(x)| > \frac{\alpha}{2}\Big\}\Big)\,d\alpha \\
&\lesssim \int_0^\infty \alpha^{p-1} \Big(\frac{\|T(g)\|_{L^{p_2}_w}}{\alpha}\Big)^{p_2} d\alpha + \int_0^\infty \alpha^{p-1} \Big(\frac{\|T(b)\|_{L^{p_1}_w}}{\alpha}\Big)^{p_1} d\alpha \\
&\lesssim \int_0^\infty \alpha^{p-p_2-1} \int_{\{\tilde{g}_{\mathcal{F}}(f)(x)\leq\alpha\}} [\tilde{g}_{\mathcal{F}}(f)(x)]^{p_2} w(x)\,dx\,d\alpha \\
&\qquad + \int_0^\infty \alpha^{p-p_1-1} \int_{\{\tilde{g}_{\mathcal{F}}(f)(x)>\alpha\}} [\tilde{g}_{\mathcal{F}}(f)(x)]^{p_1} w(x)\,dx\,d\alpha \\
&\lesssim \|f\|^{p}_{H^{p}_{\mathcal{F},w}(\mathbb{R}^N)}.
\end{aligned}
$$

Hence T is bounded from $H^p_{\mathcal{F},w}(\mathbb{R}^N)$ to $L^p_w(\mathbb{R}^N)$.

To prove the second assertion that T is bounded on $H^p_{\mathcal{F},w}(\mathbb{R}^N)$, for any given $\alpha > 0$ and $f \in H^p_{\mathcal{F},w}(\mathbb{R}^N)$, we apply the Calderón–Zygmund decomposition again to obtain

$$\begin{aligned} w(\{x : |\tilde{g}_{\mathcal{F}}(Tf)(x)| > \alpha\}) &\le w\Big(\Big\{x : |\tilde{g}_{\mathcal{F}}(Tg)(x)| > \frac{\alpha}{2}\Big\}\Big) \\ &\qquad + w\Big(\Big\{x : |\tilde{g}_{\mathcal{F}}(Tb)(x)| > \frac{\alpha}{2}\Big\}\Big) \\ &\lesssim \alpha^{-p_2}\|T(g)\|^{p_2}_{H^{p_2}_{\mathcal{F},w}(\mathbb{R}^N)} + \alpha^{-p_1}\|T(b)\|^{p_1}_{H^{p_1}_{\mathcal{F},w}(\mathbb{R}^N)} \\ &\lesssim \alpha^{-p_2}\|g\|^{p_2}_{H^{p_2}_{\mathcal{F},w}(\mathbb{R}^N)} + \alpha^{-p_1}\|b\|^{p_1}_{H^{p_1}_{\mathcal{F},w}(\mathbb{R}^N)} \\ &\lesssim \alpha^{-p_2}\int_{\{\tilde{g}_{\mathcal{F}}(f)(x)\le\alpha\}} [\tilde{g}_{\mathcal{F}}(f)(x)]^{p_2} w(x)\,dx \\ &\qquad + \alpha^{-p_1}\int_{\{\tilde{g}_{\mathcal{F}}(f)(x)>\alpha\}} [\tilde{g}_{\mathcal{F}}(f)(x)]^{p_1} w(x)\,dx, \end{aligned}$$

which, as above, implies that $\|\tilde{g}_{\mathcal{F}}(Tf)\|_{L^p_w(\mathbb{R}^N)} \lesssim \|f\|_{H^p_{\mathcal{F},w}(\mathbb{R}^N)}$, and therefore $\|Tf\|_{H^p_{\mathcal{F},w}(\mathbb{R}^N)} \lesssim \|f\|_{H^p_{\mathcal{F},w}(\mathbb{R}^N)}$ by Corollary 3.4. The proof of Theorem 1.13 is complete. □

5. Relations between different classes of weights

In this section, we clarify the relations between different classes of weights by constructing some examples and counterexamples. Our aim is to show the following:

Proposition 5.1. *For* $1 < p < \infty$, $A^{\mathrm{pro}}_p(\mathbb{R}^N) \subsetneq A^{\mathcal{F}}_p(\mathbb{R}^N) \subsetneq A_p(\mathbb{R}^N)$.

A positive measure μ on $\mathbb{R}^n$ is called doubling if there exists a constant $0 < C < \infty$, depending only on n, such that

$$\mu(2B) \le C\mu(B) \tag{5-1}$$

for all balls B.

To prove this proposition, we need the following lemmas.

Lemma 5.2. *Let* $1 < p < \infty$. *If* $a > -n$ *and* $A \ge 0$, *then* $(|x|+A)^a\,dx$ *is a doubling measure on* $\mathbb{R}^n$ *with doubling constant depending on* a *and* n, *but independent of* A.

Proof. If $A = 0$, the conclusion above is well known. If $A > 0$, following the arguments given in [Grafakos 2014, pp. 505–506], we divide all balls $B(x_0, R)$ in $\mathbb{R}^n$ into two categories: balls of type I that satisfy $|x_0| + A \ge 3R$ and type II that satisfy $|x_0| + A < 3R$.

For the balls of type I, we have

$$\int_{B(x_0,2R)} (|x| + A)^a\,dx \le \begin{cases} v_n(2R)^n(|x_0| + A + 2R)^a & \text{if } a \ge 0, \\ v_n(2R)^n(|x_0| + A - 2R)^a & \text{if } a < 0, \end{cases}$$

and

$$\int_{B(x_0,R)} (|x|+A)^a\,dx \ge \begin{cases} v_n R^n(|x_0|+A-R)^a & \text{if } a \ge 0, \\ v_n R^n(|x_0|+A+R)^a & \text{if } a < 0, \end{cases}$$

where v_n denotes the volume of the unit ball in $\mathbb{R}^n$. Since $|x_0|+A \ge 3R$, we have $|x_0|+A+2R \le 4(|x_0|+A-R)$ and $|x_0|+A-2R \ge \frac{1}{4}(|x_0|+A+R)$. The required doubling property (5-1) then follows with $C = 2^{3n}4^{|a|}$.

For balls of type II, $|x_0|+A < 3R$ implies $B(x_0,2R) \subset B(0,5R)$. Therefore

$$\int_{B(x_0,2R)} (|x|+A)^a\,dx \le \int_{B(0,5R)} (|x|+A)^a\,dx \lesssim R^{n+a}.$$

On the other hand, using the fact that $(|x|+A)^a$ is rapidly increasing if $a \ge 0$, and the inequality $|x|+A \le |x_0|+A+R < 4R$ if $a < 0$, we have

$$\begin{aligned}\int_{B(x_0,R)} (|x|+A)^a\,dx &\ge \begin{cases} \int_{B(0,R)} |x|^a\,dx & \text{if } a \ge 0, \\ \int_{B(x_0,R)} (4R)^a\,dx & \text{if } a < 0, \end{cases} \\ &\gtrsim R^{n+a}.\end{aligned}$$

This concludes the proof of Lemma 5.2. □

Lemma 5.3. *Let* $1 < p < \infty$. *If* $w_1, w_2 \in A_p(\mathbb{R}^n)$, *then* $w(x) = \min\{w_1(x), w_2(x)\}$ *is also in* $A_p(\mathbb{R}^n)$ *with* $[w]_{A_p} \le \max(1, 2^{p-2})([w_1]_{A_p} + [w_2]_{A_p})$.

Proof. This lemma slightly generalizes a result in [Grafakos 2014, p. 513], where the case of w_2 being a constant was considered. For any $Q \subset \mathbb{R}^n$,

$$\begin{aligned}&\left(\frac{1}{|Q|}\int_Q w\right)\left(\frac{1}{|Q|}\int_Q w^{-\frac{p'}{p}}\right)^{\frac{p}{p'}} \\ &\quad\le \left(\frac{1}{|Q|}\int_Q [w_1 \wedge w_2]\right)\left(\frac{1}{|Q|}\int_Q w_1^{-\frac{p'}{p}} + \frac{1}{|Q|}\int_Q w_2^{-\frac{p'}{p}}\right)^{\frac{p}{p'}} \\ &\quad\le \max(1, 2^{p-2})\left\{\left(\frac{1}{|Q|}\int_Q w_1\right) \wedge \left(\frac{1}{|Q|}\int_Q w_2\right)\right\} \\ &\qquad\qquad \cdot \left\{\left(\frac{1}{|Q|}\int_Q w_1^{-\frac{p'}{p}}\right)^{\frac{p}{p'}} + \left(\frac{1}{|Q|}\int_Q w_2^{-\frac{p'}{p}}\right)^{\frac{p}{p'}}\right\} \\ &\quad\le \max(1, 2^{p-2})\left\{\left(\frac{1}{|Q|}\int_Q w_1\right)\left(\frac{1}{|Q|}\int_Q w_1^{-\frac{p'}{p}}\right)^{\frac{p}{p'}} \right. \\ &\qquad\qquad \left. + \left(\frac{1}{|Q|}\int_Q w_2\right)\left(\frac{1}{|Q|}\int_Q w_2^{-\frac{p'}{p}}\right)^{\frac{p}{p'}}\right\} \\ &\quad\le \max(1, 2^{p-2})([w_1]_{A_p} + [w_2]_{A_p}),\end{aligned}$$

where in the second inequality we used the basic inequality

$$(a_1+a_2)^{\frac{p}{p'}} \le \max(1, 2^{p-2})(a_1^{\frac{p}{p'}} + a_2^{\frac{p}{p'}})$$

for $a_1, a_2 > 0$. Hence the required result follows. □

Proof of Proposition 5.1. By definition, it is clear that $A_p^{\text{pro}}(\mathbb{R}^N) \subset A_p^{\mathcal{F}}(\mathbb{R}^N) \subset A_p(\mathbb{R}^N)$.

Now, let us show that these inclusions are proper. For simplicity, we only consider the biparameter case on $\mathbb{R}^N = \mathbb{R}^{n_1} \times \mathbb{R}^{n_2}$, where we denote the flag $\{(0,0)\} \subset \{(0,y)\} \subset \mathbb{R}^{n_1+n_2}$ by $\mathcal{F}_1$.

We first show that $A_p^{\text{pro}}(\mathbb{R}^N) \subsetneq A_p^{\mathcal{F}_1}(\mathbb{R}^N)$. Let $1-n_2 < a < n_2(p-1)$. For $x = (x^{(1)}, \ldots, x^{(n_1)}) \in \mathbb{R}^{n_1}$, $y = (y^{(1)}, \ldots, y^{(n_2)}) \in \mathbb{R}^{n_2}$, we define

$$w(x,y) = |y|^a (|x^{(1)}| + |y|)^{-1}.$$

Since w is independent of $(x^{(2)}, \ldots, x^{(n_1)})$, for notational simplicity, we may assume $n_1 = 1$ and write x instead of $x^{(1)}$. We claim that

$$\operatorname*{ess\,sup}_{y\in\mathbb{R}^{n_2}} [w(\cdot, y)]_{A_p(\mathbb{R}^1)} = \infty, \tag{5-2}$$

$$\sup_{x\in\mathbb{R}^1} [w(x, \cdot)]_{A_p(\mathbb{R}^{n_2})} < \infty, \tag{5-3}$$

$$[w]_{A_p(\mathbb{R}^{1+n_2})} < \infty, \tag{5-4}$$

where $[\,\cdot\,]_{A_p}$ denotes the classical A_p characteristic constant. Assume (5-2), (5-3) and (5-4) hold for the moment. Then (5-3) and (5-4) imply $w \in A_p^{(1)}(\mathbb{R}^N) \cap A_p^{(2)}(\mathbb{R}^N)$, and therefore $w \in A_p^{\mathcal{F}_1}$ by Lemma 2.4; while (5-2) implies $w \notin A_p^{\text{pro}}$. Hence $A_p^{\text{pro}}(\mathbb{R}^N) \subsetneq A_p^{\mathcal{F}_1}(\mathbb{R}^N)$.

Now let us prove (5-2), (5-3) and (5-4). We prove first (5-2). Given any $y \in \mathbb{R}^{n_2}$ with $y \neq 0$, we choose an interval $I = (0, r)$ with $r = |y|^2$. Then

$$\begin{aligned}\left(\frac{1}{|I|}\int_I w(x,y)\,dx\right)&\left(\frac{1}{|I|}\int_I [w(x,y)]^{-\frac{p'}{p}}\,dx\right)^{\frac{p}{p'}} \\ &= \left(\frac{1}{r}\int_0^r (x+|y|)^{-1}\,dx\right)\left(\frac{1}{r}\int_0^r (x+|y|)^{\frac{p'}{p}}\,dx\right)^{\frac{p}{p'}} \\ &\gtrsim \frac{1}{r}\ln\left(1+\frac{r}{|y|}\right)\cdot r = \ln(1+|y|) \to +\infty,\end{aligned}$$

as $|y|$ goes to $+\infty$, which establishes (5-2).

Next, let us show (5-3). For $x = 0$, $w(0,y) = |y|^{a-1} \in A_p(\mathbb{R}^{n_2})$. For any fixed $x \neq 0$, $w_1(y) := |y|^{a-1}$ and $w_2(y) := |y|^a |x|^{-1}$ are both in $A_p(\mathbb{R}^{n_2})$, with A_p characteristic constants being independent of x. Since $w(y) \approx \min(w_1(y), w_2(y))$, (5-3) follows immediately from Lemma 5.3.

We now verify (5-4). For any $n \in \mathbb{Z}_+$, we divide all cubes $Q(x_0, l)$ (centered at x_0 of side length l) in $\mathbb{R}^n$ into two categories: cubes of type I that satisfy $|x_0| \geq 3\sqrt{n}\, l$ and type II that satisfy $|x_0| < 3\sqrt{n}\, l$. For any $Q \subset \mathbb{R}^{1+n_2}$, write $Q = Q_1 \times Q_2$, where

$$Q_1 = (x_0 - l, x_0 + l) \subset \mathbb{R} \quad \text{and} \quad Q_2 = Q_2(y_0, l) \subset \mathbb{R}^{n_2}.$$

We consider the following four cases.

Case 1: If both Q_1 and Q_2 are of type I, then for any $(x, y) \in Q$, $w(x, y) \approx |y_0|^a(|x_0| + |y_0|)^{-1}$, and hence the desired result follows easily.

Case 2: If Q_1 is of type I and Q_2 of type II, then for any $(x, y) \in Q$, we have $|x| \approx |x_0| \gtrsim |y|$ and thus $w(x, y) \approx |y|^a |x_0|^{-1}$. Moreover, $|y|^a$ is in $A_p(\mathbb{R}^{n_2})$. Hence,

$$\begin{aligned}\left(\frac{1}{|Q|}\iint_Q w(x, y)\, dx\, dy\right)&\left(\frac{1}{|Q|}\iint_Q w(x, y)^{-\frac{p'}{p}}\, dx\, dy\right)^{\frac{p}{p'}} \\ &\approx \left(\frac{1}{|Q_2|}\int_{Q_2} |y|^a\, dy\right)\left(\frac{1}{|Q_2|}\int_{Q_2} |y|^{-\frac{ap'}{p}}\, dy\right)^{\frac{p}{p'}} \leq [|y|^a]_{A_p(\mathbb{R}^{n_1})} \lesssim 1.\end{aligned}$$

Case 3: If Q_1 is of type II and Q_2 of type I, then for any $(x, y) \in Q$, we have $|y| \approx |x| + |y| \approx |y_0|$ and therefore $w(x, y) \approx |y_0|^{a-1}$. Hence the required estimate follows easily.

Case 4: If both Q_1 and Q_2 are of type II, then by Lemma 5.2,

$$\begin{aligned}\left(\frac{1}{|Q|}\iint_Q w(x, y)\, dx\, dy\right)&\left(\frac{1}{|Q|}\iint_Q w(x, y)^{-\frac{p'}{p}}\, dx\, dy\right)^{\frac{p}{p'}} \\ &\lesssim \left(\frac{1}{l^{n_2+1}}\int_{B(0,5\sqrt{n_2}\, l)} |y|^a dy \int_0^{5l} (x + |y|)^{-1}\, dx\right) \\ &\quad \times \left(\frac{1}{l^{n_2+1}}\int_{B(0,5\sqrt{n_2}\, l)} |y|^{-\frac{ap'}{p}}\, dy \int_0^{5l} (x + |y|)^{\frac{p'}{p}}\, dx\right)^{\frac{p}{p'}} \\ &\lesssim \left(\frac{1}{l^{n_2}}\int_{B(0,5\sqrt{n_2}\, l)} |y|^{a-1} dy\right)\left(l^{\frac{p'}{p} - n_2}\int_{B(0,5\sqrt{n_2}\, l)} |y|^{-\frac{ap'}{p}}\, dy\right)^{\frac{p}{p'}} \\ &\approx l^{a-1} \cdot (l^{(1-a)\frac{p'}{p}})^{\frac{p}{p'}} = 1,\end{aligned}$$

where $B(0, 5\sqrt{n_2}\, l)$ denotes the ball of radius $5\sqrt{n_2}\, l$ centered at origin of $\mathbb{R}^{n_2}$. This concludes the proof of (5-4), and hence $A_p^{\mathrm{pro}}(\mathbb{R}^N) \subsetneq A_p^{\mathcal{F}_1}(\mathbb{R}^N)$.

Finally, let us show $A_p^{\mathcal{F}_1}(\mathbb{R}^N) \subsetneq A_p(\mathbb{R}^N)$. From (5-4) and (5-2), interchanging the roles of x and y, we see that for $1 - n_1 < b < n_1(p - 1)$, $|x|^b(|y^{(1)}| + |x|)^{-1}$ is in $A_p(\mathbb{R}^N)$, but not in $A_p^{\mathcal{F}_1}(\mathbb{R}^N)$. This completes the proof of Proposition 5.1. □

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EXCEPTIONAL SEQUENCES AND SPHERICAL MODULES FOR THE AUSLANDER ALGEBRA OF $k[x]/(x^t)$

LUTZ HILLE AND DAVID PLOOG

We classify spherical modules and full exceptional sequences of modules over the Auslander algebra of $k[x]/(x^t)$. We categorify the left and right symmetric group actions on these exceptional sequences to two braid group actions: of spherical twists along simple modules, and of right mutations. In particular, every such exceptional sequence is obtained by spherical twists from a standard sequence, and likewise for right mutations.

Introduction

In this text, we study the Auslander algebras $\mathcal{A}_t$ of $\boldsymbol{k}[x]/(x^t)$. This family of finite-dimensional algebras is well known in representation theory. It also occurs for certain matrix problems, i.e., actions of linear groups on flags [Hille and Röhrle 1999, §4]. In previous work [Hille and Ploog 2019], we link $\mathcal{A}_t$ to $(t-1)$-chains of (-2)-curves on projective surfaces.

We classify exceptional and spherical modules over $\mathcal{A}_t$ in Theorem 2.2, and full exceptional sequences of modules in Theorem 4.4. Below, we just state the enumerative consequences of these classification results:

MSC2010: primary 16D90; secondary 16G20, 16S38, 18E30.
Keywords: Auslander algebra, full exceptional sequence, exceptional module, spherical module.

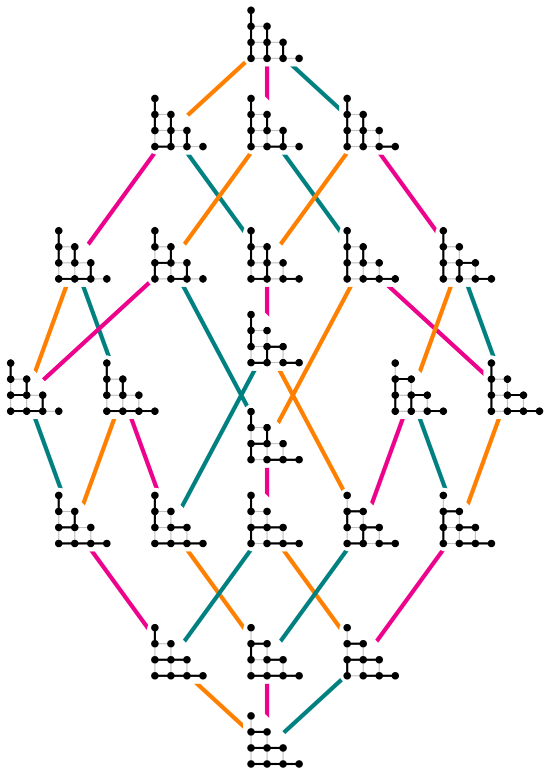


Figure 1. Right mutation graph of size-4 worm diagrams. The twenty-four worm diagrams of size 4, i.e., all full exceptional sequences of $\mathcal{A}_4$-modules. Downwards edges are right mutations: R_1, R_2, R_3. See Section 4B.

Theorem. *The numbers of the following types of objects over the algebra* $\mathcal{A}_t$ *are*

$2^t - 1$	*exceptional modules*,
$2^t - 1 - t$	2-*spherical modules*,
$t!$	*full exceptional sequences of modules*.

Moreover, we describe full exceptional sequences of modules combinatorially by *worm diagrams* in Corollary 3.6. In Theorem 4.4, we establish a natural bijection of these diagrams with the symmetric group. Hence, this group acts, from both sides, on worm diagrams, i.e., on full exceptional sequences of $\mathcal{A}_t$-modules.

We categorify both symmetric group actions to braid group actions. For the right action, this is done by right mutations of exceptional sequences; see Section 4B. For the left action, we use the twist functors along the spherical simple modules; see Section 4C. Figures 1 and 2 show these braid group actions for $\mathcal{A}_4$.

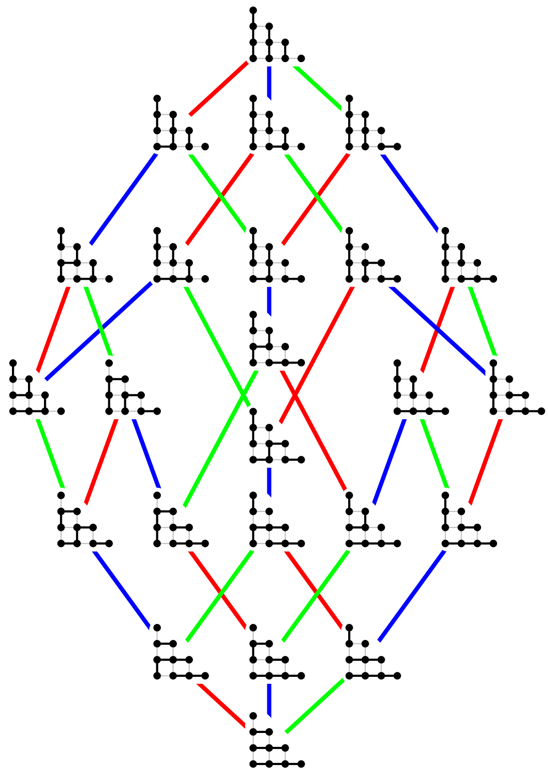


Figure 2. Spherical twist graph of size-4 worm diagrams. The twenty-four worm diagrams of size 4, i.e., all full exceptional sequences of $\mathcal{A}_4$-modules. Downwards edges are spherical twists: $\mathsf{T}_{S(1)}$, $\mathsf{T}_{S(2)}$, $\mathsf{T}_{S(3)}$. See Section 4C.

Related classification results. On terminology: a *tilting module T* in this text means a generator of the module category with $\operatorname{Ext}^{>0}(T, T) = 0$. When the additional condition $\operatorname{pd}(T) \leq 1$ is included, we say *classical tilting module*.

The algebra $\mathcal{A}_t$ is quasihereditary, and by [Brüstle et al. 1999], there are $t!$ tilting modules which are Δ-filtered. This class of modules coincides with classical tilting modules, and with τ-tilting modules; the latter have been studied in [Iyama and Zhang 2016]. See also [Eisele et al. 2018, Example 3].

Next, there are $2^{t+1} - t - 2$ bricks over $\mathcal{A}_t$, i.e., modules M with $\operatorname{Hom}(M, M) = \boldsymbol{k}$. This has been worked out as follows: the algebra $\mathcal{A}_t$ is τ-tilting finite, and for any such algebra, there is a bijection between indecomposable τ-rigid modules and bricks [Demonet et al. 2019, Theorem 4.1]. Now bricks for $\mathcal{A}_t$ are in bijection with bricks of the preprojective algebra of type A_t, and those in turn have been parametrized by join-irreducible elements of the Weyl group [Iyama et al. 2018, Theorems 1.1 and 1.2]. The combinatorics for type A are in [Iyama et al. 2018, §6.1]. We give a quick count of bricks in Corollary 2.4.

Semibricks, i.e., sets of Hom-orthogonal bricks, have been classified in [Asai 2016]; there are $(t+1)!$ of them. They correspond to support τ-tilting modules [Iyama and Zhang 2016].

Recently, tilting modules have been classified in [Geuenich 2018]. In particular, the number of basic tilting $\mathcal{A}_t$-modules is determined by an intricate recursive formula.

Conventions. We fix an algebraically closed field $\boldsymbol{k}$. All algebras, categories, and functors are over $\boldsymbol{k}$. Occasionally, we abbreviate dimensions of Hom spaces as $\hom(A,B) := \dim \operatorname{Hom}(A,B)$, and likewise for Ext^p. The shift (or translation, or suspension) functor of a triangulated category is denoted [1]. For objects A, B of a triangulated category, we write $\operatorname{Hom}^\bullet(A,B) := \bigoplus_{i\in\mathbb{Z}} \operatorname{Hom}(A,B[i])[-i]$ for their Hom complex; it is a complex of vector spaces with zero differential.

Modules are always left modules. We compose arrows in a path algebra like functions, from right to left. Given a vertex i for a bound quiver, we denote the corresponding simple, projective, and injective modules by $S(i)$, $P(i)$, $I(i)$, respectively. If M is a module, i.e., a representation of the bound quiver, we write M_i for the vector space of M at the vertex i. Here, $\otimes = \otimes_{\boldsymbol{k}}$ throughout.

The symmetric group on t letters is denoted by $\mathsf{Sym}(t)$. It is generated by simple transpositions $\tau_i := (i, i+1)$. We write $\omega_0 := \left(\begin{smallmatrix} 1 & 2 & \cdots & t \\ t & t-1 & \cdots & 1\end{smallmatrix}\right) \in \mathsf{Sym}(t)$ for the longest word. The braid group on t strands is denoted $\mathsf{Br}(t)$.

1. Definition and basic properties of $\mathcal{A}_t$

1A. ***The algebra $\mathcal{A}_t$.*** The algebra $\mathcal{A}_t$ is defined as the path algebra of the quiver with t vertices and $2t-2$ arrows

$$1 \underset{\beta}{\overset{\alpha}{\rightleftarrows}} 2 \underset{\beta}{\overset{\alpha}{\rightleftarrows}} 3 \underset{\beta}{\overset{\alpha}{\rightleftarrows}} \cdots \underset{\beta}{\overset{\alpha}{\rightleftarrows}} t-1 \underset{\beta}{\overset{\alpha}{\rightleftarrows}} t$$

bound by a zero relation $\beta\alpha = 0$ at 1, and commutativity relations $\alpha\beta = \beta\alpha$ at intermediate vertices $2, \dots, t-1$. We emphasize that there is no relation at t; this distinguishes $\mathcal{A}_t$ from the preprojective algebra of the A_t-quiver.

As is well known, $\mathcal{A}_t$ occurs as the Auslander algebra of the ring $R := \boldsymbol{k}[x]/(x^t)$. This means that R has finitely many indecomposable (finitely generated) modules — these are $M(i) := R/(x^i) = \boldsymbol{k}[x]/(x^i)$ for $i = 1, \dots, t$ — and that $\mathcal{A}_t$ is the endomorphism algebra of their direct sum: $\mathcal{A}_t = \operatorname{End}_R(M(1) \oplus \cdots \oplus M(t))$.

Moreover, $\mathcal{A}_t$ also occurs as the endomorphism algebra of a very special tilting object of geometric nature. See Appendix B and [Hille and Ploog 2019].

Remark 1.1. Reverting all arrows gives the opposite algebra, hence $\mathcal{A}_t \cong \mathcal{A}_t^{\mathrm{op}}$. In particular, the abelian categories of left and right $\mathcal{A}_t$-modules are equivalent.

1B. *The projective-injective module $P(t)$, and the rank of $\mathcal{A}_t$-modules.* By a straightforward calculation of the injective hull and of the projective cover for the simple module $S(t)$, one finds $P(t) = I(t)$. Moreover, $P(t)$ is the unique indecomposable projective-injective $\mathcal{A}_t$-module. We have $\underline{\dim}(P(t)) = (1, 2, \ldots, t)$.

Definition 1.2. The *rank* of an $\mathcal{A}_t$-module M is

$$\operatorname{rk} M := \dim M_t = \dim \operatorname{Hom}(P(t), M) = \dim \operatorname{Hom}(M, I(t)).$$

Note that by definition, the rank is additive on short exact sequences of $\mathcal{A}_t$-modules, and thus induces $\operatorname{rk} : K_0(\mathcal{A}_t) \to \mathbb{Z}$.

Remark 1.3. The subcategory of $\mathcal{A}_t$-mod of rank-0 modules is equivalent to the module category over the preprojective algebra of $\boldsymbol{k}A_{t-1}$, and in particular abelian.

1C. *Euler pairing and quadratic form.* We recall the projective resolutions of the simple $\mathcal{A}_t$-modules. In particular, $S(1), \ldots, S(t-1)$ have projective dimension 2, whereas $S(t)$ has projective dimension 1. Hence, $\mathcal{A}_t$ has global dimension 2.

Lemma 1.4. *The simple representations $S(1), \ldots, S(t)$ have projective resolutions*

$$P(1) \to P(2) \to P(1) \to S(1),$$
$$P(i) \to P(i-1) \oplus P(i+1) \to P(i) \to S(i) \quad \textit{for } i = 2, \ldots, t-1,$$
$$P(t-1) \to P(t) \to S(t).$$

The *Euler pairing* of two $\mathcal{A}_t$-modules M and N is defined as

$$\chi(M, N) := \hom(M, N) - \operatorname{ext}^1(M, N) + \operatorname{ext}^2(M, N),$$

and $\chi(M, N)$ only depends on the classes of M and N in the Grothendieck group $K_0(\mathcal{A}_t) \cong \mathbb{Z}^t$. The associated *quadratic form* is given by $q(M) := \chi(M, M)$.

Lemma 1.5. *Writing $\underline{\dim}(M) = (m_1, \ldots, m_t)$ and $\underline{\dim}(N) = (n_1, \ldots, n_t)$,*

$$\chi(M, N) = m_t n_t + \sum_{i=1}^{t-1} (m_i(n_i - n_{i+1}) + n_i(m_i - m_{i+1})).$$

Proof. Given any representation M, we can apply the resolutions of Lemma 1.4 via the horseshoe lemma to a composition series of M, and obtain a projective resolution for M (where we put $P(0) = P(t+1) = 0$):

$$\bigoplus_{i=1}^{t-1} P(i) \otimes M_i \to \bigoplus_{i=1}^{t} P(i-1) \otimes M_i \oplus P(i+1) \otimes M_i \to \bigoplus_{i=1}^{t} P(i) \otimes M_i \to M.$$

Using the functor $\mathrm{Hom}(\,\cdot\,, N)$ on this resolution produces a complex with terms

$$\bigoplus_{i=1}^{t}\mathrm{Hom}(M_i, N_i) \to \bigoplus_{i=1}^{t-1}\mathrm{Hom}(M_{i+1}, N_i)\oplus\mathrm{Hom}(M_i, N_{i+1}) \to \bigoplus_{i=1}^{t-1}\mathrm{Hom}(M_i, N_i)$$

whose cohomologies are $\mathrm{Ext}^p(M, N)$. Hence,

$$\chi(M, N) = \sum_{i=1}^{t} m_i n_i - \sum_{i=1}^{t-1}(m_{i+1}n_i + m_i n_{i+1}) + \sum_{i=1}^{t-1} m_i n_i$$

which translates to the formula of the proposition. □

Corollary 1.6. *The quadratic form of $\mathcal{A}_t$ is positive definite*:

$$q(d_1, \dots, d_t) = d_1^2 + (d_1 - d_2)^2 + (d_2 - d_3)^2 + \cdots + (d_{t-1} - d_t)^2.$$

1D. *Homomorphisms and extensions.* We next show that homomorphisms and extensions among $\mathcal{A}_t$-modules are computed explicitly by the complex

$$\mathcal{C}^\bullet(M, N) : \mathcal{C}^0(M, N) \xrightarrow{d^0} \mathcal{C}^1(M, N) \xrightarrow{d^1} \mathcal{C}^2(M, N)$$

for $M, N \in \mathcal{A}_t$-mod, with the terms already seen in the proof of Lemma 1.5

$$\bigoplus_{i=1}^{t}\mathrm{Hom}(M_i, N_i) \xrightarrow{d^0} \bigoplus_{i=2}^{t}\mathrm{Hom}(M_i, N_{i-1})\oplus\mathrm{Hom}(M_{i-1}, N_i) \xrightarrow{d^1} \bigoplus_{i=1}^{t-1}\mathrm{Hom}(M_i, N_i)$$

whose differentials are induced by the arrows of the representations M and N:

$$\begin{aligned} d^0(f_i) &= (\beta_{i-1}^N f_i - f_i\beta_i^M, \alpha_i^N f_i - f_i\alpha_{i-1}^M) && \text{for } f_i : M_i \to N_i, \\ d^1(g_i, 0) &= \alpha_{i-1}^N g_i + g_i\alpha_{i-1}^M && \text{for } g_i : M_i \to N_{i-1}, \\ d^1(0, h_i) &= \beta_i^N h_i + h_i\beta_i^M && \text{for } h_i : M_{i-1} \to N_i. \end{aligned}$$

Thus, $\mathcal{C}^\bullet(M, N)$ becomes a complex of vector spaces. Note that $\mathcal{C}^\bullet(M, N)$ is not symmetric: $\mathcal{C}^0(M, N) = \mathcal{C}^2(M, N) \oplus \mathrm{Hom}(M_t, N_t)$. In the proof of Lemma 1.5, we computed $\chi(M, N)$ abstractly, i.e., without explicit differentials. Below, we will use this information to show that $(\mathcal{C}^\bullet(M, N), d)$ really calculates $\mathrm{Ext}^p(M, N)$.

Lemma 1.7. *The functors $H^i(\mathcal{C}^\bullet(\,\cdot\,, N)) : \mathcal{A}_t\text{-mod}^{\mathrm{op}} \to \mathcal{A}_t\text{-mod}$ form a δ-functor, for a fixed $\mathcal{A}_t$-module N.*

Proof. By construction, $\mathcal{C}^\bullet(M, N)$ is covariantly functorial in N and contravariantly functorial in M. An exact sequence $M' \to M \to M''$ of modules induces an exact sequence $\mathcal{C}^\bullet(M'', N) \to \mathcal{C}^\bullet(M, N) \to \mathcal{C}^\bullet(M', N)$ of complexes. Hence, a short exact sequence $0 \to M' \to M \to M'' \to 0$ yields a long exact sequence of modules

$$0 \to \mathcal{H}^0(M'') \to \mathcal{H}^0(M) \to \mathcal{H}^0(M') \xrightarrow{\delta} \mathcal{H}^1(M'') \to \mathcal{H}^1(M) \\ \to \mathcal{H}^1(M') \xrightarrow{\delta} \mathcal{H}^2(M'') \to \mathcal{H}^2(M) \to \mathcal{H}^2(M') \to 0$$

where we set $\mathcal{H}^i(\cdot) := H^i(\mathcal{C}^\bullet(\cdot, N))$. This long exact cohomology sequence means that the $H^i(\mathcal{C}^\bullet(\cdot, N))$ form a contravariant δ-functor. □

Proposition 1.8. $\operatorname{Ext}^p(M, N) = H^i(\mathcal{C}^\bullet(M, N))$ *for* $M, N \in \mathcal{A}_t$-mod *and* $p \in \mathbb{Z}$.

Proof. Comparing the differential $d^0 : \mathcal{C}^0(M, N) \to \mathcal{C}^1(M, N)$ with morphisms of $\mathcal{A}_t$-representations gives $H^0(\mathcal{C}^\bullet(M, N)) = \ker(d^0) = \operatorname{Hom}(M, N)$ right away. Next we claim that $H^p(\mathcal{C}^\bullet(\cdot, N))$ is an erasable δ-functor, i.e., $H^p(\mathcal{C}^\bullet(P, N)) = 0$ for projective $\mathcal{A}_t$-modules and $p > 0$. For this, first take $P = P(j)$ and $N = S(l)$. Then

$$\mathcal{C}^\bullet(P(j), S(l)) = \left[P(j)_l^* \xrightarrow{d^0} P(j)_{l+1}^* \oplus P(j)_{l-1}^* \xrightarrow{d^1} P(j)_l^*\right]$$

(with the obvious modifications if $l = 1$ or $l = t$). To check that d^1 is surjective, we use three facts: generally for path algebras, the projective representation $P(j)$ corresponding to a vertex j of the quiver is obtained by following arrows emanating out of j; the special form of the quiver for $\mathcal{A}_t$; and the definition of d^1.

Since the simple modules generate $\mathcal{A}_t$-mod via extensions, the surjectivity of d^1 for all N follows, i.e., $H^2(\mathcal{C}^\bullet(P, N)) = 0$. We then get $H^1(\mathcal{C}^\bullet(P, N)) = 0$ because the Euler pairings for $\operatorname{Hom}^\bullet(M, N)$ and for $\mathcal{C}^\bullet(M, N)$ coincide. Finally, the claim follows from the universal property of derived functors [Weibel 1994, §2]. □

Proposition 1.9. *Let* M, N *be* $\mathcal{A}_t$*-modules. Then*

(1) $\hom(M, N) \geq \operatorname{ext}^2(N, M)$,

(2) $\hom(M, M) = \operatorname{ext}^2(M, M)$ *if and only if* $\operatorname{rk} M = 0$.

For a geometric proof of the crucial inequality (1), see [Hille and Ploog 2017].

Proof. (1) Consider the symmetric subcomplex $\mathcal{S}^\bullet(M, N) \subset \mathcal{C}^\bullet(M, N)$, with terms $\mathcal{S}^0(M, N) := \bigoplus_{i=1}^{t-1} \operatorname{Hom}(M_i, N_i) \subseteq \mathcal{C}^0(M, N)$ and $\mathcal{S}^p(M, N) := \mathcal{C}^p(M, N)$ for $p = 1, 2$, and the differentials of $\mathcal{C}^\bullet(M, N)$. Then $\mathcal{S}^\bullet(M, N)$ is self-dual in the sense $\mathcal{S}^\bullet(M, N) \cong \mathcal{S}^\bullet(N, M)^*[-2]$; for the isomorphism one needs to change one sign in the differential. Therefore, the following inclusion yields the claim:

$$\operatorname{Ext}^2(N,M)^* = H^2(\mathcal{S}^\bullet(N,M))^* \cong H^0(\mathcal{S}^\bullet(M,N)) \subseteq H^0(\mathcal{C}^\bullet(M,N)) = \operatorname{Hom}(M,N).$$

(2) If $\operatorname{rk} M = 0$, i.e., $M_t = 0$, then $\operatorname{End}(M) = \operatorname{Ext}^2(M, M)^*$ from $\mathcal{C}^\bullet(M, M) = \mathcal{S}^\bullet(M, M)$ and the proof of (1). Conversely, if $M_t \neq 0$, then $\mathrm{id}_M \notin H^0(\mathcal{S}^\bullet(M, N))$, so $\operatorname{Ext}^2(M, M)^* = H^0(\mathcal{S}^\bullet(M, N)) \subsetneq H^0(\mathcal{C}^\bullet(M, M)) = \operatorname{End}(M)$. □

1E. ***Serre functor and Calabi–Yau objects.*** Because $\mathcal{A}_t$ is an algebra of finite global dimension, its bounded derived category $\mathcal{D}^b(\mathcal{A}_t)$ has a Serre functor S or, equivalently, Auslander–Reiten sequences (see [Reiten and Van den Bergh 2002, Theorem I.2.4] for the equivalence). Therefore, S is the derived Nakayama functor [Happel 1988, page 37, theorem and proof].

An object $M \in \mathcal{D}^b(\mathcal{A}_t)$ is called *d-Calabi–Yau* (often abbreviated to d-CY) if $\mathsf{S}(A) \cong A[d]$, where $d \in \mathbb{Z}$.

Proposition 1.10. *The projective-injective module $P(t) \in \mathcal{D}^b(\mathcal{A}_t)$ is* 0*-CY, and the simple modules $S(1), \dots, S(t-1) \in \mathcal{D}^b(\mathcal{A}_t)$ are* 2*-CY.*

Proof. There is the unique indecomposable projective-injective module $P(t) = I(t)$, which is thus fixed by the Nakayama functor: $\mathsf{S}P(t) = I(t) = P(t)$.

The projective resolutions of the simple modules $S(1), \dots, S(t-1)$ are given by Lemma 1.4. Their injective resolutions are — as is easily checked by hand — $S(1) \to I(1) \to I(2) \to I(1)$ and $S(i) \to I(i) \to I(i-1) \oplus I(i+1) \to I(i)$ for $i = 2, \dots, t-1$. Hence, the Nakayama functor S sends $S(i)$ to $S(i)[2]$. □

Remark 1.11. It is actually true that the triangulated category $\mathcal{D}^b_0(\mathcal{A}_t)$ of rank-0 objects is a 2-CY category, i.e., it has Serre functor [2]. For a geometric proof of this fact, see [Hille and Ploog 2017]. It does not follow formally from the proposition.

1F. ***The modules $\Delta(i)$ and $\nabla(i)$.*** For any $i \in \{1, \dots, t\}$, the $\mathcal{A}_t$-representation $\nabla(i)$ is defined as follows: $\nabla(i)_j = 0$ for $j < i$ and $\nabla(i)_j = \boldsymbol{k}$ for $j \geq i$, with $\nabla(i)_j \xleftarrow{\beta_j = 1} \nabla(i)_{j+1}$ for $i \leq j < t$, and all other maps zero.

The representation $\Delta(i)$ has the same vector spaces as $\nabla(i)$ on all vertices, but with $\alpha_j = 1$ wherever possible. See Example 2.7 for visualizations of these modules. They are characterized by the resolutions $0 \to P(i-1) \to P(i) \to \Delta(i) \to 0$ and $0 \to \nabla(i) \to I(i) \to I(i-1) \to 0$. Note $\dim \Delta(i) = \dim \nabla(i) = t + 1 - i$ and $\operatorname{top} \Delta(i) = \operatorname{soc} \nabla(i) = S(i)$ and $\operatorname{soc} \Delta(i) = \operatorname{top} \nabla(i) = S(t)$.

These modules form chains of injections $\Delta(t) \hookrightarrow \Delta(t-1) \hookrightarrow \cdots \hookrightarrow \Delta(1)$ and of surjections $\nabla(1) \twoheadrightarrow \nabla(2) \twoheadrightarrow \cdots \twoheadrightarrow \nabla(t)$. We will see in Section 3 that these are full exceptional sequences, $\Delta := (\Delta(t), \dots, \Delta(1))$ and $\nabla := (\nabla(1), \dots, \nabla(t))$.

2. Exceptional and spherical modules

An object $M \in \mathcal{D}^b(\mathcal{A}_t)$ is called *exceptional* if $\operatorname{Hom}^\bullet(M, M) = \boldsymbol{k}$. And M is called *e-spherical* if $\mathsf{S}(M) \cong M[e]$ and $\operatorname{Hom}^\bullet(M, M) = \boldsymbol{k} \oplus \boldsymbol{k}[-e]$. Also recall $\operatorname{rk} M = \dim M_t = \dim \operatorname{Hom}(P(t), M)$.

Definition 2.1. A module M is called *thin* if $\underline{\dim}(M)$ has entries only zero or one.

Theorem 2.2. *Let M be an $\mathcal{A}_t$-module.*

(1) *M is exceptional if and only if M is indecomposable and thin and* $\operatorname{rk}(M) = 1$.

(2) *M is 2-spherical if and only if M is indecomposable and thin and* $\mathrm{rk}(M) = 0$.

Remark 2.3. The 0-CY module $P(t)$ has $\dim \mathrm{End}(P(t)) = t$; hence, the $\mathcal{A}_2$-module $P(2)$ is 0-spherical of rank 2.

Proof. (1) Let M be an exceptional module, with dimension vector $\underline{d} := \underline{\dim}(M)$. Then $q(\underline{d}) = \chi(M, M) = 1$, and by Corollary 1.6 this forces $d_a = \cdots = d_t = 1$ for some $a \in \{1, \dots, t\}$ and $d_i = 0$ for $i < a$. Hence, M is thin of rank 1.

Conversely, let M be an indecomposable, thin module of rank 1. Computing endomorphisms of M as a representation yields $\mathrm{End}(M) = \boldsymbol{k}$. Now Proposition 1.9 implies $\mathrm{ext}^2(M, M) < \hom(M, M) = 1$, by the assumption of $\mathrm{rk}(M) = 1$. We finally get $\mathrm{ext}^1(M, M) = 0$ from $\chi(M, M) = q(M) = 1$, as $\underline{\dim}(M)$ is of type $(0, \dots, 0, 1 \dots, 1)$, possibly without leading zeroes.

(2) Let now M be a 2-spherical module. We see $\mathrm{rk}(M) = 0$ from

$$\mathrm{Hom}(P(t), M) = \mathrm{Hom}(M[-2], P(t))^* = \mathrm{Hom}(P(t), M[-2]) = \mathrm{Ext}^{-2}(P(t), M) = 0$$

where we have used Serre duality twice: first for the 2-CY object M and then for the 0-CY object $P(t)$; see Proposition 1.10. Moreover, we have $q(M) = 2$ which, together with $\mathrm{rk}(M) = 0$, yields $\underline{\dim}(M) = (0, \dots, 0, 1, \dots, 1, 0, \dots, 0)$, possibly without leading zeroes. In particular, M is thin of rank 0.

Conversely, if M is an indecomposable, thin module of rank 0, then we again find $\mathrm{End}(M) = \boldsymbol{k}$ from checking representation endomorphisms. Proposition 1.9 now gives $\mathrm{ext}^2(M, M) = \hom(M, M) = 1$, and then $q(M) = 2$ gets us $\mathrm{Ext}^1(M, M) = 0$. It remains to show that M is 2-CY. By Proposition 1.10, the simple rank-0 modules $S(1), \dots, S(t-1)$ are 2-CY. Any simple, rank-0 module M is a consecutive extension of $S(1), \dots, S(t-1)$. Therefore, we can assume that M occurs in an extension $0 \to M' \to M \to S(i) \to 0$ with $\mathsf{S}(M') \cong M'[2]$. Moreover, because M is thin, $\mathrm{ext}^1(S(i), M') = 1$. Hence, applying the autoequivalence S to the essentially unique (up to scalars) extension leads to $\mathsf{S}(M) \cong M[2]$. □

Corollary 2.4. *An $\mathcal{A}_t$-module is a brick if and only if it is indecomposable and thin. Moreover, over $\mathcal{A}_t$ there are $2^t - 1$ exceptional modules and $2^{t+1} - t - 2$ bricks, and the number of 2-spherical modules is $2^t - t - 1$.*

Proof. ($\Longleftarrow$) Recall that M is a brick if $\mathrm{End}(M) = \boldsymbol{k}$. By the theorem, indecomposable thin modules are either 2-spherical or exceptional, and therefore bricks.

($\Longrightarrow$) We have $2 = 2\hom(M, M) \geq \hom(M, M) + \mathrm{ext}^2(M, M) \geq q(M) \geq 1$ for a brick M, using Proposition 1.9(1) and that q is positive definite. If $q(M) = 1$, then M is thin by Corollary 1.6. Otherwise, $q(M) = 2$ and $\hom(M, M) = \mathrm{ext}^2(M, M)$; hence, $\mathrm{rk}(M) = 0$ by Proposition 1.9(2), and again M is thin by Corollary 1.6.

The dimension vector of an exceptional module is $(0, \dots, 0, 1, \dots, 1)$, possibly with no leading zeroes. For each map in the representation, there are two choices,

α or β. Thus, there are 2^{i-1} exceptional modules of dimension i. Altogether, there are $\sum_{i=1}^{t} 2^{i-1} = 2^t - 1$ exceptional modules.

Any brick, i.e., an indecomposable thin module, has the dimension vector of some exceptional $\mathcal{A}_l$-module, for an $l \in \{1, \dots, t\}$. Hence, their number is given by the sum $\sum_{l=1}^{t}(2^l - 1) = 2^{t+1} - t - 2$. Finally, the number of 2-spherical modules is the difference $(2^{t+1} - t - 2) - (2^t - 1) = 2^t - t - 1$. $\square$

Lemma 2.5. *Let M and N be two exceptional $\mathcal{A}_t$-modules.*

(1) *If* $\dim M \neq \dim N$, *then* $\chi(M, N) = 0$; *otherwise*, $\chi(M, N) = 1$.

(2) *If* (M, N) *is an exceptional pair*, *i.e.*, $\mathrm{Ext}^p(N, M) = 0$ *for* $p = 0, 1, 2$, *then* $\mathrm{Ext}^2(M, N) = 0$ *and* $\hom(M, N) = \mathrm{ext}^1(M, N) \leq 1$.

Proof. (1) This follows from the formula of Lemma 1.5 and that $\underline{\dim}(M)$, $\underline{\dim}(N)$ are of the form $(0, \dots, 0, 1, \dots, 1)$, possibly without leading zeros, by Theorem 2.2.

(2) We start with Proposition 1.9(1): $\mathrm{ext}^2(M, N) \leq \hom(N, M) = 0$.

Next, assume there is a nonzero morphism $\varphi : M \to N$. Consider a vertex i with $0 \neq \varphi_i : M_i = \boldsymbol{k} \to \boldsymbol{k} = N_i$, using that M and N are thin. And again by thinness, the scalar $\varphi_i \in \boldsymbol{k}$ propagates in a unique fashion to adjacent vertices, either by 0 or by the same value φ_i. In other words, if $\mathrm{Hom}(M, N) \neq 0$, then $\hom(M, N) = 1$. Now, $\mathrm{ext}^1(M, N) = \hom(M, N) + \mathrm{ext}^2(M, N) - \chi(M, N) = \hom(M, N) \leq 1$. $\square$

The spherical twist functors $\mathsf{T}_{S(i)}$ associated to the 2-spherical simple modules $S(1), \dots, S(t-1)$ generate a subgroup $\mathsf{Br}(t) := \langle \mathsf{T}_{S(1)}, \dots, \mathsf{T}_{S(t-1)} \rangle \subset \mathrm{Aut}(\mathcal{D}^b(\mathcal{A}_t))$. This subgroup is isomorphic to the braid group on t strands; see Appendix A. We now show that the braid group action is transitive on spherical modules. This fact is interesting in itself and will be used in [Hille and Ploog 2017].

Lemma 2.6. *For a* 2*-spherical $\mathcal{A}_t$-module M, there is $b \in \mathsf{Br}(t)$ with $b(M) = S(1)$.*

Proof. By the theorem, M is a thin module. Let $i \geq 1$ be minimal with $M_i \neq 0$, and $j < t$ maximal with $M_j \neq 0$. If $i \neq j$, consider two cases:

(i) $M_i = \boldsymbol{k} \xrightarrow{\alpha} \boldsymbol{k} = M_{i+1}$. Then $\mathrm{Hom}(M, S(i)) = \boldsymbol{k}$; hence, $\mathrm{Ext}^2(M, S(i)) = \mathrm{Hom}(S(i), M)^* = 0$, and finally $\mathrm{Ext}^1(M, S(i)) = 0$ from $\chi(M, S(i)) = 1$. Put $M' := \mathsf{T}_{S(i)}^{-1}(M)$. Plugging $\mathrm{Hom}^\bullet(M, S(i)) = \boldsymbol{k}$ into the triangle describing the inverse spherical twist functor (see Appendix A), we obtain a short exact sequence $0 \to M' \to M \to S(i) \to 0$.

(ii) $M_i = \boldsymbol{k} \xleftarrow{\beta} \boldsymbol{k} = M_{i+1}$. Then $\mathrm{Hom}(S(i), M) = \boldsymbol{k}$, and $\mathrm{Ext}^1(S(i), M) = \mathrm{Ext}^2(S(i), M)) = 0$ as above. Put $M' := \mathsf{T}_{S(i)}(M)$. The spherical twist triangle reduces to the short exact sequence $0 \to S(i) \to M \to M' \to 0$.

In both cases, M' is a 2-spherical module supported on vertices $i+1, \dots, j$. Repeating this process, we see that a combination of spherical twists along $S(i)$

together with their inverses send M to a simple module. In the final step, we move this simple module via $\mathsf{Br}(t)$ to $S(1)$, using $\mathsf{T}_{S(i)}(S(i)) = S(i)[-1]$ and

$$\mathsf{T}_{S(i)}(S(i+1)) = \begin{pmatrix} S(i) \\ S(i+1) \end{pmatrix} =: S^{(i)} \quad \text{and} \quad \mathsf{T}_{S^{(i)}}(S(i+1)) = S(i)[-1]. \qquad \square$$

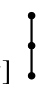
2A. ***Representing thin modules by worms.*** A nonzero, indecomposable thin representation of $\mathcal{A}_t$ is a sequence of maps $\boldsymbol{k} \xrightarrow{\alpha} \boldsymbol{k}$ and $\boldsymbol{k} \xleftarrow{\beta} \boldsymbol{k}$. Therefore, it is uniquely encoded by a word in the letters α and β, together with the last index of a nonzero vector space in the representation. For exceptional modules, the encoding is particularly simple, since the index of the last nonzero vector space is always t.

We will depict these modules by reading the word from left to right, and draw α as a line going right and β as a line going up. This we call a *worm*.

Example 2.7. The seven exceptional $\mathcal{A}_3$-modules, as representations and worms, are:

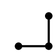
$S(3) = \nabla(3) = \Delta(3) = [0 \quad 0 \quad \boldsymbol{k}]$

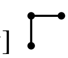
$\Delta(2) = [0 \quad \boldsymbol{k} \xrightarrow{\alpha} \boldsymbol{k}]$

$\nabla(1) = [\boldsymbol{k} \xleftarrow{\beta} \boldsymbol{k} \xleftarrow{\beta} \boldsymbol{k}]$ 

$\Delta(1) = [\boldsymbol{k} \xrightarrow{\alpha} \boldsymbol{k} \xrightarrow{\alpha} \boldsymbol{k}]$

$\nabla(2) = [0 \quad \boldsymbol{k} \xleftarrow{\beta} \boldsymbol{k}]$ 

$[\boldsymbol{k} \xrightarrow{\alpha} \boldsymbol{k} \xleftarrow{\beta} \boldsymbol{k}]$ 

$[\boldsymbol{k} \xleftarrow{\beta} \boldsymbol{k} \xrightarrow{\alpha} \boldsymbol{k}]$ 

3. Full exceptional sequences of modules

3A. ***Worm diagrams.*** We now define worm diagrams as certain collections of worms. Worms will always be conflated with exceptional modules, as explained in Section 2A. We consider $\mathbb{Z} \times \mathbb{Z}$ as a lattice grid in the obvious way.

Definition 3.1. A *worm diagram of size t* is a graph with the following properties:

(1) the vertex set is the triangle $\{(m, n) \in \mathbb{Z} \times \mathbb{Z} \mid m + n \leq t + 1 \text{ and } m, n \geq 1\}$,

(2) the edges lie on the lattice,

(3) the connected components are t worms of lengths $1, 2, \dots, t$, respectively,

(4) every worm has one vertex on the diagonal $\{(m, t + 1 - m) \mid m = 1, \dots, t\}$.

Lemma 3.2. *Let $\mathcal{E} = (E^1, \dots, E^t)$ be a worm diagram of size t. Then*

(1) $\mathrm{Ext}^p(E^j, E^i) = 0$ *for* $p = 0, 1, 2$ *if* $i < j$,

(2) $\mathrm{Hom}(E^i, E^j) = \mathrm{Ext}^1(E^i, E^j) = \boldsymbol{k}$ *and* $\mathrm{Ext}^2(E^i, E^j) = 0$ *if* $i < j$,

(3) *nonzero morphisms $E^i \to E^{i+1}$ are either injective or surjective.*

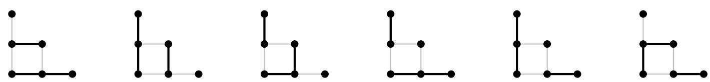
Recall that $(E^1, \dots, E^t)$ is an *exceptional sequence in $\mathcal{D}^b(\mathcal{A}_t)$* if each $E^i \in \mathcal{D}^b(\mathcal{A}_t)$ is an exceptional object and if $\mathrm{Hom}^\bullet(E^j, E^i) = 0$ whenever $i < j$. See

[Rudakov 1990] or [Huybrechts 2006, §8] for greater generality. If all E^i happen to be modules, then the vanishing conditions are just $\mathrm{Ext}^p(E^j, E^i) = 0$ for all $p \in \{0, 1, 2\}$ and $i < j$. The sequence is *full* if it generates $\mathcal{D}^b(\mathcal{A}_t)$; if all E^i are modules, this just means that the dimension vectors $\underline{\dim}(E^1), \dots, \underline{\dim}(E^t)$ form a basis of the K-group $K(\mathcal{A}_t) = \mathbb{Z}^t$.

The dimension vectors of the t worms in a worm diagram obviously span $\mathbb{Z}^t$; hence, the next statement is tantamount to clause (1) of the lemma.

Proposition 3.3. *Every worm diagram of size t gives rise to a full exceptional sequence of $\mathcal{A}_t$-modules.*

Example 3.4. There are $6 = 3!$ worm diagrams of size 3:



By the proposition, each worm diagram corresponds to a full exceptional sequence of $\mathcal{A}_3$-modules. We will see later, in Proposition 3.5, that in fact all full exceptional sequences of modules come from worm diagrams. And in Remark 4.5, the symmetric group $\mathsf{Sym}(t)$ is seen to act simply transitively on exceptional sequences of $\mathcal{A}_t$-modules; hence, there are $t!$ such sequences.

Proof of Lemma 3.2. (1), (2) Recall that the i-th worm E^i in the worm diagram $(E^1, \dots, E^t)$ ends at the point $(i, t+1-i)$ on the diagonal. Fix $i < j$, so that E^i is to the left of E^j. Let the vertex index $k \in \{2, \dots, t\}$ be minimal such that the worms coincide at vertices $k, \dots, t$, i.e., the two representations have the same α/β maps along the subquiver on this vertex set. Hence, E^i and E^j differ at the vertex $k-1$, and by the shape of worm diagrams, precisely one of the following cases occurs:

- $(E^i)_{k-1} = 0$; then $(E^j)_{k-1} \xrightarrow{\alpha} (E^j)_k$;
- $(E^j)_{k-1} = 0$; then $(E^i)_{k-1} \xleftarrow{\beta} (E^i)_k$;
- $(E^i)_{k-1} \neq 0$ and $(E^j)_{k-1} \neq 0$; then $(E^i)_{k-1} \xleftarrow{\beta} (E^i)_k$ and $(E^j)_{k-1} \xrightarrow{\alpha} (E^j)_k$.

For any $\lambda \in \boldsymbol{k}$, the map $(E^i)_t = \boldsymbol{k} \xrightarrow{\lambda} \boldsymbol{k} = (E^j)_t$ of the vector spaces of E^i and E^j in the vertex t can be uniquely extended to the left: by λ for each vertex where the maps in E^i and E^j coincide, and by 0 once they differ.

$$\begin{array}{ccccccccc} \cdots & \xrightarrow{\alpha} & \boldsymbol{k} & \xleftarrow{\beta} & \boldsymbol{k} & \xleftarrow{\beta} & \boldsymbol{k} & \xrightarrow{\alpha} & \boldsymbol{k} \\ & & \downarrow{\scriptstyle 0} & & \downarrow{\scriptstyle \lambda} & & \downarrow{\scriptstyle \lambda} & & \downarrow{\scriptstyle \lambda} \\ \cdots & \xrightarrow[\alpha]{} & \boldsymbol{k} & \xrightarrow[\alpha]{} & \boldsymbol{k} & \xleftarrow[\beta]{} & \boldsymbol{k} & \xrightarrow[\alpha]{} & \boldsymbol{k} \end{array}$$

This argument shows $\mathrm{Hom}(E^i, E^j) = \boldsymbol{k}$ and, similarly, $\mathrm{Hom}(E^j, E^i) = 0$. Moreover, we have $\chi(E^i, E^j) = \chi(E^j, E^i) = 0$, using the Euler pairing for $\mathcal{A}_t$ (Lemma 1.5) and the dimension vectors of E^i and E^j (Theorem 2.2). Next, we use the general inequality $\mathrm{ext}^2(E^i, E^j) \le \hom(E^j, E^i) = 0$ of Proposition 1.9. Combining these, we get $\mathrm{ext}^1(E^i, E^j) = \hom(E^i, E^j) + \mathrm{ext}^2(E^i, E^j) - \chi(E^i, E^j) = 1 + 0 - 0 = 1$.

This proves (2); we also know $\mathrm{ext}^1(E^j, E^i) = \mathrm{ext}^2(E^j, E^i) \le \hom(E^i, E^j) = 1$. For (1), it remains to show $\mathrm{ext}^2(E^j, E^i) = 0$. Here we employ the symmetric subcomplex $\mathcal{S}^\bullet(E^i, E^j) \subset \mathcal{C}^\bullet(E^i, E^j)$ introduced in the proof of Proposition 1.9(2). These two complexes differ just in cohomological degree 0, using $\mathrm{rk}\, E^i = \mathrm{rk}\, E^j = 1$:

$$\mathcal{C}^0(E^i, E^j) = \mathcal{S}^0(E^i, E^j) \oplus \mathrm{Hom}((E^i)_t, (E^j)_t) = \mathcal{S}^0(E^i, E^j) \oplus \boldsymbol{k}.$$

Given $0 \ne \varphi \in \mathrm{Hom}(E^i, E^j) = \boldsymbol{k}$, we have seen that $\varphi_t : (E^i)_t \to (E^j)_t$ is nonzero. The differential $d^0 : \mathcal{C}^0(E^i, E^j) \to \mathcal{C}^1(E^i, E^j)$ is not injective with kernel $H^0(\mathcal{C}^\bullet(E^i, E^j)) = \mathrm{Hom}(E^i, E^j) = \boldsymbol{k}\varphi$; hence, $H^0(\mathcal{S}^\bullet(E^i, E^j)) = 0$, i.e., $d^0|_{\mathcal{S}^0}$ is injective. By duality $\mathcal{S}^\bullet(E^i, E^j)^* = \mathcal{S}^\bullet(E^j, E^i)[-2]$ (see Proposition 1.9) we find

$$\mathrm{Ext}^2(E^j, E^i) = H^2(\mathcal{C}^\bullet(E^j, E^i)) = H^2(\mathcal{S}^\bullet(E^j, E^i)) = H^0(\mathcal{S}^\bullet(E^i, E^j))^* = 0.$$

(3) The additional feature of adjacent worms E^i, E^{i+1} is that, starting along the diagonal, they run in parallel until one of them stops. If E^i stops first, i.e., $\dim E^i < \dim E^{i+1}$, then it embeds into E^{i+1}, whereas if E^{i+1} stops first, i.e., $\dim E^i > \dim E^{i+1}$, then E^i surjects onto it. □

3B. *Filtrations of the projective-injective module.*

Proposition 3.5. *If $F^1 \subset \ldots \subset F^t = P(t)$ is a filtration such that*

(i) *each F^i is indecomposable of rank i and*

(ii) *each graded piece F^i/F^{i-1} is exceptional,*

then $(E^1, E^2, \ldots, E^t)$ is a full exceptional sequence, where $E^i := F^{t+1-i}/F^{t-i}$.

Moreover, any full exceptional sequence of $\mathcal{A}_t$-modules occurs in this way.

Proof. ($\Longrightarrow$) Assume that $F^\cdot$ is a filtration as in (i), i.e., each graded piece F^i/F^{i-1} is exceptional. Since $\underline{\dim}(P(t)) = (1, 2, \ldots, t)$, the filtration induces a worm diagram of size t, with worms $E^1, \ldots, E^t$, where $E^i = F^{t+1-i}/F^{t-i}$ is the worm ending in $(i, t+1-i)$. By Proposition 3.3, $(E^1, \ldots, E^t)$ is a full exceptional sequence.

($\Longleftarrow$) Given two $\mathcal{A}_t$-modules M, N, their *universal coextension U* is defined by the exact sequence $0 \to N \to U \to \mathrm{Ext}^1(M, N) \otimes M \to 0$ which corresponds to $\mathrm{id} \in \mathrm{End}(\mathrm{Ext}^1(M, N)) = \mathrm{Ext}^1(\mathrm{Ext}^1(M, N) \otimes M, N)$. Crucially, if (M, N) is an exceptional pair with $\mathrm{Ext}^{\ge 2}(M, N) = 0$, then $M \oplus U$ is a partial tilting module. See [Hille and Perling 2011] or [Hille and Ploog 2019, §1.2].

For an exceptional sequence of $\mathcal{A}_t$-modules $\mathcal{E} = (E^1, \dots, E^t)$, form its iterated universal coextension $T = T^1 \oplus \cdots \oplus T^t$ by $0 \to T^{i-1} \to T^i \to (E^{t+1-i})^{\oplus c_i} \to 0$ with $T^1 = E^t$ and $c_i := \mathrm{ext}^1(E^{t+1-i}, T^{i-1})$. Then T is a partial tilting module because $\mathrm{Ext}^2(E^i, E^j) = 0$ for all i, j by Lemma 2.5 and $\mathcal{A}_t$ has global dimension 2. Moreover, $E^1, \dots, E^t$ generate $\mathcal{D}^b(\mathcal{A}_t)$, hence so do $T^1, \dots, T^t$, and T is tilting.

By Lemma 2.5, we have $\hom(E^i, E^j) = \mathrm{ext}^1(E^i, E^j) \le 1$ and $\mathrm{ext}^2(E^i, E^j) = 0$ for $i < j$. Recursively applying $\mathrm{Ext}^1(E^{t+1-i}, \cdot)$ to the exact sequences defining the coextensions $T^{i-1}, T^{i-2}, \dots, T^1 = E^t$, we get

$$c_i = \mathrm{ext}^1(E^{t+1-i}, T^{i-1}) = \cdots = \mathrm{ext}^1(E^{t+1-i}, T^1) = \mathrm{ext}^1(E^{t+1-i}, E^t) \le 1.$$

Hence, in each iteration step, the coextension is either trivial or unique up to scalars.

Now by construction of iterated universal coextensions, we have $T^1 \subset \cdots \subset T^t$, and the maximal summand T^t is the universal coextension of $(E^1)^{\oplus a_1}, \dots, (E^t)^{\oplus a_t}$ with $a_i \in \{0, 1\}$. But $P(t)$ is the unique indecomposable injective-projective $\mathcal{A}_t$-module; hence, it must occur as a summand of any tilting object. This forces $a_1 = \cdots = a_t = 1$ (and subsequently $c_i = 1$ at all steps), i.e., $T^t = P(t)$.

Therefore, we find the smaller direct summands as Jordan–Hölder subquotients for the filtration $F^i = T^i$ of $P(t)$. Note $\underline{\dim}(P(t)) = (1, 2, \dots, t)$, corresponding to the triangle grid of worm diagrams. □

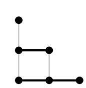
Corollary 3.6. *There is a bijection between worm diagrams of size t and full exceptional sequences of $\mathcal{A}_t$-modules.*

Corollary 3.7. *Let $(E^1, \dots, E^t)$ be a full exceptional sequence of $\mathcal{A}_t$-modules. Then* $\hom(E^i, E^j) = \mathrm{ext}^1(E^i, E^j) = 1$ *and* $\mathrm{ext}^2(E^i, E^j) = 0$ *for any $i < j$.*

Proof of Corollary 3.7. The Hom and Ext dimensions among worms have been computed in the proof of Proposition 3.3. These dimensions then apply to all full exceptional sequences of modules, by the previous corollary. □

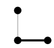
Example 3.8. Consider the standard exceptional sequence $\Delta = (\Delta(3), \Delta(2), \Delta(1))$ of $\mathcal{A}_3$-mod. Its associated iterated universal coextension and the worm diagram are

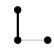
$$T = T^1 \oplus T^2 \oplus T^3 = \Delta(1) \oplus \begin{pmatrix} \Delta(2) \\ \Delta(1) \end{pmatrix} \oplus \begin{pmatrix} \Delta(3) \\ \Delta(2) \\ \Delta(1) \end{pmatrix}.$$



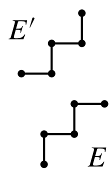
We mention in passing that the maps $\Delta(3) \to \Delta(2) \to \Delta(1)$ are all injective, so that condition (†) of [Hille and Ploog 2019, §1.3] is satisfied, i.e., T is an exact tilting object.

Example 3.9. For $t = 2$, we have $T = T^1 \oplus T^2$ with $T^2 = P(2) = \big[\boldsymbol{k} \underset{(0\ 1)}{\overset{(1\ 0)^t}{\rightleftarrows}} \boldsymbol{k}^2\big]$. There are two filtrations meeting the conditions of Proposition 3.5:

$$F^1 = E^2 := \Delta(1) = [\boldsymbol{k} \underset{0}{\overset{1}{\rightleftarrows}} \boldsymbol{k}] \subset F^2 = P(2), \quad E^1 = S(2) = [0 \underset{0}{\overset{0}{\rightleftarrows}} \boldsymbol{k}],$$ 

$$F^1 = E^2 := S(2) = [0 \underset{0}{\overset{0}{\rightleftarrows}} \boldsymbol{k}] \subset F^2 = P(2), \quad E^1 = \nabla(1) = [\boldsymbol{k} \underset{1}{\overset{0}{\rightleftarrows}} \boldsymbol{k}].$$ 

Example 3.10. The regular behavior of Corollary 3.7 only applies to modules occurring in a full exceptional sequence. Consider the exceptional modules E' and E given by the displayed zigzag worms. Then it can be immediately checked that $\hom(E', E) = 3$ and $\hom(E, E') = 2$. Obviously, longer worms can produce arbitrarily high Hom dimensions.



Arguing as in the end of proof of Lemma 3.2, we find in this case $\operatorname{Ext}^2(E', E) = H^2(\mathcal{C}^\bullet(E', E)) = H^2(\mathcal{S}^\bullet(E', E)) = H^0(\mathcal{S}^\bullet(E, E'))^* \neq 0$.

4. Group actions on exceptional sequences

Denote by $\mathcal{E}xc(t)$ the set of full exceptional sequences in $\mathcal{D}^b(\mathcal{A}_t)$, up to isomorphism, and by $m\mathcal{E}xc(t)$ the subset of sequences of modules. Let $\mathsf{Br}(t)$ be the braid group on t strands, and $\mathsf{Sym}(t)$ the symmetric group of t letters. There is a canonical surjective homomorphism $\mathsf{Br}(t) \to \mathsf{Sym}(t)$.

The braid group $\mathsf{Br}(t)$ naturally acts in two ways on $\mathcal{E}xc(t)$: first, exceptional sequences can be mutated (we will always deal with right mutations in this article). Second, the 2-spherical modules $S(1), \dots, S(t-1)$ form an A_{t-1}-chain, and thus give rise to a $\mathsf{Br}(t)$-action on the whole derived category (see Section A2), and in particular on $\mathcal{E}xc(t)$. Moreover, the symmetric group $\mathsf{Sym}(t)$ acts simply transitively on $m\mathcal{E}xc(t)$ from the left and from the right, in a combinatorial fashion.

The $\mathsf{Sym}(t)$-action on $m\mathcal{E}xc(t)$ does not extend to $\mathcal{E}xc(t)$, and the $\mathsf{Br}(t)$-actions on $\mathcal{E}xc(t)$ do not restrict to $m\mathcal{E}xc(t)$. Nevertheless, we will prove that the two braid group actions lift the symmetric group actions. In order to see this, we introduce a count of all vertical edges in a worm diagram:

$$f : m\mathcal{E}xc(t) \to \Big\{0, 1, \dots, \binom{t}{2}\Big\},$$
$$\mathcal{E} = (E^1, \dots, E^t) \mapsto f(\mathcal{E}) \text{ is the number of } \beta\text{-maps among } E^1, \dots, E^t.$$

Clearly, minimum and maximum are uniquely achieved by $f(\Delta) = 0$ (no vertical edges) and $f(\nabla) = \binom{t}{2}$ (all edges vertical), respectively.

4A. ***Symmetric group action.*** We define two permutations $\sigma(\mathcal{E}), \lambda(\mathcal{E}) \in \mathsf{Sym}(t)$ for any full exceptional sequence $\mathcal{E}$ of $\mathcal{A}_t$-modules. Mostly, we employ $\sigma(\mathcal{E})$.

Definition 4.1. Let $\mathcal{E} = (E^1, \dots, E^t)$ be a full exceptional sequence of $\mathcal{A}_t$-modules.

(1) The (*start*) *permutation* of $\mathcal{E}$ is $\sigma(\mathcal{E}) := (\sigma(E^1), \dots, \sigma(E^t)) \in \mathsf{Sym}(t)$, where $\sigma(E^i) := t + 1 - \dim E^i$ is the starting vertex of the representation E^i.

(2) The *length permutation* of $\mathcal{E}$ is $\lambda(\mathcal{E}) := (\dim E^1, \dots, \dim E^t) \in \mathsf{Sym}(t)$.

Example 4.2. Since $\sigma(\Delta(i)) = i$ and $\lambda(\Delta(i)) = t+1-i$, the exceptional sequence $\Delta = (\Delta(t), \dots, \Delta(1))$ has length permutation $\lambda(\Delta) = \mathrm{id}$ and its start permutation $\sigma(\Delta) = \binom{1\ \ 2\ \ \cdots\ t}{t\ t-1\ \cdots\ 1} = \omega_0 \in \mathsf{Sym}(t)$ is the longest word.

Lemma 4.3. *Let* $\mathcal{E} = (E^1, \dots, E^t) \in m\mathcal{E}xc(t)$ *and* $\sigma := \sigma(\mathcal{E}) \in \mathsf{Sym}(t)$.

(1) $\lambda(\mathcal{E}) = \omega_0 \cdot \sigma(\mathcal{E})$.

(2) *For* $i < j$ *fixed*, $\sigma(i) < \sigma(j) \iff (E^i)_{\sigma(j)-1} \xleftarrow{\beta} (E^i)_{\sigma(j)}$ *is a vertical edge.*

(3) $f(\mathcal{E}) = \#\{(i, j) \mid 1 \le i < j \le t,\ \sigma(i) < \sigma(j)\}$.

Proof. (1) This follows at once from $\lambda(i) = \dim E^i$, $\sigma(i) = t + 1 - \dim E^i$, and $\omega_0(i) = t + 1 - i$.

(2) Any worm diagram of size t has a unique worm of length 1; call this worm E^k. The worms to its left, $E^1, \dots, E^{k-1}$, end at vertex t in a vertical edge; and the worms to its right, $E^{k+1}, \dots, E^t$, end in a horizontal edge.

Given j, consider the worm subdiagram of size $\sigma(j)$. Its boundary diagonal $(1, \sigma(j)), (2, \sigma(j) - 1), \dots, (\sigma(j), 1)$ intersects precisely j worms, and contains the head (starting vertex) of E^j at the point $(j, \sigma(j)+1-j)$. This forces all edges left of j along the boundary to be vertical. Another worm E^i leaves a trace on the subdiagram precisely if $\sigma(i) < \sigma(j)$, and it is left of E^j if and only if $i < j$.

(3) This follows from (2). □

Theorem 4.4. *For fixed* $t \in \mathbb{N}$, *there are bijections between the following sets*:

(i) *full exceptional sequences of* $\mathcal{A}_t$*-modules*,

(ii) *ascending filtrations* $F^\cdot$ *of* $P(t)$ *with* $\operatorname{rk} F^i = i$ *and* F^i/F^{i-1} *exceptional*,

(iii) *worm diagrams of size* t,

(iv) *the symmetric group* $\mathsf{Sym}(t)$.

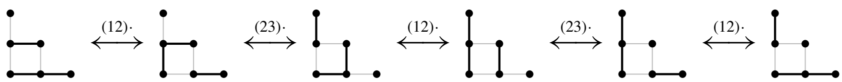
Proof. The bijection (i) ↔ (ii) was established in Proposition 3.5, and the proof of that statement contained the bijection (ii) ↔ (iii), as mentioned in Corollary 3.6.

Mapping a full exceptional sequence of modules or, equivalently, the corresponding worm diagram to its permutation is obviously injective. Moreover, every permutation comes from a worm diagram: given $\sigma \in \mathsf{Sym}(t)$, we start drawing a worm diagram with the leftmost worm, which begins in $(1, t)$ and goes $\lambda(1) = t+1-\sigma(1)$

steps downwards. Given a partially completed worm diagram, the i-th worm starts in $(i, t+1-i)$ and is of length $\lambda(i) = t+1-\sigma(i)$; its shape is determined by the worms already drawn and the definition of worm diagrams. □

Remark 4.5. Assigning start permutations induces left and right actions of the symmetric group on full exceptional sequences of modules. By the above theorem, these actions are simply transitive.

Example 4.6. We consider again the six worm diagrams of size 3. Below each worm diagram, we give its start permutation, and we show how left multiplications by transpositions move between the diagrams, e.g., $(12) \cdot \binom{1\,2\,3}{3\,2\,1} = \binom{1\,2\,3}{3\,1\,2}$.



$\binom{1\,2\,3}{3\,2\,1}$ $\binom{1\,2\,3}{3\,1\,2}$ $\binom{1\,2\,3}{2\,1\,3}$ $\binom{1\,2\,3}{1\,2\,3}$ $\binom{1\,2\,3}{1\,3\,2}$ $\binom{1\,2\,3}{2\,3\,1}$

4B. ***Braid group action from right mutations.*** Our next aim is to categorify the right action, using the well known braid group action on $\mathcal{E}xc(t)$ from mutating exceptional sequences [Rudakov 1990].

Given an exceptional pair (E', E) in $\mathcal{D}^b(\mathcal{A}_t)$, its *right mutation* $(E, \mathsf{R}E')$ is again an exceptional pair, defined by the canonical triangle

$$\mathsf{R}E' \to E' \to \operatorname{Hom}^\bullet(E', E)^* \otimes E$$

where we slightly deviate from the standard definition, by taking $\mathsf{R}E'$ as the cocone of the canonical morphism rather than the cone.

An exceptional sequence $\mathcal{E} = (E^1, \ldots, E^t)$ in $\mathcal{D}^b(\mathcal{A}_t)$ has a *right mutation at E^i*,

$$\mathsf{R}_i\mathcal{E} := (E^1, \ldots, E^{i-1}, E^{i+1}, \mathsf{R}E^i, E^{i+2}, \ldots, E^t) \quad \text{for } i = 1, \ldots, t-1,$$

and it is well known that $\mathsf{R}_i\mathcal{E}$ is again an exceptional sequence, so that we get $\mathsf{R}_i : \mathcal{E}xc(t) \xrightarrow{\sim} \mathcal{E}xc(t)$; the inverses are left mutations. Mutations satisfy the braid relations, $\mathsf{R}_i\mathsf{R}_{i+1}\mathsf{R}_i\mathcal{E} \cong \mathsf{R}_{i+1}\mathsf{R}_i\mathsf{R}_{i+1}\mathcal{E}$, leading to an action $\mathsf{Br}(t) \times \mathcal{E}xc(t) \to \mathcal{E}xc(t)$.

Lemma 4.7. *Let (E', E) be an exceptional pair of $\mathcal{A}_t$-modules with* $\hom(E', E) = \operatorname{ext}^1(E', E) = 1$ *such that nonzero morphisms $E' \to E$ are surjective. Then the right mutation $\mathsf{R}E'$ is the module given by the extension*

$$0 \to E \to \mathsf{R}E' \to \ker(E' \to E) \to 0.$$

Proof. First observe that the notation in the statement is slightly abusive but unambiguous: $\ker(E' \to E) = \ker(\varepsilon)$ for any $0 \neq \varepsilon \in \operatorname{Hom}(E', E)$. Now using $\operatorname{Ext}^{\geq 2}(E', E) = 0$ from Lemma 2.5, the long exact cohomology sequence of the triangle defining $\mathsf{R}E'$ is

$$0 \to \mathrm{Ext}^1(E', E)^* \otimes E \to H^0(\mathsf{R}E') \to E' \xrightarrow{\varepsilon} \mathrm{Hom}(E', E)^* \otimes E \to H^1(\mathsf{R}E') \to 0.$$

This exact sequence reduces to $0 \to E \to H^0(\mathsf{R}E') \to E' \xrightarrow{\varepsilon} E \to H^1(\mathsf{R}E') \to 0$ due to $\mathrm{Hom}(E', E) = \mathrm{Ext}^1(E', E) = \boldsymbol{k}$. Finally, the canonical map ε is surjective; hence, $H^1(\mathsf{R}E') = 0$ and $\mathsf{R}E'$ is indeed a module, sitting in the stated extension. □

Lemma 4.7 applies to full exceptional sequences $\mathcal{E} = (E^1, \dots, E^t)$ of modules, because $\hom(E^i, E^j) = \mathrm{ext}^1(E^i, E^j) = 1$ for all $i < j$ by Corollary 3.7.

Corollary 4.8. *Let $\mathcal{E} = (E^1, \dots, E^t) \in m\mathcal{E}xc(t)$ and $i \in \{1, \dots, t-1\}$. Then the following conditions are equivalent*:

(i) $\mathsf{R}_i\mathcal{E} \in m\mathcal{E}xc(t)$.

(ii) *There exists a surjection $E^i \twoheadrightarrow E^{i+1}$.*

(iii) *The worm E^i is longer than the worm E^{i+1}.*

Proof. Implication (ii) $\Longrightarrow$ (i) is Lemma 4.7, while (i) $\Longrightarrow$ (ii) follows from the exact sequence in its proof; (ii) $\Longrightarrow$ (iii) is obvious, and (iii) $\Longrightarrow$ (ii) is Lemma 3.2(3). □

Clause (3) of the following statement says that right mutations R_i categorify right multiplications by τ_i.

Proposition 4.9. *Let $\mathcal{E} = (E^1, \dots, E^t)$ be a full exceptional sequence of $\mathcal{A}_t$-modules with $f(\mathcal{E}) \geq 1$. If E^i is longer than E^{i+1}, then*

(1) *$\mathsf{R}_i\mathcal{E}$ is a full exceptional sequence of $\mathcal{A}_t$-modules*,

(2) $f(\mathsf{R}_i\mathcal{E}) = f(\mathcal{E}) - 1$,

(3) $\sigma(\mathsf{R}_i\mathcal{E}) = \sigma(\mathcal{E}) \cdot \tau_i$.

Proof. (1) This is the content of Corollary 4.8.

(2) $\mathsf{R}_i\mathcal{E}$ modifies only the module E^i, so we compare this module to $\mathsf{R}E^i$. Now E^i surjecting onto E^{i+1} means that the worm E^{i+1} sits as a copy in the worm E^i, i.e., the representations have the same α/β maps in degrees $j, \dots, t$, where $j := \sigma(E^{i+1}) > \sigma(E^i)$ is the starting vertex of the shorter worm. Then $(E^i)_{j-1} \xleftarrow{\beta} (E^i)_j$ is necessarily a vertical edge. The inclusion $E^{i+1} \hookrightarrow \mathsf{R}E^i$ from Lemma 4.7 shows that in the representation $\mathsf{R}E^i$, the corresponding map is α, i.e., $(\mathsf{R}E^i)_{j-1} \xrightarrow{\alpha} (\mathsf{R}E^i)_j$. Hence, $f(\mathsf{R}_i\mathcal{E}) = f(\mathcal{E}) - 1$.

(3) $\sigma(\mathsf{R}_i\mathcal{E})$ has the same values as $\sigma(\mathcal{E})$, with $\sigma(\mathcal{E})(i)$ and $\sigma(\mathcal{E})(i+1)$ interchanged. This amounts to precomposition $\sigma(\mathsf{R}_i\mathcal{E}) = \sigma(\mathcal{E}) \cdot \tau_i$. □

We are ready to show that right mutations can transform any full exceptional sequence of modules into the standard sequence $\Delta = (\Delta(t), \dots, \Delta(1))$.

Theorem 4.10. *Let $\mathcal{E}$ be a full exceptional sequence of $\mathcal{A}_t$-modules with $f(\mathcal{E}) \geq 1$, and write its length permutation $\lambda(\mathcal{E}) = \tau_{i(f)} \cdots \tau_{i(1)}$ as a minimal product of simple transpositions. Setting recursively $\mathcal{E}_0 := \mathcal{E}$ and $\mathcal{E}_j := \mathsf{R}_{i(j)}\mathcal{E}_{j-1}$, each $\mathcal{E}_j$ is a full exceptional sequence of $\mathcal{A}_t$-modules, and $\mathcal{E}_f = \Delta$.*

Proof. The basic step to mutate $\mathcal{E}$ towards Δ is this equivalence: for $1 \leq i < t$,

$$f(\sigma(\mathcal{E}) \cdot \tau_i) = f(\mathcal{E}) - 1 \quad \iff \quad E^i \twoheadrightarrow E^{i+1}.$$

Here, we identify exceptional sequences of $\mathcal{A}_t$-modules with elements of $\mathsf{Sym}(t)$ and with worm diagrams of size t, as in Theorem 4.4.

The two worm diagrams $\mathcal{E} = (E^1, \ldots, E^t)$ and $\sigma(\mathcal{E}) \cdot \tau_i =: (F^1, \ldots, F^t) \in \mathsf{Sym}(t)$ are identical, except for the pairs (E^i, E^{i+1}) and (F^i, F^{i+1}). Each pair occupies the same space in the worm diagram grid. The shorter worms have the same form, whereas the longer worms differ. There is one more vertical edge if the longer worm comes first. Since $\dim E^i > \dim E^{i+1}$ translates to $E^i \twoheadrightarrow E^{i+1}$ by Lemma 3.2(3), the equivalence is established.

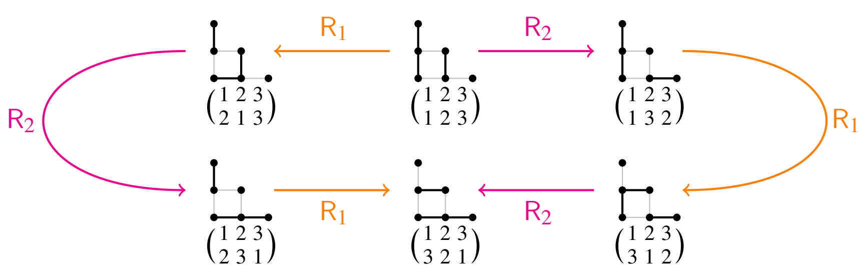
By Proposition 4.9, any surjection $E^i \twoheadrightarrow E^{i+1}$ gives rise to the mutated exceptional sequence $\mathsf{R}_i\mathcal{E}$ of modules with one less vertical edge. In this way we can proceed to obtain a sequence of mutations $\mathsf{R}_{i(f)} \cdots \mathsf{R}_{i(1)}\mathcal{E} = \Delta$ ending in the standard sequence with $f(\Delta) = 0$. The number of mutations is $f = f(\mathcal{E})$. Then

$$\omega_0 = \sigma(\Delta) = \sigma(\mathsf{R}_{i(f)} \cdots \mathsf{R}_{i(1)}\mathcal{E}) = \sigma(\mathcal{E}) \cdot \tau_{i(1)} \cdots \tau_{i(f)},$$

using $\sigma(\mathsf{R}_i\mathcal{E}) = \sigma(\mathcal{E}) \cdot \tau_i$ from Proposition 4.9. Thus, $\tau_{i(f)} \cdots \tau_{i(1)} = \omega_0\sigma(\mathcal{E}) = \lambda(\mathcal{E})$.

These two arguments combine to the statement of the theorem. □

Example 4.11. We illustrate right mutations with our running example $t = 3$. Below each worm diagram, we show its start permutation.



4C. ***Braid group action from spherical twists.*** Now we turn to the left action of $\mathsf{Sym}(t)$ on $m\mathcal{E}xc(t)$. We use spherical twist functors (see Appendix A for details) along the simple modules of rank 0, for which we introduce shorthand notation:

$$\mathsf{T}_i := \mathsf{T}_{S(i)} : \mathcal{D}^b(\mathcal{A}_t) \xrightarrow{\sim} \mathcal{D}^b(\mathcal{A}_t) \quad \text{for } i = 1, \ldots, t-1.$$

Since the T_i are autoequivalences, out of any exceptional sequence $\mathcal{E} = (E^1, \dots, E^t)$ in $\mathcal{D}^b(\mathcal{A}_t)$, we get another one: $\mathsf{T}_i\mathcal{E} := (\mathsf{T}_i(E^1), \dots, \mathsf{T}_i(E^t))$. In particular, each twist yields a bijection $\mathsf{T}_i : \mathcal{E}xc(t) \xrightarrow{\sim} \mathcal{E}xc(t)$. Spherical twists satisfy the braid relations, $\mathsf{T}_i\mathsf{T}_{i+1}\mathsf{T}_i\mathcal{E} \cong \mathsf{T}_{i+1}\mathsf{T}_i\mathsf{T}_{i+1}\mathcal{E}$, leading to an action $\mathsf{Br}(t) \times \mathcal{E}xc(t) \to \mathcal{E}xc(t)$.

In the following counterpart to Theorem 4.10, again a permutation is decomposed into transpositions $\tau_i = (i, i+1)$, but now for $\omega_0\sigma(\mathcal{E})^{-1}$ rather than $\lambda(\mathcal{E}) = \omega_0\sigma(\mathcal{E})$.

Theorem 4.12. *Let $\mathcal{E}$ be a full exceptional sequence of $\mathcal{A}_t$-modules with $f(\mathcal{E}) \geq 1$, and write the permutation $\omega_0\sigma(\mathcal{E})^{-1} = \tau_{i(f)} \cdots \tau_{i(2)}\tau_{i(1)}$ as a minimal product of simple transpositions. Setting recursively $\mathcal{E}_0 := \mathcal{E}$ and $\mathcal{E}_j := \mathsf{T}_{i(j)}\mathcal{E}_{j-1}$, each $\mathcal{E}_j$ is a full exceptional sequence of $\mathcal{A}_t$-modules, and $\mathcal{E}_f = \Delta$.*

Note that while right mutations of worm diagrams change the shape of precisely one worm, a spherical twist may modify any number. Because of this, the combinatorial details become slightly more involved.

Fix an exceptional module E, and recall that E is thin, i.e., has dimension vector $(0, \dots, 0, 1, \dots, 1)$, possibly without any zeroes at the front. We think of E as a worm crawling from the bottom left towards the top right, ending in the vertex t.

Recall that E *starts at* i if $\sigma(E) = i$, i.e., $E_i \neq 0$ and $E_{i-1} = 0$. Also note that $\dim E$ is the length of the worm; hence, $E_i \neq 0 \iff \dim E \geq t+1-i \iff \sigma(E) \geq i$. Let us introduce some graphical terminology:

- E has a *horizontal start at* i if $E_{i-1} = 0$ and $E_i \xrightarrow{\alpha} E_{i+1}$.
- E has a *vertical start at* i if $E_{i-1} = 0$ and $E_i \xleftarrow{\beta} E_{i+1}$.
- E has a *left hook at* i if $E_{i-1} \xleftarrow{\beta} E_i \xrightarrow{\alpha} E_{i+1}$.
- E has a *right hook at* i if $E_{i-1} \xrightarrow{\alpha} E_i \xleftarrow{\beta} E_{i+1}$.

Lemma 4.13. *Let E be an exceptional module, and let $S(i)$ be a simple module of rank* 0, *i.e.*, $i \in \{1, \dots, t-1\}$. *Then* $\dim \operatorname{Ext}^p(S(i), E) \leq 1$ *for all* p, *and*

$$\operatorname{Hom}(S(i), E) \neq 0 \iff E \text{ has a vertical start or a right hook at } i,$$
$$\operatorname{Ext}^2(S(i), E) \neq 0 \iff E \text{ has a horizontal start or a left hook at } i.$$

If $\operatorname{Ext}^2(S(i), E) = 0$, *then*

$$\operatorname{Ext}^1(S(i), E) \neq 0 \iff \text{either } E \text{ starts at } i+1 \text{ or } E \text{ has a right hook at } i.$$

Proof. Considering $S(i)$ and E as representations computes $\operatorname{Hom}(S(i), E)$ readily, and likewise by Serre duality $\operatorname{Ext}^2(S(i), E) = \operatorname{Hom}(E, S(i))^*$, using that $S(i)$ is

2-spherical according to Proposition 1.10:

$$\mathrm{Hom}(S(i), E) = \begin{cases} \boldsymbol{k} & \text{if } E_i \xleftarrow{\beta} E_{i+1}, \text{ and } E_{i-1} = 0 \text{ or } E_{i-1} \xrightarrow{\alpha} E_i, \\ 0 & \text{else,} \end{cases}$$

$$\mathrm{Ext}^2(S(i), E) = \begin{cases} \boldsymbol{k} & \text{if } E_i \xrightarrow{\alpha} E_{i+1}, \text{ and } E_{i-1} = 0 \text{ or } E_{i-1} \xleftarrow{\beta} E_i, \\ 0 & \text{else.} \end{cases}$$

The formulas translate to the first two statements made in the proposition.

Put $s := t + 1 - \dim E$, so that $E_s \neq 0$ and $E_{s-1} = 0$. We claim that, under the assumption $\mathrm{Ext}^2(S(i), E) = 0$,

$$\mathrm{ext}^1(S(i), E) = \begin{cases} 0 & \text{if } i \leq s-2, \\ 1 & \text{if } i = s-1, \\ 0 & \text{if } i = s, \\ \mathrm{hom}(S(i), E) & \text{if } i \geq s+1. \end{cases}$$

To see this, start with the Euler pairing $\mathrm{ext}^1(S(i), E) = \mathrm{hom}(S(i), E) - \chi(S(i), E)$, making use of the assumption. In the next step, we invoke Lemma 1.5 to write $\chi(S(i), E) = 2e_i - e_{i-1} - e_{i+1}$, where $\underline{\dim}(E) = (e_1, \dots, e_t)$. In the first two cases of the statement, $\mathrm{hom}(S(i), E) = 0$ from the formula above.

If $i = s$, i.e., the worm starts at vertex i, then we have $\mathrm{hom}(S(i), E) = 1$ because the assumption $\mathrm{ext}^2(S(i), E) = 0$ means that the first nonzero map of E is β. Then $\mathrm{ext}^1(S(i), E) = 1 - (2 - 0 - 1) = 0$. □

Corollary 4.14. *Let* $\mathcal{E} = (E^1, \dots, E^t) \in m\mathcal{E}xc(t)$ *and* $i \in \{1, \dots, t-1\}$. *Then the following conditions are equivalent*:

(1) $\mathsf{T}_i\mathcal{E} \in m\mathcal{E}xc(t)$.

(2) $\mathrm{Ext}^2(S(i), E^j) = 0$ *for all* $j = 1, \dots, t$.

(3) *The worm starting at i does so vertically.*

Proof. Implication (1) $\Longrightarrow$ (2) is Lemma A.1 and (2) $\Longrightarrow$ (1) is Corollary A.2. Since a worm starting vertically at i prevents other worms from having left hooks at i, Lemma 4.13 gives (2) $\Longleftrightarrow$ (3). □

Recall that $f(\mathcal{E})$ was defined as the number of vertical edges among all worms. We now show that a suitable spherical twist of an exceptional sequence of modules reduces the f-invariant by one. Moreover, the twist T_i categorifies the left multiplication by the transposition $\tau_i = (i, i+1) \in \mathsf{Sym}(t)$.

Proposition 4.15. *If* $\mathcal{E} = (E^1, \dots, E^t)$ *is a full exceptional sequence of* $\mathcal{A}_t$*-modules with* $f(\mathcal{E}) \geq 1$ *and the worm starting at i does so vertically*, *then*

(1) $\mathsf{T}_i\mathcal{E}$ *is a full exceptional sequence of* $\mathcal{A}_t$*-modules*,

(2) $f(\mathsf{T}_i\mathcal{E}) = f(\mathcal{E}) - 1$,

(3) $\sigma(\mathsf{T}_i\mathcal{E}) = \tau_i \cdot \sigma(\mathcal{E})$.

Proof. Statement (1) is part of Corollary 4.14.

We turn to the computation of $f(\mathsf{T}_i\mathcal{E})$. Let $E = E^j$ for some j. According to Lemma 4.13, there are the following four possibilities for $\mathrm{Hom}(S(i), E)$ and $\mathrm{Ext}^1(S(i), E)$, for which Lemma A.1 gives the exact sequence containing $\mathsf{T}_i E$:

case	$\mathrm{Hom}(S(i), E)$	$\mathrm{Ext}^1(S(i), E)$	exact sequence for $\mathsf{T}_i E$
(O)	0	0	$0 \to E \to \mathsf{T}_i E \to 0$
(H)	$\boldsymbol{k}$	0	$0 \to S(i) \to E \to \mathsf{T}_i E \to 0$
(E)	0	$\boldsymbol{k}$	$0 \to E \to \mathsf{T}_i E \to S(i) \to 0$
(HE)	$\boldsymbol{k}$	$\boldsymbol{k}$	$0 \to S(i) \to E \to \mathsf{T}_i E \to S(i) \to 0$

We examine the cases separately. In (O), the exceptional module is unchanged.

In (H), the condition $\mathrm{Hom}(S(i), E) \neq 0$ implies that E either starts vertically in i or has a right hook at i, by Lemma 4.13. However, $\mathrm{Ext}^1(S(i), E) = 0$ prevents the right hook. Hence, E starts vertically in i, and the spherical twist strips off the simple $S(i)$ from E. Thus, the number of vertical edges decreases by one.

In (E), the worm E starts at $i + 1$, and the spherical twist prolongs E by the simple $S(i)$ with a horizontal edge: $(\mathsf{T}_i E)_i = \boldsymbol{k} \xrightarrow{\alpha} \boldsymbol{k} = E_{i+1} = (\mathsf{T}_i E)_{i+1}$; this is forced by the morphism $\mathsf{T}_i E \to S(i)$. The number of vertical edges is unchanged.

In (HE), E has a right hook at i which is replaced under T_i by a left hook at i. Again, the number of vertical arrows is unchanged.

By assumption, the worm starting at i does so vertically. The shape of worm diagrams means that no worm has a left hook at i. Therefore, by Lemma 4.13 case (H) occurs exactly once, and $f(\mathsf{T}_i\mathcal{E}) = f(\mathcal{E}) - 1$.

Since case (E) occurs precisely if E starts at vertex $i + 1$, this case appears exactly once, too. We now relate $\sigma := \sigma(\mathcal{E})$ and $\sigma' := \sigma(\mathsf{T}_i\mathcal{E})$. Recall $\sigma(j) = \sigma(E^j) = t + 1 - \dim E^j$ is the starting vertex of the worm E^j. By the above, there are exactly two positions j, l where σ and σ' differ because cases (O) and (HE) do not change worm lengths, and cases (H) and (E) occur once each. Then $\sigma'(j) = i + 1 = \sigma(j) + 1$ for the unique E^j starting in i; this is case (H). In turn for case (E), the module E^l with starting vertex $i + 1$ becomes prolonged by $S(i)$, i.e., $\sigma'(l) = i = \sigma(l) - 1$. Hence, $\tau_i \cdot \sigma = (i, i + 1) \cdot \sigma(\mathcal{E}) = \sigma' = \sigma(\mathsf{T}_i\mathcal{E})$. So we have also proved (3). □

Proof of Theorem 4.12. As before, we identify exceptional sequences with worm diagrams and permutations. We start by showing, for any $i \in \{1, \dots, t - 1\}$,

$$f(\tau_i \cdot \sigma(\mathcal{E})) = f(\mathcal{E}) - 1 \quad \iff \quad \text{the worm starting at } i \text{ does so vertically.}$$

Write $\mathcal{E} = (E^1, \dots, E^t)$ and $\sigma := \sigma(\mathcal{E})$, and let E^k, E^l be the worms such that $\sigma(E^k) = i$ and $\sigma(E^l) = i + 1$. By definition, $(F^1, \dots, F^t) := \tau_i \cdot \sigma(\mathcal{E})$ is the worm diagram obtained from $\mathcal{E}$ by $\sigma(F^k) = i+1$ and $\sigma(F^l) = i$; all other worm lengths are unchanged. Recall the formula for $f(\sigma)$ from Lemma 4.3(3):

$$f(\sigma) = \#\{(j,k) \mid 1 \le j < k \le t \text{ and } \sigma(j) < \sigma(k)\},$$
$$f(\tau_i \cdot \sigma) = \#\{(j,k) \mid 1 \le j < k \le t \text{ and } \tau_i\sigma(j) < \tau_i\sigma(k)\}.$$

For j, k with $\sigma(j) \notin \{i, i+1\}$ or $\sigma(k) \notin \{i, i+1\}$, the conditions in both sets are identical: $\sigma(j) < \sigma(k) \iff \tau_i\sigma(j) < \tau_i\sigma(k)$. Thus, $|f(\sigma) - f(\tau_i\sigma)| = 1$. And $f(\sigma) = f(\tau_i\sigma) + 1$ if and only if $k < l$, i.e., the worm starting at i sits on the left of the worm starting at $i+1$. With $\sigma(E^k) = i < i+1 = \sigma(E^l)$ and $k < l$, we find that $(E^k)_{\sigma(E^l)-1} = (E^k)_i \xleftarrow{\beta} (E^k)_{i+1}$ by Lemma 4.3(2), i.e., E^k starts vertically.

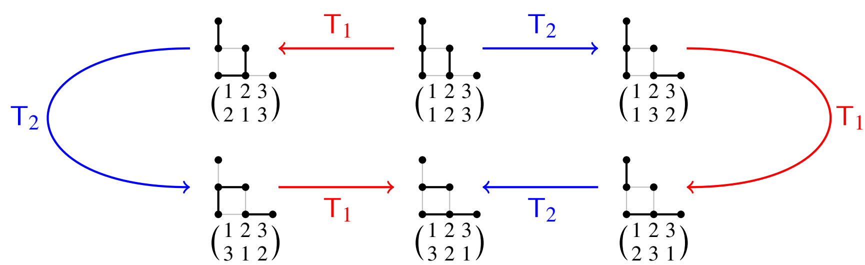
By Proposition 4.15, any vertically starting worm E^i gives rise to the twisted exceptional sequence $\mathsf{T}_i\mathcal{E}$ of modules with one fewer vertical edge. In this way we can proceed to obtain a sequence of $f = f(\mathcal{E})$ spherical twists $\mathsf{T}_{i(f)} \cdots \mathsf{T}_{i(1)}\mathcal{E} = \Delta$ ending in the standard sequence $\Delta = (\Delta(t), \ldots, \Delta(1))$. Then

$$\omega_0 = \sigma(\Delta) = \sigma(\mathsf{T}_{i(f)} \cdots \mathsf{T}_{i(1)}\mathcal{E}) = \tau_{i(f)} \cdots \tau_{i(1)} \cdot \sigma(\mathcal{E}),$$

using $\sigma(\mathsf{T}_i\mathcal{E}) = \tau_i \cdot \sigma(\mathcal{E})$ from Proposition 4.15. Hence, $\tau_{i(f)} \cdots \tau_{i(1)} = \omega_0\sigma(\mathcal{E})^{-1}$.

The theorem follows from this computation and the above equivalence. □

Example 4.16. We illustrate the proposition with our running example $t = 3$. Note how this hexagon is different from the one of Example 4.11. Below each worm diagram, we show its start permutation. This example categorifies Example 4.6, replacing left multiplications with τ_i by spherical twists T_i.



Appendix A: Spherical twist functors

Let Λ be a finite-dimensional algebra of finite global dimension, and $\mathcal{D} = \mathcal{D}^b(\Lambda)$ the bounded derived category of left Λ-modules with Serre (Nakayama) functor S.

An object S of $\mathcal{D}$ is *e-spherical* if $\mathsf{S}(S) \cong S[e]$ and $\mathrm{Hom}^\bullet(S, S) = \boldsymbol{k} \oplus \boldsymbol{k}[-e]$. Consider the complex of bimodules $S^* \otimes_{\boldsymbol{k}} S$; it corresponds to the endofunctor $\mathrm{Hom}^\bullet(S, \cdot) \otimes S$ of $\mathcal{D}$. There is the canonical evaluation morphism $\eta : S^* \otimes_{\boldsymbol{k}} S \to \Lambda$, where Λ is a bimodule in the natural way, corresponding to the identity functor.

Denoting the functor associated to cone(η) by T_S, we obtain a triangle of functors

$$\mathrm{Hom}^\bullet(S,\cdot\,)\otimes S \to \mathrm{id} \to \mathsf{T}_S \to$$

and T_S is called the *spherical twist functor* along S.

By construction, we have $\mathsf{T}_S(S) \cong S[1-e]$, and $\mathsf{T}_S(M) \cong M$ for all $M \in S^\perp = \{M \in \mathcal{D} \mid \mathrm{Hom}^\bullet(S, M) = 0\}$. These two properties remind us of reflections and can in fact be used to prove that $\mathsf{T}_S : \mathcal{D} \xrightarrow{\sim} \mathcal{D}$ is an autoequivalence [Huybrechts 2006, §8]. At one place, we will need the inverse functor, which is given by

$$\mathsf{T}_S^{-1} \to \mathrm{id} \to \mathrm{Hom}^\bullet(\,\cdot\,, S)^* \otimes S \to .$$

A1. ***Special case: modules.*** We describe a situation when the spherical twist of a module is again a module.

Lemma A.1. *Let S be a simple module, and M any module. Then $H^1(\mathsf{T}_S(M)) = \mathrm{Ext}^2(S, M) \otimes S$. Moreover, if $\mathrm{Ext}^{\geq 2}(S, M) = 0$, then $\mathsf{T}_S(M)$ is a module, and occurs in the exact sequence*

$$0 \to \mathrm{Hom}(S, M) \otimes S \to M \to \mathsf{T}_S(M) \to \mathrm{Ext}^1(S, M) \otimes S \to 0.$$

Proof. The triangle $\mathrm{Hom}^\bullet(S, M) \otimes S \to M \to \mathsf{T}_S(M) \to$ defines $\mathsf{T}_S(M) \in \mathcal{D}^b(\Lambda)$. Its long exact cohomology sequence gives $H^1(\mathsf{T}_S(M)) = \mathrm{Ext}^2(S, M) \otimes S$ right away.

If $\mathrm{Ext}^{\geq 2}(S, M) = 0$, then $\mathrm{Hom}^\bullet(S, M) = \mathrm{Hom}(S, M) \oplus \mathrm{Ext}^1(S, M)[-1]$, and the long exact cohomology sequence of the triangle is

$$0 \to H^{-1}(\mathsf{T}_S(M)) \to \mathrm{Hom}(S, M) \otimes S \xrightarrow{\varphi} M \to H^0(\mathsf{T}_S(M)) \to \mathrm{Ext}^1(S, M) \otimes S \to 0.$$

Put $h := \hom(S, M)$. The map $\varphi : S^{\oplus h} \to M$ is injective because it is the canonical evaluation and S is simple. Thus, $H^{-1}(\mathsf{T}_S(M)) = 0$ and $\mathsf{T}_S(M)$ is concentrated in degree 0, i.e., a module. □

Corollary A.2. *Let E be an exceptional $\mathcal{A}_t$-module, and let $i \in \{1, \dots, t-1\}$. If $\mathrm{Ext}^2(S(i), E) = 0$, then $\mathsf{T}_{S(i)}(E)$ is an exceptional $\mathcal{A}_t$-module.*

Proof. The algebra $\mathcal{A}_t$ has global dimension 2. Thus, the only Ext vanishing of the lemma to be checked is in degree 2. Hence, $\mathsf{T}_{S(i)}(E)$ is a module by the lemma.

Finally note that images of exceptional objects under any fully faithful functor (e.g., an autoequivalence such as the spherical twist) are again exceptional. □

A2. ***Braid relations.*** We briefly return to the general setting: if $S, S' \in \mathcal{D}$ are e-spherical objects such that $\mathrm{Hom}^\bullet(S, S') = \boldsymbol{k}[-n]$ for some n, then the twist functors T_S and $\mathsf{T}_{S'}$ satisfy the braid relations: $\mathsf{T}_S\mathsf{T}_{S'}\mathsf{T}_S \cong \mathsf{T}_{S'}\mathsf{T}_S\mathsf{T}_{S'}$. Clearly, this can be iterated to chains of e-spherical objects $S_1, \dots, S_n$ such that $\dim \mathrm{Hom}^\bullet(S_i, S_j) = 1$

if $|i-j|=1$ and zero else. Such a chain induces an action of the n-stranded braid group $\mathsf{Br}(n)$ on $\mathcal{D}$, i.e., a group homomorphism $\mathsf{Br}(n) \to \operatorname{Aut}\mathcal{D}$.

We apply this fact to the situation of this text: the $t-1$ simple modules $S(1), \dots, S(t-1)$ are 2-spherical objects of $\mathcal{D}^b(\mathcal{A}_t)$ and the only nonvanishing extensions among different simple modules are $\operatorname{Ext}^1(S(i), S(i+1)) = \boldsymbol{k}$.

Corollary A.3. *There is a braid group action* $\mathsf{Br}(t) \to \operatorname{Aut}(\mathcal{D}^b(\mathcal{A}_t))$, *mapping the braid intertwining strands i and $i+1$ to* $\mathsf{T}_{S(i)}$.

Appendix B: Dictionary algebra–geometry

The algebra $\mathcal{A}_t$ occurs in a geometric guise in our previous article [Hille and Ploog 2019]. Let X be a smooth, projective surface such that all line bundles are exceptional (this holds if X is a rational, e.g., toric, surface), and let $C_1, \dots, C_{t-1}$ be an A_{t-1}-chain of (-2)-curves in X, i.e., $C_i \cong \mathbb{P}^1$ and $C_i^2 = -2$ for all i. Then

$$\mathcal{E} = (\mathcal{O}_X(-C_1 - \cdots - C_{t-1}), \dots, \mathcal{O}_X(-C_2 - C_1), \mathcal{O}_X(-C_1), \mathcal{O}_X)$$

is an exceptional sequence in $\mathcal{D}^b(\operatorname{Coh}(X))$, and we also denote by $\mathcal{E}$ the triangulated subcategory it generates. Define an additive category $\operatorname{Coh}_{\mathcal{E}}(X) := \mathcal{E} \cap \operatorname{Coh}(X)$. Denote by T the iterated universal extension of the exceptional sequence. Then:

(1) $T \in \mathcal{E}$ is a tilting bundle such that $\operatorname{End}(T) = \mathcal{A}_t$.

(2) The derived tilting equivalence $\operatorname{RHom}(T, \cdot) : \mathcal{E} \xrightarrow{\sim} \mathcal{D}^b(\mathcal{A}_t)$ restricts to an equivalence of abelian categories $\operatorname{Hom}(T, \cdot) : \operatorname{Coh}_{\mathcal{E}}(X) \xrightarrow{\sim} \mathcal{A}_t\text{-mod}$.

Statement (2) holds more generally for self-intersection numbers ≤ -2. The tilting functor $\operatorname{Hom}(T, \cdot)$ produces right modules whereas in this article we always consider left modules. However, this is not a concern because of $\mathcal{A}_t \cong \mathcal{A}_t^{\mathrm{op}}$; see Remark 1.1. We list some geometric counterparts to algebraic notions:

sheaf $F \in \operatorname{Coh}(X) \cap \mathcal{E}$	representation $M \in \mathcal{A}_t$-mod
rank of the sheaf F	$\operatorname{rk} M = \dim M_t = \hom(P(t), M)$
locally free sheaf (vector bundle) F	M with all $M_{i-1} \xrightarrow{\alpha} M_i$ injective
torsion subsheaf of F	maximal $M' \subseteq M$ with $\alpha^i M' = 0$ for all i
exceptional sequence of line bundles $(\mathcal{O}_X(-C_1 - \cdots - C_{t-1}), \dots, \mathcal{O}_X(-C_1), \mathcal{O}_X)$	exceptional sequence of Δ-modules $(\Delta(t), \Delta(t-1), \dots, \Delta(1))$
simple sheaves in $\mathcal{E}$	simple modules
$\mathcal{O}_{C_{t-1}}(-1), \dots, \mathcal{O}_{C_2}(-1), \mathcal{O}_{C_1}$ (rank 0)	$S(1), \dots, S(t-2), S(t-1)$
$\mathcal{O}_X(-C_1 - \cdots - C_{t-1})$ (rank 1)	$S(t)$
projective objects $\mathcal{O}_X, \binom{\mathcal{O}_X(-C_1)}{\mathcal{O}_X}, \dots$	projective modules $P(1), P(2), \dots$

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THE TOPOLOGICAL BIQUANDLE OF A LINK

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To every oriented link L, we associate a topologically defined biquandle $\widehat{\mathcal{B}}_L$, which we call the topological biquandle of L. The construction of $\widehat{\mathcal{B}}_L$ is similar to the topological description of the fundamental quandle given by Matveev. We find a presentation of the topological biquandle and explain how it is related to the fundamental biquandle of the link.

1. Introduction

A biquandle is an algebraic structure with two operations that generalizes a quandle. The axioms of both structures represent an algebraic encoding of the Reidemeister moves, and study of quandles and related structures has been closely intertwined with knot theory.

It is well known that every knot has a fundamental quandle, that admits an algebraic as well as a topological interpretation. Its topological description is due to Matveev [1982], who called it *the geometric groupoid* of a knot and proved that the fundamental quandle is a complete knot invariant up to inversion (taking the mirror image and reversing orientation).

The fundamental biquandle of a knot or link, however, is purely algebraically defined. It is not clear whether it also admits a topological interpretation [Kauffman et al. 2012]. Various other issues concerning biquandles have not yet been resolved, see [Fenn et al. 2005].

To any classical oriented link, we associate a topologically defined biquandle $\widehat{\mathcal{B}}_L$, which we call the topological biquandle of the link. Our construction is similar to Matveev's construction of the geometric groupoid of a knot. The topological construction enables us to visualize the biquandle operations directly and improves our understanding of the biquandle structure. Another advantage of this construction is that it defines a functor from the (topological) category of oriented links in S^3 to the category of biquandles.

We show that the topological biquandle $\widehat{\mathcal{B}}_L$ is a quotient of the fundamental biquandle, but its structure is simpler than that of a general biquandle.

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This paper is organized as follows. In Section 2, we give the definition of a biquandle, recall some of its basic properties, define biquandle presentations and the fundamental biquandle of a link. Section 3 is the core of the paper, in which we define the topological biquandle of a link, prove that it is a biquandle and study some of its properties. In Section 4, we investigate the topological biquandle from the perspective of a link diagram. We find a presentation of the topological biquandle and show that it is a quotient of the fundamental biquandle.

2. Preliminaries

For an introduction to biquandles, we refer the reader to [Fenn et al. 2004; Hrencecin and Kauffman 2007; Kauffman and Manturov 2005].

Definition 2.1 (Biquandle axioms). A *biquandle* is a set B with two binary operations, the up operation $\urcorner$ and the down operation $\lrcorner$, such that B is closed under these operations and the following axioms are satisfied:

(1) For every $a \in B$, the maps $f_a, g_a : B \to B$ and $S : B \times B \to B \times B$, defined by $f_a(x) = x\,\overline{a}\rceil$, $g_a(x) = x\,\underline{a}\rfloor$ and $S(x, y) = (y\,\underline{x}\rfloor, x\,\overline{y}\rceil)$, are bijections.

(2) For every $a \in B$, we have $f_a^{-1}(a) = a\,\underline{f_a^{-1}(a)}\rfloor$ and $g_a^{-1}(a) = a\,\overline{g_a^{-1}(a)}\rceil$.

(3) For every $a, b, c \in B$, the equalities

$$\begin{aligned} &\text{up interchanges} && a\,\overline{b}\rceil\,\overline{c}\rceil = a\,\overline{c\,\underline{b}\rfloor}\rceil\,\overline{b\,\overline{c}\rceil}\rceil, \\ &\text{rule of five} && a\,\underline{b}\rfloor\,\overline{c\,\underline{b\,\overline{a}\rceil}\rfloor}\rceil = a\,\overline{c}\rceil\,\underline{b\,\overline{c\,\underline{a}\rfloor}\rceil}\rfloor, \\ &\text{down interchanges} && a\,\underline{b}\rfloor\,\underline{c}\rfloor = a\,\underline{c\,\overline{b}\rceil}\rfloor\,\underline{b\,\underline{c}\rfloor}\rfloor \end{aligned}$$

are valid.

A biquandle $(B, \urcorner, \lrcorner)$ in which $a\,\underline{b}\rfloor = a$ for all $a \in B$ is called a *quandle*.

It follows from the first biquandle axiom that the map $S : B \times B \to B \times B$ has an inverse. Define two new operations $\ulcorner$ and $\llcorner$ on B by

$$S^{-1}(a, b) = (b\lceil\overline{a}\,, a\lfloor\underline{b}\,)\ .$$

Remark 2.2. This "corner" notation was introduced by Kauffman [Fenn et al. 2004]. Another alternative is the "exponential notation" that was used by Fenn and Rourke [1992], and avoids brackets. One may translate between the two notations using equalities: $a^b = a\,\overline{b}\rceil$, $a^{\bar{b}} = a\lceil\overline{b}\,$, $a_b = a\,\underline{b}\rfloor$ and $a_{\bar{b}} = a\lfloor\underline{b}\,$.

Lemma 2.3. *For every $a, b \in B$, the equalities*

$$a\,\overline{b}\rceil\lceil\overline{b\,\underline{a}\rfloor} = a\lceil\overline{b}\;\overline{b\lfloor\underline{a}}\rceil = a\,\underline{b}\rfloor\lfloor\underline{b\,\overline{a}\rceil} = a\lfloor\underline{b}\;\underline{b\lceil\overline{a}}\rfloor = a$$

are valid.

Proof. We compute

$$(a,b) = S^{-1}(S(a,b)) = S^{-1}(b\underline{a}, a\overline{b}) = (a\overline{b}\,\overline{b\underline{a}}, b\underline{a}\,\underline{a\overline{b}}),$$
$$(a,b) = S(S^{-1}(a,b)) = S(b\overline{a}, a\underline{b}) = (a\underline{b}\,\underline{b\overline{a}}, b\overline{a}\,\overline{a\underline{b}})$$

and the desired equalities follow. □

Lemma 2.4. *Let X and Y be two biquandles. If $f : X \to Y$ is a biquandle homomorphism, then $f(a\overline{b}) = f(a)\overline{f(b)}$ and $f(a\underline{b}) = f(a)\underline{f(b)}$ for every $a, b \in X$.*

Proof. Let $f : X \to Y$ be a biquandle homomorphism. Choose elements $a, b \in X$ and denote $f(b\overline{a}) = x$ and $f(a\underline{b}) = y$. By Lemma 2.3 we have $a\underline{b}\,\underline{b\overline{a}} = a$, and since f is a biquandle homomorphism, it follows that $f(a\underline{b})\,\underline{f(b\overline{a})} = y\underline{x} = f(a)$. Also by Lemma 2.3, we have $b\overline{a}\,\overline{a\underline{b}} = b$, and since f is a biquandle homomorphism, it follows that $f(b\overline{a})\,\overline{f(a\underline{b})} = x\overline{y} = f(b)$. Putting those two equalities together, Lemma 2.3 gives

$$y = y\underline{x}\,\underline{x\overline{y}} = f(a)\underline{f(b)} \quad \text{and} \quad x = x\overline{y}\,\overline{y\underline{x}} = f(b)\overline{f(a)}.$$ □

The fundamental biquandle of a link is usually defined via a presentation, coming from a link diagram. Following [Ishikawa 2018], we define biquandle presentations categorically.

Definition 2.5. Let A be a set. A *free biquandle* on A is the biquandle $F_{\mathrm{BQ}}(A)$ together with an injective map $i : A \to F_{\mathrm{BQ}}(A)$, characterized by the following. For any map $f : A \to B$, where B is a biquandle, there exists a unique biquandle homomorphism $\bar{f} : F_{\mathrm{BQ}}(A) \to B$ such that $f = \bar{f} \circ i$.

For a biquandle X, let $j : A \to X$ be a map and let $\bar{j} : F_{\mathrm{BQ}}(A) \to X$ be the induced biquandle homomorphism. Let $R \subset F_{\mathrm{BQ}}(A) \times F_{\mathrm{BQ}}(A)$ be a relation on the set $F_{\mathrm{BQ}}(A)$. We say that $\langle A | R \rangle$ is a *presentation* of the biquandle X if

(1) $(\bar{j} \times \bar{j})(R) \subset \Delta_X$ (here $\Delta_X \subset X \times X$ is the diagonal),

(2) for any biquandle Y and for any map $f : A \to Y$ such that $(\bar{f} \times \bar{f})(R) \subset \Delta_Y$, there exists a unique biquandle homomorphism $\tilde{f} : X \to Y$ such that $f = \tilde{f} \circ j$.

Any classical oriented link may be given by its diagram, i.e., the image of a regular projection of the link to a plane in $\mathbb{R}^3$. A link diagram D is a directed 4-valent graph, whose vertices contain the information about the over- and under-crossings. The edges of the graph are called *semiarcs*, while the vertices are called crossings of the diagram. Denote by $A(D)$ the set of semiarcs and by $C(D)$ the set of crossings of the diagram D. In any crossing, the four semiarcs are connected by two *crossing relations*, depicted in Figure 1.

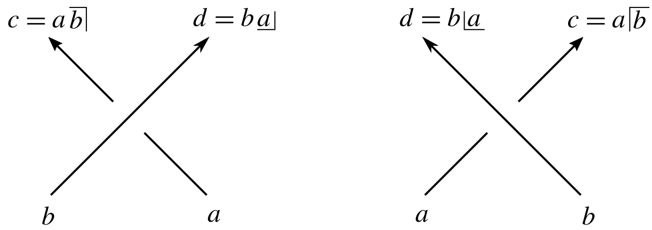

Figure 1. Crossing relations between the semiarcs of D.

Definition 2.6. The *fundamental biquandle* $\mathrm{BQ}(L)$ of a link L with a diagram D is the biquandle, given by the presentation

$$\langle A(D) \,|\, \text{crossing relations for every } c \in C(D) \rangle \,.$$

3. The topological biquandle of a link

By a link we will mean an oriented subspace of S^3, homeomorphic to a disjoint union of circles $\bigsqcup_{i=1}^{k} S^1$. For a link L, denote by N_L a regular neighborhood of L in S^3 and let $E_L = \text{closure}(S^3 - N_L)$. The orientation of L induces an orientation of its normal bundle using the right-hand rule.

Choose a 3-ball $B^3 \subset S^3$ such that $N_L \subset B^3$, then let z_0 and z_1 be two antipodal points of $S^2 = \partial B^3$. Define

$$\mathcal{B}_L = \big\{(a_0, a_1) \mid a_i : [0,1] \to E_L \text{ a path from a point on } \partial N_L \text{ to } z_i \\ \text{for } i = 0, 1 \text{ and } a_0(0) = a_1(0)\big\}.$$

If $a : [0,1] \to E_L$ is a path, we denote by $\bar{a} : [0,1] \to E_L$ the reverse path, given by $\bar{a}(t) = a(1-t)$. Given paths $a, b : [0,1] \to E_L$ with $a(1) = b(0)$, their combined path $a \cdot b$ is given by

$$(a \cdot b)(t) = \begin{cases} a(2t), & 0 \le t \le \frac{1}{2}, \\ b(2t-1), & \frac{1}{2} < t \le 1. \end{cases}$$

We say that two elements $(a_0, a_1), (b_0, b_1) \in \mathcal{B}_L$ are *equivalent* if there exists a homotopy $H_t : [0,1] \to E_L$ such that $H_0 = \overline{a_0} \cdot a_1$, $H_1 = \overline{b_0} \cdot b_1$, $H_t(0) = z_0$, $H_t(1) = z_1$ and $H_t\big(\frac{1}{2}\big) \in \partial N_L$ for all $t \in [0,1]$. It is easy to see this defines an equivalence relation on the set $\mathcal{B}_L$. The quotient set $\widehat{\mathcal{B}}_L = \mathcal{B}_L/\!\sim$ will be the underlying set of the topological biquandle of L.

Remark 3.1. Observe that every element of $\mathcal{B}_L$ is given by a pair of paths (a_0, a_1) in E_L. The homotopy class of the path a_i is an element of the fundamental quandle $Q(L)$ with the basepoint z_i for $i = 0, 1$. We thus obtained the set $\widehat{\mathcal{B}}_L$ by taking pairs of representatives of the fundamental quandle $Q(L)$, and then imposing on those pairs a new equivalence relation.

The set $\widehat{\mathcal{B}}_L$ is closely related to the group of the link L. For any point $p \in \partial N_L$, denote by m_p the loop in ∂N_L, based at p, which goes once around the meridian of L in the positive direction according to the orientation of the normal bundle. Define two maps $p_i : \mathcal{B}_L \to \pi_1(E_L, z_i)$ by $p_i(a_0, a_1) = [\overline{a_i} \cdot m_{a_i(0)} \cdot a_i]$ for $i = 0, 1$.

Lemma 3.2. *If* $(a_0, a_1) \sim (b_0, b_1)$, *then* $p_i(a_0, a_1) = p_i(b_0, b_1)$ *for* $i = 0, 1$.

Proof. Let $(a_0, a_1) \sim (b_0, b_1)$ be two equivalent elements of $\mathcal{B}_L$. Then there exists a homotopy $H_t : [0, 1] \to E_L$ such that $H_0 = \overline{a_0} \cdot a_1$, $H_1 = \overline{b_0} \cdot b_1$, $H_t(0) = z_0$, $H_t(1) = z_1$ and $H_t\left(\frac{1}{2}\right) \in \partial N_L$ for all $t \in [0, 1]$. It follows that $a_0(0)$ and $b_0(0)$ lie in the same boundary component of ∂N_L. Since $m_{a_0(0)}$ and $m_{b_0(0)}$ are two meridians of the same component of L, we may choose a homotopy $G_t : [0, 1] \to \partial N_L$ such that $G_0 = m_{a_0(0)}$, $G_1 = m_{b_0(0)}$ and $G_t(0) = G_t(1) = H_t\left(\frac{1}{2}\right)$ for $t \in [0, 1]$. Similarly, we may choose a homotopy $J_t : [0, 1] \to \partial N_L$ such that $J_0 = m_{a_1(0)}$, $J_1 = m_{b_1(0)}$ and $J_t(0) = J_t(1) = H_t\left(\frac{1}{2}\right)$ for $t \in [0, 1]$. Define a map $S_t : [0, 1] \to E_L$ by

$$S_t(u) = \begin{cases} H_t(3u/2), & 0 \le u \le \frac{1}{3}, \\ G_t(3u-1), & \frac{1}{3} \le u \le \frac{2}{3}, \\ H_t(3(1-u)/2), & \frac{2}{3} \le u \le 1. \end{cases}$$

Now S_t is a homotopy between the loops $\overline{a_0} \cdot m_{a_0(0)} \cdot a_0$ and $\overline{b_0} \cdot m_{b_0(0)} \cdot b_0$, which thus represent the same element of the fundamental group $\pi_1(E_L, z_0)$. It follows that $p_0(a_0, a_1) = p_0(b_0, b_1)$. The proof for $i = 1$ is similar. □

Corollary 3.3. *The map* p_i *induces a map* $\hat{p}_i : \widehat{\mathcal{B}}_L \to \pi_1(E_L, z_i)$ *for* $i = 0, 1$.

Denote by $[a_0, a_1] \in \widehat{\mathcal{B}}_L$ the equivalence class of the element $(a_0, a_1) \in \mathcal{B}_L$. We have found a way to associate to each element $[a_0, a_1]$ of the set $\widehat{\mathcal{B}}_L$ two elements of the fundamental groups $\pi_1(E_L, z_0)$ and $\pi_1(E_L, z_1)$, namely $\hat{p}_0[a_0, a_1]$ and $\hat{p}_1[a_0, a_1]$. Using this association, we will now define the operations on $\widehat{\mathcal{B}}_L$.

Define two binary operations (called the up- and down-operation) on $\mathcal{B}_L$ by

$$(a_0, a_1)^{(b_0, b_1)} := (a_0 \cdot p_0(b_0, b_1), a_1) \quad \text{and} \quad (a_0, a_1)_{(b_0, b_1)} := (a_0, a_1 \cdot p_1(b_0, b_1)).$$

We intend to show that these operations induce operations on the quotient space $\widehat{\mathcal{B}}_L$, and that $\widehat{\mathcal{B}}_L$ equipped with those operations forms a biquandle.

Lemma 3.4. *If* $(a_0, a_1) \sim (c_0, c_1)$ *and* $(b_0, b_1) \sim (d_0, d_1)$, *then* $(a_0, a_1)^{(b_0, b_1)} \sim (c_0, c_1)^{(d_0, d_1)}$ *and* $(a_0, a_1)_{(b_0, b_1)} \sim (c_0, c_1)_{(d_0, d_1)}$.

Proof. Let $(a_0, a_1) \sim (c_0, c_1)$ and $(b_0, b_1) \sim (d_0, d_1)$ in $\mathcal{B}_L$. There is a homotopy $H_t : [0, 1] \to E_L$ such that $H_0 = \overline{a_0} \cdot a_1$, $H_1 = \overline{c_0} \cdot c_1$, $H_t(0) = z_0$, $H_t(1) = z_1$ and $H_t\left(\frac{1}{2}\right) \in \partial N_L$ for all $t \in [0, 1]$. Since $(b_0, b_1) \sim (d_0, d_1)$, it follows by Lemma 3.2 that there exists a homotopy $G_t:[0,1]\to E_L$ such that $G_0=p_0(b_0,b_1)$, $G_1=p_0(d_0,d_1)$ and $G_t(0)=G_t(1)=z_0$ for all $t\in[0,1]$. Define a map $S_t:[0,1]\to E_L$ by

$$S_t(u)=\begin{cases}G_t(1-4u), & 0\le u\le\frac{1}{4},\\ H_t\big(2u-\frac{1}{2}\big), & \frac{1}{4}\le u\le\frac{1}{2},\\ H_t(u), & \frac{1}{2}\le u\le 1.\end{cases}$$

Now S_t is a homotopy from $\overline{a_0\cdot p_0(b_0,b_1)}\cdot a_1$ to $\overline{c_0\cdot p_0(d_0,d_1)}\cdot c_1$, for which $S_t(0)=z_0$, $S_t(1)=z_1$ and $S_t\big(\frac{1}{2}\big)\in\partial N_L$ for all $t\in[0,1]$. It follows that $(a_0,a_1)^{(b_0,b_1)}\sim(c_0,c_1)^{(d_0,d_1)}$. The proof is similar for $(a_0,a_1)_{(b_0,b_1)}\sim(c_0,c_1)_{(d_0,d_1)}$. □

Corollary 3.5. *There are induced up- and down-operations on $\widehat{\mathcal{B}}_L$, defined by*

$$[a_0,a_1]^{[b_0,b_1]}:=[a_0\cdot p_0(b_0,b_1),a_1]\quad\textit{and}\quad[a_0,a_1]_{[b_0,b_1]}:=[a_0,a_1\cdot p_1(b_0,b_1)].$$

Lemma 3.6. *The maps $f_a,g_a:\widehat{\mathcal{B}}_L\to\widehat{\mathcal{B}}_L$, defined by $f_a(x)=x^a$ and $g_a(x)=x_a$, are bijective for any $a\in\widehat{\mathcal{B}}_L$.*

Proof. Define maps $f'_a,g'_a:\widehat{\mathcal{B}}_L\to\widehat{\mathcal{B}}_L$ by $f'_a([b_0,b_1])=[a_0\cdot\overline{p_0(b_0,b_1)},a_1]$ and $g'_a([b_0,b_1])=[a_0,a_1\cdot\overline{p_1(b_0,b_1)}]$. It is easy to see that f'_a is the inverse of f_a and g'_a is the inverse of g_a, thus f_a and g_a are bijective. □

Theorem 3.7. *The set $\widehat{\mathcal{B}}_L$, equipped with the induced up- and down-operations, is a biquandle.*

Proof. For any $a,b\in\widehat{\mathcal{B}}_L$, denote $a\overline{b]}:=a^b$ and $a\underline{b]}:=a_b$. We need to show that $\widehat{\mathcal{B}}_L$ equipped with those operations satisfies all the biquandle axioms.

(1) Let $a\in\widehat{\mathcal{B}}_L$. The maps $f_a,g_a:\widehat{\mathcal{B}}_L\to\widehat{\mathcal{B}}_L$, defined by $f_a(x)=x\overline{a]}$ and $g_a(x)=x\underline{a]}$, are bijective by Lemma 3.6. The map $S:\widehat{\mathcal{B}}_L\times\widehat{\mathcal{B}}_L\to\widehat{\mathcal{B}}_L\times\widehat{\mathcal{B}}_L$ is defined by $S(a,b)=(b\underline{a]},a\overline{b]})$. Consider another map $T:\widehat{\mathcal{B}}_L\times\widehat{\mathcal{B}}_L\to\widehat{\mathcal{B}}_L\times\widehat{\mathcal{B}}_L$, defined by $T([a_0,a_1],[b_0,b_1])=\big([b_0\cdot\overline{p_0(a_0,a_1)},b_1],[a_0,a_1\cdot\overline{p_1(b_0,b_1)}]\big)$, and compute

$$\begin{aligned}&T\big(S([a_0,a_1],[b_0,b_1])\big)\\&\quad=T\big([b_0,b_1\cdot p_1(a_0,a_1)],[a_0\cdot p_0(b_0,b_1),a_1]\big)\\&\quad=\Big([a_0\cdot p_0(b_0,b_1)\cdot\overline{p_0(b_0,b_1\cdot p_1(a_0,a_1))},a_1],\\&\qquad\qquad[b_0,b_1\cdot p_1(a_0,a_1)\cdot\overline{p_1(a_0\cdot p_0(b_0,b_1),a_1)}]\Big)\\&\quad=\big([a_0\bar{b}_0m_{b_0(0)}b_0\bar{b}_0\bar{m}_{b_0(0)}b_0,a_1],[b_0,b_1\bar{a}_1m_{a_1(0)}a_1\bar{a}_1\bar{m}_{a_1(0)}a_1]\big)\\&\quad=([a_0,a_1],[b_0,b_1]).\end{aligned}$$

A similar calculation shows that $ST=id$, thus S is bijective with inverse T.

(2) Let $a = [a_0, a_1] \in \widehat{\mathcal{B}}_L$. We calculate

$$
\begin{aligned}
f_a^{-1}(a) &= [a_0, a_1]^{\overline{[a_0,a_1]}} = [a_0 \bar{a}_0 \bar{m}_{a_0(0)} a_0, a_1] = [\bar{m}_{a_0(0)} a_0, a_1],\\
a\, \underline{f_a^{-1}(a)}\rfloor &= [a_0, a_1]_{([a_0,a_1]^{\overline{[a_0,a_1]}})} = [a_0, a_1]_{[a_0\bar{a}_0\bar{m}_{a_0(0)}a_0, a_1]} = [a_0, a_1 \bar{a}_1 m_{a_1(0)} a_1]\\
&= [a_0, m_{a_1(0)} a_1].
\end{aligned}
$$

Since $a_0(0) = a_1(0)$, we have $m_{a_0(0)} = m_{a_1(0)}$ and therefore the path $\overline{\bar{m}_{a_0(0)} a_0} a_1$ is homotopic to the path $\bar{a}_0 m_{a_1(0)} a_1$. It follows that $f_a^{-1}(a) = a\, \underline{f_a^{-1}(a)}\rfloor$. The proof of $g_a^{-1}(a) = a\, \overline{g_a^{-1}(a)}\rceil$ is similar.

(3) Let $a = [a_0, a_1],\ b = [b_0, b_1]$ and $c = [c_0, c_1]$ be elements of $\widehat{\mathcal{B}}_L$. Then we have

$$
\begin{aligned}
a\, \overline{c\, \underline{b}\rfloor}\,\Big|\, \overline{b\, \overline{c}\rceil}\Big| &= (a^{c_b})^{(b^c)} = ([a_0, a_1]^{[c_0, c_1 \bar{b}_1 m_{b_1(0)} b_1]})^{[b_0 \bar{c}_0 m_{c_0(0)} c_0, b_1]}\\
&= [a_0 \bar{c}_0 m_{c_0(0)} c_0, a_1]^{[b_0 \bar{c}_0 m_{c_0(0)} c_0, b_1]}\\
&= [a_0 \bar{c}_0 m_{c_0(0)} c_0 \bar{c}_0 \bar{m}_{c_0(0)} c_0 \bar{b}_0 m_{b_0(0)} b_0 \bar{c}_0 m_{c_0(0)} c_0, a_1]\\
&= [a_0 \bar{b}_0 m_{b_0(0)} b_0 \bar{c}_0 m_{c_0(0)} c_0, a_1] = ([a_0, a_1]^{[b_0, b_1]})^{[c_0, c_1]} = a\, \overline{b}\rceil \overline{c}\rceil,
\end{aligned}
$$

$$
\begin{aligned}
a\, \underline{b}\rfloor\, \overline{c\, \underline{b\, \overline{a}\rceil}\rfloor}\Big| &= (a_b)^{c_{(b^a)}} = [a_0, a_1 \bar{b}_1 m_{b_1(0)} b_1]^{[c_0, c_1]_{[b_0 \bar{a}_0 m_{a_0(0)} a_0, b_1]}}\\
&= [a_0, a_1 \bar{b}_1 m_{b_1(0)} b_1]^{[c_0, c_1 \bar{b}_1 m_{b_1(0)} b_1]} = [a_0 \bar{c}_0 m_{c_0(0)} c_0, a_1 \bar{b}_1 m_{b_1(0)} b_1]\\
&= [a_0 \bar{c}_0 m_{c_0(0)} c_0, a_1]_{[b_0 \bar{c}_0 m_{c_0(0)} c_0, b_1]}\\
&= [a_0 \bar{c}_0 m_{c_0(0)} c_0, a_1]_{([b_0, b_1]^{[c_0, c_1 \bar{a}_1 m_{a_1(0)} a_1]})}\\
&= ([a_0, a_1]^{[c_0, c_1]})_{([b_0, b_1]^{[c_0, c_1]_{[a_0, a_1]}})} = a\, \overline{c}\rceil\, \underline{b\, \overline{c\, \underline{a}\rfloor}\rceil}\Big|.
\end{aligned}
$$

A similar calculation proves the down interchanges equality $a\, \underline{c\, \overline{b}\rceil}\Big|\, \underline{b\, \underline{c}\rfloor}\Big| = a\, \underline{b}\rfloor \underline{c}\rfloor$. Therefore $\widehat{\mathcal{B}}_L$ is a biquandle. □

Since $\widehat{\mathcal{B}}_L$ is a biquandle, there are two more operations $\ulcorner$ and $\llcorner$ on $\widehat{\mathcal{B}}_L$, defined by $S^{-1}(a, b) = (b\ulcorner\overline{a}, a\llcorner\underline{b})$. We call those operations the up-bar and the down-bar operation, respectively. It follows from the proof of Theorem 3.7 that the bar operations are computed as

$$
\begin{aligned}
[a_0, a_1] \ulcorner\overline{[b_0, b_1]} &= [a_0, a_1]^{\overline{[b_0, b_1]}} = [a_0 \cdot \overline{p_0(b_0, b_1)}, a_1] \quad \text{and}\\
[a_0, a_1] \llcorner\underline{[b_0, b_1]} &= [a_0, a_1]_{\overline{[b_0, b_1]}} = [a_0, a_1 \cdot \overline{p_1(b_0, b_1)}].
\end{aligned}
$$

Definition 3.8. Biquandle $\widehat{\mathcal{B}}_L$ is called the *topological biquandle* of the link L.

Observe that in the case of the topological biquandle, the name *biquandle* becomes further justified, since every element of $\widehat{\mathcal{B}}_L$ is represented by an ordered pair of paths (whose homotopy classes represent the elements of the fundamental quandle). We might ask ourselves which biquandles could be constructed from two quandles in a similar way. In [Horvat 2018] it is shown that given two quandles Q and K, one may construct a product biquandle with underlying set $Q \times K$, whose operations are induced by the operations on Q and K. Product biquandles are classified in [Horvat 2018, Theorem 5.3].

In the remainder of this Section, we study properties of the topological biquandle $\widehat{\mathcal{B}}_L$. It turns out that its structure is simpler than that of a general biquandle.

Lemma 3.9. *In the topological biquandle, for any $a, b, c \in \widehat{\mathcal{B}}_L$ the following hold*:

(1) *Any up-operation commutes with any down-operation.*

(2) $$a\overline{b}|\,|\overline{b} = a|\overline{b\ b}| = a\underline{b}|\,|\underline{b} = a|\underline{b\ b}| = a.$$

(3) $$a\overline{b\underline{c}|}| = a\overline{b|\underline{c}}| = a\overline{b}|, \quad a|\overline{b\underline{c}|} = a|\overline{b|\underline{c}} = a|\overline{b}\,,$$
$$a\underline{b\overline{c}|}| = a\underline{b|\overline{c}}| = a\underline{b}|, \quad a|\underline{b\overline{c}|} = a|\underline{b|\overline{c}} = a|\underline{b}\,.$$

Proof. (1) For any $[a_0, a_1], [b_0, b_1], [c_0, c_1] \in \widehat{\mathcal{B}}_L$ we have

$$([a_0, a_1]^{[b_0,b_1]})_{[c_0,c_1]} = [a_0 \cdot p_0(b_0, b_1), a_1 \cdot p_1(c_0, c_1)] = ([a_0, a_1]_{[c_0,c_1]})^{[b_0,b_1]},$$

and similar equalities hold for the up-bar and down-bar operations.

(2) Let $a, b \in \widehat{\mathcal{B}}_L,\ a = [a_0, a_1],\ b = [b_0, b_1]$, and compute

$$a\overline{b}|\,|\overline{b} = ([a_0, a_1]^{[b_0,b_1]})^{\overline{[b_0,b_1]}} = [a_0 \cdot \bar{b}_0 m_{b_0(0)} b_0 \cdot \bar{b}_0 \bar{m}_{b_0(0)} b_0, a_1] = [a_0, a_1] = a,$$

and similarly in the other three cases.

(3) We have

$$[a_0, a_1]^{([b_0,b_1]_{[c_0,c_1]})} = [a_0, a_1]^{[b_0, b_1 \cdot p_1(c_0,c_1)]} = [a_0 \cdot \bar{b}_0 m_{b_0(0)} b_0, a_1] = [a_0, a_1]^{[b_0,b_1]},$$

and similar calculations settle the other cases. $\square$

Proposition 3.10. *Let $(X, \urcorner, \lrcorner)$ be any biquandle in which the equalities $a\overline{b\underline{c}|}| = a\overline{b}|$, $a|\overline{b\underline{c}|} = a|\overline{b}$, $a\underline{b\overline{c}|}| = a\underline{b}|$ and $a|\underline{b\overline{c}|} = a|\underline{b}$ are valid for any $a, b, c \in X$. Then*

(1) *the equalities* (3) *from Lemma 3.9 are valid for any $a, b, c \in X$,*

(2) *for any $a, b \in X$ we have $a\overline{b}|\,|\overline{b} = a|\overline{b\ b}| = a\underline{b}|\,|\underline{b} = a|\underline{b\ b}| = a$,*

(3) *any up-operation on X commutes with any down-operation,*

(4) *for any $a, b, c \in X$ we have $a\overline{b\overline{c}|}| = a|\overline{c}\ \overline{b}|\overline{c}|$ and $a\underline{b\underline{c}|}| = a|\underline{c}\ \underline{b}|\underline{c}|$.*

Proof. Let X be a biquandle with the prescribed property. To prove (1), we use Lemma 2.3 to compute $a\overline{b|\underline{c}}| = a\overline{b|\underline{c\ c\overline{b}|}}| = a\overline{b}|$ and similarly for the other three cases.

To prove (2), choose elements $a, b \in X$ and use Lemma 2.3 to compute

$$a\overline{b}|\,|\overline{b} = a\overline{b}|\,|\overline{b\underline{a}|} = a, \quad a|\overline{b\ b}| = a|\overline{b\ b\underline{a}|}| = a,$$
$$a\underline{b}|\,|\underline{b} = a\underline{b}|\,|\underline{b\overline{a}|} = a, \quad a|\underline{b\ b}| = a|\underline{b\ b\overline{a}|}| = a.$$

To prove (3), choose elements $a, b, c \in X$ and use the second equality of biquandle axiom (3) to compute

$$a\,\overline{c}|\,\underline{b}| = a\,\overline{c}|\,\underline{b\,\overline{c\,\underline{a}|}|}| = a\,\underline{b}|\,\overline{c\,\underline{b\,\overline{a}|}|}| = a\,\underline{b}|\,\overline{c}|. \tag{1}$$

Now write $x = a|\overline{b}\,|\underline{c}$ and use (2) together with Equation (1) to obtain $a = x\,\underline{c}|\,\overline{b}| = x\,\overline{b}|\,\underline{c}|$, which implies $x = a|\underline{c}\,|\overline{b} = a|\overline{b}\,|\underline{c}$.

Writing $y = a|\overline{c}\,\underline{b}|$, we use (2) and the second equality of biquandle axiom (3) to compute

$$y\,\overline{c}| = y\,\overline{c\,\underline{b\,\overline{a}|}|}| = a|\overline{c}\,\underline{b}|\,\overline{c\,\underline{b\,\overline{a}|}|}| = a|\overline{c}\,\overline{c}|\,\underline{b\,\overline{c\,\underline{a}|}|}| = a\,\underline{b}|,$$

which implies $y = a\,\underline{b}|\,|\overline{c} = a|\overline{c}\,\underline{b}|$.

Finally, write $z = a\,\overline{b}|\,|\underline{c}$ and use the previously proved equality to obtain $a = z\,\underline{c}|\,|\overline{b} = z|\overline{b}\,\underline{c}|$, which implies $z = a|\underline{c}\,\overline{b}| = a\,\overline{b}|\,|\underline{c}$.

To prove (4), choose elements $x, y, z \in X$ and use the first equality of biquandle axiom (3) to compute $x\,\overline{y}|\,\overline{z\,\overline{y}|}| = x\,\overline{y\,\underline{z}|}|\,\overline{z\,\overline{y}|}| = x\,\overline{z}|\,\overline{y}|$ and putting $a = x\,\overline{y}|,\ b = z$ and $c = y$ gives $a\,\overline{b\,\overline{c}|}| = a|\overline{c}\,\overline{b}|\,\overline{c}|$. Similarly, the third equality of biquandle axiom (3) gives $x\,\underline{y}|\,\underline{z\,\underline{y}|}| = x\,\underline{y\,\overline{z}|}|\,\underline{z\,\underline{y}|}| = x\,\underline{z}|\,\underline{y}|$ and putting $a = x\,\underline{y}|,\ b = z$ and $c = y$ implies $a\,\underline{b\,\underline{c}|}| = a|\underline{c}\,\underline{b}|\,\underline{c}|$. □

Part (3) of Lemma 3.9 together with Proposition 3.10 implies:

Corollary 3.11. *Let A be a generating set of the topological biquandle $\widehat{\mathcal{B}}_L$. Any element of $\widehat{\mathcal{B}}_L$ can be expressed in the form $a\,\overline{w_1}|\,\underline{w_2}|$, where $a \in A$ and w_i is a word in $F(A)$ for $i = 1, 2$.*

4. Presentation of the topological biquandle

Recall the setting described at the beginning of Section 3. For a link L in S^3, we have chosen a regular neighborhood N_L and fixed an orientation of the normal bundle of L. We have also chosen the basepoints z_0 and z_1, which represent two antipodal points of the boundary sphere of a 3-ball neighborhood of N_L. Choose a coordinate system in which the points z_0 and z_1 have coordinates $(0, 0, 1)$ and $(0, 0, -1)$ respectively, and let D be the diagram of L obtained by projection to the plane $z = 0$.

As before, we denote by $A(D)$ the set of semiarcs and by $C(D)$ the set of crossings of the diagram D. We would like to find a presentation of the topological biquandle $\widehat{\mathcal{B}}_L$ in terms of the link diagram.

For any $a, b, c \in A(D)$, denote by $R_{a,b,c}$ the set of relations

$$R_{a,b,c} = \left\{ a\,\overline{b\,\underline{c}|}| = a\,\overline{b}|,\ a|\overline{b\,\underline{c}|} = a|\overline{b},\ a\,\underline{b\,\overline{c}|}| = a\,\underline{b}|,\ a|\underline{b\,\overline{c}|} = a|\underline{b} \right\}.$$

Theorem 4.1. *Let D be a diagram of a link L in S^3. Then*

$$\big\langle A(D)\,|\,\textit{crossing relations for each } c \in C(D),\ R_{a,b,c} \textit{ for each } a, b, c \in A(D) \big\rangle$$

is a presentation of the topological biquandle $\widehat{\mathcal{B}}_L$.

Proof. Let $R = \big\{\text{crossing relations for each } c \in C(D),\ R_{a,b,c} \text{ for each } a,b,c \in A(D)\big\}$. We will define a map $j : A(D) \to \widehat{\mathcal{B}}_L$ such that

(1) $(\bar{j} \times \bar{j})(R) \subset \Delta_{\widehat{\mathcal{B}}_L}$,

(2) for any biquandle Y and for any map $f : A(D) \to Y$ such that $(\bar{f} \times \bar{f})(R) \subset \Delta_Y$, there exists a unique biquandle homomorphism $\tilde{f} : \widehat{\mathcal{B}}_L \to Y$ such that $f = \tilde{f} \circ j$.

For a semiarc $a \in A(D)$, let $j(a) = [a_0, a_1]$, where a_0 is any path from the parallel curve to the semiarc a to z_0 that passes <u>over</u> all the other arcs of the diagram, and a_1 is a path from $a_0(0)$ to z_1 that passes <u>under</u> all the other arcs of the diagram.

<u>Proof of 1</u>. By definition of a free biquandle, there exists a unique biquandle homomorphism $\bar{j} : F_{\mathrm{BQ}}(A(D)) \to \widehat{\mathcal{B}}_L$ that extends the map j, and it is given by

$$\bar{j}(a\overline{b}|) = j(a)^{j(b)} = [a_0, a_1]^{[b_0,b_1]}, \qquad \bar{j}(a\underline{b}|) = j(a)_{j(b)} = [a_0, a_1]_{[b_0,b_1]}.$$

It follows from Lemma 2.4 that $\bar{j}$ also satisfies

$$\bar{j}(a|\overline{b}\,) = j(a)^{\overline{j(b)}} = [a_0, a_1]^{\overline{[b_0,b_1]}}, \qquad \bar{j}(a|\underline{b}\,) = j(a)_{\overline{j(b)}} = [a_0, a_1]_{\overline{[b_0,b_1]}}.$$

For any $a, b, c \in A(D)$, we use part (3) of Lemma 3.9 to compute

$$\bar{j}(a\overline{b\underline{c}|}|) = j(a)\overline{j(b)\underline{j(c)}|}| = j(a)\overline{j(b)}| = \bar{j}(a\overline{b}|),$$

and a similar computation shows that the homomorphism $\bar{j}$ preserves every relation from the set $R_{a,b,c}$.

At every positive crossing of the diagram D, the outgoing semiarcs c and d are related to the incoming semiarcs a and b by two crossing relations $c = a\overline{b}|$ and $d = b\underline{a}|$ (see the left part of Figure 1). Figure 2 shows a homotopy between $\bar{j}(a\overline{b}|)$ and $\bar{j}(c)$ and another homotopy between $\bar{j}(b\underline{a}|)$ and $\bar{j}(d)$.

At every negative crossing of the diagram D, the outgoing semiarcs c and d are related to the incoming semiarcs a and b by two relations, $c = a|\overline{b}$ and $d = b|\underline{a}$ (see the right part of Figure 1). Figure 3 shows a homotopy between $\bar{j}(a|\overline{b}\,)$ and $\bar{j}(c)$ and another homotopy between $\bar{j}(b|\underline{a}\,)$ and $\bar{j}(d)$. This shows that $(\bar{j} \times \bar{j})(R) \subset \Delta_{\widehat{\mathcal{B}}_L}$.

<u>Proof of 2</u>. Suppose Y is a biquandle and choose any map $f : A(D) \to Y$ such that $(\bar{f} \times \bar{f})(R) \subset \Delta_Y$. An element of $\widehat{\mathcal{B}}_L$ is represented by a pair (γ_0, γ_1), where γ_i is a path in E_L from a point in ∂N_L to z_i for $i = 0, 1$ and $\gamma_0(0) = \gamma_1(0)$. Project the paths γ_0, γ_1 in general position onto the plane of the diagram D. Suppose that the initial point $\gamma_0(0) = \gamma_1(0)$ lies on the parallel curve to the semiarc a and suppose that γ_0 subsequently passes <u>under</u> the semiarcs labeled by $b_1, b_2, \dots, b_m$, while γ_1 subsequently passes <u>over</u> the semiarcs labeled by $c_1, c_2, \dots, c_n$. Define

$$\tilde{f}([\gamma_0, \gamma_1]) := f(a)\overline{f(b_1)^{\epsilon_1} \cdots f(b_m)^{\epsilon_m}}|\,\underline{f(c_1)^{\phi_1} \cdots f(c_n)^{\phi_n}}|,$$

where ϵ_i denotes the sign of the crossing between γ_0 and its overlying semiarc b_i, while ϕ_i denotes the sign of the crossing between γ_1 and its underlying semiarc c_i.

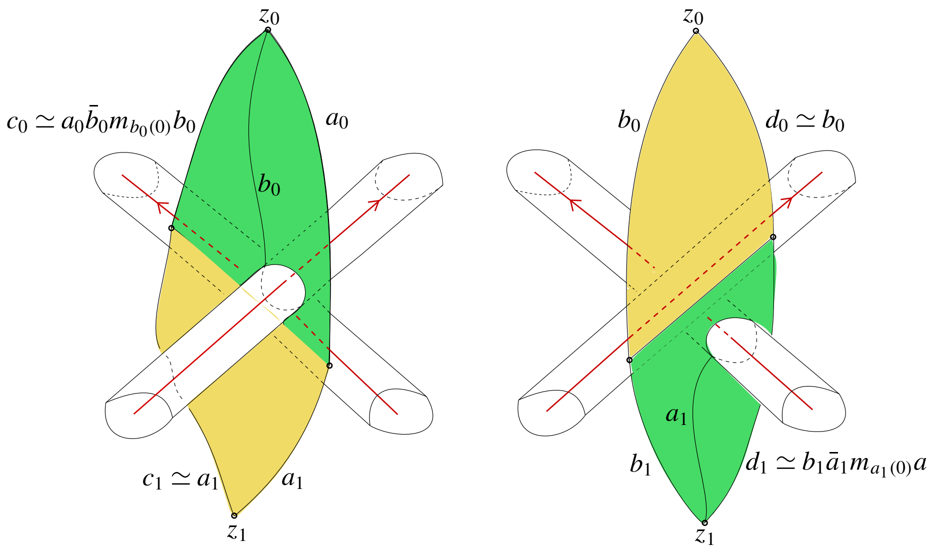

Figure 2. An illustration of the crossing relations $[a_0, a_1]^{[b_0,b_1]} = [c_0, c_1]$ and $[b_0, b_1]_{[a_0,a_1]} = [d_0, d_1]$.

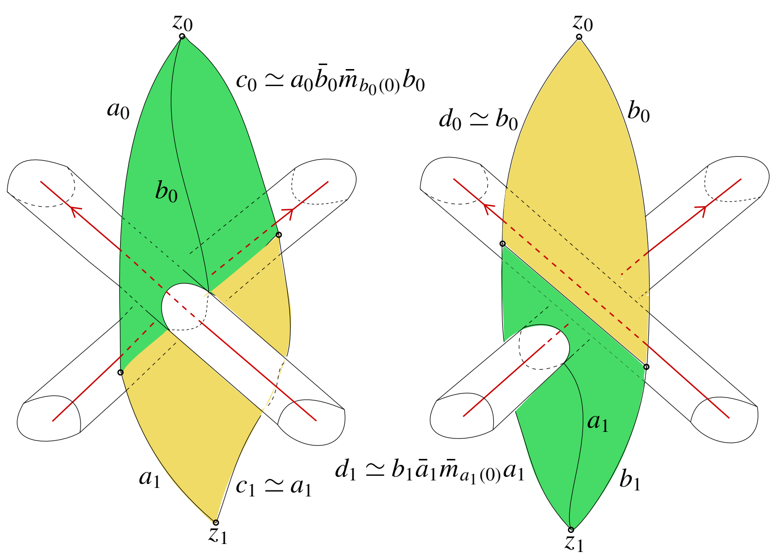

Figure 3. An illustration of the crossing relations $[a_0, a_1]^{\overline{[b_0,b_1]}} = [c_0, c_1]$ and $[b_0, b_1]_{\overline{[a_0,a_1]}} = [d_0, d_1]$.

It follows from the above definition of $\tilde{f}$ that for any $a \in A(D)$, we have $(\tilde{f} \circ j)(a) = \tilde{f}([a_0, a_1]) = f(a)$, therefore $\tilde{f} \circ j = f$. We need to show that $\tilde{f}$ is a well defined map on $\widehat{\mathcal{B}}_L$ and that it is a biquandle homomorphism. To show that $\tilde{f}$

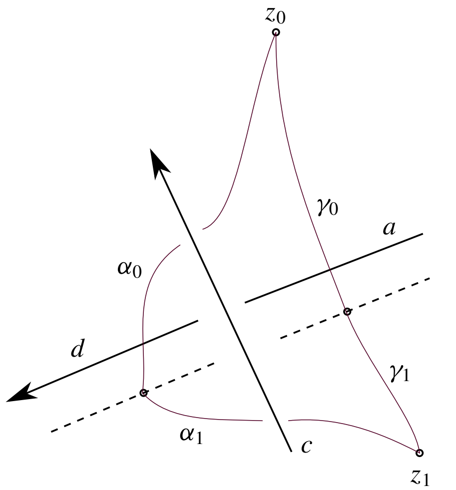

Figure 4. The invariance of $\tilde{f}$ — change of initial point.

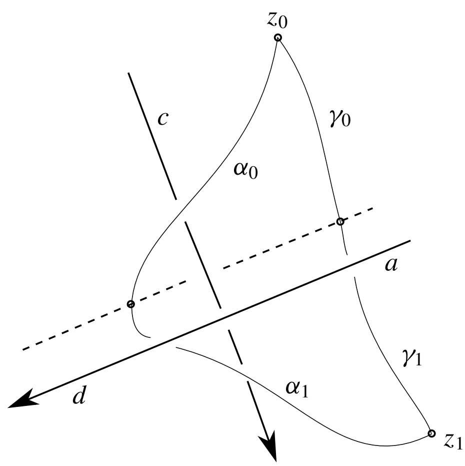

Figure 5. The invariance of $\tilde{f}$ — change of initial point.

is well defined, we have to check that any representative of the equivalence class $[\gamma_0, \gamma_1]$ gives the same value of $\tilde{f}$. During a homotopy from (γ_0, γ_1) to another representative (α_0, α_1), the following critical stages may occur:

(a) The initial point $\gamma_0(0) = \gamma_1(0)$ moves to another semiarc.

First suppose that the initial point of γ_i is at the semiarc a, while the initial point of α_i is at the semiarc d where $a\,\overline{c}\rceil = d$ (see Figure 4). Since $(\bar{f} \times \bar{f})(R) \subset \Delta_Y$, we have $f(a)\,\overline{f(c)}\rceil = f(d)$. Writing $\tilde{f}([\gamma_0, \gamma_1]) = f(a)\,\overline{w_1}\rceil\,\underline{w_2}\rfloor$, we use Lemma 2.3 to obtain $\tilde{f}([\alpha_0, \alpha_1]) = f(d)\lceil\overline{\bar{f}(c\,\underline{a}\rfloor)}\,\overline{w_1}\rceil\,\underline{w_2}\rfloor = f(a)\,\overline{f(c)}\rceil\lceil\overline{f(c)\,\underline{f(a)}\rfloor}\,\overline{w_1}\rceil\,\underline{w_2}\rfloor = f(a)\,\overline{w_1}\rceil\,\underline{w_2}\rfloor = \tilde{f}([\gamma_0, \gamma_1])$.

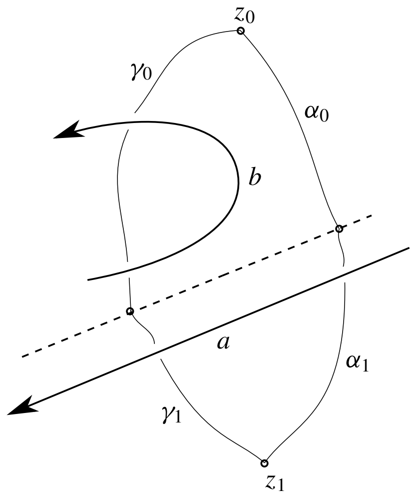

Figure 6. The invariance of $\tilde{f}$ under a homotopy — first case of (b).

Second, suppose that the initial point of γ_i is at the semiarc a, while the initial point of α_i is at the semiarc d where $a\,\underline{c}\rfloor = d$ (see Figure 5). Since $\bar{f}$ preserves the crossing relations, we have $f(a)\,\underline{f(c)}\rfloor = f(d)$. Since $\bar{f}$ preserves the relations $R_{a,b,c}$, it follows by Proposition 3.10 that any up-operation on $\bar{f}(A(D))$ commutes with any down-operation. Write $\tilde{f}([\gamma_0, \gamma_1]) = f(a)\,\overline{w_1}\rceil\,\underline{w_2}\rfloor$ and it follows that $\tilde{f}([\alpha_0, \alpha_1]) = f(d)\,\overline{w_1}\rceil\,\lfloor\underline{\bar{f}(c\,\overline{a}\rceil)}\,\underline{w_2}\rfloor = f(a)\,\underline{f(c)}\rfloor\,\lfloor\underline{f(c)\,\overline{f(a)}\rceil}\,\overline{w_1}\rceil\,\underline{w_2}\rfloor = f(a)\,\overline{w_1}\rceil\,\underline{w_2}\rfloor = \tilde{f}([\gamma_0, \gamma_1])$.

For the two remaining cases, we prove the invariance in a similar way.

(b) The arc γ_0, overcrossed by the same semiarc b twice, homotopes to an arc α_0 that is not crossed by b (or the arc γ_1, overcrossing the same semiarc b twice, homotopes to an arc α_1 that does not cross b).

For the first case, see Figure 6. We have

$$\tilde{f}([\gamma_0, \gamma_1]) = f(a)\,\overline{w_1}\rceil\,\overline{f(b)}\rceil\,\lceil\overline{f(b)}\,\overline{w_2}\rceil\,\underline{w_3}\rfloor \quad \text{and} \quad \tilde{f}([\alpha_0, \alpha_1]) = f(a)\,\overline{w_1}\rceil\,\overline{w_2}\rceil\,\underline{w_3}\rfloor.$$

Since $\bar{f}$ preserves the relations $R_{a,b,c}$, it follows by Proposition 3.10 that

$$\tilde{f}([\gamma_0, \gamma_1]) = \tilde{f}([\alpha_0, \alpha_1]).$$

For the second case, see Figure 7. We have

$$\tilde{f}([\gamma_0, \gamma_1]) = f(a)\,\overline{w_1}\rceil\,\underline{w_2}\rfloor\,\underline{f(b)}\rfloor\,\lfloor\underline{f(b)}\,\underline{w_3}\rfloor \quad \text{and} \quad \tilde{f}([\alpha_0, \alpha_1]) = f(a)\,\overline{w_1}\rceil\,\underline{w_2}\rfloor\,\underline{w_3}\rfloor.$$

Since $\bar{f}$ preserves the relations $R_{a,b,c}$, it follows by Proposition 3.10 that

$$\tilde{f}([\gamma_0, \gamma_1]) = \tilde{f}([\alpha_0, \alpha_1]).$$

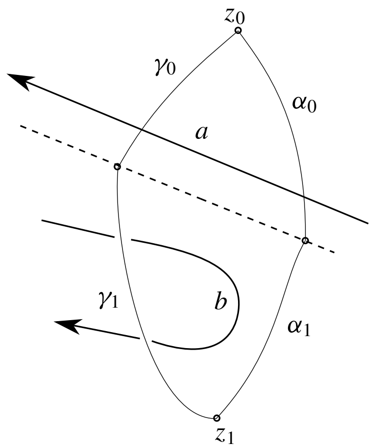

Figure 7. The invariance of $\tilde{f}$ under a homotopy — second case of (b).

(c) γ_0 passes under a crossing between two semiarcs (or γ_1 passes over a crossing between two semiarcs).

For the first case, see Figure 8. We write

$$\begin{aligned}\tilde{f}([\gamma_0,\gamma_1]) &= f(a)\,\overline{w_1|}\,\overline{f(b)|}\,\overline{f(c)|}\,\overline{w_2|}\,\underline{w_3|},\\ \tilde{f}([\alpha_0,\alpha_1]) &= f(a)\,\overline{w_1|}\,\overline{f(c)\,\underline{f(b)|}\,|}\,\overline{f(b)\,\overline{f(c)|}\,|}\,\overline{w_2|}\,\underline{w_3|}.\end{aligned}$$

Since $\bar{f}$ preserves the relations $R_{a,b,c}$, we may use the first equality of biquandle axiom (3) to compute

$$f(a)\,\overline{w_1|}\,\overline{f(c)\,\underline{f(b)|}\,|}\,\overline{f(b)\,\overline{f(c)|}\,|} = f(a)\,\overline{w_1|}\,\overline{f(b)|}\,\overline{f(c)|}$$

and therefore $\tilde{f}([\gamma_0,\gamma_1]) = \tilde{f}([\alpha_0,\alpha_1])$. The remaining cases are settled in a similar way.

To show that $\tilde{f}$ is a biquandle homomorphism, choose two elements

$$[\alpha_0,\alpha_1],\ [\beta_0,\beta_1] \in \widehat{\mathcal{B}}_L.$$

Let $\tilde{f}[\alpha_0,\alpha_1] = f(a)\,\overline{w_1|}\,\underline{w_2|}$ and $\tilde{f}[\beta_0,\beta_1] = f(b)\,\overline{z_1|}\,\underline{z_2|}$. Using Proposition 3.10, we calculate

$$\begin{aligned}\tilde{f}([\alpha_0,\alpha_1]^{[\beta_0,\beta_1]}) &= \tilde{f}[\alpha_0\bar{\beta}_0 m_{\beta_0(0)}\beta_0,\alpha_1] = f(a)\,\overline{w_1|}\,|\overline{z_1}\ \overline{f(b)|}\,\overline{z_1|}\,\underline{w_2|}\\ &= f(a)\,\overline{w_1|}\,\underline{w_2|}\,|\overline{z_1}\ \overline{f(b)|}\,\overline{z_1|} = \tilde{f}[\alpha_0,\alpha_1]\,\overline{f(b)\,\overline{z_1|}\,|},\\ &= \tilde{f}[\alpha_0,\alpha_1]\,\overline{\tilde{f}[\beta_0,\beta_1]\,|},\\ \tilde{f}([\alpha_0,\alpha_1]_{[\beta_0,\beta_1]}) &= \tilde{f}[\alpha_0,\alpha_1\bar{\beta}_1 m_{\beta_1(0)}\beta_1] = f(a)\,\overline{w_1|}\,\underline{w_2|}\,|\underline{z_2}\ \underline{f(b)|}\,\underline{z_2|}\\ &= \tilde{f}[\alpha_0,\alpha_1]\,\underline{f(b)\,\underline{z_2|}\,|} = \tilde{f}[\alpha_0,\alpha_1]\,\underline{f(b)\,\underline{z_2|}\,\overline{z_1|}\,|}\\ &= \tilde{f}[\alpha_0,\alpha_1]\,\underline{\tilde{f}[\beta_0,\beta_1]\,|},\end{aligned}$$

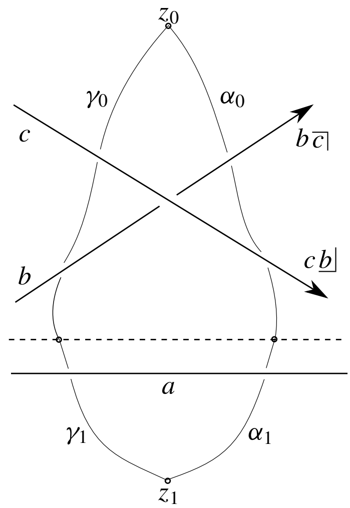

Figure 8. The invariance of $\tilde{f}$ under a homotopy — first case of (c).

thus $\tilde{f}$ is indeed a biquandle homomorphism.

To prove uniqueness of $\tilde{f}$, observe that by Corollary 3.11, any element of $\widehat{\mathcal{B}}_L$ can be written as $[\gamma_0, \gamma_1] = j(a)\,\overline{\bar{j}(w_1)|}\,\underline{\bar{j}(w_2)|}$, where $a \in A(D)$ and w_1, w_2 are elements of the free group, generated by $A(D)$. If $g : \widehat{\mathcal{B}}_L \to Y$ is any biquandle homomorphism for which $g \circ j = f$, then we have

$$g[\gamma_0, \gamma_1] = f[a_0, a_1]\,\overline{\bar{f}(w_1)|}\,\underline{\bar{f}(w_2)|} = \tilde{f}[\gamma_0, \gamma_1]. \qquad \square$$

Corollary 4.2. *For any link L, the topological biquandle $\widehat{\mathcal{B}}_L$ is a quotient of its fundamental biquandle* $\mathrm{BQ}(L)$.

Corollary 4.3. *The topological biquandle is a link invariant.*

Example 4.4. Consider the link $L = L6n1$ in the Thistlethwaite Link Table, whose diagram is depicted in Figure 9. Denoting the semiarcs of the diagram as shown in Figure 9, the fundamental biquandle of L is given by the presentation

$$\begin{aligned}\mathrm{BQ}(L) = \Big\langle a, b, c, d, e, f, g, h, i, j, k, l \;\Big|\; & l\,\overline{a|} = i,\ a\,\underline{l|} = b,\ f\,\overline{k|} = g,\ k\,\underline{f|} = l,\\ & g\,\overline{d|} = h,\ d\,\underline{g|} = a,\ c\,\overline{j|} = d,\ j\,\underline{c|} = k,\\ & i\,\overline{h|} = j,\ h\,\underline{i|} = e,\ b\,\overline{e|} = c,\ e\,\underline{b|} = f\Big\rangle,\end{aligned}$$

that reduces to

$$\begin{aligned}\mathrm{BQ}(L) = \Big\langle b, f, l \;\Big|\; & b\,\overline{f\,\underline{b|}|}\;\overline{l\,\underline{f\,\underline{b\,\overline{f\,\underline{b|}|}|}|}|}\;\underline{f\,\overline{l\,\underline{f|}|}|}\;\underline{l|} = b,\ \ f\,\overline{l\,\underline{f|}|}\;\overline{b\,\underline{l|}\,\underline{f\,\overline{l\,\underline{f|}|}|}|}\;\underline{l\,\overline{b\,\underline{l|}|}|}\;\underline{b|} = f,\\ & l\,\overline{b\,\underline{l|}|}\;\overline{f\,\underline{b|}\,\underline{l\,\overline{b\,\underline{l|}|}|}|}\;\underline{b\,\overline{f\,\underline{b|}|}|}\;\underline{f|} = l\Big\rangle.\end{aligned}$$

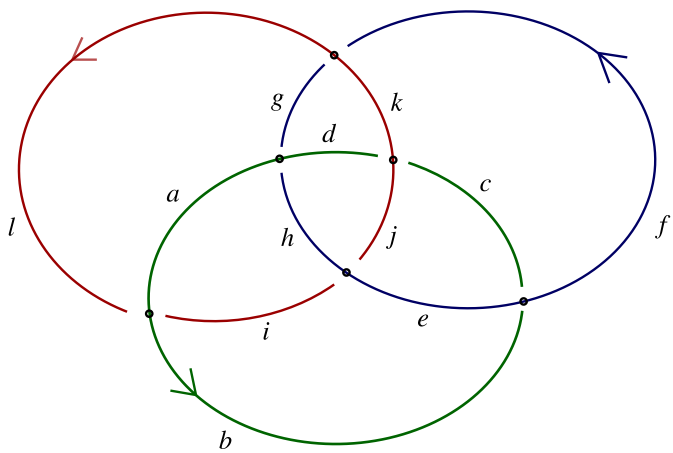

Figure 9. A diagram of the link $L6n1$ from Example 4.4.

The topological biquandle $\widehat{\mathcal{B}}_L$ is given by the presentation

$$\widehat{\mathcal{B}}_L = \Big\langle a, b, c, d, e, f, g, h, i, j, k, l \;\Big|\; l\overline{a}| = i,\ a\underline{l}| = b,\ f\overline{k}| = g,\ k\underline{f}| = l,\ g\overline{d}| = h,\ d\underline{g}| = a,\ c\overline{j}| = d,\ j\underline{c}| = k,\ i\overline{h}| = j,\ h\underline{i}| = e,\ b\overline{e}| = c,\ e\underline{b}| = f,\ R\Big\rangle,$$

where R denotes all relations $R_{x,y,z}$ for $x, y, z \in \{a, b, c, d, e, f, g, h, i, j, k, l\}$. These relations include: $x\,\overline{y|\underline{x}|}\,| = x\,\overline{y}|$, $x\,\overline{y|\underline{z}\,|\underline{w\,\overline{z}|}}\,| = x\,\overline{y}|$ and $x\,\underline{y\,\overline{z}|}| = x\,\underline{y}|$ for every $x, y, z, w \in \{b, f, l\}$. Since none of these new relations is implied from the relations in the presentation of $\mathrm{BQ}(L)$, it follows that the topological biquandle $\widehat{\mathcal{B}}_L$ is a quotient of the fundamental biquandle $\mathrm{BQ}(L)$. The presentation of the topological biquandle thus reduces to

$$\widehat{\mathcal{B}}_L = \langle b, f, l \mid b\,\overline{f}|\overline{l}|\,\underline{f}|\underline{l}| = b,\ f\,\overline{l}|\overline{b}|\underline{l}|\underline{b}| = f,\ l\,\overline{b}|\,\overline{f}|\underline{b}|\,\underline{f}| = l,\ R\rangle.$$

Remark 4.5. A presentation of the topological biquandle $\widehat{\mathcal{B}}_L$ is obtained from a presentation of the fundamental biquandle $\mathrm{BQ}(L)$ by adding relations

$$R_{a,b,c} = \left\{a\,\overline{b\,\underline{c}|}| = a\,\overline{b}|,\ a|\overline{b\,\underline{c}|} = a|\overline{b},\ a\,\underline{b\,\overline{c}|}| = a\,\underline{b}|,\ a|\underline{b\,\overline{c}|} = a|\underline{b}\right\}$$

for every ordered triple of generators (a, b, c). Seeing $\widehat{\mathcal{B}}_L$ as a subbiquandle of the fundamental biquandle $\mathrm{BQ}(L)$, we may talk about the corresponding "sections." For any $a \in \mathrm{BQ}(L)$, the section $\widehat{\mathcal{B}}_L a$ is given as $\widehat{\mathcal{B}}_L a = \{x\,\overline{a}|, x\,\underline{a}| \mid x \in \widehat{\mathcal{B}}_L\}$. The quotient set $\mathrm{BQ}(L)/\widehat{\mathcal{B}}_L$ is generated by

$$\mathrm{BQ}(L)/\widehat{\mathcal{B}}_L = \langle \widehat{\mathcal{B}}_L a\,\overline{b}|,\ \widehat{\mathcal{B}}_L a\,\underline{b}|,\ \widehat{\mathcal{B}}_L a|\overline{b},\ \widehat{\mathcal{B}}_L a|\underline{b} \mid a, b \in \mathrm{BQ}(L)\rangle.$$

Denoting by n the number of generators of $\mathrm{BQ}(L)$, the quotient set $\mathrm{BQ}(L)/\widehat{\mathcal{B}}_L$ has $4n^2$ generators, which indicates the "index" of the topological biquandle inside the fundamental biquandle. In Example 4.4, the quotient $\mathrm{BQ}(L)/\widehat{\mathcal{B}}_L$ has 36 generators.

One might question the need for the topological biquandle, when the fundamental quandle is already a complete invariant of knots up to inversion. In a more sophisticated study of links (e.g., virtual links), however, we sometimes need to combine two or more different link invariants to yield a stronger invariant. Some examples of this are the quantum enhancements using biquandles, see [Nelson et al. 2017; 2019; Nelson and Oyamaguchi 2017; Ilyutko and Manturov 2017]. In the study of virtual links, Manturov [2010] introduced the concept of parity, that induces a function on the set of crossings of any virtual link diagram. Parity allows constructions of new link invariants and also improvement of the existing invariants (e.g., Kauffman bracket). As was shown in [Ilyutko and Manturov 2017, Example 2.3], a parity of knots may be induced by a certain coloring of the fundamental biquandle of the knot. It might be possible to define other parities of virtual knots using the fundamental or topological biquandle.

The topological biquandle may just as well be defined for links in other 3-manifolds, virtual links, or higher-dimensional links, and it might lead to interesting new invariants.

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AN ENDPOINT ESTIMATE OF THE KUNZE–STEIN PHENOMENON ON SU(n, m)

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The endpoint estimates for the Kunze–Stein phenomenon associated with real rank one semisimple Lie groups and the Jacobi hypergroup were obtained by A. Ionescu and J. Liu respectively. Recently, a modified endpoint estimate was also proved for complex semisimple Lie groups by J. Liu and the author. Hence the original estimate seems not to be valid for general semisimple Lie groups with higher rank. We treat the case of SU(n, m) and obtain a modified estimate similarly to the complex case. The process using the Abel transform makes it clear why the original endpoint estimate might not be valid for general semisimple Lie groups.

1. Introduction

Let G be a noncompact connected semisimple Lie group with finite center and $1 \leq p < 2$. Then the convolution $*$ on G satisfies

$$\|f * g\|_{X_1} \leq c\|f\|_{X_2}\|g\|_{X_3}, \tag{1}$$

when the Banach spaces X_1, X_2, X_3 are $L^2(G)$, $L^p(G)$, $L^2(G)$, respectively. This inequality was established by Kunze and Stein in the case of $G = \mathrm{SL}(2, \mathbb{R})$ and by Cowling [1978] in the general case stated above. Moreover, if G is of real rank one, he deduced the Lorentz space version, that is, (1) holds when the spaces X_1, X_2, X_3 are $L^{p,w}(G)$, $L^{p,u}(G)$, $L^{p,v}(G)$, respectively, where $1 \leq p < 2$, $1 \leq u, v, w \leq \infty$, and $1+\frac{1}{w} = \frac{1}{u}+\frac{1}{v}$; see [Cowling 1997]. Ionescu [2000] proved the endpoint estimate at $p = 2$ when the spaces X_1, X_2, X_3 are $L^{2,\infty}(G)$, $L^{2,1}(G)$, $L^{2,1}(G)$, respectively. This covers Cowling's result by interpolation. For the Jacobi hypergroup $(\mathbb{R}_+, \Delta, *)$ the same endpoint inequality was obtained by J. Liu [2005]. However, if G is of higher rank, we don't know whether or not the endpoint estimate holds on G.

In this paper, as in [Kawazoe and Liu 2018], we shall obtain a modified endpoint estimate for K-bi-invariant functions on $G = \mathrm{SU}(n, m)$. Let M be a multiplier

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operator on G which will be specified later. Then we shall obtain

$$\|f * Mg\|_{L^{2,\infty}(G)} \le c\|f\|_{L^{2,1}(G)}\|g\|_{L^{2,1}(G)} \tag{2}$$

for K-bi-invariant functions f, g on G. In Theorem 4.1, when $m \ge n \ge 2$, we shall prove that (2) holds for the multiplier M whose spherical transform is given by

$$\widehat{M}(\boldsymbol{\lambda}) = \prod_{i<j} \sin^2(\lambda_i - \lambda_j)\sin^2(\lambda_i + \lambda_j). \tag{3}$$

To deduce this modified inequality, we use the inverse Abel transform expressed in terms of Euclidean fractional derivatives (see (10)) and transfer the convolution $*$ on G to the Euclidean convolution $\circledast$ on $\mathbb{R}^n$ (see (12)). According to this process, when $n = 1$, (2) holds without modification (see [Kawazoe 2018, §7]) and when $n \ge 2$, our modification with the multiplier M is essential and unavoidable (see Section 5).

2. Notations

Let $G = \mathrm{SU}(n, n+k)$ be the group of all complex $(n+m)\times(n+m)$ matrices with determinant 1 ($m = n+k$, $k \ge 0$), which leave invariant the Hermitian form $\sum_{i=1}^n x_i\bar{x}_i - \sum_{j=1}^m x_{n+j}\bar{x}_{n+j}$. Let $K = \mathrm{S}(\mathrm{U}(n)\times\mathrm{U}(m))$ and $\mathfrak{a}$ be the set of all matrices of the form

$$H_{\boldsymbol{t}} = \begin{pmatrix} 0_{n,n} & \operatorname{diag}\boldsymbol{t} & 0_{n,k} \\ \operatorname{diag}\boldsymbol{t} & & \\ & 0_{m,m} & \\ 0_{k,n} & & \end{pmatrix},$$

where $0_{p,q}$ denotes the $p \times q$ zero matrix and $\operatorname{diag}\boldsymbol{t}$ the $n\times n$ diagonal matrix with diagonal $\boldsymbol{t} = (t_1, t_2, \dots, t_n)$, $t_i \in \mathbb{R}$. Let $a_{\boldsymbol{t}} = \exp H_{\boldsymbol{t}}$ and $A = \exp\mathfrak{a} = \{a_{\boldsymbol{t}} \mid \boldsymbol{t} \in \mathbb{R}^n\}$. We identify $H_{\boldsymbol{t}}, a_{\boldsymbol{t}}$ with $\boldsymbol{t}$. In particular, functions on $\mathbb{R}^n$ are identified with functions $f(H_{\boldsymbol{t}})$ and $f(a_{\boldsymbol{t}})$ on $\mathfrak{a}$ and A, respectively, which are also denoted by $f(\boldsymbol{t})$. Let $\mathfrak{a}^*$ be the dual space of $\mathfrak{a}$ and $\alpha_i \in \mathfrak{a}^*$ be defined by $\alpha_i(H_{\boldsymbol{t}}) = t_i$. Let Σ_+ denote the set of all positive roots of $(\mathfrak{g}, \mathfrak{a})$, which consists of $\alpha_i, 2\alpha_i$ $(1 \le i \le n)$ and $\alpha_i \pm \alpha_j$ $(1 \le i < j \le n)$ with multiplicities $m_{\alpha_i} = 2k$, $m_{2\alpha_i} = 1$ and $m_{\alpha_i\pm\alpha_j} = 2$; see [Hoogenboom 1982; Meaney 1986]. We put

$$\Delta(\boldsymbol{t}) = \prod_{\alpha\in\Sigma_+}(e^{\alpha(\boldsymbol{t})} - e^{-\alpha(\boldsymbol{t})})^{m_\alpha},$$

$$\sigma_{n,k}(\boldsymbol{t}) = 2^{n(2k+1)}\prod_{i=1}^n(\sinh^{2k}(t_i)\sinh(2t_i)),$$

$$\omega_n(\boldsymbol{t}) = 2^{\frac{1}{2}n(n-1)}\prod_{i<j}(\cosh(2t_i) - \cosh(2t_j)).$$

Then $\Delta = \sigma_{n,k}\omega_n^2$ and $\Delta(\boldsymbol{t}) = O(e^{2\rho_{n,k}(\boldsymbol{t})})$, where

$$\rho_{n,k}(\boldsymbol{t}) = \tfrac{1}{2}\sum_{\alpha\in\Sigma_+} m_\alpha \alpha(\boldsymbol{t}) = \sum_{i=1}^{n} \rho_i t_i, \qquad \rho_i = k+1+2(n-i).$$

In the following, we omit the subscripts of $\sigma_{n,k}$, ω_n, $\rho_{n,k}$ for simplicity and we regard functions and operators which depend on $1 \le i < j \le n$ as identities when $n = 1$. The Weyl group W of G and the positive Weyl chamber C^+ of $\mathbb{R}^n$ are given by

$$\begin{aligned} W &= \{w \mid w\boldsymbol{t} = (\epsilon_1 t_{\sigma(1)}, \epsilon_2 t_{\sigma(2)}, \dots, \epsilon_n t_{\sigma(n)}), \sigma \in \mathrm{S}_n, \epsilon_i = \pm 1\},\\ C^+ &= \{\boldsymbol{t} \in \mathbb{R}^n \mid t_1 > t_2 > \cdots > t_n > 0\}. \end{aligned}$$

We put $\mathbb{R}^n_+ = \{\boldsymbol{t} \in \mathbb{R}^n \mid t_i \ge 0,\ 1 \le i \le n\}$. Then for K-bi-invariant functions f on G, it follows that

$$\int_G f(g)\,dg = c\int_{C^+} f(\boldsymbol{t})\Delta(\boldsymbol{t})\,d\boldsymbol{t} = \frac{c}{n!}\int_{\mathbb{R}^n_+} f(\boldsymbol{t})\Delta(\boldsymbol{t})\,d\boldsymbol{t},$$

where dg is a Haar measure on G and $d\boldsymbol{t} = dt_1 dt_2 \cdots dt_n$. Let $L^p(\Delta)$, $1 \le p \le \infty$, denote the space of K-bi-invariant functions on G with finite L^p-norm with respect to dg, and $L^{p,q}(\Delta)$ the Δ-weighted Lorentz space consisting of K-bi-invariant functions on G; see [Hunt 1966]. For a positive function w on $\mathbb{R}^n_+$, we denote by $L^p(w)$ the space of K-bi-invariant functions of G satisfying

$$\int_{\mathbb{R}^n_+} |f(\boldsymbol{t})|^p w(\boldsymbol{t})\,d\boldsymbol{t} < \infty.$$

For $\boldsymbol{\lambda} \in \mathfrak{a}^* \cong \mathbb{R}^n$, let $\phi_{\boldsymbol{\lambda}}(\boldsymbol{t})$, $\boldsymbol{t} \in \mathfrak{a} \cong \mathbb{R}^n$, denote the spherical function on G. Then it is known that, as a function of $\boldsymbol{\lambda}$, $\Delta(\boldsymbol{t})\phi_{\boldsymbol{\lambda}}(\boldsymbol{t})$ is the Fourier transform of a compactly supported function $A(\boldsymbol{s}, \boldsymbol{t})$ of $\boldsymbol{s}$ on $\mathfrak{a}$ (see [Flensted-Jensen and Ragozin 1973]):

$$\Delta(\boldsymbol{t})\phi_{\boldsymbol{\lambda}}(\boldsymbol{t}) = (2\pi)^{-n/2}\int_{C(\boldsymbol{t})} A(\boldsymbol{s}, \boldsymbol{t})e^{-i\boldsymbol{\lambda}(\boldsymbol{s})}\,d\boldsymbol{s}, \tag{4}$$

where $C(\boldsymbol{t})$ is the compact support of $A(\boldsymbol{s}, \boldsymbol{t})$ of $\boldsymbol{s}$, which depends on $\boldsymbol{t}$, and $d\boldsymbol{s}$ is a Lebesgue measure on $\mathbb{R}^n$. For a K-bi-invariant function f on G, the spherical transform $\hat{f}$ on $\mathfrak{a}^*$ and the Abel transform F_f on A are respectively defined by

$$\begin{aligned} \hat{f}(\boldsymbol{\lambda}) &= \int_{\mathbb{R}^n_+} f(\boldsymbol{t})\phi_{\boldsymbol{\lambda}}(\boldsymbol{t})\Delta(\boldsymbol{t})\,d\boldsymbol{t},\\ F_f(\boldsymbol{t}) &= e^{\rho(\boldsymbol{t})}\int_N f(a_{\boldsymbol{t}} n)\,dn, \end{aligned}$$

where dn is a normalized invariant measure on a maximal nilpotent subgroup N of G. F_f and $\hat{f}$ are W-invariant on A and $\mathfrak{a}^*$, respectively. Then it follows that

$$F_f(\boldsymbol{s}) = (2\pi)^{-n/2} \int_{\mathbb{R}^n_+} \chi_{C(\boldsymbol{t})}(\boldsymbol{s}) f(\boldsymbol{t}) A(\boldsymbol{s},\boldsymbol{t})\, d\boldsymbol{t}, \tag{5}$$

where χ_S is the characteristic function of $S \subset \mathbb{R}^n$. In particular the classical Fourier transform $\widetilde{F_f}$ of F_f coincides with the spherical transform of f:

$$\hat{f} = \widetilde{F_f}; \tag{6}$$

see [Warner 1972, Proposition 9.2.2.3]. Especially, since $\widehat{f * g} = \hat{f} \cdot \hat{g}$, it follows that

$$F_{f*g} = F_f \circledast F_g, \tag{7}$$

where $*$ and $\circledast$ denote convolutions on G and $\mathbb{R}^n$ respectively.

According to [Meaney 1986], we shall express the Abel transform F_f in terms of fractional integral operators, and its inversion formula in terms of fractional differential operators. First we define the Weyl type fractional integral operators $W_\mu^{\mathbb{R}}$ and W_μ^σ. For functions g on $\mathbb{R}$, $\mu > 0$ and $\sigma > 0$, we put

$$W_\mu^{\mathbb{R}}(g)(t) = \Gamma(\mu)^{-n} \int_t^\infty g(s)(s-t)^{\mu-1}\, ds,$$
$$W_\mu^\sigma(g)(t) = \Gamma(\mu)^{-n} \int_t^\infty g(s)(\cosh(\sigma s) - \cosh(\sigma t))^{\mu-1} d\cosh(\sigma s)$$

(see [Koornwinder 1975, §3]). As functions of μ, these operators can be analytically extended on $\mu \in \mathbf{C}$ by integration by parts. For functions g on $\mathbb{R}^n$, we put

$$\begin{aligned}\boldsymbol{W}_\mu^\sigma(g)(\boldsymbol{t}) &= \Gamma(\mu)^{-n} \int_{t_n}^\infty \cdots \int_{t_1}^\infty g(\boldsymbol{t}) \prod_{j=1}^n (\cosh(\sigma s_j) - \cosh(\sigma t_j))^{\mu-1} \\ &\qquad\qquad \times d\cosh(\sigma s_1) \cdots d\cosh(\sigma s_n) \\ &= W_\mu^{\sigma,n} \circ \cdots \circ W_\mu^{\sigma,1}(g)(\boldsymbol{t}),\end{aligned}$$

where $W_\mu^{\sigma,i}$ indicates that W_μ^σ acts on the i-th variable t_i of $\boldsymbol{t}$. Then the Abel transform F_f satisfies

$$\prod_{i<j} (\partial_j^2 - \partial_i^2) F_f(\boldsymbol{t}) = c\boldsymbol{W}_k^1 \circ \boldsymbol{W}_{1/2}^2 (f\omega)(\boldsymbol{t}) \tag{8}$$

(see [Meaney 1986, Theorem 21]) and thus, the inverse Abel transform is given as

$$f(\boldsymbol{t}) = c\omega(\boldsymbol{t})^{-1} \boldsymbol{W}_{-1/2}^2 \circ \boldsymbol{W}_{-k}^1 \Bigl(\prod_{i<j} (\partial_j^2 - \partial_i^2) F_f \Bigr)(\boldsymbol{t}). \tag{9}$$

Here, applying the relation between $W^{\mathbb{R}}_\mu$ and W^σ_μ obtained in [Kawazoe 2009, §3] to every $W^{\sigma,i}_\mu$ on the right-hand side of (9), we can express the inversion formula in terms of $W^{\mathbb{R}}_\mu$ as follows. We define for $\boldsymbol{\gamma} = (\gamma_1, \gamma_2, \dots, \gamma_n)$ in $\mathbb{R}^n$,

$$\boldsymbol{W}^{\mathbb{R}}_{\boldsymbol{\gamma}} = W^{\mathbb{R},n}_{\gamma_n} \circ \cdots \circ W^{\mathbb{R},1}_{\gamma_1},$$
$$(\operatorname{th} \boldsymbol{t})^{\boldsymbol{\gamma}} = (\operatorname{th} t_n)^{\gamma_n} \cdots (\operatorname{th} t_1)^{\gamma_1},$$

where tanh is abbreviated to th. Let $P(n)$ denote the power set of $\{1, 2, \dots, n\}$ and $P(n)' = P(n) - \{\varnothing\}$. For $I = \{i_1, i_2, \dots, i_l\} \in P(n)'$, let $\boldsymbol{t}_I = (t_{i_1}, t_{i_2}, \dots, t_{i_l})$ and

$$\int_{\boldsymbol{t}_I} f(\boldsymbol{s})\, d\boldsymbol{s}_I = \int_{t_{i_l}}^\infty \cdots \int_{t_{i_1}}^\infty f(\boldsymbol{s})\, ds_{i_1} \cdots ds_{i_l}.$$

Then it follows from Theorem 3.6 in [Kawazoe 2009] that

$$f(\boldsymbol{t}) = c\Delta^{-1/2}(\boldsymbol{t})(\operatorname{th} \boldsymbol{t})^{-(k+1/2)}\bigg(\sum_{\boldsymbol{\gamma}\in\boldsymbol{\Gamma}_1} c_{\boldsymbol{\gamma}} \boldsymbol{W}^{\mathbb{R}}_{-\boldsymbol{\gamma}} DF_f(\boldsymbol{t})(\operatorname{th} \boldsymbol{t})^{\boldsymbol{\gamma}} + \sum_{\boldsymbol{\gamma}\in\boldsymbol{\Gamma}_2, I\in P(n)'} (\operatorname{th} \boldsymbol{t})^{\boldsymbol{\gamma}} \int_{\boldsymbol{t}_I}^\infty \boldsymbol{W}^{\mathbb{R}}_{-\boldsymbol{\gamma}} DF_f(\boldsymbol{s}) A_{\boldsymbol{\gamma}}(\boldsymbol{s}_I, \boldsymbol{t}_I)\, d\boldsymbol{s}_I\bigg), \tag{10}$$

where $D = \prod_{i<j}(\partial_j^2 - \partial_i^2)$ and

$$\boldsymbol{\Gamma}_1 = \{\boldsymbol{\gamma} \in \mathbb{R}^n \mid \gamma_i = \tfrac{1}{2} + l_i,\ 1 \le l_i \le k\},$$
$$\boldsymbol{\Gamma}_2 = \{\boldsymbol{\gamma} \in \mathbb{R}^n \mid \gamma_i = l_i \text{ or } \tfrac{1}{2} + l_i,\ 1 \le l_i \le k\}.$$

Here each l_i is an integer and $l_i = 0$ when $k = 0$. Moreover, there exists a constant c such that for all $\boldsymbol{t} \in \mathbb{R}^n_+$,

$$\int_{\boldsymbol{t}_I}^\infty |A_{\boldsymbol{\gamma}}(\boldsymbol{s}_I, \boldsymbol{t}_I)|\, d\boldsymbol{s}_I \le c. \tag{11}$$

Since D is a differential operator with constant coefficients, by applying the inversion formula (10) to $f * g$, we see from (7) that

$$f * g(\boldsymbol{t}) = c\Delta^{-1/2}(\boldsymbol{t})(\operatorname{th} \boldsymbol{t})^{-(k+1/2)}\bigg(\sum_{\boldsymbol{\gamma}\in\boldsymbol{\Gamma}_1} c_{\boldsymbol{\gamma}} \boldsymbol{W}^{\mathbb{R}}_{-\boldsymbol{\gamma}} DF_f \circledast F_g(\boldsymbol{t})(\operatorname{th} \boldsymbol{t})^{\boldsymbol{\gamma}} + \sum_{\boldsymbol{\gamma}\in\boldsymbol{\Gamma}_2, I\in P(n)'} (\operatorname{th} \boldsymbol{t})^{\boldsymbol{\gamma}} \int_{\boldsymbol{t}_I}^\infty \boldsymbol{W}^{\mathbb{R}}_{-\boldsymbol{\gamma}} DF_f \circledast F_g(\boldsymbol{s}) A_{\boldsymbol{\gamma}}(\boldsymbol{s}_I, \boldsymbol{t}_I)\, d\boldsymbol{s}_I\bigg). \tag{12}$$

3. Multiplier

We shall define some multipliers which will be used to modify the endpoint estimate for the Kunze–Stein phenomenon on SU$(n, n+k)$, $n \ge 2$. Let $\widehat{M}$ and $\widetilde{M}_0$ be the functions on $\mathfrak{a}^*$ defined by

$$\widehat{M}(\boldsymbol{\lambda}) = \prod_{i<j} \sin^2(\lambda_i - \lambda_j)\sin^2(\lambda_i + \lambda_j),$$

$$\widetilde{M}_0(\boldsymbol{\lambda}) = \frac{\widehat{M}(\boldsymbol{\lambda})}{\prod_{i<j}(\lambda_i^2 - \lambda_j^2)} = \prod_{i<j} \frac{\sin^2(\lambda_i - \lambda_j)}{\lambda_i - \lambda_j}\frac{\sin^2(\lambda_i + \lambda_j)}{\lambda_i + \lambda_j}.$$

Let M denote the corresponding multiplier. Since $\widehat{M}$ is W-invariant, according to (6), we need not distinguish the multiplier M for the Fourier transform and the multiplier for the spherical transform. Let M_0 be the multiplier for the Fourier transform. Since the differential operator D corresponds to the Fourier multiplier of $\widetilde{D}(\boldsymbol{\lambda}) = \prod_{i<j}(\lambda_i^2 - \lambda_j^2)$, it follows that

$$\widehat{Mf}(\boldsymbol{\lambda}) = \widehat{M}(\boldsymbol{\lambda})\hat{f}(\boldsymbol{\lambda}) = \widetilde{M}_0(\boldsymbol{\lambda})\widetilde{D}\widetilde{F_f}(\boldsymbol{\lambda}) = (M_0 D F_f)^{\sim}(\boldsymbol{\lambda}).$$

Let χ_0 be the function on $\mathbb{R}$ defined by

$$\chi_0(x) = \begin{cases} \dfrac{\operatorname{sgn} x}{2}\sqrt{\dfrac{\pi}{2}}, & |x| < 2 \\ 0, & |x| \geq 2. \end{cases}$$

Since $\tilde{\chi}_0(\lambda) = \sin^2\lambda/(i\lambda)$, it follows that

$$\widetilde{M}_0(\boldsymbol{\lambda}) = i^{n(n-1)} \prod_{i<j} \tilde{\chi}_0(\lambda_i - \lambda_j)\tilde{\chi}_0(\lambda_i + \lambda_j).$$

Now we show that M_0 is realized in terms of convolution with a compactly supported bounded kernel.

Lemma 3.1. *For each $n \geq 2$, there exists a compactly supported bounded function m_n on $\mathbb{R}^n$ such that*

$$M_0 F = m_n \circledast F. \tag{13}$$

Proof. When $n = 2$, we put

$$m_2(x, y) = -\tfrac{1}{2}\chi_0\Big(\frac{x-y}{2}\Big)\chi_0\Big(\frac{x+y}{2}\Big).$$

Then it follows that

$$\widetilde{m}_2(\lambda_1, \lambda_2) = -\tilde{\chi}_0(\lambda_1 - \lambda_2)\tilde{\chi}_0(\lambda_1 + \lambda_2) = \widetilde{M}_0(\lambda_1, \lambda_2)$$

and thus, $M_0 F = m_2 \circledast F$. Clearly m_2 is a compactly supported bounded function on $\mathbb{R}^2$. When $n = 3$, we put

$$m_3^+(x, y, z) = \frac{i}{2}\chi_0(x)\chi_0\Big(\frac{x+y-z}{2}\Big)\chi_0\Big(\frac{x+y+z}{2}\Big),$$

$$m_3^-(x, y, z) = \frac{1}{2}\chi_0(y)\chi_0\Big(\frac{x-y-z}{2}\Big)\chi_0\Big(\frac{x-y+z}{2}\Big).$$

Then it follows that

$$\widetilde{m}_3^{+}(\lambda_1,\lambda_2,\lambda_3)=i\,\tilde{\chi}_0(\lambda_1-\lambda_2)\tilde{\chi}_0(\lambda_2-\lambda_3)\tilde{\chi}_0(\lambda_2+\lambda_3),$$
$$\widetilde{m}_3^{-}(\lambda_1,\lambda_2,\lambda_3)=\tilde{\chi}_0(\lambda_1+\lambda_2)\tilde{\chi}_0(\lambda_1-\lambda_3)\tilde{\chi}_0(\lambda_1+\lambda_3)$$

and thus, $\widetilde{m}_3^{+}\widetilde{m}_3^{-}=\widetilde{M}_0$. Hence $M_0F=m_3^{+}\circledast m_3^{-}\circledast F=m_3\circledast F$ where $m_3=m_3^{+}\circledast m_3^{-}$. Since each $m_3^{\pm}$ is a compactly supported bounded function on $\mathbb{R}^3$, it follows that m_3 is also compactly supported and bounded on $\mathbb{R}^3$. When $n\geq 4$, we see that $\widetilde{M}_0(\boldsymbol{\lambda})$ is in $L^1(\mathbb{R}^n)$ and of exponential type. Hence, by the Paley–Wiener theorem, there exists a compactly supported bounded function m_n on $\mathbb{R}^n$ satisfying (13). □

In order to obtain a modified estimate (2) by applying the inversion formula (12) to the convolution $f*Mg$, we need to estimate $\boldsymbol{W}^{\mathbb{R}}_{-\boldsymbol{\gamma}}DF_f\circledast MF_g$. We note that, when M is given by (3) and one of the entries γ_i of $\boldsymbol{\gamma}$ equals $k+\frac{1}{2}$, we cannot control the L^∞-norm of $W^{\mathbb{R}}_{-\boldsymbol{\gamma}}MF_g$; see Lemma 3.3. Hence, when $k\geq 1$, we rewrite $\boldsymbol{W}^{\mathbb{R}}_{-\boldsymbol{\gamma}}DF_f\circledast MF_g$ as $\boldsymbol{W}^{\mathbb{R}}_{-\mathbf{1}}DF_f\circledast \boldsymbol{W}^{\mathbb{R}}_{-\boldsymbol{\gamma}+\mathbf{1}}MF_g$, where $\mathbf{1}=(1,1,\dots,1)$. Each factor of this convolution is estimated as follows.

Lemma 3.2. *Let $k\geq 1$. Let $f\in L^1(\Delta)$.*

(i) *For $\mathbf{1}=(1,1,\dots,1)$,*

$$\|\boldsymbol{W}^{\mathbb{R}}_{-\mathbf{1}}DF_f\|_{L^1(\mathbb{R}^n_+)}\leq c\|f\|_{L^1(\sqrt{\Delta})}.$$

(ii) *For $\boldsymbol{\gamma}=(\gamma_1,\gamma_2,\dots,\gamma_n)$ with $1\leq\gamma_i\leq k+\frac{1}{2}$,*

$$\|\boldsymbol{W}^{\mathbb{R}}_{-\boldsymbol{\gamma}+\mathbf{1}}DF_f\|_{L^\infty(\mathbb{R}^n_+)}\leq c\|f\|_{L^1((\operatorname{th}\boldsymbol{x})^{\boldsymbol{\gamma}_k}\sqrt{\Delta})},$$

where $\boldsymbol{\gamma}_k=\big(k+\frac{1}{2}-\gamma_1,k+\frac{1}{2}-\gamma_2,\dots,k+\frac{1}{2}-\gamma_n\big)$.

Proof. It follows from (8) that

$$DF_f(\boldsymbol{t})=c(W_k^{1,n}\circ\cdots\circ W_k^{1,1})\circ(W_{1/2}^{2,n}\circ\cdots\circ W_{1/2}^{2,1})(f\omega)(\boldsymbol{t})$$
$$=c(W_k^{1,n}\circ W_{1/2}^{2,n})\circ\cdots\circ(W_k^{1,1}\circ W_{1/2}^{2,1})(f\omega)(\boldsymbol{t}). \tag{14}$$

We recall, for even functions u on $\mathbb{R}$, that $cW_k^1\circ W_{1/2}^2(u)(t)$ is the Abel transform F_u on SU$(1,1+k)$. Therefore, from Propositions 3 and 4 in [Kawazoe 2018] with $\alpha=k$ and $\rho=k+1$ for the Jacobi hypergroup it follows that

$$\|W^{\mathbb{R}}_{-1}F_u\|_{L^1(\mathbb{R}_+)}\leq c\|u\|_{L^1((\operatorname{th}x)^{2k+1}e^{(k+1)x})},$$
$$\|W^{\mathbb{R}}_{-\gamma}F_u\|_{L^\infty(\mathbb{R}_+)}\leq c\|u\|_{L^1((\operatorname{th}x)^{2k-\gamma}e^{(k+1)x})}$$

for $0\leq\gamma<k+\frac{1}{2}$. Here the weight functions satisfy $(\operatorname{th}x)^{2k+1}e^{(k+1)x}\leq\sqrt{\sigma_{1,k}}$ and $(\operatorname{th}x)^{2k-\gamma}e^{(k+1)x}=(\operatorname{th}x)^{k-1/2-\gamma}\sqrt{\sigma_{1,k}}$. Since $\prod_{i=1}^n\sqrt{\sigma_{1,k}(t_i)}=\omega(\boldsymbol{t})^{-1}\sqrt{\Delta(\boldsymbol{t})}$, applying these estimates to $W^{\mathbb{R},i}_{-\gamma_i+1}(W_k^{1,i}\circ W_{1/2}^{2,i})(f\omega)$ repeatedly (see (14)), we can deduce the desired results. □

Lemma 3.3. *Let $k \geq 1$ and $\boldsymbol{\gamma}$, $\boldsymbol{\gamma}_k$ be as above. Let $f \in L^1(\Delta)$. Then*

$$\|\boldsymbol{W}^{\mathbb{R}}_{-\boldsymbol{\gamma}+\mathbf{1}} MF_f\|_{L^\infty(\mathbb{R}^n_+)} \leq c\|f\|_{L^1((\mathrm{th}\,\boldsymbol{x})^{\boldsymbol{\gamma}_k}\sqrt{\Delta})}. \tag{15}$$

Proof. It follows from (13) and Lemma 3.2 (ii) that

$$\begin{aligned}\|\boldsymbol{W}^{\mathbb{R}}_{-\boldsymbol{\gamma}+\mathbf{1}} MF_f\|_{L^\infty(\mathbb{R}^n_+)} &= \|\boldsymbol{W}^{\mathbb{R}}_{-\boldsymbol{\gamma}+\mathbf{1}} M_0 DF_f\|_{L^\infty(\mathbb{R}^n_+)} = \|m_n \circledast \boldsymbol{W}^{\mathbb{R}}_{-\boldsymbol{\gamma}+\mathbf{1}} DF_f\|_{L^\infty(\mathbb{R}^n_+)} \\ &\leq \|m_n\|_{L^1(\mathbb{R})}\|\boldsymbol{W}^{\mathbb{R}}_{-\boldsymbol{\gamma}+\mathbf{1}} DF_f\|_{L^\infty(\mathbb{R}^n_+)} \leq c\|f\|_{L^1((\mathrm{th}\,\boldsymbol{x})^{\boldsymbol{\gamma}_k}\sqrt{\Delta})}. \quad \square\end{aligned}$$

Proposition 3.4. *Let $f, g \in L^1(\Delta)$. Suppose $k \geq 1$. Then for each $\boldsymbol{\gamma} \in \Gamma_1$ and Γ_2,*

$$\|\boldsymbol{W}^{\mathbb{R}}_{-\boldsymbol{\gamma}} DF_f \circledast MF_g\|_{L^\infty(\mathbb{R}^n_+)} \leq c\|f\|_{L^1(\sqrt{\Delta})}\|g\|_{L^1(\sqrt{\Delta})}.$$

When $k = 0$, the same estimate holds under the assumption that f, g are supported in $[1, \infty)^n$.

Proof. First we suppose that $k \geq 1$. Since $1 \leq \gamma_i \leq k + \frac{1}{2}$ for all $\boldsymbol{\gamma} = (\gamma_i) \in \Gamma_j$, $j = 1, 2$, it follows from Lemmas 3.2 (i) and 3.3 that

$$\begin{aligned}\|\boldsymbol{W}^{\mathbb{R}}_{-\boldsymbol{\gamma}} DF_f \circledast MF_g\|_{L^\infty(\mathbb{R}^n_+)} &= \|\boldsymbol{W}^{\mathbb{R}}_{-\mathbf{1}} DF_f \circledast \boldsymbol{W}^{\mathbb{R}}_{-\boldsymbol{\gamma}+\mathbf{1}} MF_g\|_{L^\infty(\mathbb{R}^n_+)} \\ &\leq \|\boldsymbol{W}^{\mathbb{R}}_{-\mathbf{1}} DF_f\|_{L^1(\mathbb{R}^n_+)}\|\boldsymbol{W}^{\mathbb{R}}_{-\boldsymbol{\gamma}+\mathbf{1}} MF_g\|_{L^\infty(\mathbb{R}^n_+)} \\ &\leq c\|f\|_{L^1(\sqrt{\Delta})}\|g\|_{L^1(\sqrt{\Delta})}.\end{aligned}$$

Next let $k = 0$. Then it follows that $\gamma_i = \frac{1}{2}$ for $\boldsymbol{\gamma} = (\gamma_i) \in \Gamma_1$ and $\gamma_i = 0$ or $\frac{1}{2}$ for $\boldsymbol{\gamma} = (\gamma_i) \in \Gamma_2$, and

$$\begin{aligned}\|\boldsymbol{W}^{\mathbb{R}}_{-\boldsymbol{\gamma}} DF_f \circledast MF_g\|_{L^\infty(\mathbb{R}^n_+)} &= \|\boldsymbol{W}^{\mathbb{R}}_{-\boldsymbol{\gamma}} DF_f \circledast m_n \circledast DF_g\|_{L^\infty(\mathbb{R}^n_+)} \\ &\leq \|\boldsymbol{W}^{\mathbb{R}}_{-\boldsymbol{\gamma}} DF_f \circledast DF_g\|_{L^\infty(\mathbb{R}^n_+)}\|m_n\|_{L^1(\mathbb{R}^n)} \\ &\leq c\|\boldsymbol{W}^{\mathbb{R}}_{-\boldsymbol{\gamma}} DF_f \circledast DF_g\|_{L^\infty(\mathbb{R}^n_+)}.\end{aligned}$$

Similarly as in the proof of Lemma 3.2, we use (14) to estimate the L^∞-norm of $\boldsymbol{W}^{\mathbb{R}}_{-\boldsymbol{\gamma}} DF_f \circledast DF_g$. We note that each $W^{2,i}_{1/2}$ is the Abel transform on SU(1, 1). For even functions u, v on $\mathbb{R}$ supported in $[1, \infty)$, let F_u, F_v denote their Abel transforms on SU(1, 1). Then, letting $\alpha = 0$ in the case of (iii) in [Kawazoe 2018, §7], we see that for $\delta = 0, \frac{1}{2}$,

$$\|W^{\mathbb{R}}_{-\delta} F_u \circledast F_v\|_{L^\infty(\mathbb{R}_+)} \leq c\|u\|_{L^1(\sqrt{\sigma_{1,k}})}\|v\|_{L^1(\sqrt{\sigma_{1,k}})}.$$

Hence, applying these estimates to $W^{\mathbb{R},i}_{-\gamma_i}\big(W^{2,i}_{1/2}(f\omega) \circledast W^{2,i}_{1/2}(g\omega)\big)$ repeatedly (see (14)), we can deduce that

$$\|\boldsymbol{W}^{\mathbb{R}}_{-\boldsymbol{\gamma}} DF_f \circledast DF_g\|_{L^\infty(\mathbb{R}_+)} \leq c\|f\|_{L^1(\sqrt{\Delta})}\|g\|_{L^1(\sqrt{\Delta})}. \tag{16}$$

Hence the desired result follows. $\square$

4. A version of the endpoint estimate

Now we shall give a version of the endpoint estimate of the Kunze–Stein phenomenon on SU(n, m).

Theorem 4.1. *Let $G = \mathrm{SU}(n, m)$ $(m \ge n \ge 2)$ and M be the multiplier defined by* (3). *Let $f, g \in L^{2,1}(\Delta)$. Then*

$$\|f * Mg\|_{L^{2,\infty}(\Delta)} \le c\|f\|_{L^{2,1}(\Delta)}\|g\|_{L^{2,1}(\Delta)}.$$

Proof. Similarly as in the proof of [Liu 2005], by the duality of Lorentz spaces, it suffices to prove that for all $h \in L^{2,1}(\Delta)$,

$$\left|\int f * Mg(\boldsymbol{x})h(\boldsymbol{x})\Delta(\boldsymbol{x})\,d\boldsymbol{x}\right| \le c\|f\|_{L^{2,1}(\Delta)}\|g\|_{L^{2,1}(\Delta)}\|h\|_{L^{2,1}(\Delta)}. \tag{17}$$

Moreover, we may suppose that f, g, h are supported in $[1, \infty)^n$. Actually, we decompose each f, g, h as the sum of the local and the global parts. Then the left-hand side of (17) is divided into 8 integrals. Any of integrals containing the local part, say f_0 where $f = f_0 + f_1$, $\mathrm{supp}(f_0) \subset [0, 1]$ and $\mathrm{supp}(f_1) \subset [1, \infty)$, is estimated as

$$\begin{aligned}\left|\int f_0 * Mg(\boldsymbol{x})h(\boldsymbol{x})\Delta(\boldsymbol{x})\,d\boldsymbol{x}\right| &= \left|M(f_0 * g * h)(0)\right| = \left|(f_0 * g) * Mh(0)\right|\\ &= \|f_0 * g\|_{L^2(\Delta)}\|Mh\|_{L^2(\Delta)}\\ &\le \|f_0\|_{L^1(\Delta)}\|g\|_{L^2(\Delta)}\|h\|_{L^2(\Delta)}\\ &\le \left(\int_{[0,1]^n}\Delta(\boldsymbol{x})\,d\boldsymbol{x}\right)^{\frac12}\|f\|_{L^2(\Delta)}\|g\|_{L^2(\Delta)}\|h\|_{L^2(\Delta)},\end{aligned}$$

because $\widehat{M}$ is bounded. Since $L^{2,1}(\Delta) \subset L^2(\Delta)$, the desired estimate follows. Now we suppose that f, g, h are supported in $[1, \infty)^n$. It follows from (12) that

$$\begin{aligned}\int f{*}Mg(\boldsymbol{x})h(\boldsymbol{x})\Delta(\boldsymbol{x})\,d\boldsymbol{x} \sim \sum_{\gamma\in\boldsymbol{\Gamma}_1}\int \boldsymbol{W}^{\mathbb{R}}_{-\boldsymbol{\gamma}}(DF_f \circledast MF_g)(\boldsymbol{x})H(\boldsymbol{x})\,d\boldsymbol{x}\\ + \sum_{\boldsymbol{\gamma}\in\boldsymbol{\Gamma}_2, S\in P(n)'}\int\left(\int_{t_S}^{\infty}\boldsymbol{W}^{\mathbb{R}}_{-\boldsymbol{\gamma}}(DF_f \circledast MF_g)(\boldsymbol{s})A_{\boldsymbol{\gamma}}(s_S, \boldsymbol{x}_S)\,d\boldsymbol{s}_S\right)H(\boldsymbol{x})\,d\boldsymbol{x},\end{aligned}$$

where $H(\boldsymbol{x}) = h(\boldsymbol{x})\sqrt{\Delta(\boldsymbol{x})}$. Since

$$\|\boldsymbol{W}^{\mathbb{R}}_{-\boldsymbol{\gamma}}(DF_f \circledast MF_g)\|_{L^\infty(\mathbb{R}^n_+)} \le c\|f\|_{L^1(\sqrt{\Delta})}\|g\|_{L^1(\sqrt{\Delta})}$$

by Proposition 3.4, it follows from (11) that

$$\left|\int f * g(\boldsymbol{x})h(\boldsymbol{x})\Delta(\boldsymbol{x})\,d\boldsymbol{x}\right| \le c\|f\|_{L^1(\sqrt{\Delta})}\|g\|_{L^1(\sqrt{\Delta})}\|h\|_{L^1(\sqrt{\Delta})}. \tag{18}$$

If a function a is supported in $[1,\infty)^n$, then it follows that

$$\|a\|_{L^1(\sqrt{\Delta})} \le c\|a\|_{L^1(e^{\rho(x)})} \le c\|a\|_{L^{2,1}(e^{2\rho(x)})} \le c\|a\|_{L^{2,1}(\Delta)};$$

see [Ionescu 2000, Lemma 3; Kawazoe and Liu 2018, Lemma 2]. Therefore, (17) follows from (18). □

5. A remark on the Abel transform

In the process of obtaining the modified endpoint estimate in Theorem 4.1 the key is (15) if $k \ge 1$ and (16) if $k = 0$. When $n = 1$, since M and D are identity operators, these inequalities hold and thus, the original endpoint estimate follows without modification; see [Kawazoe 2018, §7]. Similarly, when $n \ge 2$ and $k \ge 1$, if $f \in L^1(\Delta)$, which is supported in $[1,\infty)^n$, satisfies

$$\|\boldsymbol{W}^{\mathbb{R}}_{-\boldsymbol{\gamma}+\boldsymbol{1}} F_f\|_{L^\infty(\mathbb{R}^n_+)} \le c\|f\|_{L^1(\sqrt{\Delta})}, \tag{19}$$

then the endpoint estimate holds without modification. We note that $\boldsymbol{\gamma}-\boldsymbol{1}$ for $\boldsymbol{\gamma} \in \Gamma_2$ have the opportunity to be $(0, 0, \dots, 0)$. Therefore, to obtain the endpoint estimate without modification by our process, at least, $f \in L^1(\Delta)$, which is supported in $[1,\infty)^n$, satisfies

$$\|F_f\|_{L^\infty(\mathbb{R}^n_+)} \le c\|f\|_{L^1(\sqrt{\Delta})}. \tag{20}$$

We calculate the Abel transform F_f explicitly and show that the estimate (20) might be not true.

First we obtain the kernel function $A(\boldsymbol{s},\boldsymbol{t})$ of $\Delta(\boldsymbol{t})\phi_{\boldsymbol{\lambda}}(\boldsymbol{t})$; see (4). The spherical function $\phi_{\boldsymbol{\lambda}}(\boldsymbol{t})$ on $\mathrm{SU}(n, n+k)$ is explicitly given by

$$\phi_{\boldsymbol{\lambda}}(\boldsymbol{t}) = \frac{c}{\prod_{i<j}(\lambda_i^2-\lambda_j^2)}\frac{\det(\phi_{\lambda_i}(t_j))}{\omega(\boldsymbol{t})},$$

where $\phi_\lambda(t)$ is the spherical function on $\mathrm{SU}(1, 1+k)$; see [Hoogenboom 1982, §4; Meaney 1986, (13)]. Then

$$\Delta(\boldsymbol{t})\phi_{\boldsymbol{\lambda}}(\boldsymbol{t}) = \frac{c\sigma(\boldsymbol{t})\omega(\boldsymbol{t})}{\prod_{i<j}(\lambda_i^2-\lambda_j^2)}\det(\phi_{\lambda_i}(t_j)).$$

Since $\sigma(\boldsymbol{t}) = 2^{n(2k+1)}\prod_{i=1}^n(\sinh^{2k}(t_i)\sinh(2t_i)) = \sigma_{1,k}(t_1)\cdots\sigma_{1,k}(t_n)$ and, as a function of λ_i, $\sigma_{1,k}(t_j)\phi_{\lambda_i}(t_j)$ is the Fourier transform of a compactly supported function on $\mathbb{R}_+$ such as

$$\sigma_{1,k}(t_j)\phi_{\lambda_i}(t_j) = \int_0^{t_j} A_{k,0}(s,t_j)\cos(\lambda_i s)\,ds$$

(see [Koornwinder 1975, (2.16)]), it follows that

$$\sigma(\boldsymbol{t})\det(\phi_{\lambda_i}(t_j)) = \int_0^{t_1}\int_0^{t_2}\cdots\int_0^{t_n} A_{k,0}(s_1,t_1)A_{k,0}(s_2,t_2)\cdots A_{k,0}(s_n,t_n) \times \det(\cos(\lambda_i s_j))\,ds_n\cdots ds_2\,ds_1$$

(see [Meaney 1985, (5.10)]). Let us suppose that $n=2$. Then we see that

$$\begin{aligned}
&\det(\cos(\lambda_i s_j))\\
&= \begin{vmatrix}\cos(\lambda_1 s_1) & \cos(\lambda_1 s_2)\\ \cos(\lambda_2 s_1) & \cos(\lambda_2 s_2)\end{vmatrix} = \begin{vmatrix}\cos(\lambda_1 s_1) & \cos(\lambda_1 s_2)\\ \cos(\lambda_2 s_1)-\cos(\lambda_1 s_1) & \cos(\lambda_2 s_2)-\cos(\lambda_1 s_2)\end{vmatrix}\\
&= \tfrac12(\lambda_1^2-\lambda_2^2)\\
&\quad\times\begin{vmatrix}\cos(\lambda_1 t_1) & \cos(\lambda_1 t_2)\\ \dfrac{\sin\big(\frac12(\lambda_2+\lambda_1)s_1\big)}{\frac12(\lambda_2+\lambda_1)}\dfrac{\sin\big(\frac12(\lambda_2-\lambda_1)s_1\big)}{\frac12(\lambda_2-\lambda_1)} & \dfrac{\sin\big(\frac12(\lambda_2+\lambda_1)s_2\big)}{\frac12(\lambda_2+\lambda_1)}\dfrac{\sin\big(\frac12(\lambda_2-\lambda_1)s_2\big)}{\frac12(\lambda_2-\lambda_1)}\end{vmatrix}.
\end{aligned}$$

On the other hand, we note that

$$\begin{aligned}
&\frac{1}{2\pi}\iint_{|u+v|\le t_1,\,|u-v|\le t_2}\frac{\pi}{2}e^{-i(\lambda_1 u+\lambda_2 v)}\,du\,dv\\
&\quad=\frac12\frac{1}{\sqrt{2\pi}}\int_{|s|\le t_1}\sqrt{\frac{\pi}{2}}e^{-i\left(\frac12(\lambda_1+\lambda_2)s\right)}\,ds\frac{1}{\sqrt{2\pi}}\int_{|t|\le t_2}\sqrt{\frac{\pi}{2}}e^{-i\left(\frac12(\lambda_1-\lambda_2)t\right)}\,dt\\
&\quad=\frac12\frac{\sin\big(\frac12(\lambda_2+\lambda_1)t_1\big)}{\frac12(\lambda_2+\lambda_1)}\frac{\sin\big(\frac12(\lambda_2-\lambda_1)t_2\big)}{\frac12(\lambda_2-\lambda_1)}.
\end{aligned}$$

Hence, if we set

$$\chi_{s,t}(x,y)=\begin{cases}\frac{\pi}{2}, & |x-y|\le s,\ |x+y|\le t,\\ 0, & \text{otherwise,}\end{cases}$$

then we see that

$$\det(\cos(\lambda_i s_j)) = (\lambda_1^2-\lambda_2^2)\begin{vmatrix}\cos(\lambda_1 s_1) & \cos(\lambda_1 s_2)\\ \tilde\chi_{s_1,s_1}(\lambda_1,\lambda_2) & \tilde\chi_{s_2,s_2}(\lambda_1,\lambda_2)\end{vmatrix}.$$

Therefore, it follows that

$$\Delta(\boldsymbol{t})\phi_{\boldsymbol\lambda}(\boldsymbol{t}) = c\omega(\boldsymbol{t})\int_0^{t_1}\int_0^{t_2}A_{k,0}(s_1,t_1)A_{k,0}(s_2,t_2) \times\begin{vmatrix}\cos(\lambda_1 s_1) & \cos(\lambda_1 s_2)\\ \tilde\chi_{s_1,s_1}(\lambda_1,\lambda_2) & \tilde\chi_{s_2,s_2}(\lambda_1,\lambda_2)\end{vmatrix}\,ds_2\,ds_1.$$

Here, regarding $A_{k,0}(s_1, t_1)$ as an even function of s_1, we see that

$$\begin{aligned}\int_0^{t_1}\int_0^{t_2} A_{k,0}(s_1,t_1)A_{k,0}(s_2,t_2)\cos(\lambda_1 s_1)\tilde{\chi}_{s_2,s_2}(\lambda_1,\lambda_2)\,ds_1\,ds_2 \\ = \sqrt{\frac{\pi}{2}}\mathcal{F}_1(\chi_{t_1}A_{k,0}(\cdot,t_1))(\lambda_1)\int_0^{t_2} A_{k,0}(s_2,t_2)\tilde{\chi}_{s_2,s_2}(\lambda_1,\lambda_2)\,ds_2 \\ = \left(\sqrt{\frac{\pi}{2}}\int_0^{t_2} A_{k,0}(s,t_2)(\chi_{t_1}A_{k,0}(\cdot,t_1))\circledast_1\chi_{s,s}\,ds\right)^{\sim}(\lambda_1,\lambda_2),\end{aligned}$$

where $\mathcal{F}_1$ and $\circledast_1$ denote respectively the Fourier transform and the convolution with respect to the first variable. Hence the above function is the Fourier transform of

$$\sqrt{\frac{\pi}{2}}\int_0^{t_2} A_{k,0}(s,t_2)\left(\int_{-\infty}^{\infty}(\chi_{t_1}A_{k,0})(u,t_1)\chi_{s,s}(x_1-u,x_2)\,du\right)ds.$$

Since $|x_1-u+x_2|<s$ and $|x_1-u-x_2|<s$ yield that $x_1+x_2-s<u<x_1-x_2+s$ and $x_2<s$, this integral is equal to

$$H(x_1,x_2,t_1,t_2)=\sqrt{\frac{\pi}{2}}\int_{x_2}^{t_2} A_{k,0}(s,t_2)\left(\int_{x_1+x_2-s}^{x_1-x_2+s}(\chi_{t_1}A_{k,0})(u,t_1)\,du\right)ds. \tag{21}$$

Finally, we can deduce that

$$\Delta(\boldsymbol{t})\phi_{\boldsymbol{\lambda}}(\boldsymbol{t}) = c\omega(\boldsymbol{t})(H(\cdot\,,\,\cdot\,,t_1,t_2)-H(\cdot\,,\,\cdot\,,t_2,t_1))^{\sim}(\lambda_1,\lambda_2) \tag{22}$$

and thus,

$$A(\boldsymbol{x},\boldsymbol{t}) = c\omega(t_1,t_2)(H(x_1,x_2,t_1,t_2)-H(x_1,x_2,t_2,t_1)). \tag{23}$$

It is quite clear that, as a function of (x_1,x_2), this function is supported on $[-(t_1+t_2), t_1+t_2]\times[-(t_1+t_2), t_1+t_2]$. Since $A_{k,0}(s,t)$ on $\mathbb{R}_+^2$ satisfies

$$|A_{k,0}(s,t)|\le ce^{1/2t}\sinh t(\cosh t-\cosh s)^{k-1/2}\sim(\mathrm{th}\,t)^{k-1/2}\sqrt{\sigma_{1,k}(t)}$$

(see [Koornwinder 1975, (2.19)]), it follows from (21) and (23) that

$$|A(\boldsymbol{x},\boldsymbol{t})|\le ct_1t_2(\mathrm{th}\,t_1)^{k-1/2}(\mathrm{th}\,t_2)^{k-1/2}\sqrt{\Delta}(\boldsymbol{t}).$$

Hence we see from (5) that

$$\|F_f\|_{L^\infty(\mathbb{R}_+^n)}\le c\|f\|_{L^1(x_1x_2\sqrt{\Delta}(\boldsymbol{x}))}.$$

Therefore, (20) might be not true.

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MABUCHI METRICS AND PROPERNESS OF THE MODIFIED DING FUNCTIONAL

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In this paper, we study Mabuchi metrics on Fano manifolds. We prove that Mabuchi metrics exist if and only if the modified Ding functional is proper modulo the automorphism group. As an application, we establish a criterion for the existence of Mabuchi metrics on Fano group compactifications.

1. Introduction

The existence of canonical metrics has been a fundamental and longstanding problem in Kähler geometry. On Fano manifolds, Kähler–Einstein metrics have been studied extensively. The most remarkable progress is the resolution of Yau–Tian–Donaldson conjecture which relates the existence of Kähler–Einstein metrics to the K-stability of the Fano manifold [Tian 2015; Chen et al. 2015a; 2015b; 2015c]. It has been known early in the 1980s that the existence of Kähler–Einstein metrics fails when the Fano manifold has nonvanishing Futaki invariant. In this case, other canonical metrics, such as extremal metrics and Kähler–Ricci solitons have attracted much attention.

Mabuchi [2001a; 2001b; 2002; 2003] studied a generalized Kähler–Einstein metric, which is neither an extremal metric nor a Kähler–Ricci soliton. Following [Yao 2017], we call this metric the *Mabuchi metric* for simplicity. Let M be a compact Fano manifold of complex dimension n. Let

$$\omega = \sqrt{-1} g_{i\bar{j}}\, dz^i \wedge d\bar{z}^j \in 2\pi c_1(M)$$

be a Kähler metric and h_ω be its Ricci potential. ω is a Mabuchi metric if

$$X_\omega := -\sqrt{-1} g^{i\bar{j}} \frac{\partial e^{h_\omega}}{\partial \bar{z}^j} \frac{\partial}{\partial z^i} \tag{1-1}$$

is holomorphic [Mabuchi 2001a]. The uniqueness of Mabuchi metrics has been proved in [Mabuchi 2003]. Recently, Donaldson [2017] introduced a new GIT

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(geometric invariant theory) picture, in which the corresponding moment map is given by the Ricci potential. Then Yao [2017] observed that in this picture X_ω is holomorphic if and only if ω is a critical point of the norm square of the moment map, given by the following energy

$$\mathscr{E}^D(\omega) = \int_M (e^{h_\omega} - 1)^2 \omega^n. \tag{1-2}$$

This brings new interest in the study of Mabuchi metrics. On toric Fano manifolds, the notion of relative Ding stability has been introduced by Yao [2017]. He has also established the existence of Mabuchi metrics when the toric Fano manifold is relatively Ding stable. The purpose of this paper is to discuss the existence of Mabuchi metrics on general Fano manifolds through properness of energy functionals.

According to [Mabuchi 2001a], if ω is a Mabuchi metric, then (1-1) coincides with the extremal vector field [Futaki and Mabuchi 1995]. To state the main results, we first recall notions on the extremal vector field. Denote by $\mathrm{Aut}_0(M)$ the identity component of its holomorphic transformation group. Its Lie algebra $\eta(M)$ consists of all holomorphic vector fields on M. $\mathrm{Aut}_0(M)$ admits a semidirect decomposition

$$\mathrm{Aut}_0(M) = \mathrm{Aut}_r(M) \propto R_u,$$

where $\mathrm{Aut}_r(M) \subset \mathrm{Aut}_0(M)$ is a reductive group and R_u is the unipotent radical of $\mathrm{Aut}_0(M)$. Denote by $\eta_r(M)$ the reductive part of $\eta(M)$. For any $v \in \eta(M)$, let K_v be the one parameter group generated by the image part $\mathrm{Im}(v)$. For a Kähler metric $\omega_0 \in 2\pi c_1(M)$, by Hodge theorem, there is a unique normalized potential given by

$$i_v\omega_0 = \sqrt{-1}\bar\partial\theta_v(\omega_0), \qquad \int_M \theta_v(\omega_0)\omega_0^n = 0. \tag{1-3}$$

Then $\theta_v(\omega)$ is real valued if and only if ω is K_v-invariant. For any

$$\phi \in \mathscr{H}_v(\omega_0) := \{\phi \in C^\infty(M) \mid \omega_\phi := \omega_0 + \sqrt{-1}\partial\bar\partial\phi > 0,\ \phi \text{ is } K_v\text{-invariant}\},$$

the normalized potential $\theta_v(\omega_\phi) = \theta_v(\omega_0) + v(\phi)$. Denoted by $\mathrm{Fut}(v)$ the Futaki invariant of $v \in \eta(M)$. The extremal vector field X is the holomorphic vector field uniquely determined by [Futaki and Mabuchi 1995]

$$\mathrm{Fut}_X(v) := \mathrm{Fut}(v) + \int_M \theta_v(\omega_0)\theta_X(\omega_0)\omega_0^n = 0, \quad \text{for all } v \in \eta(M). \tag{1-4}$$

Moreover, $X \in \eta_c(M)$, the center of $\eta_r(M)$ and K_X lies in a compact Lie group.

From now on, we assume that ω_0 is K_X-invariant unless otherwise claimed. As pointed by Mabuchi [2003], both $\min_M \theta_X(\omega_\phi)$ and $\max_M \theta_X(\omega_\phi)$ are independent of the choice of $\omega_\phi \in 2\pi c_1(M)$. For convenience, we write

$$c_X := \min_M\{1 - \theta_X(\omega_\phi)\}, \quad C_X := \max_M\{1 - \theta_X(\omega_\phi)\}.$$

By [Mabuchi 2001a], Mabuchi metrics exist only if $c_X > 0$, and $\omega_\phi \in 2\pi c_1(M)$ is a Mabuchi metric if

$$\text{Ric}(\omega_\phi) - \omega_\phi = \sqrt{-1}\partial\bar{\partial}\log(1-\theta_X(\omega_\phi)). \tag{1-5}$$

Tian [1997] introduced the notion of properness of energy functionals as an analytic characterization of existence of Kähler-Einstein metrics. When the automorphism group of M is not discrete, a notion of properness modulo a subgroup of $\text{Aut}_0(M)$ was reformulated [Cao et al. 2005; Darvas and Rubinstein 2017; Tian 1996; Zhou and Zhu 2008]. In particular, Darvas and Rubinstein [2017] established a properness principle and solved Tian's properness conjecture. It is natural to ask the analogous problem for Mabuchi metrics. By [Mabuchi 2001b], the Mabuchi metric is a critical point of the following *modified Ding functional*

$$\mathfrak{D}_X(\phi) = -\frac{1}{V}\int_0^1\int_M \dot{\phi}_s(1-\theta_X(\omega_{\phi_s}))\,\omega_{\phi_s}^n \wedge ds - \log\left(\frac{1}{V}\int_M e^{h_0-\phi}\omega_0^n\right), \tag{1-6}$$

where $V = \int_M \omega_0^n$, $\{\phi_s\}_{s\in[0,1]}$ is any smooth path in $\mathcal{H}_X(\omega_0)$ joining 0 and ϕ, and h_0 is the Ricci potential of ω_0, normalized by

$$\int_M e^{h_0}\omega_0^n = \int_M \omega_0^n.$$

In view of [Cao et al. 2005; Darvas and Rubinstein 2017; Tian 1997; 1996; Zhou and Zhu 2008], we have the following definition of properness.

Definition 1.1. Suppose H^c is a reductive subgroup (which is the complexification of a compact Lie group H) of $\text{Aut}_0(M)$ which contains K_X. The modified Ding functional $\mathfrak{D}_X(\cdot)$ is said to be *proper modulo H^c* if there exists an increasing function $f(t) \geq -c$ for $t \in \mathbb{R}$ and some constant $c \geq 0$ such that $\lim_{t\to+\infty} f(t) = +\infty$ and

$$\mathfrak{D}_X(\phi) \geq \inf_{\sigma\in H^c} f(I_X(\phi_\sigma) - J_X(\phi_\sigma)),$$

where ϕ_σ is defined by $\sigma^*(\omega_\phi) = \omega_0 + \sqrt{-1}\partial\bar{\partial}\phi_\sigma$. I_X and J_X are modified Aubin functionals (see Section 2B).

Our first main result is the following properness theorem.

Theorem 1.2. *Suppose $c_X > 0$ and $\text{Aut}_0^X(M)$ is the centralizer of K_X^c in $\text{Aut}_0(M)$. Then M admits Mabuchi metrics if and only exists $C, C' > 0$, such that*

$$\mathfrak{D}_X(\phi) \geq C \inf_{\sigma\in\text{Aut}_0^X(M)} J_X(\phi_\sigma) - C', \quad \textit{for all } \phi \in \mathcal{H}_X(\omega_0).$$

Remark 1.3. One can show that the existence of Mabuchi metric implies the properness of $\mathfrak{D}_X(\cdot)$ modulo the automorphism group of M following the arguments for Kähler–Ricci solitons [Cao et al. 2005]. However, the theorem gives an optimal properness can be obtained by using the properness principle of Darvas and Rubinstein [2017].

Remark 1.4. Suppose ω_0 is a Mabuchi metric on M. We can define

$$\Lambda_{1,X}=\Big\{u\in C^\infty(M)\;\Big|\;\triangle_{\omega_0}u-\frac{X}{1-\theta_X(\omega_0)}u=-u\Big\}. \tag{1-7}$$

Then by the similar argument as in [Wang et al. 2016, Lemma 3.2], one can show that the properness modulo $\mathrm{Aut}_0^X(M)$ is equivalent to the properness for Kähler potentials that are perpendicular to $\Lambda_{1,X}$ with respect to the weighted inner product

$$(\varphi,\psi)=\int_M \varphi\psi(1-\theta_X(\omega_0))\omega_0^n.$$

The properness condition can be verified for some special Fano manifolds. A characterization for the properness of the modified Ding functional on toric Fano manifolds has been given by [Nakamura 2017]. We consider more general Fano group compactifications by using the ideas of [Li et al. 2018], in which the modified K-energy is discussed. Let G be a connected, complex reductive group of dimension n, we call M a *(biequivariant) compactification of* G if it admits a holomorphic $G\times G$ action on M with an open and dense orbit isomorphic to G as a $G\times G$-homogeneous space [Alexeev and Katzarkov 2005; Delcroix 2017a]. (M, L) is called a *polarized compactification* of G if L is a $G\times G$-linearized ample line bundle on M. In particular, when $L=-K_M$, we call M a *Fano group compactification*. We establish the criterion for the existence of Mabuchi metrics on Fano group compactifications.

Theorem 1.5. *Let $(M,-K_M)$ be a Fano compactification of G and P be the associated polytope. Then M admits Mabuchi metrics if and only if $c_X>0$ and*

$$\boldsymbol{b}_X-4\rho\in\Xi, \tag{1-8}$$

where

$$\boldsymbol{b}_X=\frac{1}{V}\int_{2P_+} y[1-\theta_X(y)]\pi(y)\,dy,$$

$$\pi(y)=\prod_{\alpha\in\Phi_+}\langle\alpha,y\rangle^2,\quad V=\int_{2P_+}\pi(y)\,dy,$$

Ξ is the relative interior of the cone generated by positive roots Φ_+, $\rho=\frac{1}{2}\sum_{\alpha\in\Phi_+}\alpha$ and $\theta_X(y)$ is the normalized potential of X viewed as a function on $2P_+$, which will be described in Lemma 4.2 below. For notation on group compactifications, see *Section 2C.*

The paper is organized as follows: In Section 2, we first review some preliminaries on energy functionals and the definition of properness modulo an automorphism group. Then we recall basic properties of polarized compactifications. Theorem 1.2 will be proved in Section 3. In Section 4, we obtain Theorem 1.5. The sufficient part will be proved by the verification of properness of the modified Ding functional.

2. Preliminaries

In this section, we first review the notions of energy functionals associated to Mabuchi metrics. Then we recall the basic knowledge for group compactifications for later use.

2A. ***Reduction to the complex Monge–Ampère equations.*** It is clear that (1-5) is equivalent to the following equation

$$\omega_\phi^n(1-\theta_X(\omega_\phi)) = \omega_0^n e^{h_0-\phi}. \tag{2-1}$$

We consider the following continuity path

$$\omega_{\phi_t}^n(1-\theta_X(\omega_{\phi_t})) = \omega_0^n e^{h_0-t\phi_t}, \quad t\in[0,1]. \tag{2-2}$$

Let $\mathfrak{I} := \{t\in[0,1] \mid \text{(2-2) has a solution for } t\}$. Then $\mathfrak{I}$ is open by the implicit function theorem. For the starting point $t=0$, we have

Theorem 2.1. *When $c_X>0$,* (2-2) *has a solution at $t=0$.*

Since we did not find a reference for this result, we give a proof of it for completeness in the Appendix. Hence, $0\in\mathfrak{I}$ and there exists an $\epsilon_0>0$ such that (2-2) has a solution for $t\in[0,\epsilon_0]$. For the closedness of $\mathfrak{I}$, it suffices to establish the C^0-estimate of (2-2). The following lemmas will be used later.

Lemma 2.2. *Let ϕ_t be a solution of* (2-2) *at t. Then the first eigenvalue of $-L_t$ for*

$$L_t := \triangle_{\omega_{\phi_t}} - \frac{X}{1-\theta_X(\omega_{\phi_t})} + t \tag{2-3}$$

is nonnegative for $t\in[0,1]$ and equals 0 *only if $t=1$. Consequently, we have the following weighted Poincaré inequality*:

$$\int_M |\bar\partial\psi|^2_{\omega_{\phi_t}}(1-\theta_X(\omega_{\phi_t}))\omega_{\phi_t}^n \geq t\left[\int_M \psi^2(1-\theta_X(\omega_{\phi_t}))\omega_{\phi_t}^n - \frac{1}{V}\left(\int_M \psi(1-\theta_X(\omega_{\phi_t}))\omega_{\phi_t}^n\right)^2\right]. \tag{2-4}$$

for any K_X-invariant $\psi\in C^{1,\alpha}$.

Remark 2.3. We remark that L_t is self-dual on the space of real-valued K_X-invariant functions, equipped with the weighted inner product (see [Mabuchi 2003, Lemma 2.1])

$$\langle f,g\rangle_t := \int_M f L_t(g)(1-\theta_X(\omega_{\phi_t}))\omega_{\phi_t}^n.$$

Proof of Lemma 2.2. Without loss of generality, we may choose a local coframe $\{\Theta^i\}_{i=1}^n$ such that $\omega_{\phi_t} = \sqrt{-1}\sum_{i=1}^n \Theta^i \wedge \bar{\Theta}^i$. Suppose $L_t\psi = -\lambda\psi$. Then

$$
\begin{aligned}
\text{(2-5)}\quad & \lambda \int_M \psi_{,i}\psi_{,\bar{i}}(1-\theta_X(\omega_{\phi_t}))\omega_{\phi_t}^n \\
&= -\int_M \left[\left(\triangle_{\omega_{\phi_t}} - \frac{X}{1-\theta_X(\omega_{\phi_t})} + t\right)\psi\right]_{,i} \psi^{,i}(1-\theta_X(\omega_{\phi_t}))\omega_{\phi_t}^n \\
&= -\int_M \psi_{,j\bar{j}i}\psi_{,\bar{i}}(1-\theta_X(\omega_{\phi_t}))\omega_{\phi_t}^n + \int_M X^j_{,i}\psi_{,\bar{i}}\psi_{,j}\omega_{\phi_t}^n + \int_M X^i\psi_{,ij}\psi_{,\bar{j}}\omega_{\phi_t}^n \\
&\quad + \int_M \frac{X(\psi)\theta_X(\omega_{\phi_t})_{,i}}{[1-\theta_X(\omega_{\phi_t})]^2}\psi_{,\bar{i}}(1-\theta_X(\omega_{\phi_t}))\omega_{\phi_t}^n - t\int_M \psi_{,i}\psi_{,\bar{i}}(1-\theta_X(\omega_{\phi_t}))\omega_{\phi_t}^n,
\end{aligned}
$$

here and below, we denote $\phi_{,i}$ for covariant derivatives with respect to ω_{ϕ_t}, similar conventions are used for covariant derivatives of other tensors.

By the Ricci identity and integration by parts, we have

$$
\begin{aligned}
&-\int_M \psi_{,j\bar{j}i}\psi_{,\bar{i}}(1-\theta_X(\omega_{\phi_t}))\omega_{\phi_t}^n \\
&= -\int_M \psi_{,ij\bar{j}}\psi_{,\bar{i}}(1-\theta_X(\omega_{\phi_t}))\omega_{\phi_t}^n + \int_M \psi_{,\bar{j}}\psi_{,\bar{i}}\,\mathrm{Ric}_{i\bar{j}}(1-\theta_X(\omega_{\phi_t}))\omega_{\phi_t}^n \\
&= \int_M \psi_{,ij}\psi_{,\bar{i}\bar{j}}(1-\theta_X(\omega_{\phi_t}))\omega_{\phi_t}^n - \int_M X^i\psi_{,ij}\psi_{,\bar{j}}\omega_{\phi_t}^n \\
&\qquad\qquad + \int_M \psi_{,j}\psi_{,\bar{i}}\,\mathrm{Ric}_{i\bar{j}}(1-\theta_X(\omega_{\phi_t}))\omega_{\phi_t}^n.
\end{aligned}
$$

Substituting this into (2-5) and using (2-2), it follows that

$$
\begin{aligned}
&\lambda\int_M \psi_{,i}\psi_{,\bar{i}}(1-\theta_X(\omega_{\phi_t}))\omega_{\phi_t}^n \\
&\quad = \int_M \psi_{,ij}\psi_{,\bar{i}\bar{j}}(1-\theta_X(\omega_{\phi_t}))\omega_{\phi_t}^n + (1-t)\int_M \psi_{,\bar{i}}\psi_{,j}g_{i\bar{j}}(0)(1-\theta_X(\omega_{\phi_t}))\omega_{\phi_t}^n,
\end{aligned}
$$

where $\omega_0 = \sqrt{-1}g_{i\bar{j}}(0)\Theta^i \wedge \bar{\Theta}^j$. □

2B. *Energy functionals.* Recall that the Aubin's functionals are given by

$$
I(\phi) = \int_M \phi(\omega_0^n - \omega_\phi^n), \qquad J(\phi) = \int_0^1\int_M \dot{\phi}_s(\omega_0^n - \omega_{\phi_s}^n)\wedge ds,
$$

where $\{\phi_s\}_{s\in[0,1]}$ is any smooth path in $\mathcal{H}_X(\omega_0)$ joining 0 and ϕ. It is known [Tian 2012] that

$$
\text{(2-6)}\qquad 0 \le \frac{1}{n}J(\phi) \le I(\phi) - J(\phi) \le nJ(\phi).
$$

To deal with Mabuchi metrics, the following modified functionals were introduced in [Mabuchi 2003]:

$$I_X(\phi) = \int_M \phi[(1-\theta_X(\omega_0))\omega_0^n - (1-\theta_X(\omega_\phi))\omega_\phi^n],$$

$$J_X(\phi) = \int_0^1 \int_M \dot{\phi}_s \big[(1-\theta_X(\omega_0))\omega_0^n - (1-\theta_X(\omega_{\phi_s}))\omega_{\phi_s}^n\big] \wedge ds.$$

By [Mabuchi 2003, Remark A.1.9], when $c_X > 0$,

$$0 \le I_X(\phi) \le (n+2)(I_X(\phi) - J_X(\phi)) \le (n+1)I_X(\phi). \tag{2-7}$$

Lemma 2.4. *There are positive constants* $c_1, c_2 > 0$ *such that*

$$c_1 I(\phi) \le I_X(\phi) - J_X(\phi) \le c_2 I(\phi). \tag{2-8}$$

Proof. Take a path $\phi_s = s\phi$. Then

$$\begin{aligned}\frac{d}{ds}[I_X(\phi_s) - J_X(\phi_s)] &= -s \int_M \phi \cdot \left(\triangle_{\omega_{\phi_s}} - \frac{X}{1-\theta_X(\omega_{\phi_s})}\right)\phi \cdot (1-\theta_X(\omega_{\phi_s}))\,\omega_{\phi_s}^n \\ &= s \int_M |\partial\phi|^2_{\omega_{\phi_s}} (1-\theta_X(\omega_{\phi_s}))\,\omega_{\phi_s}^n,\end{aligned}$$

Note that

$$\frac{d}{ds}[I(\phi_s) - J(\phi_s)] = s\int_M |\partial\phi|^2_{\omega_{\phi_s}}\,\omega_{\phi_s}^n.$$

When $c_X > 0$, it follows that

$$0 \le c_X \frac{d}{ds}[I(\phi_s) - J(\phi_s)] \le \frac{d}{ds}[I_X(\phi_s) - J_X(\phi_s)] \le C_X \frac{d}{ds}[I(\phi_s) - J(\phi_s)].$$

Thus the lemma follows from (2-6). □

For convenience, we write the modified Ding functional (1-6) as $\mathcal{D}_X(\phi) = \mathcal{N}(\phi) + \mathcal{D}_X^0(\phi)$, where

$$\mathcal{N}(\phi) = -\log\left(\frac{1}{V}\int_M e^{h_0-\phi}\omega_0^n\right), \tag{2-9}$$

$$\mathcal{D}_X^0(\phi) = -\frac{1}{V}\int_0^1\int_M \dot{\phi}_s(1-\theta_X(\omega_{\phi_s}))\,\omega_{\phi_s}^n \wedge ds. \tag{2-10}$$

It is known that $\mathcal{N}(\cdot)$ is convex with respect to geodesics [Berndtsson 2015]. In the later proof of Theorem 1.2, we need the convexity of $\mathcal{D}_X(\cdot)$.

Lemma 2.5. *The functional* $\mathcal{D}_X^0(\cdot)$ *satisfies*:

1. *When* $c_X > 0$, $\mathcal{D}_X^0(\cdot)$ *is monotonic, that is for any* $\phi_0 \le \phi_1$, $\mathcal{D}_X^0(\phi_0) \ge \mathcal{D}_X^0(\phi_1)$.
2. $\mathcal{D}_X^0(\cdot)$ *is affine along any* $C^{1,1}$*-geodesic connecting two smooth potentials in* $\mathcal{H}_X(\omega_0)$.

Proof. To see (1), by definition we have

$$\mathcal{D}_X^0(\phi_1) = \mathcal{D}_X^0(\phi_0) - \frac{1}{V}\int_0^1\int_M \dot{\phi}_s(1-\theta_X(\omega_{\phi_s}))\,\omega_{\phi_s}^n \wedge ds,$$

where ϕ_s is any smooth path in $\mathcal{H}_X(\omega_0)$ joining ϕ_0 and ϕ_1. Take in particular $\phi_s = s(\phi_1-\phi_0)+\phi_0$ and note that $c_X > 0$; we have

$$\mathcal{D}_X^0(\phi_1) = \mathcal{D}_X^0(\phi_0) - \frac{1}{V}\int_0^1\int_M (\phi_1-\phi_0)(1-\theta_X(\omega_{\phi_s}))\,\omega_{\phi_s}^n \wedge ds \le \mathcal{D}_X^0(\phi_0).$$

Next we prove (2). Let $\{\phi_t\}$ be the $C^{1,1}$-geodesic connecting $\phi_0, \phi_1 \in \mathcal{H}_X(\omega_0)$. By [Chen 2000], $\{\phi_t\}$ can be approximated by a family of smooth ϵ-geodesic $\{\phi_t^\epsilon \mid t \in \Omega\}$ in $\mathcal{H}_X(\omega_0)$ connecting ϕ_0 and ϕ_1, satisfying

$$\left(\frac{\partial^2}{\partial\tau\partial\bar{\tau}}\phi_t^\epsilon - \left|\bar{\partial}\left(\frac{\partial\phi_t^\epsilon}{\partial\tau}\right)\right|^2_{\omega_{\phi_t}}\right)(\omega_0+\sqrt{-1}\partial\bar{\partial}\phi_t^\epsilon)^n = \epsilon\cdot\omega_0^n, \tag{2-11}$$

on $M\times\Omega$, where $\Omega := [0,1]\times S^1 \subset \mathbb{C}$ and $t = \mathrm{Re}(\tau)$. For each ϵ, we have

$$\frac{\partial}{\partial\tau}\mathcal{D}_X^0(\phi_t^\epsilon) = -\frac{1}{V}\int_M \frac{\partial}{\partial\tau}\phi_t^\epsilon(1-\theta_X(\omega_{\phi_t^\epsilon}))\,\omega_{\phi_t^\epsilon}^n.$$

It follows that

$$\begin{aligned}\frac{\partial^2}{\partial\tau\partial\bar{\tau}}\mathcal{D}_X^0(\phi_t^\epsilon) = &-\frac{1}{V}\int_M \frac{\partial^2\phi_t^\epsilon}{\partial\tau\partial\bar{\tau}}(1-\theta_X(\omega_{\phi_t^\epsilon}))\,\omega_{\phi_t^\epsilon}^n\\ &+\frac{1}{V}\int_M \frac{\partial\phi_t^\epsilon}{\partial\tau}\frac{\partial\theta_X(\omega_{\phi_t^\epsilon})}{\partial\bar{\tau}}\,\omega_{\phi_t^\epsilon}^n\\ &-\frac{\sqrt{-1}}{V}\int_M \frac{\partial\phi_t^\epsilon}{\partial\tau}(1-\theta_X(\omega_{\phi_t^\epsilon}))\,n\omega_{\phi_t^\epsilon}^{n-1}\wedge\partial\bar{\partial}\frac{\partial\phi_t^\epsilon}{\partial\bar{\tau}}.\end{aligned} \tag{2-12}$$

Recall that $\theta_X(\omega_{\phi_t^\epsilon}) = \theta_X(\omega_0) + X(\phi_t^\epsilon)$. One gets

$$\frac{1}{V}\int_M \frac{\partial\phi_t^\epsilon}{\partial\tau}\frac{\partial\theta_X(\omega_{\phi_t^\epsilon})}{\partial\bar{\tau}}\,\omega_{\phi_t^\epsilon}^n = \frac{1}{V}\int_M \frac{\partial\phi_t^\epsilon}{\partial\tau}X^i\left(\frac{\partial\phi_t^\epsilon}{\partial\bar{\tau}}\right)_{,i}\omega_{\phi_t^\epsilon}^n.$$

On the other hand, by integration by parts, we have

$$\begin{aligned}&\frac{\sqrt{-1}}{V}\int_M \frac{\partial\phi_t^\epsilon}{\partial\tau}(1-\theta_X(\omega_{\phi_t^\epsilon}))\,n\omega_{\phi_t^\epsilon}^{n-1}\wedge\partial\bar{\partial}\frac{\partial\phi_t^\epsilon}{\partial\bar{\tau}}\\ &=\frac{\sqrt{-1}}{V}\left[\int_M \bar{\partial}\frac{\partial\phi_t^\epsilon}{\partial\tau}(1-\theta_X(\omega_{\phi_t^\epsilon}))\,n\omega_{\phi_t^\epsilon}^{n-1}\wedge\partial\frac{\partial\phi_t^\epsilon}{\partial\bar{\tau}} - \int_M \frac{\partial\phi_t^\epsilon}{\partial\tau}\bar{\partial}\theta_X(\omega_{\phi_t^\epsilon})\,n\omega_{\phi_t^\epsilon}^{n-1}\wedge\partial\frac{\partial\phi_t^\epsilon}{\partial\bar{\tau}}\right]\\ &=-\frac{1}{V}\int_M\left|\bar{\partial}\left(\frac{\partial\phi_t^\epsilon}{\partial\tau}\right)\right|^2_{\omega_{\phi_t}}(1-\theta_X(\omega_{\phi_t^\epsilon}))\,\omega_{\phi_t^\epsilon}^n + \frac{1}{V}\int_M \frac{\partial\phi_t^\epsilon}{\partial\tau}X^i\left(\frac{\partial\phi_t^\epsilon}{\partial\bar{\tau}}\right)_{,i}\omega_{\phi_t^\epsilon}^n.\end{aligned}$$

Plugging these into (2-12), by (2-11), we have

$$\frac{\partial^2}{\partial\tau\partial\bar{\tau}}\mathcal{D}_X^0(\phi_t^\epsilon) = -\epsilon < 0.$$

Thus $\mathscr{D}^0_X(\cdot)$ is concave along ϕ^ϵ_t. Let $\epsilon \to 0$. Then $\sqrt{-1}\partial\bar{\partial}_\tau\mathscr{D}^0_X(\phi^\epsilon_t)$ converges weakly to $\sqrt{-1}\partial\bar{\partial}_\tau\mathscr{D}^0_X(\phi_t)$ as Monge–Ampère measures. It follows that

$$\sqrt{-1}\partial\bar{\partial}_\tau\mathscr{D}^0_X(\phi_t) = 0;$$

thus $\mathscr{D}^0_X(\phi_t)$ is affine as desired. □

Remark 2.6. Indeed, one can improve Lemma 2.5(2) to any bounded geodesic in finite energy spaces $\mathscr{E}^1_{K_X}(M)$. See [Berman and Witt Nyström 2014, Proposition 2.17], where we take $g(t) = 1 - t$ in their settings.

2C. ***Group compactifications.*** As an application of Theorem 1.2, we will study the existence of Mabuchi metrics on group compactifications by testing properness of the modified Ding functional. The existence of Kähler–Einstein metrics on these manifolds has been solved by [Delcroix 2017a] by using the continuity method, while the properness of K-energy was studied in [Li et al. 2018]. We will prove Theorem 1.5 by ideas therein later. In this subsection, we recall some facts of group compactifications from [Delcroix 2017a; Li et al. 2018].

2C1. *Notation on Lie groups.* Choose a maximal compact subgroup K of G such that G is its complexification. Let T be a chosen maximal torus of K and T^c its complexification. Then T^c is the maximal algebraic torus of G. Denote their Lie algebras by the corresponding Fraktur lower case letters. Assume that Φ is the root system of (G, T^C) and W is the Weyl group. Choose a set of positive roots Φ_+. Set $\rho = \frac{1}{2}\sum_{\alpha\in\Phi_+}\alpha$ and let Ξ be the relative interior of the cone generated by Φ_+. Let J be the complex structure of G. Then

$$\mathfrak{g} = \mathfrak{k} \oplus J\mathfrak{k}.$$

Set $\mathfrak{a} = J\mathfrak{t}$, it can be decomposed as a toric part and a semisimple part:

$$\mathfrak{a} = \mathfrak{a}_t \oplus \mathfrak{a}_{ss},$$

where $\mathfrak{a}_t := \mathfrak{z}(\mathfrak{g}) \cap \mathfrak{a}$ and $\mathfrak{a}_{ss} := \mathfrak{a} \cap [\mathfrak{g}, \mathfrak{g}]$. We extend the Killing form on $\mathfrak{a}_{ss}$ to a scalar product $\langle\cdot,\cdot\rangle$ on $\mathfrak{a}$ such that $\mathfrak{a}_t$ is orthogonal to $\mathfrak{a}_{ss}$. The positive roots Φ_+ define a positive Weyl chamber $\mathfrak{a}_+ \subset \mathfrak{a}$, and a positive Weyl chamber $\mathfrak{a}^*_+$ on $\mathfrak{a}^*$, where

$$\mathfrak{a}^*_+ := \{y \mid \alpha(y) := \langle\alpha, y\rangle > 0,\ \forall\alpha \in \Phi_+\},$$

it coincides with the dual of $\mathfrak{a}_+$ under $\langle\cdot,\cdot\rangle$. For later use, we fix a Lebesgue measure dy on $\mathfrak{a}^*$ which is normalized by the lattice of the characters of T^c.

2C2. *$K\times K$-invariant Kähler metrics.* Let Z be the closure of T^c in M. It is known that $(Z, L|_Z)$ is a polarized toric manifold with a W-action, and $L|_Z$ is a W-linearized ample toric line bundle on Z [Alexeev and Brion 2004a; 2004b; Alexeev and Katzarkov 2005; Delcroix 2017a]. Let $\omega_0 \in 2\pi c_1(L)$ be a $K\times K$-invariant

Kähler form induced from (M, L) and P be the polytope associated to $(Z, L|_Z)$, which is defined by the moment map associated to ω_0. Then P is a W-invariant Delzant polytope in $\mathfrak{a}^*$. By the $K\times K$-invariance, for any

$$\phi \in \mathcal{H}_{K\times K}(\omega_0) := \bigl\{\phi \in C^\infty(M) \mid \omega_\phi > 0,\ \phi \text{ is } K\times K\text{-invariant}\bigr\},$$

the restriction of ω_ϕ on Z is a toric Kähler metric. It induces a smooth strictly convex function ψ_ϕ on $\mathfrak{a}$, which is W-invariant [Azad and Loeb 1992; Delcroix 2017a].

By the KAK-decomposition [Knapp 1996, Theorem 7.39], for any $g \in G$, there are $k_1, k_2 \in K$ and $x \in \mathfrak{a}$ such that $g = k_1 \exp(x) k_2$. Here x is uniquely determined up to a W-action. This means that x is unique in $\bar{\mathfrak{a}}_+$. Thus there is a bijection between smooth $K\times K$-invariant functions Ψ on G and smooth W-invariant functions on $\mathfrak{a}$ which is given by

$$\Psi(\exp(\cdot)) = \psi(\cdot) : \mathfrak{a} \to \mathbb{R}.$$

Clearly when a W-invariant ψ is given, Ψ is well-defined. In the following, we will not distinguish ψ and Ψ. The following KAK-integral formula can be found in [Knapp 1986, Proposition 5.28] (see also [Hu and Yan 2005]).

Proposition 2.7. *Let dV_G be a Haar measure on G and dx the Lebesgue measure on $\mathfrak{a}$. Then there exists a constant $C_H > 0$ such that for any $K\times K$-invariant, dV_G-integrable function ψ on G,*

$$\int_G \Psi(g)\, dV_G = C_H \int_{\mathfrak{a}_+} \psi(x) \boldsymbol{J}(x)\, dx,$$

where $\boldsymbol{J}(x) = \prod_{\alpha\in\Phi_+} \sinh^2 \alpha(x)$.

Without loss of generality, we can normalize $C_H = 1$ for simplicity.

Next we recall local holomorphic coordinates on G used in [Delcroix 2017a]. By the standard Cartan decomposition, we can decompose $\mathfrak{g}$ as

$$\mathfrak{g} = (\mathfrak{t} \oplus \mathfrak{a}) \oplus \bigl(\textstyle\bigoplus_{\alpha\in\Phi} V_\alpha\bigr),$$

where $V_\alpha = \{X \in \mathfrak{g} \mid \mathrm{ad}_H(X) = \alpha(H)X,\ \forall H \in \mathfrak{t}\oplus\mathfrak{a}\}$, the root space of complex dimension 1 with respect to α. By [Helgason 1978], one can choose $X_\alpha \in V_\alpha$ such that $X_{-\alpha} = -\iota(X_\alpha)$ and $[X_\alpha, X_{-\alpha}] = \alpha^\vee$, where ι is the Cartan involution and $\alpha^\vee$ is the dual of α by the Killing form. Let $E_\alpha := X_\alpha - X_{-\alpha}$ and $E_{-\alpha} := J(X_\alpha + X_{-\alpha})$. Denote by $\mathfrak{k}_\alpha$, $\mathfrak{k}_{-\alpha}$ the real line spanned by E_α, $E_{-\alpha}$, respectively. Then we have the Cartan decomposition of $\mathfrak{k}$:

$$\mathfrak{k} = \mathfrak{t} \oplus \bigl(\textstyle\bigoplus_{\alpha\in\Phi_+} (\mathfrak{k}_\alpha \oplus \mathfrak{k}_{-\alpha})\bigr).$$

Denote by r the dimension of T, and choose a real basis $\{E^0_1, \dots, E^0_r\}$ of $\mathfrak{t}$. Then $\{E^0_1, \dots, E^0_r\}$ together with $\{E_\alpha, E_{-\alpha}\}_{\alpha\in\Phi_+}$ forms a real basis of $\mathfrak{k}$, which is indexed by $\{E_1, \dots, E_n\}$, which can also be regarded as a complex basis of $\mathfrak{g}$. For any $g \in G$, we define local coordinates $\{z^i_{(g)}\}_{i=1,\dots,n}$ on a neighborhood of g by

$$(z^i_{(g)}) \to \exp(z^i_{(g)} E_i) g.$$

It is easy to see that $\theta^i|_g = dz^i_{(g)}|_g$, where θ^i is the dual of E_i, which is a right-invariant holomorphic 1-form. Thus $\bigwedge_{i=1}^n (dz^i_{(g)} \wedge d\bar{z}^i_{(g)})|_g$ is also a right-invariant (n, n)-form, which defines a Haar measure dV_G.

The derivations of the $K\times K$-invariant function ψ in the above local coordinates was computed by Delcroix [2017a, Theorem 1.2] as follows.

Lemma 2.8. *Let ψ be a $K \times K$ invariant function on G. Then for any $x \in \mathfrak{a}_+$,*

$$E^0_i(\psi)|_{\exp(x)} = d\psi(\mathrm{Im}(E^0_i))|_x, \quad 1 \le i \le r, \qquad E_{\pm\alpha}(\psi)|_{\exp(x)} = 0.$$

Lemma 2.9. *Let ψ be a $K\times K$-invariant function on G. Then for any $x \in \mathfrak{a}_+$, the complex Hessian matrix of ψ in the above coordinates is diagonal by blocks, and equal to*

$$\mathrm{Hess}_{\mathbb{C}}(\psi)(\exp(x)) = \begin{pmatrix} \frac{1}{4}\mathrm{Hess}_{\mathbb{R}}(\psi)(x) & 0 & & 0 \\ 0 & M_{\alpha_{(1)}}(x) & & 0 \\ 0 & 0 & \ddots & \vdots \\ \vdots & \vdots & & 0 \\ 0 & 0 & & M_{\alpha_{((n-r)/2)}}(x) \end{pmatrix}, \tag{2-13}$$

where $\Phi_+ = \{\alpha_{(1)}, \dots, \alpha_{((n-r)/2)}\}$ is the set of positive roots and

$$M_{\alpha_{(i)}}(x) = \tfrac{1}{2}\langle \alpha_{(i)}, \nabla\psi(x)\rangle \begin{pmatrix} \coth \alpha_{(i)}(x) & \sqrt{-1} \\ -\sqrt{-1} & \coth \alpha_{(i)}(x) \end{pmatrix}.$$

By (2-13) in Lemma 2.9, we see that a ψ induced by some ω_ϕ is convex on $\mathfrak{a}$. The complex Monge–Ampère measure is given by $\omega^n = (\sqrt{-1}\partial\bar{\partial}\psi_\phi)^n = \mathrm{MA}_{\mathbb{C}}(\psi_\phi)\, dV_G$, where

$$\mathrm{MA}_{\mathbb{C}}(\psi_\phi)(\exp(x)) = \frac{1}{2^{r+n}} \mathrm{MA}_{\mathbb{R}}(\psi_\phi)(x) \frac{1}{\boldsymbol{J}(x)} \prod_{\alpha\in\Phi_+} \langle \alpha, \nabla\psi_\phi(x)\rangle^2. \tag{2-14}$$

2C3. *Legendre functions.* By the convexity of ψ_ϕ on $\mathfrak{a}$, the gradient $\nabla\psi_\phi$ defines a diffeomorphism from $\mathfrak{a}$ to the interior of the dilated polytope $2P$.[1] Let $P_+ := P \cap \bar{\mathfrak{a}}^*_+$. Then by the W-invariance of ψ_ϕ and P, the restriction of $\nabla\psi_\phi$ on $\mathfrak{a}_+$ is a diffeomorphism from $\mathfrak{a}_+$ to the interior of $2P_+$. Let u_G be the standard Guillemin function on $2P$ [Guillemin 1994]. Set

$$\mathscr{C}_W = \big\{ u \mid u \text{ is strictly convex, } u - u_G \in C^\infty(\overline{2P}) \text{ and } u \text{ is } W\text{-invariant} \big\}.$$

[1] We remark that the moment map is given by $\frac{1}{2}\nabla\psi_\phi$, whose image is P.

It is known that for any $K\times K$-invariant $\omega=\sqrt{-1}\partial\bar\partial\psi\in 2\pi c_1(L)$, its Legendre function u is given by

$$u(y(x))=x^i y_i(x)-\psi(x),\quad y_i(x)=\psi_{,i}(x)=\frac{\partial\psi}{\partial x_i} \tag{2-15}$$

and is a function in $\mathscr{C}_W$ (see [Abreu 1998]). By a similar argument to that in [Guan 1999] for toric manifolds, we have:

Lemma 2.10. *For any $\phi_0,\phi_1\in\mathscr{H}_{K\times K}(\omega_0)$, there exists a geodesic $\{\phi_t\}_{t\in[0,1]}$ in $\mathscr{H}_{K\times K}(\omega_0)$ joining them, and the Legendre function of ψ_ϕ is given by*

$$u_{\phi_t}=(1-t)u_{\phi_0}+tu_{\phi_1}.$$

3. Proof of the properness theorem

We always assume $c_X>0$ in this section.

3A. We first prove the properness modulo an arbitrary reductive subgroup $H^c$of $\mathrm{Aut}_0(M)$ which contains K_X implies the existence of Mabuchi metrics. It will be proved by steps as for Kähler–Ricci solitons [Cao et al. 2005; Tian and Zhu 2000].

First, we have:

Lemma 3.1. *Let ϕ_t be a solution of* (2-2) *at t. If $I_X(\phi_t)$ is uniformly bounded, then there is a uniform constant C such that*

$$|\phi_t|\le C,\quad \textit{for all }\ t\in[0,1].$$

Proof. This estimate was essentially obtained in [Mabuchi 2003]. Here we will give a different proof following the arguments of [Tian and Zhu 2000]. In view of Kołodziej's L^∞-estimate [1998] for the complex Monge–Ampère equation, it suffices to obtain the L^p-estimate of $e^{-t\phi_t}$ for some $p>1$.

By the assumption, $0\le I_X(\phi_t)\le C_1$ for some uniform C_1. By (2-2), we have

$$\int_M e^{h_0-t\phi_t}\omega_0^n=\int_M(1-\theta_X(\omega_{\phi_t}))\,\omega_{\phi_t}^n=\int_M e^{h_0}\omega_0^n,$$

thus

$$\inf_M\phi_t\le 0\le\sup_M\phi_t.$$

While by (2-2),

$$-t\int_M\phi_t\omega_{\phi_t}^n=-t\int_M\phi_t\frac{e^{h_0-t\phi_t}}{1-\theta_X(\omega_{\phi_t})}\,\omega_0^n\ge -C_2t\int_{\{\phi_t\ge0\}}\phi_te^{-t\phi_t}\omega_0^n\ge -C_3.$$

Thus

$$t\int_M\phi_t\,\omega_0^n\le C_4. \tag{3-1}$$

Let $\Gamma(\cdot,\cdot)$ be the Green function of ω_0. Then by $\triangle_{\omega_0}\phi_t > -n$, $\Gamma + C_\Gamma \geq 0$ for some $C_\Gamma > 0$. By (3-1) and Green's formula, we have

$$t\sup_M \phi_t \leq \frac{t}{V}\int_M \phi_t\,\omega_0^n - \frac{t}{V}\min_M\left(\int_M (\Gamma(x,\cdot)+C_\Gamma)\triangle_{\omega_0}\phi_t\,\omega_0^n\right) \leq C_5. \tag{3-2}$$

By the boundedness of $I_X(\phi_t)$, we have

$$-\frac{1}{V}\int_M \phi_t\,\omega_{\phi_t}^n \leq C_1 - \frac{1}{V}\int_M \phi_t\,\omega_0^n \leq C_6. \tag{3-3}$$

Moreover,

$$\begin{aligned}-t\int_{\{\phi_t\leq 0\}} \phi_t\,\omega_{\phi_t}^n &= -t\int_M \phi_t\,\omega_{\phi_t}^n + t\int_{\{\phi_t\geq 0\}} \phi_t\,\omega_{\phi_t}^n \\ &\leq tVC_6 + t\int_{\{\phi_t\geq 0\}} \phi_t \frac{e^{h_0 - t\phi_t}}{1-\theta_X(\omega_{\phi_t})}\,\omega_0^n \leq C_7.\end{aligned} \tag{3-4}$$

By (3-2), there is a uniform $C > 0$ such that $\hat{\phi}_t := \phi_t - C/t \leq -1$. By (3-4), it follows that

$$-t\int_M \phi_t(1-\theta_X(\omega_{\phi_t}))\,\omega_{\phi_t}^n \leq -t\int_{\{\phi_t\leq 0\}} \phi_t(1-\theta_X(\omega_{\phi_t}))\,\omega_{\phi_t}^n \leq C_X C_7,$$

and consequently,

$$-t\int_M \hat{\phi}_t(1-\theta_X(\omega_{\phi_t}))\,\omega_{\phi_t}^n \leq C_8. \tag{3-5}$$

On the other hand,

$$\begin{aligned}\int_M \left|\bar{\partial}(-\hat{\phi}_t)^{\frac{p+1}{2}}\right|^2_{\omega_{\phi_t}} \omega_{\phi_t}^n &= \frac{n(p+1)^2}{4p}\int_M (-\hat{\phi}_t)^p(\omega_{\phi_t}^n - \omega_{\phi_t}^{n-1}\wedge\omega_0) \\ &\leq \frac{n(p+1)^2}{4p}\int_M (-\hat{\phi}_t)^p\,\omega_{\phi_t}^n.\end{aligned}$$

Recall that $0 < c_X < 1-\theta_X(\omega_{\phi_t}) < C_X$. Combining the above inequality with (2-4),

$$\begin{aligned}&\int_M (-\hat{\phi}_t)^{p+1}(1-\theta_X(\omega_{\phi_t}))\omega_{\phi_t}^n \\ &\leq \frac{Cp}{t}\int_M (-\hat{\phi}_t)^p(1-\theta_X(\omega_{\phi_t}))\,\omega_{\phi_t}^n + \frac{1}{V}\left(\int_M (-\hat{\phi}_t)^{(p+1)/2}(1-\theta_X(\omega_{\phi_t}))\,\omega_{\phi_t}^n\right)^2 \\ &\leq \frac{Cp}{t}\int_M (-\hat{\phi}_t)^p(1-\theta_X(\omega_{\phi_t}))\,\omega_{\phi_t}^n \\ &\qquad + \frac{1}{V}\left(\int_M (-\hat{\phi}_t)^p(1-\theta_X(\omega_{\phi_t}))\,\omega_{\phi_t}^n\right)\left(\int_M (-\hat{\phi}_t)(1-\theta_X(\omega_{\phi_t}))\,\omega_{\phi_t}^n\right) \\ &\leq \frac{C'p}{t}\int_M (-\hat{\phi}_t)^p(1-\theta_X(\omega_{\phi_t}))\,\omega_{\phi_t}^n,\end{aligned}$$

where we used (3-5) in the last line. By iteration and using (3-5), we have

$$\int_M (-\hat{\phi}_t)^{p+1}(1-\theta_X(\omega_{\phi_t}))\,\omega_{\phi_t}^n \le \frac{C'^p(p+1)!}{t^p}\int_M (-\hat{\phi}_t)(1-\theta_X(\omega_{\phi_t}))\,\omega_{\phi_t}^n \le \frac{c^{p+1}(p+1)!}{t^{p+1}}.$$

Thus for $0<\epsilon<1/c$,

$$\int_M e^{-t\epsilon\hat{\phi}_t}(1-\theta_X(\omega_{\phi_t}))\,\omega_{\phi_t}^n = \sum_{p=0}^{+\infty}\frac{(t\epsilon)^p}{p!}\int_M (-\hat{\phi}_t)^p(1-\theta_X(\omega_{\phi_t}))\,\omega_{\phi_t}^n \le \frac{1}{1-c\epsilon}.$$

It follows that

$$\begin{aligned}\int_M e^{-t(1+\epsilon)\phi_t}\omega_0^n &= \int_M e^{-t(1+\epsilon)\phi_t}e^{-h_0-t\phi_t}(1-\theta_X(\omega_{\phi_t}))\,\omega_{\phi_t}^n\\ &\le C_9\int_M e^{-t\epsilon\hat{\phi}_t}(1-\theta_X(\omega_{\phi_t}))\,\omega_{\phi_t}^n \le C.\end{aligned}$$

Then the lemma then follows from Kołodziej's result. □

Lemma 3.2 [Li 2007]. *Fix $\epsilon_0 \in (0,1)$. Then the modified Ding functional $\mathfrak{D}_X(\phi_t)$ is uniformly bounded from above for $t>\epsilon_0$.*

The proof follows from the above and the next lemmas.

Lemma 3.3. *For any solution ϕ_t of* (2-2) *with $t<1$,*

$$\min_{\sigma\in H^c}\{I_X((\phi_t)_\sigma)-J_X((\phi_t)_\sigma)\} = I_X(\phi_t)-J_X(\phi_t).$$

Proof. We will use the argument of Tian [2012] to prove this lemma. For any $Y\in\mathfrak{h}^c$, let $\sigma(s)$ be the one parameter group generated by $\mathrm{Re}(Y)$ with $\sigma(0)=\mathrm{id}$. For a solution ϕ_t of (2-2), set $\phi_{t\,s}=(\phi_t)_{\sigma(s)}$. Note that (2-2) is equivalent to

$$h_t+(1-t)\phi_t = \log(1-\theta_X(\omega_{\phi_t}))+c_t,$$

where h_t is the normalized Ricci potential of ω_{ϕ_t} and c_t is a constant depending on t. Thus

$$\begin{aligned}\text{(3-6)}\quad &\frac{\partial}{\partial s}\Big|_{s=0}(I_X-J_X)(\phi_{t\,s})\\ &= \int_M \frac{\partial}{\partial s}\Big|_{s=0}\phi_{t\,s,\bar{k}}\phi_{t,i}g^{i\bar{k}}(1-\theta_X(\omega_{\phi_t}))\,\omega_{\phi_t}^n\\ &= -\frac{1}{1-t}\int_M Y^i\left[h_{t,i}+\frac{\theta_X(\omega_{\phi_t})_{,i}}{1-\theta_X(\omega_{\phi_t})}\right](1-\theta_X(\omega_{\phi_t}))\,\omega_{\phi_t}^n\\ &= -\frac{1}{1-t}\int_M Y(h_t)\omega_{\phi_t}^n+\frac{1}{1-t}\left(\int_M Y(h_t)\theta_X(\omega_{\phi_t})\,\omega_{\phi_t}^n-\int_M Y^i\theta_X(\omega_{\phi_t})_{,i}\,\omega_{\phi_t}^n\right).\end{aligned}$$

Recall that $\theta_Y(\omega_{\phi_t})$ satisfies

$$\triangle_{\omega_{\phi_t}}\theta_Y(\omega_{\phi_t})+Y(h_t)+\theta_Y(\omega_{\phi_t})=\text{const.},$$

thus

$$\int_M Y(h_t)\theta_X(\omega_{\phi_t})\,\omega_{\phi_t}^n=-\int_M\theta_X(\omega_{\phi_t})\theta_Y(\omega_{\phi_t})\,\omega_{\phi_t}^n-\int_M\theta_X(\omega_{\phi_t})\triangle_{\omega_{\phi_t}}\theta_Y(\omega_{\phi_t})\,\omega_{\phi_t}^n.$$

Substituting this into (3-6) and by integration by parts, yields

$$\text{(3-7)}\quad \frac{\partial}{\partial s}\Big|_{s=0}(I_X-J_X)(\phi_{t\,s})=-\frac{1}{1-t}\int_M Y(h_t)\,\omega_{\phi_t}^n-\frac{1}{1-t}\int_M\theta_X(\omega_{\phi_t})\theta_Y(\omega_{\phi_t})\,\omega_{\phi_t}^n$$
$$=0.$$

The last equality follows from (1-4). This shows that $s=0$ is a critical point of $(I_X-J_X)(\phi_{t\,s})$.

To prove the lemma, it suffices to show that $(I_X-J_X)(\phi_{t\,s})$ is convex with respect to s. It is direct to check that

$$\text{(3-8)}\qquad \frac{\partial^2}{\partial s^2}\phi_{t\,s}=\left|\bar\partial\left(\frac{\partial}{\partial s}\phi_{t\,s}\right)\right|^2_{\omega_{\phi_{t\,s}}}.$$

Thus $\phi_{t\,s}$ gives a geodesic in the space of Kähler potentials. In the following, we denote $\phi_s=\phi_{t\,s}$ for fixed t for simplicity and $\omega_{\phi_{t\,s}}=\sqrt{-1}g_{i\bar j}(s)dz^i\wedge d\bar z^j$. Then

$$\text{(3-9)}\qquad \frac{\partial}{\partial s}\triangle_{\omega_{\phi_s}}\phi_s=-g^{i\bar k}g^{\bar j l}\cdot\phi_{s,\bar k l}\phi_{s,\bar j i}+\triangle_{\omega_{\phi_s}}\dot\phi_s.$$

Note that

$$\text{(3-10)}\quad \frac{d}{ds}(I_X-J_X)(\phi_s)=-\int_M\dot\phi_s\triangle_{\omega_{\phi_s}}\phi_s(1-\theta_X(\omega_{\phi_s}))\,\omega_{\phi_s}^n+\int_M\dot\phi_s X(\phi_s)\,\omega_{\phi_s}^n.$$

We want to differentiate the above equality. For the first term, we have by (3-9)

$$\begin{aligned}&\frac{d}{ds}\int_M\dot\phi_s\triangle_{\omega_{\phi_s}}\phi_s(1-\theta_X(\omega_{\phi_s}))\,\omega_{\phi_s}^n\\&=\int_M\ddot\phi_s\triangle_{\omega_{\phi_s}}\phi_s(1-\theta_X(\omega_{\phi_s}))\,\omega_{\phi_s}^n-\int_M X^i\dot\phi_{s,i}\triangle_{\omega_{\phi_s}}\phi_s\dot\phi_s\,\omega_{\phi_s}^n\\&\quad+\int_M\dot\phi_s\triangle_{\omega_{\phi_s}}\dot\phi_s\triangle_{\omega_{\phi_s}}\phi_s(1-\theta_X(\omega_{\phi_s}))\,\omega_{\phi_s}^n+\int_M\dot\phi_s\triangle_{\omega_{\phi_s}}\dot\phi_s(1-\theta_X(\omega_{\phi_s}))\,\omega_{\phi_s}^n\\&\qquad\qquad-\int_M\dot\phi_s(\dot\phi_{s,l\bar k}\phi_{s,i\bar j})g^{i\bar k}g^{l\bar j}(1-\theta_X(\omega_{\phi_s}))\,\omega_{\phi_s}^n.\end{aligned}$$

Substituting (3-8) into the first term and by integration by parts, it follows that

$$
\begin{aligned}
(3\text{-}11)\quad & \frac{d}{ds}\int_M \dot\phi_s \triangle_{\omega_{\phi_s}}\phi_s(1-\theta_X(\omega_{\phi_s}))\,\omega_{\phi_s}^n \\
&= -\int_M \dot\phi_s\dot\phi_{s,i}(\triangle_{\omega_{\phi_s}}\phi_s)_{,\bar k}g^{i\bar k}(1-\theta_X(\omega_{\phi_s}))\,\omega_{\phi_s}^n \\
&\qquad -\int_M \dot\phi_s\dot\phi_{s,l\bar k}\phi_{s,i\bar j}g^{i\bar k}g^{l\bar j}(1-\theta_X(\omega_{\phi_s}))\,\omega_{\phi_s}^n \\
&\qquad\qquad +\int_M \dot\phi_s\triangle_{\omega_{\phi_s}}\dot\phi_s(1-\theta_X(\omega_{\phi_s}))\,\omega_{\phi_s}^n \\
&= \int_M \dot\phi_{s,l}\dot\phi_{s,\bar k}\phi_{s,i\bar j}g^{l\bar j}g^{i\bar k}(1-\theta_X(\omega_{\phi_s}))\,\omega_{\phi_s}^n - \int_M \dot\phi_s X^i\dot\phi_{s,l}\phi_{s,i\bar j}g^{l\bar j}\,\omega_{\phi_s}^n \\
&\qquad\qquad +\int_M \dot\phi_s\triangle_{\omega_{\phi_s}}\dot\phi_s(1-\theta_X(\omega_{\phi_s}))\,\omega_{\phi_s}^n \\
&= \int_M \dot\phi_{s,l}\dot\phi_{s,\bar k}(\phi_{s,i\bar j}-g_{i\bar j})g^{i\bar k}g^{l\bar j}(1-\theta_X(\omega_{\phi_s}))\,\omega_{\phi_s}^n \\
&\qquad -\int_M \dot\phi_s X^i\dot\phi_{s,l}\phi_{s,i\bar j}g^{l\bar j}\,\omega_{\phi_s}^n + \int_M X^i\dot\phi_{s,i}\dot\phi_s\,\omega_{\phi_s}^n,
\end{aligned}
$$

where $g_{i\bar j}=g_{i\bar j}(s)$. The second term in (3-10) gives

$$
\frac{d}{ds}\int_M \dot\phi_s X^i\phi_{s,i}\,\omega_{\phi_s}^n = \int_M \ddot\phi_s X^i\phi_{s,i}\,\omega_{\phi_s}^n + \int_M \dot\phi_s X^i\dot\phi_{s,i}\,\omega_{\phi_s}^n + \int_M \dot\phi_s X^i\phi_{s,i}\triangle_{\omega_{\phi_s}}\dot\phi_s\,\omega_{\phi_s}^n.
$$

Substituting (3-8) into the above equality and by integration by parts again, we have

$$
(3\text{-}12)\quad \frac{d}{ds}\int_M \dot\phi_s X^i\phi_{s,i}\,\omega_{\phi_s}^n = -\int_M \dot\phi_s\dot\phi_{s,l}(X^i\phi_{s,i})_{,\bar j}g^{l\bar j}\,\omega_{\phi_s}^n + \int_M \dot\phi_s X^i\dot\phi_{s,i}\,\omega_{\phi_s}^n.
$$

Combining (3-10)–(3-12), we get

$$
\frac{d^2}{ds^2}(I_X-J_X)(\phi_s) = \int_M \dot\phi_{s,\bar k}\dot\phi_{s,l}g_{i\bar j}(0)g^{i\bar k}g^{l\bar j}(1-\theta_X(\omega_{\phi_s}))\,\omega_{\phi_s}^n \ge 0. \qquad \square
$$

3B. The converse part of Theorem 1.2 can be proved by using the properness principle of [Darvas and Rubinstein 2017]. Since the pluripotential theory for Mabuchi will be used, we first recall some results in [Berman and Witt Nyström 2014].

Let T be the (closed) torus generated by the imaginary part of X. Let $\mathrm{PSH}_T(\omega_0)$ be the set of T-invariant ω_0-plurisubharmonic functions. According to [Berman and Witt Nyström 2014], for any continuous nonnegative function g and $\phi\in\mathrm{PSH}_T(\omega_0)$, one can define a g-Monge–Ampère measure $\mathrm{MA}_g(\phi)$ and the measure has weak continuity. When ϕ is smooth, $\mathrm{MA}_g(\phi)=\mathrm{MA}(\phi)g(m_\phi)$, where m_ϕ is the moment map of the torus action with respect to ω_ϕ. In particular, when $g(t)=e^t$, it corresponds to the case of Kähler–Ricci solitons; when $g(t) = 1 - t$, it corresponds to the case of Mabuchi metrics. Based on the pluripotential theory of g-Monge–Ampère measure, the existence and uniqueness theory for Kähler–Ricci solitons is obtained by a variational approach. The approach also applies to Mabuchi metrics. Write $\omega_0 = \sqrt{-1}\partial\bar{\partial}\psi_0$ locally. Following [Berman and Witt Nyström 2014], we call $\phi \in \mathrm{PSH}_T(\omega_0)$ a *weak Mabuchi metric* if

$$\mathrm{MA}_g(\phi) = e^{-(\psi_0+\phi)}. \tag{3-13}$$

Let $\mathscr{E}^1_T(M)$ be the set of T-invariant metrics with finite energy [Berman et al. 2013]. Then by the same argument as in [Berman and Witt Nyström 2014] with the modified Ding energy $\mathscr{D}_X(\cdot)$ in this paper, we have

Proposition 3.4. *$\phi \in \mathscr{E}^1_T(M)$ is a weak Mabuchi metric if and only if it minimizes the modified Ding functional $\mathscr{D}_X(\cdot)$.*

Proof of the converse part of Theorem 1.2. We take $\mathscr{R} = \mathscr{H}_X(\omega_0)$, $d = d_1$ as in [Darvas and Rubinstein 2017, Definition 4.2], $F = \mathscr{D}_X(\cdot)$ and $G = \mathrm{Aut}^X_0(M)$ in the setting of [Darvas and Rubinstein 2017, §3].

Suppose ω_0 is the Mabuchi metric and $\mathrm{Iso}_0(M, \omega_0)$ is the identity component of the corresponding isometry group. By a Calabi–Matsushima type theorem of Mabuchi [2002], we have

$$\mathfrak{aut}^X(M) = \mathfrak{iso}(M, \omega_0) \oplus J\,\mathfrak{iso}(M, \omega_0), \tag{3-14}$$

where $\mathfrak{aut}^X(M)$ and $\mathfrak{iso}(M, \omega_0)$ are Lie algebras of $\mathrm{Aut}^X_0(M)$ and $\mathrm{Iso}_0(M, \omega_0)$, respectively. We will check that $\mathscr{D}_X(\cdot)$, $\mathrm{Aut}^X(M)$ satisfy (P1)–(P7) in the Hypothesis 3.2 of [Darvas and Rubinstein 2017], which are enough for the "existence ⇒ properness" direction:

(P1) This is confirmed by [Berndtsson 2015, Theorem 1.1] and Lemma 2.5(2).

(P2) This can be shown by using Lemma 2.5(1) and Lemmas 5.15, 5.20, 5.29 of [Darvas and Rubinstein 2017], where we replace $AM_X(\cdot)$ and $F^X(\cdot)$ in [Darvas and Rubinstein 2017] by $-\mathscr{D}^0_X(\cdot)$ and $\mathscr{D}_X(\cdot)$, respectively. The monotonicity of $-\mathscr{D}^0_X(\cdot)$ is confirmed by Lemma 2.5(1). The proof then follows exactly those in [Darvas and Rubinstein 2017].

(P3) This can be proved similarly to [Berman and Witt Nyström 2014, Theorem 1.3] by using Proposition 3.4, we will finish it in the proof of (P5).

(P4) This is [Darvas and Rubinstein 2017, Lemma 5.9].

(P5) We mainly use the arguments of [Berman and Witt Nyström 2014] by taking $g(t) = 1 - t$ in the g-Monge–Ampère equation there. By Corollary 2.9 and Theorem 2.18 of [Berman and Witt Nyström 2014], we see that any weak solution ω_ϕ is locally bounded and minimizes $\mathscr{D}_X(\cdot)$. Hence any two weak solution ω_{ϕ_0}

and ω_{ϕ_1} can be connected by a bounded geodesic $\phi_t \subset \mathrm{PSH}_T(\omega_0)$. By Remark 2.6 and [Berndtsson 2015, Theorem 1.2], $\mathcal{D}_X(\phi_t)$ is affine and there is a family of $\{\sigma_t\} \subset \mathrm{Aut}_0(M)$ such that $\omega_{\phi_t} = \sigma_t^*(\omega_{\phi_0})$. In particular, we can take $\omega_{\phi_0} = \omega_0$, the *smooth* Mabuchi metric on M. Thus for any t, ω_{ϕ_t} is a *smooth* Mabuchi metric. This confirms (P3).

It remains to show that $\{\sigma_t\} \subset \mathrm{Aut}_0^X(M)$. Write $\omega_0 = \sqrt{-1}\partial\bar{\partial}\psi_0$ locally and denoted by $\mathrm{MA}(\phi)$ the Monge–Ampére operator of $\psi_0 + \phi$. Since ω_{ϕ_t} is smooth, (3-13) reduces to

$$\mathrm{MA}(\phi_t)(1 - \theta_X(\omega_{\phi_t})) = e^{-\psi_0 - \phi_t},$$

which is equivalent to

$$\sigma_t^*(\mathrm{MA}(\phi_0)(1 - \theta_{\sigma_{t*}^{-1}X}(\omega_{\phi_0})) = \sigma_t^*(e^{-\psi_0 - \phi_0})$$

since $\omega_{\phi_t} = \sigma_t^*(\omega_{\phi_0})$. Thus

$$\sigma_{t*}^{-1} X = X$$

for all t which proves $\{\sigma_t\} \subset \mathrm{Aut}_0^X(M)$. Thus (P5) is proved.

(P6) This can be shown exactly as in [Darvas and Rubinstein 2017, Theorem 8.1], by using (3-14) instead of [Darvas and Rubinstein 2017, Proposition 6.10];

(P7) This follows from the cocycle condition of $\mathcal{D}_X(\cdot)$.

The theorem then follows from the second part of [Darvas and Rubinstein 2017, Theorem 3.4]. □

4. Existence criterion on Fano group compactifications

In this section, we will prove Theorem 1.5. Let M be a group compactification and ω_0 be a $K \times K$-invariant Kähler metric in $2\pi c_1(M)$. Assume $\omega_0 = \sqrt{-1}\partial\bar{\partial}\psi_0$ on G. For $\phi \in \mathcal{H}_{K\times K}(\omega_0)$, we will write ψ_ϕ in short for $\psi_0 + \phi$ and u_ϕ the Legendre function of ψ_ϕ.

4A. ***Reduction of the modified Ding functional.*** We will give a formula of $\mathcal{D}_X(\phi)$ in terms of ϕ and u_ϕ. First, we compute the Futaki invariant of a vector field in $\mathfrak{z}(\mathfrak{g})$.

Lemma 4.1. *Let Y be a vector field of the form*

$$Y = \sqrt{-1} Y^i E_i^0, \quad 1 \le i \le r \tag{4-1}$$

for some $Y^i \in \mathbb{C}$ such that $\alpha_i Y^i = 0$ for any $\alpha \in \Phi$. Then

$$\mathrm{Fut}(Y) = -V \cdot Y^i \boldsymbol{b}_i, \tag{4-2}$$

where $\boldsymbol{b} = (1/V)\int_{2P_+} y\pi(y)\,dy$ is the barycenter of $2P_+$ with respect to the measure $\pi(y)\,dy$.

Proof. Since $Y \in \mathfrak{z}(\mathfrak{g})$, it is $K \times K$-invariant, so is its potential. Recall that

$$\mathrm{Fut}(Y) = -\int_M \hat{\theta}_Y(\omega_0)\,\omega_0^n, \tag{4-3}$$

where $\hat{\theta}_Y(\omega_0)$ is the potential of Y normalized by

$$\int_M \hat{\theta}_Y(\omega_0) e^{h_0} \omega_0^n = 0. \tag{4-4}$$

By $\omega_0 = \sqrt{-1}\partial\bar{\partial}\psi_0$ and Lemma 2.8, it is not hard to see that

$$\hat{\theta}_Y(\omega_0) = Y^i \frac{\partial}{\partial x^i}\psi_0 + C, \quad \text{for all } x \in \mathfrak{a}_+, \tag{4-5}$$

where C is a constant determined by (4-4). On the other hand, we have

$$\begin{aligned}\int_{\mathfrak{a}_+} Y^i \frac{\partial}{\partial x^i}\psi_0 e^{h_0} \det(\psi_{0,ij}) \prod_{\alpha\in\Phi_+} \langle \alpha, \nabla\psi_0\rangle^2\, dx &= \int_{\mathfrak{a}_+} Y^i \frac{\partial}{\partial x^i}\psi_0 e^{-\psi_0} \boldsymbol{J}(x)\, dx \\ &= -\int_{\mathfrak{a}_+} Y^i \frac{\partial}{\partial x^i}(e^{-\psi_0}\boldsymbol{J}(x))\, dx.\end{aligned} \tag{4-6}$$

Here we used the fact that

$$Y^i \frac{\partial}{\partial x^i}\boldsymbol{J}(x) = 2\boldsymbol{J}(x) \sum_{\alpha\in\Phi_+} Y^i \alpha_i \cdot \coth\langle \alpha, x\rangle \equiv 0.$$

Note that when M is Fano, $4\rho \in \mathrm{Int}(2P_+)$ (see [Delcroix 2017b, Remark 4.10] or [Li et al. 2018, §3.2]), by [Delcroix 2017a, Proposition 2.10]. Hence, we have

$$e^{-\psi_0}\boldsymbol{J}(x) = e^{4\rho(x)-\psi_0} \prod_{\alpha\in\Phi_+} \Big(\frac{1-e^{-2\alpha(x)}}{2}\Big)^2 \to 0, \quad x \to \infty \text{ in } \mathfrak{a}_+.$$

Also recall the fact that $\boldsymbol{J}(x) = 0$ on $\partial(\mathfrak{a}_+)$. By integration by parts in (4-6), we see that

$$\int_{\mathfrak{a}_+} Y^i \frac{\partial}{\partial x^i}\psi_0 e^{h_0} \det(\psi_{0,ij}) \prod_{\alpha\in\Phi_+} \langle \alpha, \nabla\psi_0\rangle^2\, dx = 0.$$

Thus by Proposition 2.7, we get $C = 0$ in (4-5). Equation (4-2) then follows from (4-3). □

Then we use (1-4) to determine the potential of the extremal vector field X.

Lemma 4.2. *Under the coordinates chosen in Section 2C, the extremal field X, when restricted on Z, can be expressed as*

$$X = \sqrt{-1} X^i E_0^i, \quad 1 \le i \le r \tag{4-7}$$

for some $X^i \in \mathbb{R}$ *such that* $\alpha(X) = 0$, *for all* $\alpha \in \Phi$. *Furthermore*, *the* X^i *are determined by the condition*

$$\int_{2P_+} v^i y_i (1 - \theta_X(y))\pi(y)\, dy = 0, \quad \textit{for all } v \in \mathfrak{z}(\mathfrak{g}), \tag{4-8}$$

where $\theta_X(y) = X^i y_i - X^i \boldsymbol{b}_i$.

Proof. Since the Futaki invariant is a character on $\eta_r(M)$, it suffices to consider (1-4) for all $v \in \mathfrak{z}(\eta_r(M)) \subset \mathfrak{z}(\mathfrak{g})$. We may assume X is of the form (4-7). Since K_X lies in a compact group, we have $X^i \in \mathbb{R}$.

For $\phi \in \mathcal{H}_{K\times K}(\omega_0)$ and $v \in \eta_c(M)$, $\theta_v(\omega_\phi)$ is $K\times K$-invariant, so it can be written as

$$\theta_v(\omega_\phi) = v^i \frac{\partial \psi_\phi}{\partial x^i} + c_v,$$

where v^i and c_v are constants with $v^i \alpha_i = 0$ for any $\alpha \in \Phi_+$. By the second equality of (1-3), the potential is determined by

$$\theta_v(y) = v^i y_i - v^i \boldsymbol{b}_i. \tag{4-9}$$

Let $r_z = \dim(\mathfrak{z}(\mathfrak{g}))$ and suppose $E_1^0, \dots, E_{r_z}^0$ is a basis of $\mathfrak{z}(\mathfrak{g})$. We claim that the extremal vector field X is given by $X = \sum_1^{r_z} \sqrt{-1} X^i E_i^0 \in \mathfrak{z}(\mathfrak{g})$ such that

$$\boldsymbol{b}_i = \frac{1}{V}\left(\int_{2P_+} y_i y_j \pi(y)\, dy - V \boldsymbol{b}_i \boldsymbol{b}_j\right) X^j, \quad 1 \le i, j \le r_z. \tag{4-10}$$

In view of (4-9) and Lemma 4.1, it is direct to check that X given by (4-10) satisfies (1-4). Hence X must be extremal by the uniqueness. To see that (4-10) has a unique solution, it suffices to check that the matrix (a_{ij}) given by

$$a_{ij} = \frac{1}{V}\int_{2P_+} y_i y_j \pi(y)\, dy - \boldsymbol{b}_i \boldsymbol{b}_j$$

is invertible. In fact, for any vector $v = (v^i)$, consider the convex function $f_v(y) = (v^i y_i)^2$. By Jensen's inequality,

$$v^i v^j a_{ij} = \frac{1}{V}\int_{2P_+} [v(y)]^2 \pi(y)\, dy - [v(\boldsymbol{b})]^2 \ge 0,$$

with equality if and only if $f_v(y)$ is affine on $2P_+$. However, this forces $v = 0$, thus $(a_{ij}) > 0$. □

Proposition 4.3. *For* $\phi \in \mathcal{H}_{K\times K}(\omega_0)$, *the modified Ding functional is given by*

$$\mathcal{D}_X(\phi) = \mathcal{L}_X(u_\phi) + \mathcal{F}(u_\phi) + \text{const.},$$

where u_ϕ is the Legendre function of ψ_ϕ and

$$\mathcal{L}_X(u_\phi) = \frac{1}{V}\int_{2P_+} u_\phi(y)\pi(y)[1-\theta_X(y)]\,dy - u_\phi(4\rho), \tag{4-11}$$

$$\mathcal{F}(u_\phi) = -\log\biggl(\int_{\mathfrak{a}_+} e^{-\psi_\phi}\boldsymbol{J}(x)\,dx\biggr) + u_\phi(4\rho). \tag{4-12}$$

Proof. By (1-6), Proposition 2.7 and (2-14), it follows that[2]

$$\begin{aligned}\mathcal{D}^0_X(\phi) &= -\frac{1}{V}\int_0^1\int_{\mathfrak{a}_+}\dot\phi_s[1-\theta_X(\omega_{\phi_s})]\det(\psi_{\phi_s,ij})\prod_{\alpha\in\Phi_+}\langle\alpha,\nabla\psi_{\phi_s}\rangle^2\,dx\wedge ds + \text{const.},\\ \mathcal{N}(\phi) &= -\log\biggl(\frac{1}{V}\int_{\mathfrak{a}_+} e^{-\psi_\phi}\boldsymbol{J}(x)\,dx\biggr).\end{aligned} \tag{4-13}$$

By differentiation with Legendre transformations, we have $\dot u_s(y_s(x)) = -\dot\psi_s(x)$. Then by (4-13), $\mathcal{D}^0(\phi)$ equals

$$\int_0^1\int_{2P_+}\dot u_s[1-\theta_X(y)]\pi(y)\,dy\wedge ds = \int_{2P_+} u_\phi[1-\theta_X(y)]\pi(y)\,dy + \text{const.} \qquad \square$$

Remark 4.4. The functionals

$$\begin{aligned}\mathcal{L}_X(u) &= \frac{1}{V}\int_{2P_+} u(y)\pi(y)[1-\theta_X(y)]\,dy - u(4\rho),\\ \mathcal{F}(u) &= -\log\biggl(\int_{\mathfrak{a}_+} e^{-\psi}\boldsymbol{J}(x)\,dx\biggr) + u(4\rho),\end{aligned}$$

where ψ is the Legendre function of u, are well-defined on

$$\mathcal{C}'_W = \bigl\{u \in C^0(\overline{2P})\cap C^\infty(2P) \mid u \text{ is strictly convex, } W\text{-invariant}\bigr\}.$$

First, we deal with the case when $u \in C^\infty(\overline{2P})\cap\mathcal{S}_W$. In this case, we can choose the function U_δ constructed in [Donaldson 2002, Proposition 3.3.11]. Then $u_\delta = u + U_\delta \in \mathcal{C}_W$ and u_δ converges uniformly to u on $\overline{2P}$. On the other hand, let ψ, ψ_δ be the Legendre functions of u, u_δ. It follows ψ_δ converges uniformly to ψ. Hence, by definition,

$$\mathcal{L}_X(u_\delta)\to\mathcal{L}_X(u) \quad\text{and}\quad \mathcal{F}(u_\delta)\to\mathcal{F}(u) \qquad \text{as } \delta\to 0^+. \tag{4-14}$$

Thus $\mathcal{L}_X(u)$ and $\mathcal{F}(u)$ are well-defined.

For an arbitrary $u\in\mathcal{C}'_W$, consider $u^c(y) = u(cy)|_{2P}$ for $c\in(0,1)$. Then $u^c \in C^\infty(\overline{2P})\cap\mathcal{C}'_W$. Let ψ^c be the Legendre functions of u^c. As before, as $c\to 1^-$, we

[2] Since we have assumed $C_H = 1$, it follows that $V := \int_M \omega_0^n = \int_{2P_+}\pi(y)\,dy$ by Proposition 2.7. Similarly $\int_{2P_+}[1-\theta_X(y)]\pi(y)\,dy = V$.

have that u^c and ψ^c converge uniformly to u and ψ, respectively. Again, we have

$$\mathcal{L}_X(u^c) \to \mathcal{L}_X(u) \quad \text{and} \quad \mathcal{F}(u^c) \to \mathcal{F}(u) \qquad \text{as } c \to 1^-. \tag{4-15}$$

Hence, $\mathcal{L}_X(u)$ and $\mathcal{F}(u)$ are well-defined. Moreover, by (4-14) and (4-15), it follows that

$$\inf_{u\in\mathcal{C}'_W} \mathcal{D}_X(u) = \inf_{u\in\mathcal{C}_W} \mathcal{D}_X(u) \tag{4-16}$$

as proved in [Donaldson 2002, Proposition 3.3.11] for K-energy.

4B. ***The linear part.*** In this part, we deal with the linear part $\mathcal{L}_X(\cdot)$. First, we introduce the spaces of normalized functions. Let O be the origin of $\mathfrak{a}^*$. Note that $\mathfrak{a}_t^*$ is the fixed point set of the W-action. Thus $\nabla u(O) \in \mathfrak{a}_t$ for any $u \in \mathcal{C}_W$. We normalize $u \in \mathcal{C}_W$ by

$$\hat{u}(y) = u(y) - \langle \nabla u(O), y\rangle - u(O).$$

Clearly $\hat{u} \in \mathcal{C}_W$ and

$$\min_{2P} \hat{u} = \hat{u}(O) = 0. \tag{4-17}$$

The subset of normalized functions in $\mathcal{C}_W$ will be denoted by $\hat{\mathcal{C}}_W$.

Proposition 4.5. *Under the assumption* $c_X > 0$ *and* (1-8), *there exists a constant* $\lambda > 0$ *such that*

$$\mathcal{L}_X(u) \ge \lambda \int_{2P_+} u\pi(y)[1-\theta_X(y)]\,dy, \quad \textit{for all } u \in \hat{\mathcal{C}}_W. \tag{4-18}$$

Proof. Suppose the proposition is not true. Then there is a sequence $\{u_k\} \subset \hat{\mathcal{C}}_W$ such that

$$\mathcal{L}_X(u_k) \to 0 \quad \text{and} \quad \int_{2P_+} u_k\pi(y)[1-\theta_X(y)]\,dy = 1. \tag{4-19}$$

By $c_X > 0$ and the argument of [Li et al. 2018, Lemma 6.1], the second equality implies there is a subsequence (still denoted by $\{u_k\}$) which converges locally uniformly to some $u_\infty \in \hat{\mathcal{C}}_W$.

For any $u \in \mathcal{C}_W$, by convexity, we have

$$u - \langle \nabla u(\boldsymbol{b}_X), y - \boldsymbol{b}_X\rangle - u(\boldsymbol{b}_X) \ge 0. \tag{4-20}$$

Thus

$$\begin{aligned}
(4\text{-}21)\quad &\mathscr{L}_X(u)\\
&= \frac{1}{V}\int_{2P_+}[u-\langle\nabla u(\boldsymbol{b}_X),\,y-\boldsymbol{b}_X\rangle-u(\boldsymbol{b}_X)]\pi(y)[1-\theta_X(y)]\,dy\\
&\qquad+\frac{1}{V}\int_{2P_+}[\langle\nabla u(\boldsymbol{b}_X),\,y-\boldsymbol{b}_X\rangle+u(\boldsymbol{b}_X)]\pi(y)[1-\theta_X(y)]\,dy-u(4\rho)\\
&= \frac{1}{V}\int_{2P_+}[u-\langle\nabla u(\boldsymbol{b}_X),\,y-\boldsymbol{b}_X\rangle-u(\boldsymbol{b}_X)]\pi(y)[1-\theta_X(y)]\,dy+u(\boldsymbol{b}_X)\\
&\qquad\qquad-u(4\rho)\\
&\ge \frac{1}{V}\int_{2P_+}[u-\langle\nabla u(\boldsymbol{b}_X),\,y-\boldsymbol{b}_X\rangle-u(\boldsymbol{b}_X)]\pi(y)[1-\theta_X(y)]\,dy\\
&\qquad\qquad+\langle\nabla u(4\rho),\boldsymbol{b}_X-4\rho\rangle\\
&\ge 0,
\end{aligned}$$

where the last inequality follows from (1-8), (4-20) and the fact that $\nabla u(4\rho)\in\mathfrak{a}_+$. Applying the above inequality to u_k, by (4-19), we have

$$(4\text{-}22)\quad 0\le\int_{2P_+}[u_k-\langle\nabla u_k(\boldsymbol{b}_X),\,y-\boldsymbol{b}_X\rangle-u_k(\boldsymbol{b}_X)]\pi(y)[1-\theta_X(y)]\,dy\to 0,$$

$$(4\text{-}23)\quad 0\le\langle\nabla u_k(4\rho),\boldsymbol{b}_X-4\rho\rangle\to 0.$$

By (4-22), we see that u_∞ must be affine linear. Since $u_k(O)=0$, we have $u_\infty(y)=\xi^i y_i$ for some $(\xi^i)\in\bar{\mathfrak{a}}_+$. Since u_∞ is normalized and O lies in the interior of $2P_+\cap\mathfrak{a}_+^*$, it holds that $\xi\in\mathfrak{a}_{ss}$. Otherwise u_∞ is not nonnegative. Substituting u_∞ into (4-23), we see that $\langle\xi,\boldsymbol{b}_X-4\rho\rangle=0$. But $\xi\in\bar{\mathfrak{a}}_+$ and $\boldsymbol{b}_X-4\rho\in\Xi$. Hence $\xi^i=0$ and consequently $u_\infty(y)\equiv 0$.

Since $u_k(4\rho)\to u_\infty(4\rho)=0$, by (4-11) and the second line of (4-19), we have $\mathscr{L}_X(u_k)\to 1$ by the second line of (4-19), which is a contradiction. □

Yao [2017] uses (4-18) to define the “uniform relative Ding stability” in the toric case. In [Yao 2017], it is shown the condition $c_X>0$ is a necessary condition of (4-18). Since those arguments can be generalized to group compactifications with no difficulties, we omit the details.

Proposition 4.6. *Inequality* (4-18) *can not hold if* $c_X\le 0$.

4C. ***Sufficiency.*** We first show the sufficient part of Theorem 1.5 using Theorem 1.2. It suffices to prove the following theorem.

Theorem 4.7. *If* $c_X>0$ *and* (1-8) *hold, then the modified Ding functional is proper modulo* $Z(G)$. *Consequently,* M *admits Mabuchi metrics, by Theorem 1.2.*

First we have the following lemma on the nonlinear part.

Lemma 4.8. *For any $\phi \in \mathcal{H}_{K\times K}(\omega_0)$, let*

$$\tilde{\psi}_\phi := \psi_\phi - 4\rho_i x^i, \quad x \in \mathfrak{a}_+.$$

Then

$$\mathcal{F}(u_\phi) = -\log\left(\int_{\mathfrak{a}_+} e^{-(\tilde{\psi}_\phi - \inf_{\mathfrak{a}_+}\tilde{\psi}_\phi)} \prod_{\alpha\in\Phi_+}\left(\frac{1-e^{-2\alpha_i x^i}}{2}\right)^2 dx\right). \tag{4-24}$$

Consequently, for any $c > 0$,

$$\mathcal{F}(u_\phi) \geq \mathcal{F}\left(\frac{u_\phi}{1+c}\right) - n\cdot\log(1+c). \tag{4-25}$$

Proof. Since ψ_ϕ is convex, so is $\tilde{\psi}_\phi$. Thus if $x^* \in \mathfrak{a}_+$ satisfies $\nabla\psi_\phi(x^*) = 4\rho$, then

$$\tilde{\psi}_\phi(x) \geq \tilde{\psi}_\phi(x^*) = \inf_{\mathfrak{a}_+}\tilde{\psi}_\phi.$$

By the definition of Legendre transformation, we have

$$\psi_\phi(x) + u_\phi(4\rho) = \psi_\phi(x) + 4x^{*i}\rho_i - \psi_\phi(x^*) = \psi_\phi(x) - \inf_{\mathfrak{a}_+}\tilde{\psi}_\phi.$$

Substituting this into (4-12), it follows that

$$\begin{aligned}
\mathcal{F}(u_\phi) &= -\log\left(\int_{\mathfrak{a}_+} e^{-(\psi_\phi + u_\phi(4\rho))}\boldsymbol{J}(x)\,dx\right)\\
&= -\log\left(\int_{\mathfrak{a}_+} e^{-(\tilde{\psi}_\phi - \inf_{\mathfrak{a}_+}\tilde{\psi}_\phi)} e^{-4\rho_i x^i}\boldsymbol{J}(x)\,dx\right)\\
&= -\log\left(\int_{\mathfrak{a}_+} e^{-(\tilde{\psi}_\phi - \inf_{\mathfrak{a}_+}\tilde{\psi}_\phi)} \prod_{\alpha\in\Phi_+}\left(\frac{1-e^{-2\alpha_i x^i}}{2}\right)^2 dx\right).
\end{aligned}$$

This proves (4-24).

Then we prove (4-25). For $u_c(y) = \frac{1}{1+c}u(y)$, its Legendre function $\psi_c(x) = \frac{1}{1+c}\psi((1+c)x)$ satisfies $\tilde{\psi}_c(x) = \frac{1}{1+c}\tilde{\psi}((1+c)x)$. In particular,

$$-\inf_{\mathfrak{a}_+}\tilde{\psi}_c(x) = -\frac{1}{1+c}\inf_{\mathfrak{a}_+}\tilde{\psi}.$$

By the above relations and (4-24), one gets

$$\begin{aligned}
&\mathcal{F}(u_c)\\
&\quad= -\log\left(\int_{\mathfrak{a}_+} e^{-\frac{1}{1+c}(\tilde{\psi}_\phi((1+c)x) - \inf_{\mathfrak{a}_+}\tilde{\psi}_\phi)} \prod_{\alpha\in\Phi_+}\left(\frac{1-e^{-2\alpha_i x^i}}{2}\right)^2 dx\right)\\
&\quad= -\log\left(\int_{\mathfrak{a}_+} e^{-\frac{1}{1+c}(\tilde{\psi}_\phi(x) - \inf_{\mathfrak{a}_+}\tilde{\psi}_\phi)} \prod_{\alpha\in\Phi_+}\left(\frac{1-e^{-\frac{2}{1+c}\alpha_i x^i}}{2}\right)^2 dx\right) + r\cdot\log(1+c).
\end{aligned}$$

Note that $\#\Phi = (n-r)/2$. Combining the above inequality and relations

$$\log(1+c) \geq \log(1-e^{-t}) - \log(1-e^{-t/(1+c)}) \geq 0, \quad \text{for all } t \geq 0, c \geq 0$$

and

$$\mathcal{F}(u) \geq -\log\biggl(\int_{\mathfrak{a}_+} e^{-\frac{1}{1+c}(\tilde{\psi}_\phi(x) - \inf_{\mathfrak{a}_+} \tilde{\psi}_\phi)} \prod_{\alpha\in\Phi_+} \Bigl(\frac{1-e^{-2\alpha_i x^i}}{2}\Bigr)^2 \, dx\biggr),$$

we have (4-25). □

Proposition 4.9. *Suppose $c_X > 0$ and* (1-8) *holds. Then there are positive constants c and C such that*

$$\mathcal{D}_X(u) \geq c\int_{2P_+} u[1-\theta_X(y)]\pi(y)\,dy - C, \quad \textit{for all } u \in \hat{\mathscr{C}}_W. \tag{4-26}$$

Proof. Let $\omega_0 = \sqrt{-1}\partial\bar{\partial}\psi_0$ be a fixed smooth background metric with h_0 its normalized Ricci potential. Let u_0 be the Legendre function of ψ_0. Define a function A by

$$A(y) = \frac{V}{\int_{\mathfrak{a}_+} e^{-\psi_0}\boldsymbol{J}(x)\,dx} e^{h_0(\nabla u_0(y))}, \quad y(x) = \nabla\psi_0(x).$$

It is clear that

$$\int_{\mathfrak{a}_+} e^{-\psi_0}\boldsymbol{J}(x)\,dx = \int_M e^{h_0}\omega_0^n = V.$$

Hence, A is a bounded smooth function.

Let

$$\mathcal{D}_A(u_\phi) := \mathcal{D}_A^0(u_\phi) + \mathcal{N}(\phi), \quad \text{for all } \phi \in \mathcal{H}_{K\times K}(\omega_0),$$

where

$$\mathcal{D}_A^0(u) := \frac{1}{V}\int_{2P_+} uA(y)\pi(y)\,dy.$$

It is obvious that u_0 is a critical point of $\mathcal{D}_A(\cdot)$. On the other hand, along any geodesic, $\mathcal{D}_A^0(\cdot)$ is affine by Lemma 2.10 and $\mathcal{N}(\cdot)$ is convex by [Berndtsson 2015, Theorem 1.1]. Hence,

$$\mathcal{D}_A(u) \geq \mathcal{D}_A(u_0), \quad \text{for all } u \in \mathscr{C}_W.$$

Furthermore, by a similar argument as in Remark 4.4, we can extend $\mathcal{D}_A(\cdot)$ to a functional defined on $\mathscr{C}'_W$. Moreover, analogous to (4-16), we have

$$\min_{u\in\mathscr{C}'_W} \mathcal{D}_A(u) = \mathcal{D}_A(u_0). \tag{4-27}$$

Rewrite $\mathcal{D}_A(\cdot) = \mathcal{L}_A(\cdot) + \mathcal{F}(\cdot)$, where

$$\mathcal{L}_A(u) := \frac{1}{V}\int_{2P_+} uA(y)\pi(y)\,dy - u(4\rho).$$

By Proposition 4.5 and the boundedness of A, it is clear that for any $\delta > 0$

$$\begin{aligned}\mathcal{L}_X(u) - \mathcal{L}_A(u) &= \int_{2P_+} u(1-\theta_X(y) - A(y))\pi(y)\,dy \\ &\le C_A \int_{2P_+} u[1-\theta_X(y)]\pi(y)\,dy \\ &\le \frac{C_A(1+\delta)}{\lambda}\mathcal{L}_X(u) - C_A\delta \int_{2P_+} u[1-\theta_X(y)]\pi(y)\,dy,\end{aligned}$$

for all $u \in \hat{\mathscr{C}}_W$ and some constant $C_A > 0$. Thus

$$\mathcal{L}_X(u) \ge \frac{\lambda}{\lambda + C_A(1+\delta)}\Big[\mathcal{L}_A(u) + C_A\delta \int_{2P_+} u[1-\theta_X(y)]\pi(y)\,dy\Big],$$

for all $u \in \hat{\mathscr{C}}_W$. Hence, taking $C = C_A(1+\delta)/\lambda$, we have for any $u \in \hat{\mathscr{C}}_W$,

$$\begin{aligned}&\mathcal{D}_X(u) \\ &\ge \mathcal{L}_A\Big(\frac{u}{1+C}\Big) + \mathcal{F}(u) + \frac{C_A\delta}{1+C}\int_{2P_+} u[1-\theta_X(y)]\pi(y)\,dy \\ &\ge \mathcal{L}_A\Big(\frac{u}{1+C}\Big) + \mathcal{F}\Big(\frac{u}{1+C}\Big) + \frac{C_A\delta}{1+C}\int_{2P_+} u[1-\theta_X(y)]\pi(y)\,dy \\ &\quad - n\log(1+C) \\ &= \mathcal{D}_A\Big(\frac{u}{1+C}\Big) + \frac{C_A\delta}{1+C}\int_{2P_+} u[1-\theta_X(y)]\pi(y)\,dy - n\log(1+C),\end{aligned} \tag{4-28}$$

where we used (4-25). By using (4-27)

$$\mathcal{D}_A\Big(\frac{u}{1+C}\Big) \ge \mathcal{D}_A(u_0).$$

Thus, combining with (4-28), we have

$$\mathcal{D}_X(u) \ge \frac{C_A\delta}{1+C}\int_{2P_+} u[1-\theta_X(y)]\pi(y)\,dy + \big(\mathcal{D}_A(u_0) - n\log(1+C)\big). \qquad \square$$

To use Theorem 1.2, we introduce the following normalization: for any $\phi \in \mathcal{H}_{K\times K}(\omega_0)$, let u_ϕ be the Legendre function of ψ_ϕ. Take a $v \in \eta_c(M)$ such that $\mathrm{Re}(v) = -\nabla u_\phi(O)$. Let $\sigma_v(t)$ be the one parameter group generated by $\mathrm{Re}(v)$. Then $\sigma_v(t) \in Z(G)$. It follows that

$$(\sigma_v(1))^*\omega_\phi = \omega_0 + \sqrt{-1}\partial\bar{\partial}\hat{\phi}$$

induces a $K\times K$-invariant Kähler potential $\hat{\phi}$. Since we may also normalize $\psi_{\hat{\phi}}$ so that $\psi_{\hat{\phi}}(O) = 0$, the Legendre function $u_{\hat{\phi}}$ of $\psi_{\hat{\phi}}$ is given by

$$u_{\hat{\phi}}(y) = u_\phi(y) - \langle \nabla u_\phi(O), y\rangle - u_\phi(O), \tag{4-29}$$

which satisfies $u_{\hat{\phi}} \in \hat{\mathscr{C}}_W$. Then we have:

Lemma 4.10. *Under the above normalization, we have* $\mathscr{D}_X(u_{\hat{\phi}}) = \mathscr{D}_X(u_\phi)$.

Proof. Let $a^i = -\mathrm{Re}(u_{\phi,i}(O))$; then $(a^i) \in \mathfrak{a}_t$ and consequently $\alpha(a) = 0$ for all $\alpha \in \Phi$. On the other hand, we have

$$\psi_{\hat{\phi}}(x) = \psi_\phi(x-a) + u_\phi(O).$$

Taking the change of variables $x \to (x-a)$ in (4-24), by the above relations, we see that $\mathscr{F}(u_\phi) = \mathscr{F}(u_{\hat{\phi}})$. By $(a^i) \in \mathfrak{a}_t$ and (4-8), $\mathscr{L}_X(a^i y_i - u_\phi(O)) = 0$. Hence, by (4-29) $\mathscr{L}_X(u_\phi) = \mathscr{L}_X(u_{\hat{\phi}})$. The lemma is proved. □

The following lemma is analogous to [Li et al. 2018, Lemma 4.14; Wang et al. 2016, Lemma 3.4], we omit the proof.

Lemma 4.11. *There exists a uniform* $C_J > 0$ *such that*

$$\left| J_X(\hat{\phi}) - \int_{2P_+} u_{\hat{\phi}}[1-\theta_X(y)]\pi(y)\,dy \right| \le C_J, \quad \text{for all } \phi \in \mathscr{H}_{K\times K}(\omega_0),$$

where $u_{\hat{\phi}} \in \hat{\mathscr{C}}_W$ *and* $\psi_{\hat{\phi}}$ *is the Legendre function of* $u_{\hat{\phi}}$.

Proof of Theorem 4.7. For any $\phi \in \mathscr{H}_{K\times K}(\omega_0)$, there exists $\sigma \in Z(G)$ such that

$$\sigma^*\omega_\phi = \omega_0 + \sqrt{-1}\partial\bar{\partial}\hat{\phi}$$

as above. Applying Proposition 4.9, we have

$$\mathscr{D}_X(u_{\hat{\phi}}) \ge \delta \int_{2P_+} u_{\hat{\phi}}\pi\,dy - C_\delta.$$

Thus by Proposition 4.3 and Lemmas 4.10, 4.11,

$$\mathscr{D}_X(\phi) = \mathscr{D}_X(\hat{\phi}) = \mathscr{D}_X(u_{\hat{\phi}}) \ge \delta \cdot J_X(\hat{\phi}) - C_J - C_\delta.$$

The theorem then follows from (2-7). □

4D. *Necessity.* To complete the proof of Theorem 1.5, we will show that (1-8) is also a necessary condition of the existence of Mabuchi metrics. It is equivalent to show that

$$\langle \xi, \boldsymbol{b}_X - 4\rho \rangle > 0, \quad \text{for all } \xi \in \mathfrak{a}_+. \tag{4-30}$$

We will adopt the method used in [Delcroix 2017a].

By the $K\times K$-invariance, (2-1) can be reduced to the following Monge–Ampére equation on $\mathfrak{a}_+$,

$$\det(\psi_{0,ij} + \phi_{ij}) \prod_{\alpha\in\Phi_+} \langle \alpha, \nabla(\psi_0+\phi)\rangle^2 = C \cdot \frac{e^{-(\psi_0+\phi-\log \boldsymbol{J})}}{1-\theta_X(\omega_0) - X(\phi)}. \tag{4-31}$$

Suppose ϕ is a solution, for any $\xi \in \mathfrak{a}_+$, we have

$$\begin{aligned}
0 &= -\int_{\mathfrak{a}_+} \xi^i \frac{\partial}{\partial x^i} e^{-(\psi_0+\phi-\log \boldsymbol{J})} \\
&= \int_{\mathfrak{a}_+} \xi^i e^{-(\psi_0+\phi-\log \boldsymbol{J})} \frac{\partial(\psi_0+\phi-\log \boldsymbol{J})}{\partial x^i} \\
&= \int_{\mathfrak{a}_+} \xi^i \det(\psi_{0,ij}+\phi_{,ij}) \Big(\prod_{\alpha\in\Phi_+} \langle\alpha, \nabla(\psi_0+\phi)\rangle^2\Big)[1-\theta_X(\omega_\phi)] \frac{\partial(\psi_0+\phi-\log \boldsymbol{J})}{\partial x^i} \\
&< V\int_{2P_+} \xi^i (y_i-4\rho_i)\pi(y)[1-\theta_X(y)]\,dy \\
&= V\cdot\langle\xi, \boldsymbol{b}_X-4\rho\rangle,
\end{aligned}$$

where in the fourth line we used the fact that for any $\xi, x \in \mathfrak{a}_+$

$$-\xi^i \frac{\partial}{\partial x^i} \log \boldsymbol{J} = -2\sum_{\alpha\in\Phi_+} \alpha(\xi)\cdot \coth\alpha(x) < -2\sum_{\alpha\in\Phi_+} \alpha(\xi) = -4\rho(\xi).$$

Then we have (4-30).

Appendix: Proof of Theorem 2.1

In this appendix, we solve (2-2) at $t=0$. Following [Zhu 2000] for the Kähler–Ricci soliton case, we introduce the following path,

$$(1-\theta_X(\omega_{\phi_t}))^t \omega^n_{\phi_t} = e^{h_0}\omega_0^n, \quad t \in [0, 1]. \tag{A-1}$$

Set $\mathfrak{I} := \{t \in [0, 1] \mid \text{(A-1) has a solution for } t\}$. The Calabi–Yau theorem implies that $0 \in \mathfrak{I}$. We shall prove $\mathfrak{I}$ is both open and closed in [0, 1].

Openness. Define a functional

$$J_t(\phi) = \int_0^1\int_M \dot\phi_s (1-\theta_X(\omega_{\phi_s}))^t\, \omega^n_{\phi_s} \wedge ds,$$

where ϕ_s is any smooth path joining ϕ and 0 in $\mathcal{H}_X(\omega_0)$. It is standard to show that $J_t(\cdot)$ is well-defined. Thus by taking $\phi_s = s\phi$, we have

$$J_t(\phi) = \int_0^1\int_M \phi (1-\theta_X(\omega_{s\phi_s}))^t\, \omega^n_{s\phi} \wedge ds.$$

Replacing h_0 by $h_0 + J_t(\phi_t)$ in (A-1), we have the operator L_t defined by

$$L_t(\psi) := \triangle_{\omega_{\phi_t}}\psi - \frac{tX(\psi)}{1-\theta_X(\omega_{\phi_t})} - \int_M \psi(1-\theta_X(\omega_{\phi_t}))^t\, \omega^n_{\phi_t}, \quad \text{for all } \psi \in \mathcal{H}_X(\omega_0).$$

Then for any K_X-invariant smooth real functions f and g, it is easy to see

$$\int_M L_t(f)g(1-\theta_X(\omega_{\phi_t}))^t\omega_{\phi_t}^n = \int_M fL_t(g)(1-\theta_X(\omega_{\phi_t}))^t\omega_{\phi_t}^n. \tag{A-2}$$

Lemma A.1. *Suppose ϕ_t is a smooth solution of* (A-1) *for some $t \in [0, 1)$. Then, the first eigenvalue of L_t is positive.*

Proof. Suppose λ is the first eigenvalue and ψ is an eigenfunction. Then by $L_t\psi = -\lambda\psi$,

$$\lambda\int_M \psi(1-\theta_X(\omega_{\phi_t}))^t\omega_{\phi_t}^n = \int_M \psi(1-\theta_X(\omega_{\phi_t}))^t\omega_{\phi_t}^n \cdot \int_M \psi(1-\theta_X(\omega_{\phi_t}))^t\omega_{\phi_t}^n.$$

By the assumption $c_X > 0$, if $\psi \equiv c$ for some constant $c \neq 0$, so $\lambda > 0$. Thus we may assume that $\psi \not\equiv$ const. below.

As before, we may choose a local coframe $\{\Theta^i\}$ such that

$$\omega_{\phi_t} = \sqrt{-1}\sum_{i=1}^n \Theta^i \wedge \bar{\Theta}^i.$$

By (3-2) and integration by parts, it follows that

$$\begin{aligned} \lambda\int_M &\psi_{,i}\psi_{,\bar{i}}(1-\theta_X(\omega_{\phi_t}))^t\omega_{\phi_t}^n \\ &= -\int L_t(\psi)_{,i}\psi_{,\bar{i}}(1-\theta_X(\omega_{\phi_t}))^t\omega_{\phi_t}^n \\ &= -\int_M \psi_{,j\bar{j}i}\psi_{,\bar{i}}(1-\theta_X(\omega_{\phi_t}))^t\omega_{\phi_t}^n + t\int_M \frac{X^j_{,i}\psi_{,j}\psi_{,\bar{i}}}{1-\theta_X(\omega_{\phi_t})}(1-\theta_X(\omega_{\phi_t}))^t\omega_{\phi_t}^n \\ &\qquad + t\int_M \frac{\bar{X}^{\bar{j}}X^i\psi_{,i}\psi_{,\bar{j}}}{(1-\theta_X(\omega_{\phi_t}))^2}(1-\theta_X(\omega_{\phi_t}))^t\omega_{\phi_t}^n \\ &\qquad\qquad + \int_M \frac{X^j\psi_{,\bar{i}}\psi_{,ij}}{1-\theta_X(\omega_{\phi_t})}(1-\theta_X(\omega_{\phi_t}))^t\omega_{\phi_t}^n. \end{aligned} \tag{A-3}$$

By the Ricci identity and integration by parts, the first term on the right-hand side

$$\begin{aligned} -\int_M &\psi_{,j\bar{j}i}\psi_{,\bar{i}}(1-\theta_X(\omega_{\phi_t}))^t\omega_{\phi_t}^n \\ &= -\int_M (\psi_{,ij\bar{j}} - R^p_{j\ i\bar{j}}\psi_{,p})\psi_{,\bar{i}}(1-\theta_X(\omega_{\phi_t}))^t\omega_{\phi_t}^n \\ &= \int_M \mathrm{Ric}_{i\bar{p}}\,\psi_{,p}\psi_{,\bar{i}}(1-\theta_X(\omega_{\phi_t}))^t\omega_{\phi_t}^n + \int_M \psi_{,ij}\psi_{,\bar{i}\bar{j}}(1-\theta_X(\omega_{\phi_t}))^t\omega_{\phi_t}^n \\ &\qquad - t\int_M \psi_{,ij}\psi_{,\bar{i}}X^j(1-\theta_X(\omega_{\phi_t}))^{t-1}\omega_{\phi_t}^n. \end{aligned}$$

Plugging the above equality into (A-3), one gets

$$\text{(A-4)}\quad \lambda\int_M \psi_{,i}\psi_{,\bar{i}}(1-\theta_X(\omega_{\phi_t}))^t\omega_{\phi_t}^n = \int_M\left(\mathrm{Ric}_{i\bar{j}}+\frac{tX_{\bar{j},i}}{1-\theta_X(\omega_{\phi_t})}\right)\psi_{,j}\psi_{,\bar{i}}(1-\theta_X(\omega_{\phi_t}))^t\omega_{\phi_t}^n + \int_M \psi_{,ij}\psi_{,\bar{i}\bar{j}}(1-\theta_X(\omega_{\phi_t}))^t\omega_{\phi_t}^n + t\int_M \frac{\overline{X}^{\bar{j}}X^i\psi_{,i}\psi_{,\bar{j}}}{(1-\theta_X(\omega_{\phi_t}))^2}(1-\theta_X(\omega_{\phi_t}))^t\omega_{\phi_t}^n.$$

On the other hand, by (A-1),

$$\mathrm{Ric}_{i\bar{j}}(\omega_{\phi_t}) = g_{i\bar{j}}(t) - t\left[\frac{X_{i,\bar{j}}}{1-\theta_X(\omega_{\phi_t})}+\frac{\overline{X}_{,i}X_{,\bar{j}}}{(1-\theta_X(\omega_{\phi_t}))^2}\right].$$

Plugging this into (A-4), one gets

$$\lambda\int_M \psi_{,i}\psi_{,\bar{i}}(1-\theta_X(\omega_{\phi_t}))^t\omega_{\phi_t}^n = \int_M g_{i\bar{j}}(0)\psi_{,\bar{i}}\psi_{,j}(1-\theta_X(\omega_{\phi_t}))^t\omega_{\phi_t}^n + \int_M \psi_{,ij}\psi_{,\bar{i}\bar{j}}(1-\theta_X(\omega_{\phi_t}))^t\omega_{\phi_t}^n.$$

Since $\psi\not\equiv$ const., it must hold that $\lambda>0$. □

The openness then follows from the above lemma and implicit function theorem.

Closedness. For the closeness, it suffices to establish the a priori estimates for (A-1).

First, we prove the C^0-estimate.

Proposition A.2. *Let ϕ_t be a solution of* (A-1) *at t. Then there exists a uniform constant C such that $|\phi_t|\le C$.*

Proof. Consider the equation

$$\text{(A-5)}\qquad \det(g_{i\bar{j}}(t))(1-\theta_X(\omega_{\phi_t}))^t = \det(g_{i\bar{j}}(0))e^{h_0+J_t(\phi_t)}.$$

By integration,

$$\int_M (1-\theta_X(\omega_{\phi_t}))^t\omega_{\phi_t}^n = e^{J_t(\phi_t)}V,$$

we have

$$J_t(\phi_t) = \log\int_M (1-\theta_X(\omega_{\phi_t}))^t\omega_{\phi_t}^n - \log V.$$

This implies

$$\text{(A-6)}\qquad t\log c_X \le J_t(\phi_t)\le t\log C_X.$$

Equation (A-5) can be rewritten as

$$\det(g_{i\bar{j}}(t)) = \det(g_{i\bar{j}}(0))e^{\hat{f}_t},$$

where $\hat{f}_t := h_0 + J_t(\phi_t) - t\log(1-\theta_X(\omega_{\phi_t}))$. Let $\hat{\phi}_t = \phi_t - c_t$. Then $\sup_M \hat{\phi}_t = -1$. Since

$$|\hat{f}_t| \le \|h_0\|_{C^0} + 2\max\{|\log c_X|, |\log C_X|\},$$

by the argument for the C^0-estimate in [Tian 1996], we see that $|\hat{\phi}_t| \le C'$ for some uniform $C' > 0$. On the other hand,

$$\text{(A-7)}\quad c_t \int_0^1 \int_M (1-\theta_X(\omega_{s\phi_t}))^t \omega_{s\phi_t}^n \wedge ds = J_t(\phi_t) - \int_0^1 \int_M \hat{\phi}_t (1-\theta_X(\omega_{s\phi_t}))^t \omega_{s\phi_t}^n \wedge ds.$$

Combining (A-6), (A-7) and the fact that $0 < c_x \le 1-\theta_X(\omega_{s\phi_t}) \le C_X$, one gets a uniform constant $\hat{C}$ such that $|c_t| \le \hat{C}$. This implies

$$|\phi_t| \le |\hat{\phi}_t| + \hat{C} \le C' + \hat{C}. \qquad \square$$

Next we consider the C^2-estimate.

Proposition A.3. *Let* $\phi = \phi_t$ *be a solution of* (A-1) *at* t. *Then there exist two uniform positive constants* C *and* c *such that*

$$n + \triangle_{\omega_0}\phi \le C e^{c(\phi_t - \inf_M \phi_t)}.$$

Proof. Following the computations of [Zhu 2000, Section 6], at the point where $(n+\triangle_{\omega_0}\phi)e^{-c\phi}$ takes its maximum, we have

$$\triangle_{\omega_0} \log(1-\theta_X(\omega_\phi)) = -\frac{\triangle_{\omega_0}\theta_X(\omega_\phi)}{1-\theta_X(\omega_\phi)} - \frac{|\partial\theta_X(\omega_\phi)|^2}{(1-\theta_X(\omega_\phi))^2} \le C_1(n+\triangle_{\omega_0}\phi) + C_2$$

for some constants C_1, C_2 independent of ϕ. Then as in [Zhu 2000, (6.2)], we see that at this point,

$$\begin{aligned}\text{(A-8)}\quad & \triangle_{\omega_\phi}((n+\triangle_{\omega_0}\phi)e^{-c\phi}) \\ & \ge e^{-c\phi}\big(\triangle_{\omega_0}(h_0 - t\log(1-\theta_X(\omega_\phi))) - n^2 \inf_{l\ne k} R_{i\bar{i}l\bar{l}}\big) \\ & \qquad + (c + \inf_{l\ne i} R_{i\bar{i}l\bar{l}})(n+\triangle_{\omega_0}\phi)e^{-c\phi}\left(\sum_i \frac{1}{1+\phi_{,i\bar{i}}}\right) - cn(n+\triangle_{\omega_0}\phi)e^{-c\phi} \\ & \ge -e^{-c\phi}(C_3 + cC_4(n+\triangle_{\omega_0}\phi)) + C_5 e^{-c\phi}(n+\triangle_{\omega_0}\phi)^{n/(n-1)}\end{aligned}$$

for sufficiently large constant c and some uniform constants C_3–C_5. The proposition then follows from (A-8) in a standard way. $\square$

The higher order estimates then follow from nonlinear elliptic equation theory and we omit the details.

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A GENERALIZATION OF MALOO'S THEOREM ON FREENESS OF DERIVATION MODULES

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Let A be a Noetherian local k-domain (k is a Noetherian ring) whose derivation module $\mathrm{Der}_k(A)$ is finitely generated as an A-module, and let $\mathfrak{P}_{A/k} \subset A$ be the corresponding maximally differential ideal. A theorem due to Maloo states that if A is regular and height $\mathfrak{P}_{A/k} \leq 2$, then $\mathrm{Der}_k(A)$ is A-free. In this note we prove the following generalization: if $\mathrm{projdim}_A(\mathrm{Der}_k(A)) < \infty$ and grade $\mathfrak{P}_{A/k}$ = height $\mathfrak{P}_{A/k} \leq 2$, then $\mathrm{Der}_k(A)$ is A-free. We provide several corollaries — to wit, the cases where A contains a field of positive characteristic, A is Cohen–Macaulay, or A is a factorial domain — as well as examples with $\mathrm{Der}_k(A)$ having infinite projective dimension. Moreover, our result connects to the Herzog–Vasconcelos conjecture, raised for algebras essentially of finite type over a field of characteristic zero, which we show to be true if depth $A \leq 2$ in a much more general context.

1. Motivation: Maloo's theorem

The investigation about either necessary or sufficient conditions for the freeness of derivation modules, in the algebrogeometric setting of local rings which are essentially of finite type over a field of characteristic zero, has attracted attention for decades. One of the natural reasons is the fact that derivations can be realized as tangent vector fields on the given algebraic variety. Several conjectures have been proposed on the theme, such as the famous Zariski–Lipman conjecture, which remains open in the nongraded 2-dimensional case, and the so-called Herzog–Vasconcelos conjecture, which is homological in nature and, unlike the former, is known to be true in a few specific situations.

Beyond the traditional context of localizations of affine rings, the problem of understanding freeness of derivation modules of more general Noetherian local algebras has been poorly tackled and is, at present, far from being well understood.

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One of the few results in this direction is given in [Maloo 1999, Theorem 4] in the case of (commutative, unital) Noetherian *regular* local algebras. In order to state Maloo's theorem, let k be a Noetherian ring and let A be a Noetherian regular local k-domain for which the A-module $\mathrm{Der}_k(A)$ formed by the k-derivations of A is finitely generated. Let $\mathfrak{P}_{A/k}$ be the corresponding maximally differential ideal (it exists and, in the local case, is unique). Assume that $\mathfrak{P}_{A/k}$ has height at most 2. Then $\mathrm{Der}_k(A)$ is free as an A-module.

In the present paper our main goal is to generalize Maloo's theorem. After invoking in Section 2 a couple of preparatory facts, due to Maloo himself and to Lequain, we give in Section 3 our central result (Theorem 3.1) which establishes the following: Let k be a Noetherian ring and let A be a Noetherian local k-domain such that $\mathrm{Der}_k(A)$ is a finitely generated A-module and $\operatorname{grade}\mathfrak{P}_{A/k} = \operatorname{height}\mathfrak{P}_{A/k} \leq 2$. If $\operatorname{projdim}_A(\mathrm{Der}_k(A)) < \infty$ then $\mathrm{Der}_k(A)$ is free as an A-module.

From this result we derive corollaries where we get rid of the hypothesis $\operatorname{grade}\mathfrak{P}_{A/k} = \operatorname{height}\mathfrak{P}_{A/k}$. Namely, if A is a Noetherian local k-domain such that $\mathrm{Der}_k(A)$ is a finitely generated A-module of finite projective dimension and $\operatorname{height}\mathfrak{P}_{A/k} \leq 2$, then $\mathrm{Der}_k(A)$ is a free A-module in the following cases:

- k is a field of positive characteristic contained in A (Corollary 3.3),
- A is Cohen–Macaulay (Corollary 3.5),
- A is a factorial domain (Corollary 3.6).

Note that the last two corollaries independently recover Maloo's theorem (which we state as Corollary 3.8), since a regular ring A is necessarily Cohen–Macaulay, factorial, and satisfies the property that all finitely generated A-modules have finite projective dimension. It is also worth mentioning that factorial non-Cohen–Macaulay domains of characteristic zero do exist (see Remark 3.7).

In Remark 3.9 we point out, for completeness, that the converse of Maloo's result is false; we give an instance in characteristic $p > 0$, and we mention that there exists a difficult example in characteristic zero constructed by Maloo.

In Section 4 we employ our results in order to present explicit examples of hypersurface rings A over a field k, in characteristic zero as well as in prime characteristic, satisfying the property that

$$\operatorname{projdim}_A(\mathrm{Der}_k(A)) = \infty.$$

An auxiliary tool is Lemma 4.1, which furnishes a set of generators together with a test for the nonfreeness of $\mathrm{Der}_k(A)$ in this setting. We are also able to describe the ideal $\mathfrak{P}_{A/k}$ in the examples.

Section 5 deals with the aforementioned Herzog–Vasconcelos conjecture, which precisely predicts that if k is a field with $\operatorname{char} k = 0$ and A is a local ring which is essentially of finite type over k, with the property that $\operatorname{projdim}_A(\mathrm{Der}_k(A)) < \infty$, then $\mathrm{Der}_k(A)$ must be free as an A-module. Herzog provides an excellent survey [Herzog 1994] on homological problems related to certain modules (we point out that in [Vasconcelos 1985, p. 373] there is also a related conjecture which says that under the above conditions the ring A must be a complete intersection). The Herzog–Vasconcelos conjecture has been settled in a few specific cases, and its hypotheses force A to be a normal domain (as well as Gorenstein if A is Cohen–Macaulay; see Remark 5.1). Our contribution is Corollary 5.2, which is stated in greater generality and solves the problem in the case where depth $A \leq 2$. As a consequence, the conjecture is true for the local ring of any point of an affine algebraic surface over a ground field of arbitrary characteristic. We finish the paper by illustrating Corollary 5.2 in Example 5.3, which gives a three-dimensional non-Cohen–Macaulay normal domain A, essentially of finite type over a field k with char $k = 0$, such that $\mathrm{Der}_k(A)$ has infinite projective dimension over A.

2. Preliminaries and auxiliary results

All rings in this paper are tacitly assumed to be commutative, unital, and Noetherian. If A is a ring and M is an A-module, a *derivation* of A into M is an additive map $\Delta : A \to M$ such that

$$\Delta(ab) = a\Delta(b) + b\Delta(a) \quad \text{for all } a, b \in A.$$

We denote by $\mathrm{Der}(A, M)$ the set of all derivations of A into M, which is an A-module in a natural way. If A is a k-algebra via a ring homomorphism $\psi : k \to A$, an element of $\mathrm{Der}(A, M)$ is a *k-derivation* if it vanishes on the image of ψ (a typical situation is when ψ is an inclusion). The set formed by all k-derivations of A into M is denoted by $\mathrm{Der}_k(A, M)$, which is seen to be an A-submodule of $\mathrm{Der}(A, M)$. If $\Omega_{A/k}$ is the module of Kähler k-differentials of A, it is well known that

$$\mathrm{Hom}_A(\Omega_{A/k}, M) \simeq \mathrm{Der}_k(A, M).$$

We refer, e.g., to [Matsumura 1986, Chapter 9]. In the case $M = A$ we simplify the notation to $\mathrm{Der}_k(A)$ (which is then the A-dual of $\Omega_{A/k}$). If for instance A is a polynomial ring $k[X_1, \ldots, X_n]$ — or a localization thereof — then $\mathrm{Der}_k(A)$ is a free A-module on the partial derivations $\partial_1, \ldots, \partial_n$.

We invoke a few specific concepts and facts that will play a fundamental role in the sequel.

Definition 2.1. Given a k-algebra A, we say that an ideal $\mathfrak{a} \subseteq A$ is $\mathrm{Der}_k(A)$-*differential* (*differential*, for short) if

$$\Delta(\mathfrak{a}) \subseteq \mathfrak{a} \quad \text{for all } \Delta \in \mathrm{Der}_k(A).$$

Remark 2.2. By Zorn's lemma, the family

$$\mathfrak{F}_{A/k} = \{\mathfrak{b} \mid \mathfrak{b} \text{ is a proper differential ideal of } A\}$$

contains maximal elements. If A is local, then $\mathfrak{F}_{A/k}$ has a unique maximal element [Maloo 1997, p. 82], the so-called *maximally differential ideal* of the k-algebra A, denoted herein by $\mathfrak{P}_{A/k}$. This ideal has interesting properties; besides the results given in the present paper, we mention for example [Brumatti and Lequain 1994; Singh 1983], as well as the connection between $\mathfrak{P}_{A/k}$ and Hironaka's concept of permissibility [Seibt 1980, Theorem 1.2]. On the other hand, certain features of this ideal are quite subtle, for instance its behavior under completion [de Souza Doering and Lequain 1986; Patil and Singh 1983].

Lemma 2.3 [Maloo 1997, Theorem 5]. *If A is a local k-algebra such that* $\mathrm{Der}_k(A)$ *is a finitely generated A-module, then* $\mathrm{Der}_k(A)/\mathfrak{P}_{A/k}\,\mathrm{Der}_k(A)$ *is free as an $A/\mathfrak{P}_{A/k}$-module. In particular, if* $\mathfrak{P}_{A/k} = (0)$, *then* $\mathrm{Der}_k(A)$ *is free as an A-module.*

Lemma 2.4 [Lequain 1971, Theorem 1.4]. *Let $(A, \mathfrak{m})$ be a local k-algebra.*

(i) *If $A/\mathfrak{P}_{A/k}$ has positive characteristic, then* $\operatorname{rad}\mathfrak{P}_{A/k} = \mathfrak{m}$.

(ii) *If $A/\mathfrak{P}_{A/k}$ has characteristic zero, then $\mathfrak{P}_{A/k}$ is prime.*

3. Main result and corollaries

If A is a ring, by a *finite* A-module we shall mean, as usual, a finitely generated A-module, and the *grade* of an ideal $\mathfrak{a} \subset A$ is the number $\operatorname{grade}\mathfrak{a}$ defined as the maximal length of an A-sequence contained in $\mathfrak{a}$. Recall that $\operatorname{grade}\mathfrak{a}$ is bounded above by the height of $\mathfrak{a}$. Basic facts can be found in [Bruns and Herzog 1998].

In the sequel, k denotes a ring. A *k-domain* is an integral domain with a structure of k-algebra. Our central result is the following:

Theorem 3.1. *Let A be a local k-domain such that* $\mathrm{Der}_k(A)$ *is a finite A-module and* $\operatorname{grade}\mathfrak{P}_{A/k} = \operatorname{height}\mathfrak{P}_{A/k} \le 2$. *If* $\operatorname{projdim}_A(\mathrm{Der}_k(A)) < \infty$, *then* $\mathrm{Der}_k(A)$ *is free as an A-module.*

Proof. For simplicity we write $\mathfrak{P} = \mathfrak{P}_{A/k}$ (which exists and is unique, as mentioned in Remark 2.2) and $D = \mathrm{Der}_k(A)$. We may suppose that $D \neq 0$. As recalled in Section 2, if $\Omega = \Omega_{A/k}$ is the module of Kähler k-differentials of A, we have $\mathrm{Hom}_A(\Omega, M) \simeq \mathrm{Der}_k(A, M)$ for every A-module M.

If p stands for the characteristic of the residue ring $A/\mathfrak{P}$, we distinguish two cases:

(i) $p > 0$. Let $\mathfrak{m}$ be the maximal ideal of A. By Lemma 2.4(i), we have $\operatorname{rad}\mathfrak{P} = \mathfrak{m}$. Hence, $\dim A = \operatorname{height}\mathfrak{P} \le 2$, which yields

$$\operatorname{depth} A \le 2.$$

On the other hand, we may assume that depth $A \geq 1$, as otherwise the domain A must a field K; hence, $D = \mathrm{Der}_k(K)$ is a (finite-dimensional) K-vector space and we are done. Let $a \in \mathfrak{m}$ be a nonzero element. Applying $\mathrm{Hom}_A(\Omega, \cdot)$ to the short exact sequence

$$0 \to A \xrightarrow{\cdot a} A \to A/(a) \to 0$$

we get an exact sequence of derivation modules

$$0 \to D \xrightarrow{\cdot a} D \to \mathrm{Der}_k(A, A/(a)).$$

In particular, a is D-regular and the quotient D/aD can be regarded as a submodule of $\mathrm{Der}_k(A, A/(a))$. Now if $\{a, b\} \subset \mathfrak{m}$ is an A-sequence, then in order to conclude that $\{a, b\}$ is a D-sequence it suffices to show that b is $\mathrm{Der}_k(A, A/(a))$-regular. Also note that $D/(a, b)D \neq 0$ because of Nakayama's lemma. Applying $\mathrm{Hom}_A(\Omega, \cdot)$ to the exact sequence

$$0 \to A/(a) \xrightarrow{\cdot b} A/(a)$$

we obtain an exact sequence

$$0 \to \mathrm{Der}_k(A, A/(a)) \xrightarrow{\cdot b} \mathrm{Der}_k(A, A/(a))$$

as needed. Thus, we have shown that depth $D \geq$ depth A. Since $\mathrm{projdim}_A D < \infty$, the Auslander–Buchsbaum formula forces D to be free.

(ii) $p = 0$. According to Lemma 2.4(ii), the ideal $\mathfrak{P}$ is prime. Consider the local ring $(A_{\mathfrak{P}}, \mathfrak{P}A_{\mathfrak{P}})$. First we claim that the $A_{\mathfrak{P}}$-module $D_{\mathfrak{P}} = D \otimes_A A_{\mathfrak{P}}$ is free. Note that $D_{\mathfrak{P}}$ may not be isomorphic to $\mathrm{Der}_k(A_{\mathfrak{P}})$ since we are not requiring $\Omega_{A/k}$ to be finitely presented.

Let $\boldsymbol{a}$ be an A-sequence of maximal length contained in $\mathfrak{P}$. By hypothesis, this length is at most 2. Of course we may assume that $D_{\mathfrak{P}} \neq 0$. Using the same argument employed in the previous case (i), we get that $\boldsymbol{a}$ is a D-sequence. Hence,

$$\boldsymbol{a}/\mathbf{1} \subset \mathfrak{P}A_{\mathfrak{P}}$$

is a $D_{\mathfrak{P}}$-sequence [Bruns and Herzog 1998, Corollary 1.1.3(a)], and we obtain

$$\text{depth } D_{\mathfrak{P}} \geq \text{grade } \mathfrak{P} = \text{height } \mathfrak{P} = \dim A_{\mathfrak{P}} \geq \text{depth } A_{\mathfrak{P}}.$$

The hypothesis $\mathrm{projdim}_A D < \infty$ yields $\mathrm{projdim}_{A_{\mathfrak{P}}} D_{\mathfrak{P}} < \infty$ and then the Auslander–Buchsbaum formula guarantees the freeness of $D_{\mathfrak{P}}$, as claimed.

We proceed to prove that D itself is free as an A-module. As a matter of notation, if $(B, \mathfrak{n})$ is a local domain, then we denote by $\nu_B(N)$ and $\mathrm{rank}_B N$ the minimal number of generators and the generic rank of a finite B-module N, respectively. The former is the dimension of the $B/\mathfrak{n}$-vector space $N/\mathfrak{n}N$, and the latter is the dimension of the L-vector space $N \otimes_B L$, where $L = B_{(0)}$ (the fraction field of B).

It is a standard fact that $\nu_B(N) \geq \operatorname{rank}_B N$, with equality if and only if N is a free B-module.

As the domains A and $A_{\mathfrak{P}}$ have clearly the same field of fractions, it is easy to see that $\operatorname{rank}_A D = \operatorname{rank}_{A_{\mathfrak{P}}} D_{\mathfrak{P}}$, and since the $A_{\mathfrak{P}}$-module $D_{\mathfrak{P}}$ is free, we get

$$\operatorname{rank}_A D = \nu_{A_{\mathfrak{P}}}(D_{\mathfrak{P}}).$$

Therefore, in order to prove that D is free, it suffices to verify that $\nu_{A_{\mathfrak{P}}}(D_{\mathfrak{P}}) = \nu_A(D)$. To this end, we apply Lemma 2.3, which gives

$$D/\mathfrak{P}D \simeq (A/\mathfrak{P})^{\oplus r}$$

for some integer $r \geq 1$. Thus,

$$\nu_A(D) = \nu_A(D/\mathfrak{P}D) = \nu_{A/\mathfrak{P}}(D/\mathfrak{P}D) = r.$$

On the other hand, if we denote

$$\kappa(\mathfrak{P}) = A_{\mathfrak{P}}/\mathfrak{P}A_{\mathfrak{P}}$$

(the residue field of $A_{\mathfrak{P}}$), we can write

$$\nu_{A_{\mathfrak{P}}}(D_{\mathfrak{P}}) = \nu_{A_{\mathfrak{P}}}(D_{\mathfrak{P}}/\mathfrak{P}D_{\mathfrak{P}}) = \nu_{A_{\mathfrak{P}}/\mathfrak{P}A_{\mathfrak{P}}}(D_{\mathfrak{P}}/\mathfrak{P}D_{\mathfrak{P}}) = \nu_{\kappa(\mathfrak{P})}(\kappa(\mathfrak{P})^{\oplus r}) = r$$

so that $\nu_{A_{\mathfrak{P}}}(D_{\mathfrak{P}}) = \nu_A(D)$, as needed. □

Remark 3.2. If we assume that $k \subset A$ and

$$\mathfrak{P}_{A/k} \cap k = (0)$$

(e.g., if the subring k is a field), then we have a natural embedding

$$k \hookrightarrow A/\mathfrak{P}_{A/k}$$

and hence $\operatorname{char}(A/\mathfrak{P}_{A/k}) = \operatorname{char} k$. Now notice that, in the case (i) of the proof of Theorem 3.1, the hypothesis $\operatorname{grade} \mathfrak{P}_{A/k} = \operatorname{height} \mathfrak{P}_{A/k}$ is not needed. An immediate byproduct of these observations is Corollary 3.3 below.

Corollary 3.3. *Let A be a local domain containing a field k with* $\operatorname{char} k > 0$, *such that* $\operatorname{Der}_k(A)$ *is a finite A-module and* $\operatorname{height} \mathfrak{P}_{A/k} \leq 2$. *If* $\operatorname{projdim}_A(\operatorname{Der}_k(A)) < \infty$, *then* $\operatorname{Der}_k(A)$ *is free as an A-module.*

We believe that Corollary 3.3 holds in the case $\operatorname{char} k = 0$ as well. It is easy to see that the issue relies on the following question, for which we expect a negative answer.

Question 3.4. Let k be a field with $\operatorname{char} k = 0$. Is it possible for a local k-domain A, with $\operatorname{Der}_k(A)$ a finite A-module with finite projective dimension, to be such that $\operatorname{grade} \mathfrak{P}_{A/k} = 1$ and $\operatorname{height} \mathfrak{P}_{A/k} = 2$?

It is a standard fact that in a Cohen–Macaulay local ring A we have grade $\mathfrak{a} =$ height $\mathfrak{a}$ for every ideal $\mathfrak{a} \subset A$. Thus, we also readily derive from Theorem 3.1 the following consequence.

Corollary 3.5. *Let A be a Cohen–Macaulay local k-domain such that* $\mathrm{Der}_k(A)$ *is a finite A-module and* height $\mathfrak{P}_{A/k} \leq 2$. *If* $\mathrm{projdim}_A(\mathrm{Der}_k(A)) < \infty$, *then* $\mathrm{Der}_k(A)$ *is free as an A-module.*

Furthermore, we consider the class of factorial domains, also called unique factorization domains. We mention en passant that, among several important properties, one of the nice features of a factorial local domain $(B, \mathfrak{n})$ with depth $B \geq 2$ is that its punctured spectrum $\mathrm{Spec}(B) \setminus \{\mathfrak{n}\}$ has trivial Picard group (the same happens to Spec B itself).

Corollary 3.6. *Let A be a factorial local k-domain such that* $\mathrm{Der}_k(A)$ *is a finite A-module and* height $\mathfrak{P}_{A/k} \leq 2$. *If* $\mathrm{projdim}_A(\mathrm{Der}_k(A)) < \infty$, *then* $\mathrm{Der}_k(A)$ *is free as an A-module.*

Proof. Write $\mathfrak{P}_{A/k} = \mathfrak{P}$. If $\mathfrak{P} = (0)$, then $\mathrm{Der}_k(A)$ is free by Lemma 2.3. If height $\mathfrak{P} = 1$, then (since A is a domain) we must have grade $\mathfrak{P} =$ height $\mathfrak{P}$, and the assertion follows from Theorem 3.1. So we may assume that height $\mathfrak{P} = 2$. Moreover, by part (i) in the proof of Theorem 3.1 (since this part does not depend on the condition grade $\mathfrak{P} =$ height $\mathfrak{P}$), we are reduced to the case where $\mathrm{char}(A/\mathfrak{P}) = 0$, so that $\mathfrak{P}$ is prime by Lemma 2.4(ii). Therefore, we can guarantee that $\mathfrak{Q} \subset \mathfrak{P}$ for some prime ideal $\mathfrak{Q} \subset A$ with

$$\text{height}\, \mathfrak{Q} = 1.$$

Since A is factorial, we have $\mathfrak{Q} = (a)$ for some (prime) element a [Matsumura 1986, Theorem 20.1]. It follows that any given

$$b \in \mathfrak{P} \setminus (a)$$

is a non-zero-divisor of $A/(a)$, i.e., $\{a, b\} \subset \mathfrak{P}$ is an A-sequence and hence grade $\mathfrak{P} \geq 2$, which forces grade $\mathfrak{P} = 2 =$ height $\mathfrak{P}$, so that we can once again apply Theorem 3.1. □

Remark 3.7. In virtue of the cases treated in Corollaries 3.3 and 3.5, it is natural to ask about the existence of factorial non-Cohen–Macaulay domains of characteristic zero (and dimension necessarily greater than or equal to 3, since a factorial — hence normal — domain of dimension 2 is Cohen–Macaulay). This is a nontrivial problem but fortunately such rings do exist, as shown by [Freitag and Kiehl 1974, Theorem 5.8], which thus justifies our Corollary 3.6. We also refer the reader to the survey given in [Lipman 1975].

Finally, recall that every regular local ring A is a factorial Cohen–Macaulay domain, and that every finite A-module has finite projective dimension. Thus, both Corollaries 3.5 and 3.6 independently recover [Maloo 1999, Theorem 4], which we state below.

Corollary 3.8. *Let A be a regular local k-algebra such that* $\mathrm{Der}_k(A)$ *is a finite A-module and* $\mathrm{height}\,\mathfrak{P}_{A/k} \leq 2$. *Then* $\mathrm{Der}_k(A)$ *is free as an A-module.*

This result can be illustrated simply by taking A as the local ring of a nonsingular point of an affine algebraic (or algebroid) surface over a perfect field k of any characteristic.

Remark 3.9. As expected, the converse of Corollary 3.8 does not hold. A simple example is the nonregular 2-dimensional local domain

$$A = k[X, Y, Z]_{(X,Y,Z)}/(XY - Z^p)$$

where k is a field with $\mathrm{char}\, k = p > 0$. Letting x, y, z denote the residue classes of the variables, the A-module $\mathrm{Der}_k(A)$ is seen to be free, a basis being $\{\Delta_1, \Delta_2\}$, where

$$\Delta_1 = (p-1)x\partial_x + y\partial_y, \qquad \Delta_2 = \partial_z.$$

The case of characteristic zero is much harder, but [Maloo 1997, p. 84] presents a 1-dimensional nonregular Noetherian local ring containing a field k with $\mathrm{char}\, k = 0$, such that $\mathrm{Der}_k(A)$ is a finite free A-module.

Remark 3.10. One of the ingredients used by Maloo in the proof of his theorem is [Maloo 1999, Lemma 3], which he proves essentially by using that $\mathrm{depth}(\mathrm{Der}_k(A)) \geq \min\{2, \mathrm{depth}\, A\}$ (this is easy to see in the special situation where the differential module $\Omega_{A/k}$ is a finite A-module, and can be derived from [Bruns and Herzog 1998, Exercise 1.4.19]). However, no proof of this property in generality was given therein. The argument is, indeed, basic — relies on the fact that $\mathrm{Der}_k(A)$ is a dual — and is supplied in the proof of our Theorem 3.1. Later on, in Corollary 5.2, this general fact will be used crucially.

4. Examples: derivation modules with infinite projective dimension

Our goal in this section is to apply our results in order to furnish explicit examples of algebras over a field k, in characteristic zero as well as in prime characteristic, whose module of k-derivations has infinite projective dimension. Note that this could not be achieved solely by means of Maloo's theorem (Corollary 3.8).

In order to satisfactorily clarify the examples, which will be built on hypersurface rings, we provide first a (characteristic-free) useful tool. As in the proof of Theorem 3.1, we use $\mathrm{rank}(\cdot)$ and $\nu(\cdot)$ to denote rank and minimal number of generators of finite modules over a specified base ring, respectively.

Lemma 4.1. *Let k be an arbitrary field and let S be the localization of a polynomial ring over k at the ideal generated by the indeterminates. Let* $\{\partial_1, \dots, \partial_n\}$ *be the natural free basis of* $\mathrm{Der}_k(S)$. *For a noninvertible* $f \in S$ *such that* $\partial_j(f) \neq 0$ *for some* j, *let* $\mathfrak{J} \subset S$ *be the ideal generated by the (ordered, signed) set* $\{\partial_1(f), \dots, \partial_n(f), f\}$, *giving rise to a free presentation*

$$S^m \xrightarrow{\phi} S^{n+1} \to \mathfrak{J} \to 0$$

where we regard ϕ *as a matrix (taken in the canonical bases). Let* ϕ' *be the submatrix of* ϕ *resulting from deletion of its last row, and if* $A = S/(f)$, *let* ϕ_A *be the matrix formed by the nonzero columns of the matrix* $\phi' \otimes \mathrm{Id}_A$ *obtained by reducing the entries of* ϕ' *modulo* f. *We have*:

(i) $\mathrm{Der}_k(A)$ *is generated as an A-module by the derivations corresponding to the column-vectors of* ϕ_A.

(ii) *If* f *is irreducible and* $\nu_A(\mathrm{Der}_k(A)) \geq n$, *then* $\mathrm{Der}_k(A)$ *cannot be free as an A-module.*

Proof. (i) Consider the tangential idealizer

$$T_{S/k}(f) = \{\Delta \in \mathrm{Der}_k(S) \mid \Delta(f) \in (f)\},$$

which is a submodule of $\mathrm{Der}_k(S)$, also known as the module of logarithmic derivations of f. By [Miranda-Neto 2017, Proposition 2.3], the derivations corresponding to the column-vectors of ϕ' generate $T_{S/k}(f)$ as an S-module. Now, if as above $A = S/(f)$, there is an isomorphism of A-modules

$$\mathrm{Der}_k(A) \simeq T_{S/k}(f)/f\,\mathrm{Der}_k(S)$$

[Miranda-Neto 2016, Proposition 2.6], where clearly

$$f\,\mathrm{Der}_k(S) = (f)\partial_1 \oplus \cdots \oplus (f)\partial_n \simeq f S^n.$$

Therefore, under the natural identification, the A-module $\mathrm{Der}_k(A)$ can generated by the derivations given by the (nonzero) column-vectors of $\phi' \otimes \mathrm{Id}_A$.

(ii) It suffices to show that the rank of the A-module $\mathrm{Der}_k(A)$ is at most $n-1$. This is certainly known (notably in characteristic zero) but it is instructive to write down an independent, general proof. As the ideal $(f) \subset S$ is prime and f is not killed by some ∂_j, we can easily check that

$$T_{S/k}(f) :_S \mathrm{Der}_k(S) = (f),$$

which means that (f) lies in the support of the S-module $\mathfrak{C} = \mathrm{Der}_k(S)/T_{S/k}(f)$. Because $\mathfrak{C}$ is also an A-module, isomorphic to the cokernel of the injection

$\iota : \mathrm{Der}_k(A) \hookrightarrow A^n$ given by

$$\mathrm{Der}_k(A) \simeq T_{S/k}(f)/f\,\mathrm{Der}_k(S) \subset \mathrm{Der}_k(S)/f\,\mathrm{Der}_k(S) \simeq S^n/fS^n = A^n,$$

we get that $(0) \subset A$ lies in the support of $\mathfrak{C} \simeq A^n/\iota(\mathrm{Der}_k(A))$. This yields $\mathrm{rank}_A\,\mathfrak{C} > 0$ and consequently

$$\mathrm{rank}_A(\mathrm{Der}_k(A)) = n - \mathrm{rank}_A\,\mathfrak{C} < n$$

as needed. □

Example 4.2. Let k be a field with $\mathrm{char}\,k = 3$ and let A be the 2-dimensional local domain $A = S/(f)$, where $S = k[X, Y, Z]_{(X,Y,Z)}$ and

$$f = X^2Y + XYZ + Z^3.$$

Consider the Jacobian ideal

$$\mathfrak{J} = (\partial_X(f), \partial_Y(f), \partial_Z(f), f) = (-XY + YZ, X^2 + XZ, XY, f) \subset S.$$

The given generators yield, explicitly, a (minimal) free presentation of the form

$$S^4 \xrightarrow{\phi} S^4 \to \mathfrak{J} \to 0$$

where

$$\phi = \begin{pmatrix} X & X & Z^2 & 0 \\ Y & 0 & Y^2 & -f \\ Z & X-Z & Z^2 & 0 \\ 0 & 0 & -Y & X^2+XZ \end{pmatrix}.$$

Reducing, modulo f, the matrix ϕ' (with notation as in Lemma 4.1) and denoting by x, y, z the residue classes of the variables, Lemma 4.1(i) guarantees that $\mathrm{Der}_k(A)$ can be generated by the derivations corresponding to the columns of the matrix

$$\phi_A = \begin{pmatrix} x & x & z^2 \\ y & 0 & y^2 \\ z & x-z & z^2 \end{pmatrix}$$

which are seen to be minimal generators. Thus,

$$\nu_A(\mathrm{Der}_k(A)) = 3 = \dim S$$

so that $\mathrm{Der}_k(A)$ is not free as an A-module by Lemma 4.1(ii). The condition $\mathrm{height}\,\mathfrak{P}_{A/k} \leq 2$ is automatic since $\dim A = 2$ (here we clearly have $\mathfrak{P}_{A/k} = \mathfrak{m}$). By Corollary 3.3 — or, alternatively, by Corollary 3.5 — we get

$$\mathrm{projdim}_A(\mathrm{Der}_k(A)) = \infty.$$

Remark 4.3. The first-named author claimed in [Miranda-Neto 2017, Example 2.10(ii)] that, if as above $\operatorname{char} k = 3$ and $f = X^2Y + XYZ + Z^3$, then the ideal $\mathfrak{J} = (\mathfrak{G}, f) = (\partial_X(f), \partial_Y(f), \partial_Z(f), f)$ satisfies, in particular, $\nu(\mathfrak{J}) = 3$, by implicitly assuming that it coincides with the gradient ideal $\mathfrak{G}$. However, this is not true, since the conductor of f into $\mathfrak{G}$ is the proper ideal

$$\mathfrak{G} : (f) = (Y, X^2 + XZ)$$

so that $f \notin \mathfrak{G}$ (for a weighted polynomial of weight δ, this pathology may only occur if $\operatorname{char} k$ divides δ). Precisely, by Example 4.2, $\mathfrak{J}$ has 4 minimal generators, and moreover, it can be easily verified that the kernel of the presentation map ϕ is free of rank 1, which yields that $\mathfrak{J}$ has projective dimension 2. As a consequence of this correction, f is *not* a free divisor (i.e., its logarithmic derivation module cannot be free) by [Miranda-Neto 2017, Proposition 2.7].

Example 4.4. Let us investigate an example in higher dimension. Let k be a field with $\operatorname{char} k = 0$. Consider the 3-dimensional local domain

$$A = k[X, Y, Z, W]_{(X,Y,Z,W)}/(X^3 + XY^3 + YZ + Y^2W)$$

and write $A = k[x, y, z, w]_{(x,y,z,w)}$, in terms of the residue classes of the variables modulo the defining equation of A. After computing a free presentation matrix of the Jacobian ideal (built from the natural generators as in Lemma 4.1), deleting its last row and taking images in A, we obtain the matrix

$$\phi_A = \begin{pmatrix} 0 & -y & 0 & -x & 3xy^2 + z + 2yw \\ 0 & 0 & -y & -3y & -3x^2 - y^3 \\ -y & 3x^2 & z & 0 & 0 \\ 1 & y^2 & 3xy + 2w & 7xy + 3w & 0 \end{pmatrix}$$

whose columns give generators for the A-module $\operatorname{Der}_k(A)$, by Lemma 4.1(i). Such generators are seen to be minimal. Thus,

$$\nu_A(\operatorname{Der}_k(A)) = 5 > 4 = \dim S$$

and hence, $\operatorname{Der}_k(A)$ is not free as an A-module, by Lemma 4.1(ii).

Notice, moreover, that the maximal ideal $\mathfrak{m} = (x, y, z, w) \subset A$ is not differential. In fact, if

$$\Delta = -y\partial_z + \partial_w$$

is the derivation corresponding to the first column of ϕ_A, then

$$\Delta(w) = 1 \notin \mathfrak{m}$$

which implies $\mathfrak{P}_{A/k} \neq \mathfrak{m}$. Since $\mathfrak{P}_{A/k}$ is prime (by Lemma 2.4(ii)) and $\dim A = 3$, we get height $\mathfrak{P}_{A/k} \leq 2$ (here indeed we have $\mathfrak{P}_{A/k} = (x, y, z)$, so that, precisely, height $\mathfrak{P}_{A/k} = 2$). By Corollary 3.5, we conclude that

$$\operatorname{projdim}_A(\operatorname{Der}_k(A)) = \infty.$$

Remark 4.5. In the case of a *complete* local algebra of characteristic zero, there is a serious constraint imposed on its structure if the maximally differential ideal is not equal to the maximal ideal. To be more precise, let $(A, \mathfrak{m})$ be a local k-algebra whose $\mathfrak{m}$-adic completion $\hat{A}$ satisfies $\operatorname{char} \hat{A} = 0$ and

$$\mathfrak{P}_{\hat{A}/k} \neq \widehat{\mathfrak{m}}$$

(a word of caution: the ideal $\mathfrak{P}_{\hat{A}/k}$ may differ from the completion of $\mathfrak{P}_{A/k}$ [de Souza Doering and Lequain 1986; Patil and Singh 1983]), or what amounts to the same, there exists $\vartheta \in \operatorname{Der}_k(\hat{A})$ such that $\vartheta(\widehat{\mathfrak{m}}) \nsubseteq \widehat{\mathfrak{m}}$. Then, by [Zariski 1965, Lemma 4], we have that $\hat{A}$ is a power series ring

$$\hat{A} = \mathfrak{A}[\![T]\!]$$

in 1 indeterminate T over a suitable subring $\mathfrak{A} \subset \{a \in \hat{A} \mid \vartheta(a) = 0\} \subset \hat{A}$. As a consequence, we get that if $\hat{A}$ cannot be expressed as a power series ring over a subring $\mathfrak{A} \subset \hat{A}$, then height $\mathfrak{P}_{\hat{A}/k} = \dim A$.

5. Connection to the Herzog–Vasconcelos conjecture

We recall below a well known — but mostly open — conjecture in the algebrogeometric setting of localizations of affine rings over a field containing the rationals, independently raised by Herzog and Vasconcelos. Notice that, if A is such a k-algebra, then the module of differentials $\Omega_{A/k}$ is automatically a finite A-module and hence so is its A-dual $\operatorname{Der}_k(A)$.

Conjecture (Herzog and Vasconcelos). Let k be a field with $\operatorname{char} k = 0$, and let A be a local ring which is essentially of finite type over k. If $\operatorname{projdim}_A(\operatorname{Der}_k(A)) < \infty$, then $\operatorname{Der}_k(A)$ is free as an A-module.

If as above A is a localization of a finite-type algebra over a field, $\operatorname{Der}_k(A)$ can be regarded as a module of second-order syzygies (being isomorphic to the kernel of the A-linear map of free modules induced by a Jacobian matrix corresponding to A), and therefore, in case A is Cohen–Macaulay with $\dim A \leq 2$, the conjecture is true and follows trivially from the Auslander–Buchsbaum formula. Apart from this easy instance, the problem has been settled in a few situations, to wit, quasihomogeneous complete intersections with isolated singularity [Herzog 1994, Theorem 2.4], Stanley–Reisner rings [Brumatti and Simis 1995], and Buchsbaum affine semigroup rings [Müller and Patil 1999].

Remark 5.1. In the setting above, the celebrated Zariski–Lipman conjecture predicts that A must be regular if $\operatorname{Der}_k(A)$ is free [Lipman 1965]. As in [Herzog

1994, p. 6], we may combine the two conjectures and ask whether A is regular if $\operatorname{projdim}_A(\operatorname{Der}_k(A)) < \infty$. By [Scheja and Storch 1972, Satz 9.1], the finiteness of $\operatorname{projdim}_A(\operatorname{Der}_k(A))$ forces A to be a normal domain, and according to [Herzog 1981, Corollary 3.3] it also implies

$$\operatorname{Hom}_A\Big(\bigwedge^d \operatorname{Der}_k(A), A\Big) \simeq A$$

where $d = \dim A \geq 1$ — the rank of $\operatorname{Der}_k(A)$ in this case. But, if moreover A is Cohen–Macaulay, the dual module above is isomorphic to a canonical module of A, so that A is in fact Gorenstein (it is conjectured in [Vasconcelos 1985, p. 373] that A must be a complete intersection). This observation gives an analogue, in the case of the Herzog–Vasconcelos conjecture, of the statement [Hochster 1977, Remark 2] to the effect that if the Zariski–Lipman conjecture admits a Cohen–Macaulay counterexample, then there is also a Gorenstein counterexample.

Here, our contribution to the Herzog–Vasconcelos problem is Corollary 5.2 below, which is essentially contained in the proof of Theorem 3.1 and solves the conjecture in case depth $A \leq 2$. Our statement is indeed more general since the k-algebra A is not necessarily essentially of finite type, and moreover k — which is allowed to have any characteristic — is not required to be a field.

Corollary 5.2. *Let A be a local algebra over a ring k such that* $\operatorname{Der}_k(A)$ *is a finite A-module. Assume that* depth $A \leq 2$. *If* $\operatorname{projdim}_A(\operatorname{Der}_k(A)) < \infty$, *then* $\operatorname{Der}_k(A)$ *is free as an A-module.*

Proof. If depth $A = 0$, then by the Auslander–Buchsbaum equality, the hypothesis $\operatorname{projdim}_A(\operatorname{Der}_k(A)) < \infty$ yields that $\operatorname{Der}_k(A)$ is free. Now assume that depth A is either 1 or 2. Thus, just as in part (i) in the proof of Theorem 3.1, we readily derive that a maximal A-sequence is necessarily a $\operatorname{Der}_k(A)$-sequence, so that $\operatorname{depth}(\operatorname{Der}_k(A)) \geq \operatorname{depth} A$ and once again the Auslander–Buchsbaum formula does the job. □

In particular, we get that the Herzog–Vasconcelos conjecture is true for the local ring A of any point of an affine algebraic surface over a ground field k of arbitrary characteristic. If $\operatorname{char} k = 0$ as in the original statement, this follows alternatively from the fact (recalled in Remark 5.1) that a ring satisfying the conditions of the conjecture must be normal.

We close the paper by working out an instance in higher dimension satisfying the property that the corresponding module of derivations has infinite projective dimension — which, by the preceding discussion, occurs automatically if the ring is nonnormal. It follows that, in order to produce an interesting example by means of Corollary 5.2, we need to start from a (non-Cohen–Macaulay) normal domain. Using Serre's normality criterion it is easy to see, for instance, that if B is a local isolated singularity (i.e., B is a local ring which is locally regular at the nonmaximal prime ideals) with $\operatorname{depth}(B) \geq 2$, then B is a normal domain.

Example 5.3. Let X, Y, Z, T, U, V be indeterminates over a field k with $\operatorname{char} k = 0$. Let $(S, \mathfrak{M})$ denote the localization of the polynomial ring $k[X, Y, Z, T, U, V]$ at the ideal generated by the indeterminates. Set $A = S/\mathfrak{I}$, where $\mathfrak{I} \subset S$ is the ideal generated by the 7 polynomials

$$XT - YZ, \qquad XV - YU, \qquad ZV - TU, \qquad X^3 + Z^3 + U^3,$$
$$X^2Y + Z^2T + U^2V, \qquad XY^2 + ZT^2 + UV^2, \qquad Y^3 + T^3 + V^3.$$

This is a particular situation of the example given by [Roberts 2010, §6], where it is stated that (the completion of) A is a normal domain. Let us indicate how to verify this feature in the present case. Denote by Θ the Jacobian matrix of the given generators of $\mathfrak{I}$. We have $\operatorname{height} \mathfrak{I} = 3$ (hence A is 3-dimensional). The ideal $I_3(\Theta)$ generated by the minors of order 3 of Θ satisfies

$$\operatorname{rad}(I_3(\Theta) + \mathfrak{I}) = \mathfrak{M},$$

and therefore, A is an isolated singularity. Since $\operatorname{projdim}_S A = 4$, the Auslander–Buchsbaum formula gives

$$\operatorname{depth} A = 2,$$

and thus, A is indeed a (non-Cohen–Macaulay) normal domain.

Since A is a domain which is essentially of finite type over a field containing the rationals, the rank of $\theta = \Theta \otimes \operatorname{Id}_A$ (i.e., the Jacobian matrix with entries taken modulo $\mathfrak{I}$) is known to be equal to the height of $\mathfrak{I}$, and then, as

$$\operatorname{Der}_k(A) \simeq \ker\bigl(A^6 \xrightarrow{\theta} A^7\bigr)$$

we get $\operatorname{rank}(\operatorname{Der}_k(A)) = 6 - \operatorname{height} \mathfrak{I} = 3$.

Now, let $T_{S/k}(\mathfrak{I})$ be the S-module formed by the $\Delta \in \operatorname{Der}_k(S)$ such that $\Delta(\mathfrak{I}) \subset \mathfrak{I}$. We can employ the method presented in [Miranda-Neto 2011, §2] in order to describe generators for $T_{S/k}(\mathfrak{I})$, and recall the fact that $\operatorname{Der}_k(A) \simeq T_{S/k}(\mathfrak{I})/\mathfrak{I}\operatorname{Der}_k(S)$ [Miranda-Neto 2016, Proposition 2.6]. Thus, writing x, y, z, t, u, v for the residue classes of the indeterminates, we obtain that the A-module $\operatorname{Der}_k(A)$ is (minimally) generated by the derivations corresponding to the columns of the matrix

$$\varphi = \begin{pmatrix} 0 & 0 & x & y & -zt & 0 & -uv & -u^2 & 0 & -z^2 \\ x & y & 0 & 0 & -t^2 & 0 & -v^2 & -uv & 0 & -zt \\ 0 & 0 & z & t & xy & -uv & 0 & 0 & -u^2 & x^2 \\ z & t & 0 & 0 & y^2 & -v^2 & 0 & 0 & -uv & xy \\ 0 & 0 & u & v & 0 & zt & xy & x^2 & z^2 & 0 \\ u & v & 0 & 0 & 0 & t^2 & y^2 & xy & zt & 0 \end{pmatrix}$$

so that $\nu(\mathrm{Der}_k(A)) = 10 > \mathrm{rank}(\mathrm{Der}_k(A))$ and hence $\mathrm{Der}_k(A)$ cannot be free as an A-module. By Corollary 5.2, we finally obtain that

$$\mathrm{projdim}_A(\mathrm{Der}_k(A)) = \infty.$$

Notice that this cannot be detected by means of the results given in Section 3; indeed, in this example we have height $\mathfrak{P}_{A/k} = 3 > 2$, since $\mathfrak{P}_{A/k}$ equals the maximal ideal of A, as we can immediately observe from the structure of φ.

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τ-TILTING FINITE GENTLE ALGEBRAS ARE REPRESENTATION-FINITE

PIERRE-GUY PLAMONDON

We show that a gentle algebra over a field is τ-tilting finite if and only if it is representation-finite. The proof relies on the "brick-τ-tilting correspondence" of Demonet, Iyama, and Jasso and on a combinatorial analysis.

1. Introduction and main result

The theory of τ-tilting was introduced in [Adachi et al. 2014] as a far-reaching generalization of classical tilting theory for finite-dimensional associative algebras. One of the main classes of objects in the theory is that of *τ-rigid modules*: a module M over an algebra Λ is τ-rigid if the space of morphisms $\mathrm{Hom}_\Lambda(M, \tau M)$ vanishes, where τ is the Auslander–Reiten translation. In [Demonet et al. 2019], conditions were established for an algebra Λ to admit only finitely many isomorphism classes of indecomposable τ-rigid modules. Such an algebra is called *τ-tilting finite*.

An obvious sufficient condition for an algebra to be τ-tilting finite is for it to be representation-finite. This is not a necessary condition: for instance, if k is a field, then the algebra $k\langle x, y\rangle/(x^2, y^2, xy, yx)$ is representation-infinite (since it is a string algebra in the sense of [Butler and Ringel 1987] and admits at least one band, namely xy^{-1}), but it is τ-tilting finite (since it is local). Our aim in this note is to prove that, for a certain class of algebras called *gentle algebras*, representation-finiteness and τ-tilting finiteness are equivalent conditions.

Gentle algebras form a subclass of the class of string algebras. They enjoy a simple definition in terms of generators and relations: a gentle algebra is a finite-dimensional algebra isomorphic to a quotient of a path algebra of a finite quiver Q by an ideal I generated by paths of length two, satisfying the condition that for every vertex v of Q, the minimal full subquiver with relation of $\overline{Q} = (Q, I)$ containing v and all arrows attached to v is a full subquiver with relations of the one depicted below, where dotted lines indicate relations and where the $\bullet$ vertices may not all be distinct:

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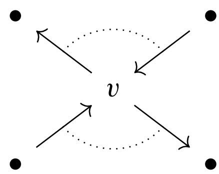
Keywords: representation theory, τ-tilting theory, finite representation type, gentle algebras.



Despite their simple definition, gentle algebras are encountered in many different contexts. They were introduced in [Assem and Skowroński 1987] in the study of iterated tilted algebras of type $\tilde{A}_m$, but have recently appeared in connection with dimer models [Bocklandt 2012; Broomhead 2012], enveloping algebras of some Lie algebras [Huerfano and Khovanov 2006], cluster algebras and categories arising from triangulated surfaces [Labardini-Fragoso 2009; Assem et al. 2010], m-Calabi–Yau tilted algebras [García Elsener 2017; 2018], nonkissing complexes of grids and associated objects [McConville 2017; Garver and McConville 2018; Palu et al. 2017; Brüstle et al. 2019], noncommutative nodal curves [Burban and Drozd 2018], and partially wrapped Fukaya categories [Haiden et al. 2017; Lekili and Polishchuk 2019]. Surface models have been introduced to study the category representations of a gentle algebra and associated categories [Baur and Simões 2018; Opper et al. 2018; Palu et al. 2018].

In this note, we prove the following theorem on gentle algebras. It is proved for Schurian gentle algebras in [Demonet et al. $\geq$ 2019] (see also [Demonet 2017]).

Theorem 1.1. *A gentle algebra is τ-tilting finite if and only if it is representation-finite.*

The proof of the theorem uses the "brick-τ-tilting correspondence" of [Demonet et al. 2019] (recalled in Section 2), and applies a reduction of any gentle algebra to two classes of examples (studied in Section 3).

Conventions and a note on terminology. All algebras in this paper are finite-dimensional over a base field k, which is arbitrary. We compose arrows in quivers from left to right: if $1 \xrightarrow{\alpha} 2 \xrightarrow{\beta} 3$ is a quiver, then $\alpha\beta$ is a path, while $\beta\alpha$ is not. For any arrow α of a quiver, we denote its source by $s(\alpha)$ and its target by $t(\alpha)$; we extend this notation naturally to the formal inverse α^{-1} of α.

In order to keep this note short, the notions of strings, bands, and string modules from [Butler and Ringel 1987] will be used freely and without further introduction. We note that the above convention for composition of arrows differs from the one used in [Butler and Ringel 1987].

2. The "brick-τ-tilting correspondence" and two reduction results

We will be using two results, Corollaries 2.3 and 2.4, allowing us to reduce the number of vertices of our bound quivers. They will both follow from the following consequence of the *brick-τ-tilting correspondence*. Recall that a *brick* is a module whose endomorphism algebra is a division algebra.

Theorem 2.1 [Demonet et al. 2019, Theorem 1.4]. *A finite-dimensional algebra* Λ *is* τ*-tilting finite if and only if there are only finitely many isomorphism classes of* Λ*-modules which are bricks.*

Corollary 2.2. *Let* Λ *and* Λ' *be two finite-dimensional algebras, and assume that there exists a fully faithful functor* $F : \operatorname{mod} \Lambda \to \operatorname{mod} \Lambda'$. *If* Λ' *is* τ*-tilting finite, then so is* Λ.

Proof. If B is a brick over Λ, then FB is a brick over Λ', since $\operatorname{End}_\Lambda(B)$ is isomorphic to $\operatorname{End}_{\Lambda'}(FB)$. Moreover, two bricks B and B' over Λ are isomorphic if and only if FB and FB' are isomorphic. Therefore, if Λ admits infinitely many bricks, then so does Λ'. The result then follows from Theorem 2.1. □

Corollary 2.3 (first reduction [Demonet et al. 2017, Theorem 5.12(d)]). *If* Λ *is* τ*-tilting finite and* I *is an ideal in* Λ, *then* Λ/I *is* τ*-tilting finite.*

Proof. Apply Corollary 2.2 to $\cdot \otimes_{\Lambda/I} \Lambda/I : \operatorname{mod} \Lambda/I \to \operatorname{mod} \Lambda$. □

Corollary 2.4 (second reduction). *If* Λ *is* τ*-tilting finite and* $e \in \Lambda$ *is an idempotent, then* $e\Lambda e$ *is* τ*-tilting finite.*

Proof. Apply Corollary 2.2 to $\operatorname{Hom}_{e\Lambda e}(\Lambda e, \cdot) : \operatorname{mod} e\Lambda e \to \operatorname{mod} \Lambda$. Alternatively, apply [Pilaud et al. 2018, Theorem 1.1] for a proof which does not use the brick-τ-tilting correspondence. □

Remark 2.5. In practice, Corollary 2.3 implies that erasing arrows or vertices from a τ-tilting finite algebra yields another τ-tilting finite algebra, and Corollary 2.4 implies that erasing a vertex v and replacing any path of length two without relation of the form

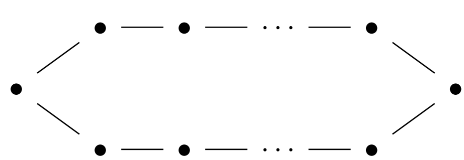
$$u \xrightarrow{\alpha} v \xrightarrow{\beta} w$$

by a "shortcut" arrow $u \xrightarrow{[\alpha\beta]} w$ also preserves τ-tilting finiteness.

3. Two classes of examples

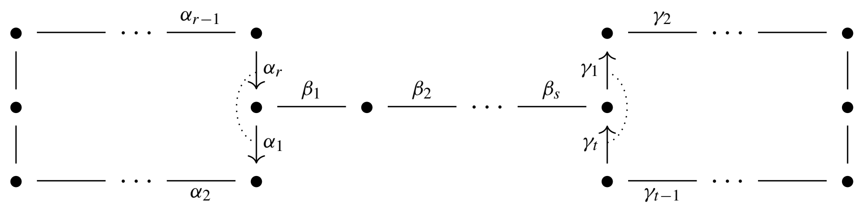
Our strategy to prove Theorem 1.1 will be to reduce any gentle algebra of infinite-representation type to one of the two classes of examples presented in this section.

Example 3.1 (type $\tilde{A}_m$). Let Q be a quiver of type $\tilde{A}_m$, that is to say, an orientation of the following diagram with $m+1$ vertices, where $m \geq 1$:



The representation theory of the path algebra $\Lambda = kQ$ is very well understood in this case; see for instance [Assem et al. 2006, §VIII.2]. In particular, this algebra is τ-tilting infinite.

Example 3.2. The second class of examples that we will consider will be given by the path algebras of quivers Q defined by any orientation of the diagram



modulo the relations $\alpha_r\alpha_1$ and $\gamma_t\gamma_1$ (note that the orientations of α_1, α_r, γ_1, and γ_t are imposed, while those of other arrows can be arbitrary). We allow $r = 1$ (in which case $\alpha_1 = \alpha_r$ is a loop whose square vanishes); we allow the same for t. We also allow $s = 0$; in this case, we require that the cycle on the left and the cycle on the right are not both oriented cycles; otherwise, the algebra would be infinite-dimensional.

Proposition 3.3. *The algebras defined in Example 3.2 are τ-tilting infinite.*

Proof. Let Λ be an algebra in the class defined in Example 3.2.

We first deal with the case where $s = 0$. In this case, let v be the vertex common to both cycles. Let $e = 1 - e_v$. Then the algebra $e\Lambda e$ is of type $\tilde{A}_m$, so it is τ-tilting infinite. By Corollary 2.4, Λ is τ-tilting infinite.

Assume, therefore, that $s \geq 1$. We will construct an infinite family of bricks for Λ; by the brick-τ-tilting correspondence (see Theorem 2.1), this will imply that Λ is τ-tilting infinite.

Let $b' = \alpha_1\alpha_2^{\delta_2}\cdots\alpha_{r-1}^{\delta_{r-1}}\alpha_r$ be the string corresponding to the cycle on the left, $b'' = \gamma_1\gamma_2^{\zeta_2}\cdots\gamma_{t-1}^{\zeta_{t-1}}\gamma_t$ be the one corresponding to the cycle on the right, and $\omega = \beta_1^{\varepsilon_1}\cdots\beta_s^{\varepsilon_s}$ be the middle string followed from left to right, where the δ_i, ε_i, and ζ_i are the appropriate signs.

Define $b = (b')^{\varepsilon_1}\omega(b'')^{\varepsilon_1}\omega^{-1}$. We claim that the string module defined by b is a brick. To prove this, we need to prove that the only substring of b appearing both on top of and at the bottom of b is b itself, so that the endomorphism ring of the string module is isomorphic to the base field k (using the description of all morphisms between string modules obtained in [Crawley-Boevey 1989]). Here, we say that a substring σ' of a string σ is *on top of* σ if the arrows in σ adjacent to σ' are leaving σ', and that it is *at the bottom of* σ if the arrows in σ adjacent to σ' are entering σ'.

Note first that the middle copy of ω is neither on top of nor at the bottom of b. Indeed, if $\varepsilon_1 = 1$, then ω is not at the bottom, since the first arrow of $(b'')^{\varepsilon_1}$ is direct, and ω is not on top, since the last arrow of $(b')^{\varepsilon_1}$ is direct; if $\varepsilon_1 = -1$, then ω is not at the bottom, since the last arrow of $(b')^{\varepsilon_1}$ is inverse, and ω is not on top, since the last arrow of $(b'')^{\varepsilon_1}$ is inverse.

Next, let us deal with the substrings of length 0 of b. The starting point of b is on top if $\varepsilon_1 = 1$ or at the bottom if $\varepsilon_1 = -1$. It appears twice more in b: at the end of b' and the end of b. At the end of b' it is neither on top nor at the bottom, and at the end of b it is on top if $\varepsilon_1 = 1$ or at the bottom if $\varepsilon_1 = -1$. Therefore, this vertex does not occur both on top and at the bottom of b. The other vertices appearing several times in b are the vertices of ω and the starting/ending points of b''. The former appear either twice at the top or twice at the bottom of b. The latter cannot be both on top and at the bottom, since it appears in the middle of paths of length two of the following form: if $\varepsilon_1 = 1$, then these paths are $\beta_s^{\varepsilon_s}\gamma_1$ and $\gamma_t\beta_s^{-\varepsilon_s}$, and if $\varepsilon_1 = -1$, then they are $\beta_s^{\varepsilon_s}\gamma_t^{-1}$ and $\gamma_1^{-1}\beta_s^{-\varepsilon_s}$. In both cases the middle vertices are either on top of b or at the bottom of b, but not both. Thus, no substring of length zero appears both at the top and the bottom of b.

Assume that there is a substring ρ of length at least one, different from b, which appears both on top and at the bottom of b. Since the only arrows of b that are used twice are those of ω, ρ has to be a substring of ω and of ω^{-1}. Since ω does not go twice through the same vertex, the only substring both on top and at the bottom of ω is ω itself. Hence, $\rho = \omega$. But we saw above that the middle substring ω is neither on top nor at the bottom of b. This is a contradiction.

Thus, the string module defined by b is a brick.

Using the above arguments, one can also check that all powers of b define bricks as well. Thus, Λ admits infinitely many pairwise nonisomorphic bricks, and by the brick-τ-tilting correspondence (see Theorem 2.1), it is τ-tilting infinite. □

4. Proof of the main theorem

We now prove Theorem 1.1. Let $\overline{Q} = (Q, I)$ be a gentle bound quiver. Assume that the algebra $\Lambda = kQ/I$ is of infinite representation type. Let us show that it is τ-tilting infinite.

By [Butler and Ringel 1987], there exists a band b on $\overline{Q}$. Our strategy will be to reduce to one of the two cases in the following lemma.

Lemma 4.1. *The algebra Λ is τ-tilting infinite if $\overline{Q}$ admits a band b satisfying one of the following conditions*:

(1) *b does not go through the same vertex twice* (*except for the starting and ending points of b*) *or*

(2) *b has the form $b = b'\omega b''\omega^{-1}$, where*

- *b' and b'' are strings such that $s(b') = t(b')$ and $s(b'') = t(b'')$,*
- *$(b')^2$ and $(b'')^2$ are not strings,*

- *ω is a possibly trivial string,*
- *none of b', b'', and ω go through the same vertex twice (except for the endpoints of b' and b''), and*
- *the only vertices that b', b'', and ω may have in common are their ending points.*

Proof. Let I be the ideal generated by all arrows and vertices through which b does not go. If we are in case (1), then Λ/I is isomorphic to the path algebra of a quiver of type $\tilde{A}_m$. These algebras are τ-tilting infinite, so the result follows from Corollary 2.3. If we are in case (2), then Λ/I is isomorphic to an algebra in the class defined in Example 3.2. By Proposition 3.3, these are τ-tilting infinite, so the result follows again from Corollary 2.3. □

To prove Theorem 1.1, it is therefore sufficient to show that a band as in Lemma 4.1 always exists.

Let b be a band of minimal length on $\overline{Q}$. If b does not go through the same vertex twice (except at its endpoints), then by Lemma 4.1(1), the theorem is proved.

Assume, therefore, that there is a vertex u through which b passes twice. Up to cyclic reordering of b, we can assume that this vertex is the starting point of b. Up to choosing another such vertex u, we can also assume that $b = b'b''$, with b' and b'' nontrivial strings starting and ending at u and such that b' does not go through the same vertex twice (except at its endpoints). Note that, by minimality of b, the string b' cannot be a band; that is, $(b')^2$ cannot be a string. The same is true for b''.

Lemma 4.2. *Let $b = b'b''$ be as above. Then b' and b'' cannot have a vertex in common apart from their starting and ending points.*

Proof. Assume that b' and b'' have another vertex in common, and let v be such a vertex. Write $b' = \alpha_1^{\delta_1} \cdots \alpha_r^{\delta_r}$ and $b'' = \beta_1^{\varepsilon_1} \cdots \beta_s^{\varepsilon_s}$, where the α_i and β_i are arrows and the δ_i and ε_i are ± 1, and assume that $s(\alpha_j^{\delta_j}) = v = t(\beta_k^{\varepsilon_k})$, with $i \neq 1, r$ and $j \neq 1, s$. By minimality of b, $\alpha_j^{\delta_j}\alpha_{j+1}^{\delta_{j+1}} \cdots \alpha_r^{\delta_r}\beta_1^{\varepsilon_1} \cdots \beta_k^{\varepsilon_k}$ cannot be a band. This implies that $\delta_j = \varepsilon_k$ and that the composition of $\alpha_j^{\delta_j}$ and $\beta_k^{\varepsilon_k}$ is a relation in $\overline{Q}$. But then $\alpha_{j-1}^{-\delta_{j-1}}\alpha_{j-2}^{-\delta_{j-2}} \cdots \alpha_1^{-\delta_1}\beta_1^{\varepsilon_1} \cdots \beta_k^{\varepsilon_k}$ is a band, since $\beta_k^{\varepsilon_k}$ cannot be in a relation both with $\alpha_j^{\delta_j}$ and with $\alpha_{j-1}^{\delta_{j-1}}$. This again contradicts the minimality of b. □

Now, if b'' does not go twice through the same vertex (except for its endpoints), then we are in case (2) of Lemma 4.1 with ω trivial, and the theorem is proved. Assume thus that b'' does go twice through a vertex v outside its endpoints (or three times through v if it is the endpoint of b''). Up to choosing another vertex v, we can assume that there is a substring $b''' = \beta_j^{\varepsilon_j}\beta_{j+1}^{\varepsilon_{j+1}} \cdots \beta_k^{\varepsilon_k}$ of b'' which starts and ends in v, does not go through the same vertex twice outside its endpoints, and is such that $\omega := \beta_1^{\varepsilon_1} \cdots \beta_{j-1}^{\varepsilon_{j-1}}$ does not go through the same vertex twice.

If β_k and β_{j-1} form a relation of $\overline{Q}$, then β_j and β_k cannot form a relation, since there is at most one involving β_k and β_{j-1}, β_j are distinct. Thus, b''' is a band with no repeated vertices (except for its endpoints), and we have reduced to case (1) of Lemma 4.1, proving the theorem.

If, on the other hand, β_k and β_{j-1} do not form a relation, then $b'\omega b'''\omega^{-1}$ is a band satisfying the conditions of case (2) of Lemma 4.1.

This finishes the proof of Theorem 1.1.

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YAMABE EQUATION ON SOME COMPLETE NONCOMPACT MANIFOLDS

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We consider the Yamabe equation on a complete noncompact Riemannian manifold and find some geometric conditions on the manifold such that the Yamabe problem admits a bounded positive solution.

1. Introduction

Let (M, g) be a complete Riemannian manifold of dimension $n \geq 3$. The Yamabe problem on a compact Riemannian manifold without boundary consists of finding a constant scalar curvature metric $\tilde{g}$ which is pointwise conformally related to g. It is well known that this problem is equivalent to showing the existence of a positive solution to the equation

$$\Delta_g u - \frac{n-2}{4(n-1)} R_g u + K u^{(n+2)/(n-2)} = 0,$$

if one sets $\tilde{g} = u^{4/(n-2)} g$. Usually, one writes this equation as

$$\Delta_g u - c(n) R_g u + K u^{p-1} = 0 \quad \text{on } M, \tag{1-1}$$

where Δ_g is the Laplace-Beltrami operator associated with g, R_g is the scalar curvature of g, $c(n) = (n-2)/(4(n-1))$, $p = 2n/(n-2)$, and K is a constant satisfying $K = c(n) R_{\tilde{g}}$, where $R_{\tilde{g}}$ is the scalar curvature of $\tilde{g}$. As is well known, the existence of minimizing solution to the Yamabe problem on a compact manifold was established through the combined works of Yamabe [1960], Trudinger [1968], Aubin [2001] and Schoen [1984].

Yau [1982] and Kazdan [1985] suggested the study of (1-1) in a noncompact complete manifold. This study was proposed again in the book by Aubin [2001]. For the case where (M, g) is a noncompact complete manifold with nonpositive scalar curvature, Aviles and McOwen [1988] have established some existence results. However, the understanding on the case where (M, g) is of nonnegative scalar curvature is still rather limited. Some existence and nonexistence results on

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the case (M, g) of positive scalar curvature have been established in [Kim 1996; Zhang 2003; 2004; Grosse 2013; Jin 1988]. S. Kim [1996; 1997] introduced a functional $Y_\infty(M)$ (which may be called the Yamabe constant at infinity) to study the Yamabe problem on a complete noncompact manifold and got an existence result merely under the assumption $Y(M) < Y_\infty(M)$ for such a manifold (M, g) with positive scalar curvature. However, Zhang [2003] found a gap in Kim's proof, and fixed the gap under an additional assumption on the volume growth of geodesic balls. Zhang [2004] also studied the existence of positive solutions of (1-1) with K a prescribed nonnegative function under certain conditions. N. Grosse [2013] studied the existence of positive solutions of (1-1) by assuming (M, g) is of bounded geometry (here bounded geometry means g is complete and the curvature tensor and all its covariant derivatives are bounded) via weighted Sobolev embeddings.

In this paper, we focus on the solvability of the Yamabe problem on a complete noncompact Riemannian manifold without the nonnegativity assumption on its scalar curvature, and intend to improve and generalize some results obtained in [Zhang 2003; Kim 1997]. More concretely, first, we try to prove a similar existence result to that in [Zhang 2003] under weaker assumptions on the volume growth of geodesic balls without the assumption that the scalar curvature of (M, g) is nonnegative. Then, we try to replace the hypothesis on the volume growth of geodesic balls of M by some other geometric hypotheses to derive some existence results.

In order to state our results, we need to clarify some notation. Generally, (M, g) denotes a complete noncompact manifold with $\dim(M) \geq 3$. O is a fixed point in M and $d(x) = d(x, O)$ denotes the distance from O to any $x \in M$ with respect to g, R_m is the curvature tensor, $\mathrm{inj}(M)$ is the injective radius of M and $\mathrm{V}_g(B_r(x))$ denotes the volume of $B_r(x)$. Let $Y(M)$ and $Y_\infty(M)$ be the Yamabe constant and the Yamabe constant at infinity on M, respectively.

Throughout this article, we always assume M satisfies the following conditions:

$$Y(M) < Y_\infty(M) \quad \text{and} \quad Y_\infty(M) > 0. \tag{1-2}$$

It is worth pointing out that $Y_\infty(M) > 0$ implies that $Y(M) > -\infty$ by Theorem 1.7 in [Grosse and Nardmann 2014]. Now we are ready to state our main results.

Theorem 1.1. *Let (M, g) be a complete noncompact Riemannian manifold of dimension $n \geq 3$ satisfying* (1-2). *Suppose that there exists a positive constant C such that $R_g \geq -Cd(x)^{-2}$ when $d(x)$ is large . Then there exists a constant $\rho_0(n, Y(M), Y_\infty(M)) > 0$ such that, if $\mathrm{V}_g(B(O, r)) \leq Cr^{n+\rho}$ for all large r, where ρ is a number with $\rho < \rho_0$, then the Yamabe equation* (1-1) *admits a positive solution u with $K = 1, 0, -1$ corresponding to $Y(M)$ being positive*, 0, *and negative, respectively. Moreover, with $\alpha = \alpha(n, \rho) > 0$, we have*

$$\lim_{d(x)\to\infty} d(x)^\alpha u(x) = O(1).$$

The method we used here is inspired by Zhang [2003] and Kim [1996]. Under the control condition on volume growth stated in the above theorem, we can derive a priori decay estimates of the "approximate solutions $\{u_i\}$" (see the details in Proposition 2.2). Hence, it follows that, if the sequence $\{u_i\}$ blows up, then the blow up points must lie in a compact subset of M.

Remark 1.2. In the case $\rho < 0$ and the scalar curvature of (M, g) is nonnegative, we have

$$\lim_{d(x)\to\infty} d(x)^{(n-2)/2}u(x) = o(1),$$

which is just the main result in [Zhang 2003].

Remark 1.3. There are a lot of manifolds satisfying the condition $Y(M) < Y_\infty(M)$, such that M is not locally conformally flat and there exists a compact subset M_0 such that $M\backslash M_0$ admits a conformal map to S^n (see [Schoen and Yau 1988; Kim 1996]). Zhang [2003] constructed a explicit example on a warped product manifold.

By the volume comparison theorem, the following corollary is an immediate consequence of Theorem 1.1.

Corollary 1.4. *Let (M, g) be a complete noncompact Riemannian manifold of dimension $n \geq 3$ with nonnegative Ricci curvature. Suppose $Y(M) < Y_\infty(M)$. Then the Yamabe equation admits a positive solution u with $K = 1$ and*

$$\lim_{d(x)\to\infty} d(x)^{(n-2)/2}u(x) = O(1).$$

It is natural to ask what happens without the assumption on volume growth. In this situation, one will encounter a new difficulty that, if $\{u_i\}$ blows up, maybe the blow up points tend to infinity of M. To overcome this difficulty, we need to analyze the convergence of the pointed manifolds induced by $\{u_i\}$ under the pointed Cheeger–Gromov topology by providing certain suitable conditions, then we discuss the blowup behavior of u_i on the limit pointed manifold. We obtain the following results.

Theorem 1.5. *Let (M, g) be a complete noncompact Riemannian manifold of dimension $n \geq 3$ satisfying* (1-2). *Assume $|\operatorname{Ric}(M)| \leq C_0$ and $\operatorname{inj}(M) \geq i_0$, where C_0 and i_0 are positive constants. Then* (1-1) *has a positive solution with $K = 1, 0, -1$ corresponding to $Y(M)$ being positive*, 0, *and negative*, *respectively. Moreover*,

$$\lim_{d(x)\to\infty} u(x) = O(1).$$

If we do not have an a priori positive lower bound on the injective radius, by [Anderson 1989; 1990] we can also get the following conclusion.

Theorem 1.6. *Let (M, g) be a complete noncompact Riemannian manifold of dimension $n \geq 3$ satisfying* (1-2). *Suppose*

(i) *there exist positive constants* C_0, v_0 *and* C *such that*

$$|\operatorname{Ric}(M)| \le C_0, \quad \mathrm{V}_g(B(p,1)) \ge v_0 \quad \textit{for any } p \in M,$$
$$\textit{and} \quad \int_M |R_m|^{n/2} d\mathrm{V}_g \le C, \quad \textit{respectively};$$

(ii) *the length of the shortest inessential* (*null-homotopic*) *geodesic loops*, *denoted by* l_M, *is positive*, *i.e.*, $l_M \ge l > 0$, *or* M *is an odd-dimensional*, *oriented manifold.*

Then, *the Yamabe equation* (1-1) *has a positive solution.*

The paper is organized as follows: In Section 2, we recall some basic notation, prove some basic facts about the Yamabe functional and discuss the variational approach as in the compact case. In Section 3, we give the proof of Theorem 1.1. In Section 4 we prove Theorems 1.5 and 1.6 by analyzing the blowup behavior of $\{u_j\}$ under the pointed Cheeger–Gromov topology.

2. Some basic notation and known results

In this section, we will recall some basic notation and definitions such as the Yamabe constants $Y(M)$ and $Y_\infty(M)$. Then we discuss the existence of "smooth approximate solutions u_i" corresponding to the exhaustion of M. The main methods and techniques used in this section can be found in the survey paper [Lee and Parker 1987]. For the sake of clarity and completeness, we shall still write it down. Finally, we recall the definition of pointed Cheeger–Gromov topology.

Yamabe constant on noncompact manifold. For any $\upsilon \in C_c^\infty(M)\backslash\{0\}$, define

$$E_g(\upsilon) = \int_M (|\nabla \upsilon|^2 + c(n) R_g \upsilon^2)\, d\mathrm{V}_g,$$

where $c(n) = (n-2)/(4(n-1))$. Then the Yamabe constant of (M, g) is defined by

$$Y(M) = \inf\left\{ \frac{E_g(\upsilon)}{\|\upsilon\|^2_{L^p(g)}} \;\middle|\; \upsilon \in C_c^\infty(M)\backslash\{0\} \right\}.$$

Kim [1996; 1997] defined a new functional called the Yamabe constant at infinity for noncompact manifolds as follows: choose an exhaustion $\{K_i\}_{i\in\mathbb{N}}$ of M, which is composed of bounded sets, and define

$$Y_\infty(M) = \lim_{i\to\infty} Y(M\backslash K_i).$$

Obviously $Y_\infty(M)$ does not depend on the exhaustion we choose.

Lemma 2.1. *For any complete noncompact manifold M, it always holds that*

$$-c(n)\|(R_g)_-\|_{L^{n/2}} \le Y(M) \le Y_\infty(M) \le \Lambda,$$

where $\Lambda = (n(n-2))/4\omega_n^{2/n}$ is the best Sobolev constant on $\mathbb{R}^n$ and $(R_g)_-$ is the negative part of the scalar curvature on M.

Proof. The first inequality is derived from the Hölder inequality and the second holds evidently by the definition of $Y(M)$ and $Y_\infty(M)$.

In order to prove the inequality on the right hand side, we need to make the following arguments. Let

$$u_\alpha = \left(\frac{\alpha}{\alpha^2+|x|^2}\right)^{(n-2)/2}.$$

It is well-known that we may obtain the best Sobolev constant in $\mathbb{R}^n$ by this family $\{u_\alpha\}$. In other words,

$$\int_{\mathbb{R}^n} |\nabla u_\alpha|^2\,dx = \Lambda\left(\int_{\mathbb{R}^n} u_\alpha^p\,dx\right)^{2/p}.$$

For any $q \in M\backslash K_i$, we choose the normal coordinates around q. It is well-know that, in the normal coordinates, $d\mathrm{V}_g = (1+O(r))$. Given $\epsilon > 0$, let B_ϵ denote the ball of radius ϵ in $\mathbb{R}^n$. We choose a smooth radial cutoff function $0 \le \eta(r) \le 1$ which is supported in $B_{2\epsilon}$ and with $\eta \equiv 1$ on B_ϵ. Setting $\varphi = \eta u_\alpha$, we have

$$\begin{aligned}\int_{\mathbb{R}^n} |\nabla\varphi|^2\,dx &= \int_{B_{2\epsilon}} \big(\eta^2|\nabla u_\alpha|^2 + 2\eta u_\alpha\langle\nabla\eta, \nabla u_\alpha\rangle + u_\alpha^2|\nabla\eta|^2\big)\,dx \\ &\le \int_{\mathbb{R}^n} |\nabla u_\alpha|^2\,dx + C\int_{A_\epsilon} (u_\alpha|\nabla u_\alpha| + u_\alpha^2)\,dx,\end{aligned} \tag{2-1}$$

where A_ϵ denotes the annulus $B_{2\epsilon}\backslash B_\epsilon$. Since

$$u_\alpha \le \alpha^{(n-2)/2} r^{2-n} \quad \text{and} \quad |\nabla u_\alpha| \le (n-2)\alpha^{(n-2)/2} r^{1-n},$$

then, for fixed ϵ, the second term on the right hand side of inequality (2-1) is $O(\alpha^{n-2})$ as $\alpha \to 0$. For the first term of (2-1), we have

$$\begin{aligned}\int_{\mathbb{R}^n} |\nabla u_\alpha|^2\,dx &= \Lambda\left(\int_{B_\epsilon} u_\alpha^p\,dx + \int_{\mathbb{R}^n\backslash B_\epsilon} u_\alpha^p\,dx\right)^{2/p} \\ &\le \Lambda\left(\int_{B_{2\epsilon}} \varphi^p\,dx + \int_{\mathbb{R}^n\backslash B_\epsilon} \alpha^n r^{-2n}\,dx\right)^{2/p} \\ &\le \Lambda\left(\int_{B_{2\epsilon}} \varphi^p\,dx\right)^{2/p} + O(\alpha^{n-2}).\end{aligned}$$

Therefore, on M, we have

$$\int_{B_{2\epsilon}} (|\nabla\varphi|^2 + c(n)R_g\varphi^2)\, dV_g \\ \le (1+C\epsilon)\left(\Lambda\|\varphi\|^2_{L^p} + C\alpha^{n-2} + C\int_0^{2\epsilon}\int_{S_r} u_\alpha^2 r^{n-1}\, d\omega\, dr\right).$$

The last term on the right hand side of the above inequality is actually bounded by a constant multiple of α. Obviously,

$$\int_0^{2\epsilon} u_\alpha^2 r^{n-1}\, dr = \alpha^2 \int_0^{2\epsilon/\alpha} \sigma^{n-1}(\sigma^2+1)^{2-n}\, d\sigma,$$

and noting that $\sigma^2 \le \sigma^2 + 1 \le 2\sigma^2$ for $\sigma \ge 1$ we can see that

$$C_1\left(C + \alpha^2\int_1^{2\epsilon/\alpha} \sigma^{3-n}\, d\sigma\right) \le \alpha^2 \int_0^{2\epsilon/\alpha} \sigma^{n-1}(\sigma^2+1)^{2-n}\, d\sigma \\ \le C_2\left(C + \alpha^2\int_1^{2\epsilon/\alpha} \sigma^{3-n}\, d\sigma\right).$$

A simple computation shows

$$\alpha^2\int_1^{2\epsilon/\alpha} \sigma^{3-n}\, d\sigma \le \begin{cases} \alpha & \text{if } n = 3, \\ -\alpha^2\log\alpha & \text{if } n = 4, \\ \alpha^2 & \text{if } n \ge 5. \end{cases}$$

Thus, choosing first ϵ and then α small, we can arrange that

$$\frac{E_g(\varphi)}{\|\varphi\|^2_{L^p}} \le (1+C\epsilon)(\Lambda + C\alpha).$$

Since ϵ and α can be arbitrarily small, it follows that

$$\frac{E_g(\varphi)}{\|\varphi\|^2_{L^p}} \le \Lambda. \qquad \square$$

Note that the proof of the above lemma does not assume that the injective radius of M has a positive lower bound.

The variational approach. In this subsection, let $B_r(O)$ denote the geodesic ball centered at O with radius r on M (M is noncompact), where O is a fixed point in M. Denote

$$Y_j = \inf_{\varphi\in W_0^{1,2}(B_j(O))\setminus\{0\}} \left\{\frac{E_g(\varphi)}{\|\varphi\|^2_{L^p(g)}}\right\}.$$

We have the following proposition:

Proposition 2.2. *Assume $Y_j < \Lambda$. Then, the following Dirichlet problem admits a positive solution u_j with $\|u_j\|_{L^p} = 1$:*

$$\Delta u_j - c(n) R_g u_j + Y_j u_j^{p-1} = 0, \quad \text{in } B_j(O), \tag{2-2}$$

$$u_j = 0, \quad \text{on } \partial B_j(O). \tag{2-3}$$

To prove this proposition, we need to establish some lemmas. First, for $s \in (2, p]$, we define

$$Q_s(u) = \frac{E_g(u)}{\|u\|^2_{L^s(g)}} \quad \text{and} \quad \lambda_s = \inf\{Q_s(u) \mid u \in W_0^{1,2}(B_j(O)) \backslash \{0\}\}.$$

Lemma 2.3 [Aubin 1976]. *For $Q_s(u)$ and λ_s defined as above, we always have*

$$\limsup_{s \to p} \lambda_s \le Y_j.$$

Moreover, if $\lambda_s \ge 0$, then $\lambda_s \to Y_j$.

Lemma 2.4. *For any $s \in (2, p)$, there exists $u_s \in C^\infty(\bar{B}_j(O))$, $u_s > 0$ in $B_j(O)$, $u_s = 0$ on $\partial B_j(O)$ and $\|u_s\|_{L^s} = 1$ such that $Q_s(u_s) = \lambda_s$ and the following equation is satisfied*:

$$\Delta u_s - c(n) R_g u_s + \lambda_s u_s^{s-1} = 0. \tag{2-4}$$

Proof. Take a minimizing sequence $\{u_i\} \subset W_0^{1,2}(B_j(O)) \backslash \{0\}$ such that $Q_s(u_i) \to \lambda_s$. Since $Q_s(|u|) \le Q_s(u)$ and $Q_s(tu) = Q_s(u)$, we can assume $u_i \ge 0$ and $\|u_i\|_{L^s} = 1$. Then we have

$$Q_s(u_i) = E_g(u_i) = \|\nabla u_i\|_2^2 + c(n) \int_{B_j(O)} R_g u_i^2 \, d\mathrm{V}_g \to \lambda_s.$$

Hence we have $\|\nabla u_i\|^2_{L^2} \le c_1 + c_2 \|u_i\|^2_{L^2}$. By the Hölder inequality, we also have

$$\|u_i\|^2_{L^2} \le C(\mathrm{V}_g(B_j(O)) \|u_i\|^2_{L^s} = C(\mathrm{V}_g(B_j(O)).$$

Therefore, $\{u_i\}$ is a bounded sequence in $W_0^{1,2}(B_j(O)$. Then, neglecting a subsequence, there exists $u_s \in W_0^{1,2}(B_j(O))$ such that $\{u_i\}$ converges weakly to u_s in $W^{1,2}(B_j(O))$. On the other hand, we also know that $W^{1,2} \hookrightarrow L^r$ is compactly embedded when $0 \le r < p$. Hence we have

$$\|\nabla u_s\|_{L^2} \le \liminf_{i \to \infty} \|\nabla u_i\|_{L^2}, \tag{2-5}$$

$$\int R_g u_i^2 \, d\mathrm{V}_g \to \int R_g u_s^2 \, d\mathrm{V}_g, \tag{2-6}$$

$$\|u_s\|_{L^s} = \lim_{i \to \infty} \|u_i\|_{L^s} = 1. \tag{2-7}$$

Combining the above three inequalities we infer

$$Q_s(u_s) \le \liminf_{i\to\infty} Q_s(u_i) = \lambda_s.$$

Then, the definition of λ_s tells us $Q_s(u_s) = \lambda_s$. This means that u_s is the weak solution of (2-4). Using an L^p estimate and the Schauder estimate (see [Gilbarg and Trudinger 1998]), we take a standard boot-strapping argument to deduce $u_s \in C^{2,\alpha}(\bar{B}_j(O))$.

Since $u_i \ge 0$, it follows that $u_s \ge 0$. Hence, it is easy to see that there exist some constant $c \ge 0$ such that $\Delta u_s - cu_s \le 0$. By the maximal principle, we have $u_s > 0$ in $B_j(O)$. Since t^{s-1} is a smooth function when $t > 0$, it follows that u_s^{s-1} is a smooth function. Hence, the standard elliptic theory tells us that $u_s \in C^\infty(\bar{B}_j(O))$. □

Lemma 2.5. *The set $\{u_s \mid s_0 \le s < p\}$ is uniformly bounded with respect to s for some constant $s_0 \in (2,\ p)$.*

Proof. Each u_s satisfies Equation (2-4) and $u_s = 0$ on $\partial B_j(O)$. Let $b > 0$ be a constant which will be determined later. Multiplying both sides of (2-4) by u_s^{1+2b} and integrating by parts, we obtain

$$\int_{B_j(O)} \big(\langle \nabla u_s,\ (1+2b)u_s^{2b}\nabla u_s\rangle + c(n)R_g u_s^{2+2b}\big)\, d\mathrm{V}_g = \lambda_s \int_{B_j(O)} u_s^{s+2b}\, d\mathrm{V}_g.$$

If we set $w = u_s^{1+b}$, then the above equality can be written as

$$\frac{1+2b}{(1+b)^2}\int_{B_j(O)} |\nabla w|^2\, d\mathrm{V}_g = \int_{B_j(O)} \big(\lambda_s w^2 u_s^{s-2} - c(n)R_g w^2\big)\, d\mathrm{V}_g.$$

Now, applying the sharp Sobolev inequality, for any $\epsilon > 0$, there exists some $C(\epsilon)$ such that

$$\begin{aligned} \|w\|_{L^p}^2 &\le \frac{(1+\epsilon)}{\Lambda}\int_{B_j(O)} |\nabla w|^2 d\mathrm{V}_g + C(\epsilon)\int_{B_j(O)} w^2\, d\mathrm{V}_g \\ &\le (1+\epsilon)\frac{(1+b)^2}{1+2b}\int_{B_j(O)} \frac{\lambda_s}{\Lambda} w^2 u_s^{s-2}\, d\mathrm{V}_g + C'(\epsilon)\|w\|_{L^2}^2 \\ &\le (1+\epsilon)\frac{(1+b)^2}{1+2b}\frac{\lambda_s}{\Lambda}\|w\|_{L^p}^2 \|u_s\|_{L^{n(s-2)/2}}^{s-2} + C'(\epsilon)\|w\|_{L^2}^2. \end{aligned} \tag{2-8}$$

Since $s < p$, we have $(s-2)n/2 < s$. By the Hölder inequality, we have

$$\|u_s\|_{L^{n(s-2)/2}} \le C(s)\|u_s\|_{L^s} = C(s),$$

where $C(s) \to 1$ as s tends to p.

Now, we need to consider the following two cases:

Case 1: $0 \le Y_j < \Lambda$. In this case we have $\lambda_s \ge 0$. Moreover, by Lemma 2.3 we know that there exists some $s_0 \in (0, p)$ such that $\lambda_s/\Lambda \le \mu < 1$ for any $s \in [s_0, p)$. Thus, we can choose ϵ and b small enough such that

$$(1+\epsilon)\frac{(1+b)^2}{1+2b}\frac{\lambda_s}{\Lambda} < 1.$$

So, it follows from (2-8) that

$$\|w\|_{L^p}^2 \le C\|w\|_{L^2}^2.$$

Case 2: $Y_j < 0$. For this case the same result holds obviously. Indeed, as Y_j is less than zero, it follows from Lemma 2.3 that there exists some $s_0 \in (0, p)$, such that $\lambda_s < 0$ for any $s \in [s_0, p)$. We apply the Hölder inequality to derive

$$\|w\|_{L^2} = \|u_s\|_{L^{2(1+b)}}^{1+b} \le C\|u_s\|_{L^s}^{1+b} \le C.$$

Therefore, we have that $\|w\|_{L^p} = \|u_s\|_{L^{p(1+b)}}^{1+b}$ is bounded uniformly with respect to s. By L^p estimates and the Sobolev embedding theorem, we know that the lemma is true. □

Proof of Proposition 2.2. By Lemma 2.5, we know u_s is uniformly bounded in $C^{k,\alpha}(\bar{B}_j(O))$. Hence, there exists a subsequence of $\{u_s\}$ which converges to a solution of (2-2) and (2-3). □

Pointed Cheeger–Gromov topology. At the last part of this section, we recall the definition of convergence of manifolds under the pointed Cheeger–Gromov topology.

Definition 2.6 (see [Petersen 2006]). A sequence of pointed complete Riemann manifolds is said to converge in pointed $C^{m,\alpha}$ Cheeger–Gromov topology

$$(M_i, p_i, g_i) \to (M, p, g)$$

if for every $R > 0$ we can find a domain $B_R(p) \subset \Omega \subset M$ and embeddings $F_i : \Omega \to M_i$ for large i such that $F_i(\Omega) \supset B_R(p_i)$ and $F_i^* g_i \to g$ on Ω in the $C^{m,\alpha}$ topology.

Note that $C^{m,\alpha}$ type convergence implies pointed Gromov–Hausdorff convergence.

3. Proof of Theorem 1.1

We proceed now to the proof of Theorem 1.1, which will be divided into four steps. The basic idea we used here is to employ the finite domain exhaustion of M and then consider the subsolution sequence u_i of Yamabe equations corresponding to this exhaustion. A crucial step is to establish a decay estimate of u_i near infinity.

Step 1. By the condition $Y(M) < Y_\infty(M)$ and Lemma 2.1, we have $Y(M) < \Lambda$. On the other hand, by the definition of Y_j, we know that $\{Y_j\}$ converges decreasingly to $Y(M)$. So, when j is large enough, we have $Y_j < \Lambda$. Using Proposition 2.2, we know there is a positive solution u_j solving

$$\begin{aligned} \Delta u_j - c(n)R_g u_j + Y_j u_j^{p-1} &= 0, \quad \text{in } B_j(O), \\ u_j &= 0, \quad \text{on } \partial B_j(O). \end{aligned}$$

Next, we extend u_j to the whole manifold by defining $u_j(x) = 0$ when $x \notin B_j(O)$. The extended function, we still denote it by u_j, is continuous and a subsolution to the equation

$$\Delta u - c(n)R_g u + Y_j u^{p-1} = 0, \quad \text{on } M.$$

Step 2. In this step, we will establish an a priori decay estimate for $\{u_j\}$.

Lemma 3.1. *There exists a $\rho_0(n, Y(M), Y_\infty(M)) > 0$, such that for any $\rho < \rho_0$, if $\mathrm{V}_g(B(O, r)) \le Cr^{n+\rho}$ for all large r, we have*

$$\lim_{d(x)\to\infty} \lim_{j\to\infty} d(x)^\alpha u_j(x) = O(1),$$

where ρ can be negative and $\alpha = \alpha(\rho, n) > 0$.

Proof. Given $R > 1$, first we fix a point $x_0 \in M$ such that $d(x_0) = 2R^2$, then we scale the metric by $\tilde g = g/R^4$. Let d_1, ∇_1, $R_{\tilde g}$, Δ_1 and $d\mathrm{V}_{\tilde g}$ be the corresponding distance, gradient, scalar curvature, Laplace–Beltrami operator and volume element with respect to the rescaled manifold $(M, \tilde g)$. Define $v_j(x) = R^{n-2}u_j(x)$. Since

$$\Delta u_j - c(n)R_g u_j + Y_j u_j^{p-1} \ge 0, \quad \text{on } M.$$

A direct computation shows

$$\Delta_1 v_j - c(n)R_{\tilde g} v_j + Y_j v_j^{p-1} = R^{n+2}\big(\Delta u_j - c(n)R_g u_j + Y_j u_j^{p-1}\big) \ge 0, \tag{3-1}$$

$$\int_{d_1(x_0,x)\le 1} v_j^p \, d\mathrm{V}_{\tilde g} = \int_{d(x_0,x)\le R^2} u_j^p \, d\mathrm{vol}_g \le \int_M u_j^p \, d\mathrm{V}_g = 1. \tag{3-2}$$

Take $\varphi \in C^\infty[0, \infty)$ such that $0 \le \varphi \le 1$ and $|\varphi'(r)| \le C$, which satisfies $\varphi(r) = 1$ when $r \in \big[0, \frac12\big]$, $\varphi(r) = 0$ when $r \in [1, \infty)$. Let $G(s) = s^\beta$ and define

$$F(t) = \int_0^t G'(s)^2 \, ds = \frac{\beta^2}{2\beta - 1} t^{2\beta-1}.$$

By a simple computation, we see that, as $\beta > 1$,

$$sF(s) \le s^2 G'(s)^2 = \beta^2 G(s)^2. \tag{3-3}$$

Let $\eta(x) = \varphi(d_1(x_0, x))$; we know the support $\mathrm{spt}(\eta^2 F(v)) \subseteq M \setminus B_{R^2/2}(O)$. We multiply (3-1) by $\eta^2 F(v)$ and then integrate by parts to obtain that, for some

$\epsilon > 0$,

$$(1-\epsilon)\int |\nabla_1 v|^2 G'(v)^2\eta^2\, d\mathrm{V}_{\tilde g} \le \beta^2\epsilon^{-1}\int |\nabla_1\eta|^2 G(v)^2\, d\mathrm{V}_{\tilde g} - \frac{\beta^2}{2\beta-1}\int c(n)R_{\tilde g}G(v)^2\eta^2\, d\mathrm{V}_{\tilde g} + Y_j\int v^{p-2}vF(v)\, d\mathrm{V}_{\tilde g},$$

where ϵ may be chosen arbitrarily small. By the condition $R_g \ge -Cd^{-2}(x, O)$, we have that, when R is large enough, $R_{\tilde g} \ge -C$. Hence, from the above inequality it follows that

$$\|\nabla_1(G(v)\eta)\|^2_{L^2} + \int c(n)R_{\tilde g}(G(v)\eta)^2\, d\mathrm{V}_{\tilde g} \le C\beta^2\|\nabla_1\eta\|^2_{L^\infty}\int G(v)^2\, d\mathrm{V}_{\tilde g} + \frac{Y_j}{1-\epsilon}\int v^{p-1}F(v)\eta^2\, d\mathrm{V}_{\tilde g}. \tag{3-4}$$

Next, we need to consider the following two cases:

Case 1. $Y(M) \ge 0$. Since Y_j converges decreasingly to $Y(M)$, it follows that $Y_j \ge 0$. On the other hand, by the assumption $Y_\infty(M) > 0$ and the fact $Y(M\backslash B_r(O))$ increases with respect to r, we have $Y(M\backslash B_r(O) > 0$ when r is large enough. Let

$$C_0 = \frac{1}{Y(M\backslash B_{R^2/2}(O))}.$$

It is easy to see that $C_0 > 0$ as R is large. Since $\mathrm{spt}(\eta^2F(v)) \subseteq M\backslash B_{R^2/2}(O)$, by the definition of the Yamabe quotient we have

$$\|G(v)\eta\|^2_{L^p} \le C_0\|\nabla_1(G(v)\eta)\|^2_{L^2} + C_0\int_{d_1(x_0,x)\le 1} c(n)R_{\tilde g}[G(v)\eta]^2\, d\mathrm{V}_{\tilde g}.$$

Here, all the norms were taken on the domain $d_1(x_0, x) \le 1$ with respect to the rescaled metric $\tilde g$. By the fact that $Y_j \ge 0$ and (3-3), we obtain

$$\begin{aligned}\|G(v)\eta\|^2_{L^p} &\le CC_0\beta^2\|\nabla_1\eta\|^2_{L^\infty}\int G(v)^2\, d\mathrm{V}_{\tilde g} + C_0Y_j(\beta^2+\epsilon)\int v^{p-2}G(v)^2\eta^2\, d\mathrm{V}_{\tilde g}\\ &\le CC_0\beta^2\|\nabla_1\eta\|^2_{L^\infty}\int G(v)^2\, d\mathrm{V}_{\tilde g} + C_0Y_j(\beta^2+\epsilon)\|G(v)\eta\|^2_{L^p}\Big(\int v^p\, d\mathrm{V}_{\tilde g}\Big)^{2/n}\\ &\le CC_0\beta^2\|\nabla_1\eta\|^2_{L^\infty}\int G(v)^2\, d\mathrm{V}_{\tilde g} + C_0Y_j(\beta^2+\epsilon)\|G(v)\eta\|^2_{L^p}.\end{aligned} \tag{3-5}$$

Here we have used inequality (3-2) in the last inequality.

By the assumption $Y(M) < Y_\infty(M)$, we have, when R sufficiently large,

$$Y(M) < Y(M\backslash B_{R^2/2}(O)).$$

Noting $Y_j \downarrow Y(M)$ as $j \to \infty$, we have that, when j is large enough,

$$Y_j < Y(M \backslash B_{R^2/2}(O)) = \frac{1}{C_0}. \tag{3-6}$$

Hence, there exists $\beta_0 > 1$ such that, for all j and small enough ϵ,

$$(\beta_0^2 + \epsilon) C_0 Y_j < 1. \tag{3-7}$$

Substitute (3-7) into (3-5) to obtain

$$\|v^{\beta_0}\eta\|_{L^p}^2 \le C\|\nabla_1 \eta\|_{L^\infty}^2 \int v^{2\beta_0} d\mathrm{V}_{\tilde{g}}. \tag{3-8}$$

By the definition of η and the Hölder inequality, we infer from (3-8),

$$\begin{aligned}\left(\int_{B_1(x_0,1/2)} v^{2n\beta_0/(n-2)}\, d\mathrm{V}_{\tilde{g}}\right)^{(n-2)/n} &\le \|v^{\beta_0}\eta\|_{L^p}^2 \le C\int_{B_1(x_0,1)} v^{2\beta_0}\, d\mathrm{V}_{\tilde{g}} \\ &\le C\left(\int_{B_1(x_0,1)} v^p\, d\mathrm{V}_{\tilde{g}}\right)^{\beta_0(n-2)/n} \big(\mathrm{V}_{\tilde{g}}(B_1(x_0,1))\big)^{n-(n-2)\beta_0/n} \\ &\le C\big(\mathrm{V}_{\tilde{g}}(B_1(x_0,1))\big)^{n-(n-2)\beta_0/n}.\end{aligned} \tag{3-9}$$

Now, we proceed to a consideration of the possible growth rate of volumes of geodesic balls such that the Yamabe equation (1-1) on M is solvable. If $\mathrm{V}_g(B(O,r)) \le Cr^{n+\rho}$ for all r large, then we have

$$\mathrm{V}_{\tilde{g}}(B_1(x_0,1))) = \frac{\mathrm{V}_g(B_{R^2}(x_0))}{R^{2n}} \le \frac{\mathrm{V}_g(B_{4R^2}(O))}{R^{2n}} \le CR^{2\rho}.$$

Therefore, we obtain

$$\left(\int_{B_1(x_0,1/2)} v^{2n\beta_0/(n-2)}\, d\mathrm{V}_{\tilde{g}}\right)^{(n-2)/n} \le CR^{2\rho[n-(n-2)\beta_0]/n}. \tag{3-10}$$

Subsequently we will use a standard Moser iteration argument to finish the proof the lemma. Given $0 < r_2 < r_1 < \frac{1}{2}$, by taking $G(v) = v^\beta$ we have

$$\begin{aligned}&\int_{B_1(x_0,r_1)} v^{p-2}G(v)^2\, d\mathrm{V}_{\tilde{g}} \\ &\le \left(\int_{B_1(x_0,r_1)} v^{2n\beta_0/(n-2)}\, d\mathrm{V}_{\tilde{g}}\right)^{2/(n\beta_0)} \left(\int_{B_1(x_0,r_1)} G(v)^{2n\beta_0/(n\beta_0-2)}\, d\mathrm{V}_{\tilde{g}}\right)^{(n\beta_0-2)/(n\beta_0)} \\ &\le \left(\int_{B_1(x_0,r_1)} v^{2n\beta_0/(n-2)}\, d\mathrm{V}_{\tilde{g}}\right)^{2/(n\beta_0)} \left(\int_{B_1(x_0,r_1)} G(v)^{(2n\delta)/(n-2)}\, d\mathrm{V}_{\tilde{g}}\right)^{(n-2)/(n\delta)},\end{aligned}$$

where

$$\delta = \frac{(n-2)\beta_0}{n\beta_0 - 2} < 1.$$

Therefore, by combining (3-10) with the above inequality we have

(3-11)
$$\int_{B_1(x_0,r_1)} v^{p-2}G(v)^2\,dV_{\tilde g} \le C R^{\frac{4\rho}{n-2}\frac{n-(n-2)\beta_0}{n\beta_0}} \left(\int_{B_1(x_0,r_1)} G(v)^{\frac{2n\delta}{n-2}}\,dV_{\tilde g}\right)^{(n-2)/(n\delta)}.$$

Noting that
$$\frac{n\delta}{n-2} = \frac{n\beta_0}{n\beta_0-2} > 1,$$
we use again the Hölder inequality to obtain

$$\text{(3-12)}\quad \begin{aligned} \int_{B_1(x_0,r_1)} & G(v)^2\,dV_{\tilde g} \\ &\le \left(\int_{B_1(x_0,r_1)} G(v)^{2n\delta/(n-2)}\,dV_{\tilde g}\right)^{(n-2)/(n\delta)} V_{\tilde g}(B_1(x_0,1))^{(n\delta-n+2)/(n\delta)} \\ &\le C\left(\int_{B_1(x_0,r_1)} G(v)^{2n\delta/(n-2)}\,dV_{\tilde g}\right)^{(n-2)/(n\delta)} R^{4\rho/(n\beta_0)}. \end{aligned}$$

For $0 < r_2 < r_1 < \frac{1}{2}$, we choose η to be a radial function, supported in $B_1(x_0, r_1)$, such that $\eta = 1$ if $x \in B_1(x_0, r_2)$ and $|\nabla_1\eta| \le 2/(r_1 - r_2)$. We also note that (3-5) remains valid for such η and any fixed $\beta > 1$, i.e.,

$$\text{(3-13)}\quad \begin{aligned} \|G(v)\eta\|^2_{L^p} \le C C_0\beta^2 \|\nabla_1\eta\|^2_{L^\infty} & \int G(v)^2\,dV_{\tilde g} \\ & + C_0 Y_j(\beta^2+\epsilon)\int v^{p-2}G(v)^2\eta^2\,dV_{\tilde g}. \end{aligned}$$

Substituting (3-11) and (3-12) into the right hand side of (3-13), we obtain

$$\text{(3-14)}\qquad \|G(v)\chi_{r_2}\|_{L^{2n/(n-2)}} \le C\frac{R^{2\rho/(n\beta_0)}\beta}{r_1-r_2}\|G(v)\chi_{r_1}\|_{L^{2n\delta/(n-2)}}.$$

Here χ_{r_i} is the characteristic function of $B_1(x_0, r_i)$.

By taking $\beta = \delta^{-m}$ and $r_m = r_1(2+2^{-m})/4$, the standard Moser iteration shows that
$$\|v\|_{L^\infty(B_1(x_0,r_1/2))} \le C R^{2\rho\delta/(n\beta_0(1-\delta))} = C R^{(n-2)\rho/(n(\beta_0-1))}.$$

Note that, if $(n-2)\rho/(n(\beta_0-1)) < n-2$, i.e., $\rho < n(\beta_0-1)$,
$$u_j(x_0) = \frac{v_j(x_0)}{R^{n-2}} \le C d^{-\alpha}(x_0),$$
where
$$\alpha = \frac{n-2}{2} - \frac{(n-2)\rho}{2n(\beta_0-1)}.$$

From the above arguments, we know that ρ_0 can be chosen as $n(\beta_0-1)$. Here, β_0 should be chosen such that (3-7) holds as well as $\beta_0 < n/(n-2)$. So, by a simple computation, we have

$$\rho_0=\min\left(n\sqrt{\frac{Y_\infty}{Y(M)}}-n,\ \frac{2n}{n-2}\right).$$

Case 2. $Y(M)<0$. In this case, we have $Y_j\le 0$ when j is sufficiently large, since $\{Y_j\}$ converges decreasingly to $Y(M)$. Thus we can directly drop the last term in (3-4). Then (3-5) turns out to be

$$\|G(v)\eta\|_{L^p}^2\le CC_0\beta^2\|\nabla_1\eta\|_{L^\infty}^2\int G(v)^2\,dV_{\tilde{g}}. \tag{3-15}$$

For the present situation, we may directly choose $\rho_0=2n/(n-2)$ and take the same argument as in Case 1 to deduce

$$\lim_{d(x)\to\infty}\lim_{j\to\infty}d(x)^\alpha u_j(x)=O(1),$$

where $\alpha=(n-2/(4n))(2n-\rho(n-2))$, completing the proof of Lemma 3.1. □

Step 3. Now we turn to showing $\{u_j\}$ is uniformly bounded with respect to j. For this purpose, we prove it by contradiction. If not, then there exists a subsequence $\{k\}\subseteq\{j\},\ z_k\in M$, such that

$$u_k(z_k)=\max u_k\triangleq m_k\to+\infty.$$

By Lemma 3.1, we know there exists a sufficiently large R_0 such that $z_k\in B_{R_0}(O)$. Thus we can assume $z_k\to z_0$. Take a normal coordinate system at z_0. It is well-known that, in the normal coordinate system, we have

$$g_{ij}(x)=\delta_{ij}+O(|x|^2),\quad\text{and}\quad\det(g_{ij}(x))=1+O(|x|^2).$$

Denote the coordinates of z_k at this atlas by x_k. Then, $x_k\to 0$ as $k\to\infty$. With respect to this coordinate chart, u_k satisfies the following equation:

$$\frac{1}{\sqrt{\det g}}\partial_i(\sqrt{\det g}\,g^{ij}\partial_j u_k)-c(n)R_g(x)u_k+Y_k u_k^{p-1}=0 \tag{3-16}$$

Without loss of generality, we may assume the above equation can be defined in $\{x:|x|<1\}$. Now define

$$v_k=m_k^{-1}u_k(\delta_k x+x_k),$$

where $\delta_k=m_k^{1-p/2}\to 0$. Then v_k can be defined on the ball centered at 0 with radius $\rho_k=(1-|x_k|)/\delta_k\to\infty$ in $\mathbb{R}^n$. Moreover, v_k satisfies

$$\frac{1}{b_k}\partial_i(b_k a_k^{ij}\partial_j v_k)-c_k v_k+Y_k v_k^{p-1}=0, \tag{3-17}$$

where

$$a_k^{ij}(x) = g^{ij}(\delta_k x + x_k) \to \delta_{ij}, \tag{3-18}$$

$$b_k(x) = \sqrt{\det g(\delta_k x + x_k)} \to 1, \tag{3-19}$$

$$c_k(x) = c(n) m_k^{2-p} R_g(\delta_k x + x_k) \to 0. \tag{3-20}$$

The above convergence is actually C^1 uniform convergence on any finite domain of $\mathbb{R}^n$. Noting that

$$0 \le v_k \le v_k(0) = 1,$$

by L^p and Schauder estimates we obtain that, for any $R > 0$, there exist $C(R) > 0$ and $k(R) > 0$, such that

$$\|v_k\|_{C^{2,\alpha}(\bar{B}_R)} \le C(R), \quad \text{for all } k \ge k(R).$$

Picking $R_m \to +\infty$, we make a standard diagonal argument to show that there exists a subsequence $\{v_m\}$, such that $v_m \to v \in C^2(\mathbb{R}^n)$ with respect to the C^2-norm on every $\overline{B}_{R_m}$. Let $m \to \infty$. In view of Equations (3-17)–(3-20) we know that v is a nonnegative solution of

$$\Delta v + Y(M) v^{p-1} = 0, \tag{3-21}$$

with $v(0) = 1$. By the maximal principle, we have $v > 0$.

By changing of the variables, we obtain

$$\int_{|x| \le \frac{1}{2}\delta_k^{-1}} v_k^p b_k \, dx = \int_{B_{1/2}(x_k)} u_k^p \sqrt{\det g} \, dx \le \|u_k\|_{L^p}^p = 1. \tag{3-22}$$

Since $\{v_m^p b_m\}$ converges to v^p uniformly on any bounded domain in $\mathbb{R}^n$, by Fatou's lemma we obtain

$$\int_{\mathbb{R}^n} v^p dx \le 1. \tag{3-23}$$

Similarly, we have

$$\int_{|x| \le \frac{1}{2}\delta_k^{-1}} |\nabla v_k|^2 b_k \, dx = \int_{B_{1/2}(x_k)} |\nabla u_k|^2 \sqrt{\det g} \, dx \le \|\nabla u_k\|_{L^2(B_{R_0}(O))}^2. \tag{3-24}$$

By L^p estimate, we have

$$\|u_k\|_{W^{2,2n/(n+2)}(B_{R_0}(O))} \le C.$$

Then the Sobolev embedding theorem yields

$$\|\nabla u_k\|_{L^2(B_{R_0}(O))} \le C.$$

Combining the above inequality and (3-24), by Fatou's lemma again we obtain

$$\int_{\mathbb{R}^n} |\nabla v|^2\,dx < \infty. \tag{3-25}$$

Choose $\eta \in C_0^\infty(\mathbb{R}^n)$ such that $0 \le \eta \le 1$, $\eta = 1$ when $x \in B_1(0)$, $\eta = 0$ when $x \in \mathbb{R}^n \backslash B_2(0)$. Define

$$v_R(x) = \eta\Big(\frac{x}{R}\Big)v(x).$$

Then, obviously we have

$$\int_{\mathbb{R}^n} (|\nabla(v - v_R)|^2 + |v - v_R|^p)\,dx \to 0, \quad \text{as } R \to \infty. \tag{3-26}$$

Multiplying (3-21) by v_R and integrating by parts, we get

$$\int_{\mathbb{R}^n} \nabla v \cdot \nabla v_R\,dx = Y(M)\int_{\mathbb{R}^n} v^{p-1} v_R\,dx. \tag{3-27}$$

In view of (3-26), we let $R \to \infty$ in (3-27) to obtain

$$\int_{\mathbb{R}^n} |\nabla v|^2\,dx = Y(M)\int_{\mathbb{R}^n} v^p\,dx. \tag{3-28}$$

Now, by virtue of (3-23), (3-28) and the Sobolev inequality we get

$$\Lambda\bigg(\int_{\mathbb{R}^n} v^p\,dx\bigg)^{2/p} \le \int_{\mathbb{R}^n} |\nabla v|^2\,dx = Y(M)\int_{\mathbb{R}^n} v^p\,dx. \tag{3-29}$$

So we have

$$\Lambda \le Y(M)\bigg(\int_{\mathbb{R}^n} v^p\,dx\bigg)^{2/n} \le Y(M). \tag{3-30}$$

This contradicts the assumption $Y(M) < \Lambda$.

Step 4. The convergence of $\{u_j\}$.

By the standard elliptic theory, u_j is uniformly bounded in $C^{k,\alpha}$, for all $k \in \mathbb{N}$. Hence, there exists a subsequence of $\{u_j\}$ which converges to u satisfying

$$\Delta u - c(n)R_g u + Y(M)u^{p-1} = 0.$$

However, we do not know whether or not $u \neq 0$. The next theorem tells us that, under the hypothesis $Y(M) < Y_\infty(M)$, there holds such a $u \not\equiv 0$.

Proposition 3.2. *Assume that u is the limit function of $\{u_j\}$ as above. If $Y(M) < Y_\infty(M)$, then $u \not\equiv 0$.*

Proof. We prove this proposition by contradiction. If $u \equiv 0$, then we know u_j converge to 0 on any compact set of M. For any fixed R, let $\eta(r)$ be a smooth function such that $\eta(r) = 1$ when $r \geq 2R$, $\eta(r) = 0$ when $r \leq \frac{3}{2}R$. Then we have

$$
\begin{aligned}
(3\text{-}31)\quad & \int_M (|\nabla u_j|^2 + c(n) R_g u_j^2)\, d\mathrm{V}_g \\
&= \int_{M\setminus B_R} (|\nabla u_j|^2 + c(n) R_g u_j^2)\, d\mathrm{V}_g + \int_{B_R} (|\nabla u_j|^2 + c(n) R_g u_j^2)\, d\mathrm{V}_g \\
&= \int_{M\setminus B_R} (|\nabla \eta u_j|^2 + c(n) R_g \eta^2 u_j^2)\, d\mathrm{V}_g + \int_{B_{2R}\setminus B_R} (|\nabla u_j|^2 + c(n) R_g u_j^2)\, d\mathrm{V}_g \\
&\quad - \int_{B_{2R}\setminus B_R} (|\nabla \eta u_j|^2 + c(n) R_g \eta^2 u_j^2)\, d\mathrm{V}_g + \int_{B_R} (|\nabla u_j|^2 + c(n) R_g u_j^2)\, d\mathrm{V}_g \\
&\geq Y(M\setminus B_R)\Big(\int_{M\setminus B_R} |\eta u_j|^p\, d\mathrm{V}_g\Big)^{2/p} + \int_{B_{2R}\setminus B_R} (|\nabla u_j|^2 + c(n) R_g u_j^2)\, d\mathrm{V}_g \\
&\quad - \int_{B_{2R}\setminus B_R} (|\nabla \eta u_j|^2 + c(n) R_g \eta^2 u_j^2)\, d\mathrm{V}_g + \int_{B_R} (|\nabla u_j|^2 + c(n) R_g u_j^2)\, d\mathrm{V}_g,
\end{aligned}
$$

and

$$
(3\text{-}32)\qquad \int_{M\setminus B_R} |\eta u_j|^p\, d\mathrm{V}_g = 1 - \int_{B_{2R}} u_j^p\, d\mathrm{V}_g + \int_{B_{2R}\setminus B_R} (\eta u_j)^p\, d\mathrm{V}_g.
$$

Substitute (3-32) into (3-31), then let $j \to \infty$ to get

$$Y(M) \geq Y(M\setminus B_R).$$

Since the above inequality holds for any fixed R, let $R \to \infty$, we obtain

$$
(3\text{-}33)\qquad Y(M) \geq Y_\infty(M).
$$

So we have

$$Y(M) = Y_\infty(M),$$

which contradicts to the hypothesis. □

By Proposition 3.2 we know $u \not\equiv 0$. Using the maximal principle, we obtain $u(x) > 0$. Now after a suitable dilation, we can obtain a positive solution to (1-1) with $K = 1, 0, -1$ when $Y(M)$ is positive, 0, and negative, respectively. This completes the proof.

4. Proof of Theorems 1.5 and 1.6

In this section, we will study the blowup behavior of $\{u_i\}$ under the pointed Cheeger–Gromov topology. First of all, we prove a uniform estimate of u_j near the boundary.

The method used here is the Giorgi–Nash–Moser iteration just as in the argument in Step 2 of Section 3.

Let u_j be the positive solution obtained in Proposition 2.2 and

$$U_j = \left\{x \in B_j(O) \mid d(x, \partial B_j(O)) < \tfrac{1}{8}\right\}.$$

In order to prove Theorem 1.5 and 1.6, we need to establish the following theorem.

Theorem 4.1. *There exists a positive constant C which does not depend on j such that $u_j(x) \le C$ for all $x \in U_j$ when j is large enough.*

Proof. Extend u_j to the whole manifold by defining $u_j(x) = 0$ when $x \notin B_j(O)$. The extended function, still denoted by u_j, is continuous and satisfies

$$\Delta u_j - c(n) R_g u_j + Y_j u_j^{p-1} \ge 0 \quad \text{on } M. \tag{4-1}$$

Let $G(s) = s^\beta$ and define

$$F(t) = \int_0^t G'(s)^2\, ds = \frac{\beta^2}{2\beta - 1} t^{2\beta-1}.$$

By a simple computation, we have that, as $\beta > 1$,

$$s F(s) \le s^2 G'(s)^2 = \beta^2 G(s)^2. \tag{4-2}$$

Take $\varphi \in C^\infty[0, \infty)$ such that $0 \le \varphi \le 1$, $\varphi(r) = 1$ when $r \in [0, 1/2]$, $\varphi(r) = 0$ when $r \in [1, \infty)$, and $|\varphi'(r)| \le C$. For any fixed $x_j \in \partial B_j(O)$, let $\eta(x) = \varphi(d(x_j, x))$. Obviously, $\operatorname{spt}(\eta^2 F(v)) \subseteq M \setminus B_{j/2}(O)$. Multiplying the both side of (4-1) by $\eta^2 F(v)$ and integrating by parts yields that, for some $\epsilon > 0$,

$$\begin{aligned}\|\nabla(G(u_j)\eta)\|_{L^2}^2 &+ \int c(n) R_g (G(u_j)\eta)^2\, d\mathrm{V}_g \\ &\le C\beta^2 \|\nabla\eta\|_{L^\infty}^2 \int G(u_j)^2\, d\mathrm{V}_g + (\beta^2 + \epsilon) Y_j \int u_j^{p-2} G(u_j)^2 \eta^2\, d\mathrm{V}_g,\end{aligned}$$

where ϵ can be chosen arbitrary small.

Since $Y(M \backslash B_r(O))$ is increasing with respect to r, we infer from the assumption $Y_\infty(M) > 0$ that $Y(M \backslash B_r(O)) > 0$ when r is large. Let

$$C_j = \frac{1}{Y(M \backslash B_{j/2}(O))}.$$

Noting $\operatorname{spt}(\eta^2 F(u_j)) \subseteq M \setminus B_{j/2}(O)$, by the definition of the Yamabe quotient we have

$$\|G(u_j)\eta\|_{L^p}^2 \le C_j \|\nabla(G(u_j)\eta)\|_{L^2}^2 + C_j \int_{B_1(x_j)} c(n) R_g [G(u_j)\eta]^2\, d\mathrm{V}_g. \tag{4-3}$$

By a similar argument with that in Step 2 of Section 3, we derive from the above inequality

$$
\begin{aligned}
\text{(4-4)}\quad & \|G(u_j)\eta\|_{L^p}^2 \\
& \le CC_j\beta^2\|\nabla\eta\|_{L^\infty}^2 \int G(u_j)^2\, d\mathrm{V}_g + C_jY_j(\beta^2+\epsilon)\int u_j^{p-2}G(u_j)^2\eta^2\, d\mathrm{V}_g \\
& \le CC_j\beta^2\|\nabla\eta\|_{L^\infty}^2 \int G(u_j)^2\, d\mathrm{V}_g + C_jY_j(\beta^2+\epsilon)\|G(u_j)\eta\|_{L^p}^2.
\end{aligned}
$$

By the hypothesis, we have

$$\lim_{j\to+\infty} C_jY_j = \frac{Y(M)}{Y_\infty(M)} < 1.$$

Hence, we can choose β_0 sufficiently close to 1, j sufficiently large and ϵ sufficiently small such that

$$(\beta_0^2+\epsilon)C_jY_j \le \lambda < 1. \tag{4-5}$$

Substituting (4-5) into (4-4) leads to

$$\|u_j^{\beta_0}\eta\|_{L^p}^2 \le C\int |\nabla\eta|^2 u_j^{2\beta_0}\, d\mathrm{V}_g. \tag{4-6}$$

By the definition of η and the Hölder inequality

$$
\begin{aligned}
\left(\int_{B_{1/2}(x_j)} u_j^{2n\beta_0/(n-2)}\, d\mathrm{vol}_g\right)^{(n-2)/n} & \le \|u_j^{\beta_0}\eta\|_{L^p}^2 \le C\int_{B_1(x_j)} u_j^{2\beta_0}\, d\mathrm{V}_g \\
& \le C(\mathrm{V}_g(B_1(x_j)))^{n-(n-2)\beta_0/n} \le C.
\end{aligned}
$$

Here we have used the volume comparison theorem in the above inequality. Then, by almost the same iteration argument as in the previous section we can show that

$$\|u_j\|_{L^\infty(B_{r_1/2}(x_j))} \le C,$$

where $r_1 < \frac{1}{2}$ is any fixed positive number, completing the proof. □

Proof of Theorem 1.5. It is sufficient to show that $\{u_j\}$ is uniformly bounded on any given compact set on M. If not, then the following two situations appear.

Case 1. The sequence $\{u_j\}$ blows up at the "interior" of M, i.e., there exists a subsequence $\{k\} \subseteq \{j\}$, $z_k \in M$, such that

$$u_k(z_k) = \max u_k \triangleq m_k \to +\infty,$$

where $z_k \in K$ and $K \subseteq M$ is a compact subset. By the same arguments as in Step 3 of Section 3, we know this is impossible.

Case 2. The sequence $\{u_j\}$ blows up at "infinity" of M, i.e., there exists a subsequence $\{k\} \subseteq \{j\}$, $z_k \in M$, such that

$$u_k(z_k) = \max u_k \triangleq m_k \to +\infty,$$

where $z_k \to \infty$. If this case occurs, we can not choose a normal coordinate system at "infinity" just as in Case 1. To overcome this difficulty, we consider the sequence of pointed manifold (M, z_i, g). By Theorem 1.1 and Remark 2.4 in [Anderson 1990], we know there exists a subsequence denoted by $\{z_j\}$ such that $\{(M, z_i, g)\}$ converges in the $C^{1,\alpha}$ topology to a complete pointed Riemann manifold $(M_\infty, z_\infty, g_\infty)$ under the assumption $|\operatorname{Ric}| \leq c$ and $\operatorname{inj}(M) \geq a > 0$.

Take a normal coordinate system $\{x_i\}$ around z_∞ on M_∞. Without loss of generality, we can assume this coordinate chart is defined on $B_{1/16}(z_\infty)$. By Definition 2.6, we know there exist F_i such that $F_i(z_\infty) = z_i$, $F_i(B_{1/16}(z_\infty)) \subset B_{1/8}(z_i)$ when i is sufficiently large, and $F_i^* g \to g_\infty$ on $B_{1/16}(z_\infty)$ in the $C^{1,\alpha}$ topology. Moreover, by Theorem 4.1, we have $B_{1/8}(z_i) \subset B_i(O)$ when i is large enough. Define

$$F_i^* g = g_i \quad \text{and} \quad v_j = u_j \circ F_j. \tag{4-7}$$

Then v_j satisfies the following equation on $B_{1/16}(z_\infty)$:

$$\Delta_{g_j} v_j - c(n)(R_g \circ F_j) v_j + Y_j v_j^{p-1} = 0. \tag{4-8}$$

Let $\tilde{v}_k = m_k^{-1} v_k(\delta_k x)$, where m_k and δ_k are the same as in Case 1. Obviously, the definition domain of $\tilde{v}_j$ is the ball centered at 0 with radius $\rho_k = 1/(16\delta_k) \to \infty$ in $\mathbb{R}^n$. Moreover $\tilde{v}_k$ satisfies

$$\frac{1}{\tilde{b}_k} \partial_i (\tilde{b}_k \tilde{a}_k^{ij} \partial_j \tilde{v}_k) - \tilde{c}_k \tilde{v}_k + Y_k \tilde{v}_k^{p-1} = 0, \tag{4-9}$$

where

$$\tilde{a}_k^{ij}(x) = g_k^{ij}(\delta_k x) \to \delta_{ij}, \tag{4-10}$$

$$\tilde{b}_k(x) = \sqrt{\det g_k(\delta_k x)} \to 1, \tag{4-11}$$

$$\tilde{c}_k(x) = c(n) m_k^{2-p} (R_g \circ F_k)(\delta_k x) \to 0. \tag{4-12}$$

Here,

$$0 \leq \tilde{v}_k \leq \tilde{v}_k(0) = 1. \tag{4-13}$$

By L^p estimate we obtain that, for any $R > 0$ and $q > 0$, there exist $C(R) > 0$ and $k(R) > 0$ such that

$$\|\tilde{v}_k\|_{W^{2,q}(B_R)} \leq C(R), \quad \text{for all } k \geq k(R).$$

The Sobolev embedding theorem yields $\tilde{v}_k \in C^{1,\alpha}(B_R(0))$. Hence, by taking a subsequence we get

$$\tilde{v}_k \to v \quad \text{in } C^{1,\alpha}.$$

It is easy to see that v is a $C^{1,\alpha}$ weak solution of

$$\Delta v + Y(M) v^{p-1} = 0 \quad \text{in } B_R(0).$$

Since $v \le 1$, the standard elliptic theory tells us that v is smooth.

Choosing $R_m \to +\infty$ and taking a standard diagonal argument we know that there exists a subsequence $\{v_m\}$ such that $v_m \to v$ with respect to the $C^{1,\alpha}$ norm on every compact subset in $\mathbb{R}^n$. Letting $m \to \infty$, in view of (4-9)–(4-12) we know that v is a nonnegative solution with $v(0) = 1$ of the following equation:

$$\Delta v + Y(M) v^{p-1} = 0. \tag{4-14}$$

The maximal principle yields $v > 0$.

Similarly, we have

$$\int_{\mathbb{R}^n} v^p \, dx \le 1 \quad \text{and} \quad \int_{\mathbb{R}^n} |\nabla v|^2 \, dx < \infty.$$

For the present situation, it is easy to see that v also satisfies (3-26)–(3-30). Thus we can get the same contradiction.

From now on we know $\{u_j\}$ is uniformly bounded on M. By the standard elliptic theory, u_j is uniformly bounded in $C^{2,\alpha}$ on any compact set $K \subseteq M$. Hence, there exists a subsequence which converges to u satisfying

$$\Delta u - c(n) R_g u + Y(M) u^{p-1} = 0.$$

By Proposition 3.2 again, we know u is a positive solution. Then, by a suitable scaling we can obtain a positive solution to (1-1) with $K = 1, 0, -1$ when $Y(M)$ is positive, 0, and negative, respectively, thus completing the proof. □

Proof of Theorem 1.6. By Theorem 2.6 in [Anderson 1990], we know pointed manifolds (M_i, z_i, g_i) satisfying the condition (i) in Theorem 1.6 will converge in the pointed Gromov–Hausdorff topology, to an n dimensional orbifold (V, g) with a finite number of singular points, each having a neighborhood homeomorphic to the cone $C(S^{n-1}/\Gamma)$ with Γ a finite subgroup of $O(n)$. Furthermore, this convergence is $C^{1,\alpha}$ off the singular points. However, if these manifolds satisfy the additional condition (ii) in Theorem 1.6, then the singularities of this orbifold do not arise, see Theorem A′ in [Anderson 1989], Remark 2.7 and Corollary 2.8 in [Anderson 1990]. All in all, we have that the (M_i, z_i, g_i) converge in the $C^{1,\alpha}$ topology to a complete pointed Riemann manifold $(M_\infty, z_\infty, g_\infty)$. The proof of this theorem is exactly the same as the proof of Theorem 1.5. □

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WEIGHTED INFINITESIMAL UNITARY BIALGEBRAS ON ROOTED FORESTS AND WEIGHTED COCYCLES

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In this paper, we define a new coproduct on the space of decorated planar rooted forests to equip it with a weighted infinitesimal unitary bialgebraic structure. We introduce the concept of Ω-cocycle infinitesimal bialgebras of weight λ and then prove that the space of decorated planar rooted forests $H_{\mathrm{RT}}(X, \Omega)$, together with a set of grafting operations $\{B^+_\omega \mid \omega \in \Omega\}$, is the free Ω-cocycle infinitesimal unitary bialgebra of weight λ on a set X, involving a weighted version of a Hochschild 1-cocycle condition. As an application, we equip a free cocycle infinitesimal unitary bialgebraic structure on the undecorated planar rooted forests, which is the object studied in the well-known (noncommutative) Connes–Kreimer Hopf algebra.

1. Introduction

An infinitesimal bialgebra is a module A which is simultaneously an algebra (possibly without a unit) and a coalgebra (possibly without a counit) such that the coproduct Δ is a derivation of A in the sense that

(1) $$\Delta(ab) = a \cdot \Delta(b) + \Delta(a) \cdot b \quad \text{for } a, b \in A.$$

When an infinitesimal bialgebra has an antipode, it will be called an infinitesimal Hopf algebra. Infinitesimal bialgebras, first introduced by Joni and Rota [1979], are in order to give an algebraic framework for the calculus of Newton divided differences. The basic theory of infinitesimal bialgebras and infinitesimal Hopf algebras was developed in [Aguiar 2000; 2001; 2004]. Furthermore, infinitesimal bialgebras

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are also closely related to associative Yang–Baxter equations, Drinfeld's doubles, pre-Lie algebras and Drinfeld's Lie bialgebras [Aguiar 2001]. Recently, Wang and Wang [2014] generalized Aguiar's results by studying the Drinfeld's double for braided infinitesimal Hopf algebras in Yetter–Drinfeld categories. Another different version of infinitesimal bialgebras and infinitesimal Hopf algebras was defined by Loday and Ronco [2006] and further studied by Foissy [2009; 2010], in the sense that

$$\Delta(ab) = a \cdot \Delta(b) + \Delta(a) \cdot b - a \otimes b \quad \text{for } a, b \in A. \tag{2}$$

In 2010, the relationship between classical rime solutions of the Yang–Baxter equation and Bézout operators was investigated by Ogievetsky and Popov [2010], who turned the associative Yang–Baxter equation [Bai et al. 2012a; 2012b] into a general structure, called the nonhomogeneous associative classical Yang–Baxter equation. Surprisingly, in the spirit of the well-known fact that a solution of the associative Yang–Baxter equation gives an infinitesimal bialgebra [Aguiar 2000], Ogievetsky and Popov [2010] clarified an algebraic meaning of the nonhomogeneous associative classical Yang–Baxter equation, involving a coproduct given by

$$\Delta_r(a) := a \cdot r - r \cdot a - \lambda(a \otimes 1) \quad \text{for } a \in A. \tag{3}$$

Here $\lambda \in \boldsymbol{k}$ and $r \in A \otimes A$ is a solution of the nonhomogeneous associative classical Yang–Baxter equation. Note that, by [Ogievetsky and Popov 2010], Equation (3) satisfies

$$\Delta_r(ab) = a \cdot \Delta_r(b) + \Delta_r(a) \cdot b + \lambda(a \otimes b) \quad \text{for } a, b \in A, \tag{4}$$

which is precisely a uniform version of the two compatibilities — Equations (1) and (2). Such an algebraic structure was called an infinitesimal unitary bialgebra of weight λ in [Gao and Zhang 2018; Zhang et al. 2018]. We would like to point out that weighted infinitesimal unitary bialgebras have a close connection with pre-Lie algebras. For example, Aguiar [2004] constructed a pre-Lie algebra from an infinitesimal bialgebra of weight zero. Motivated by Aguiar's construction, a pre-Lie algebra from a weighted infinitesimal unitary bialgebra was derived in [Gao and Zhang 2018].

The rooted forest is a significant object studied in algebra and combinatorics. One of the most important examples is the Connes–Kreimer Hopf algebra of rooted forests, which was introduced and studied extensively in [Connes and Kreimer 1998; Grossman and Larson 1989; Hoffman 2003; Kreimer 1998; Moerdijk 2001]. In particular, the Connes–Kreimer Hopf algebra serves as a "baby model" of Feynman diagrams in the algebraic approach of the renormalization in quantum field theory [Brouder and Frabetti 2003; Brouder et al. 2010; Connes and Kreimer 2000; Guo et al. 2011; 2017; Guo and Zhang 2008]. It is also related to many other Hopf algebras built on rooted forests, such as those studied by Foissy [2002a; 2002b] and

Holtkamp [2003], Grossman and Larson [1989], Loday and Ronco [1998]. One reason for the significance of these algebraic structures on rooted forests is that most of them possess universal properties, involving a Hochschild 1-cocycle, which have interesting applications in renormalization. For example, the Connes–Kreimer Hopf algebra of rooted forests inherits its algebra structure from the initial object in the category of (commutative) algebras with a linear operator [Foissy 2002a; Moerdijk 2001]. Recently this universal property of rooted forests was generalized in [Zhang et al. 2016] in terms of decorated planar rooted forests, and the universal property of Loday–Ronco Hopf algebra was investigated in [Zhang and Gao 2019] in terms of decorated planar binary trees.

The concept of algebras with (one or more) linear operators was first introduced by Kurosh [1960] but forgotten until it was rediscovered by Guo [2009], who constructed the free objects of such algebras in terms of various combinatorial objects, such as Motzkin paths, rooted forests and bracketed words. There such structure was called an Ω-operated algebra, where Ω is a set to index the linear operators. See also [Bokut et al. 2010; Gao and Guo 2017; Guo 2012; Guo et al. 2013]. It has been observed that the decorated planar rooted forests $H_{\mathrm{RT}}(\Omega)$ whose vertices are decorated by a set Ω, together with a set of grafting operations $\{B_\omega^+ \mid \omega \in \Omega\}$, is a free object on the empty set in the category of Ω-operated algebras [Kreimer and Panzer 2013; Zhang et al. 2016]. Particularly, the noncommutative Connes–Kreimer Hopf algebra H_{RT} of planar rooted forests equipped with the grafting operation B^+ is a free operated algebra [Guo 2009].

As a related result, an infinitesimal unitary bialgebra of weight zero on rooted forests has been established in [Gao and Wang 2019]. Using an infinitesimal version of the Hochschild 1-cocycle condition, they showed that the space of decorated planar rooted forests is the free cocycle infinitesimal unitary bialgebra of weight zero. However, this infinitesimal 1-cocycle condition is not a real Hochschild 1-cocycle condition. It is almost a natural question to wonder whether we can construct an infinitesimal (unitary) bialgebra of weight λ on decorated rooted forests, by using a Hochschild 1-cocycle condition. The present paper gives a positive answer to this question. Namely, we first propose the concept of weighted Ω-cocycle infinitesimal unitary bialgebras, involving a weighted version of a Hochschild 1-cocycle condition. Then we prove that the space of decorated planar rooted forests $H_{\mathrm{RT}}(X, \Omega)$ is the free objects in this category, provided suitable operations are equipped. This freeness characterization of decorated planar rooted forests gives an algebraic explanation of the fundamental roles played by these combinatorial objects.

Structure of the Paper. In Section 2, we recall the concept of a weighted infinitesimal (unitary) bialgebra and show that some well-known algebras possess a weighted infinitesimal (unitary) bialgebra.

In Section 3, after summarizing concepts and basic facts on decorated rooted forests, we construct a new coproduct by a weighted version of a Hochschild 1-cocycle condition (Equation (13)) on decorated planar rooted forests $H_{\mathrm{RT}}(X, \Omega)$ to equip it with a new coalgebra structure (Theorem 3.8). Further $H_{\mathrm{RT}}(X, \Omega)$ can be turned into an infinitesimal unitary bialgebra of weight λ with respect to the concatenation product and the empty tree as its unit (Theorem 3.9).

In Section 4, under the framework of operated algebras, we propose the concept of weighted Ω-cocycle infinitesimal unitary bialgebras (Definition 4.3(a)), involving a weighted 1-cocycle condition. Having this concept in hand, we prove that $H_{\mathrm{RT}}(X, \Omega)$ is the free Ω-cocycle infinitesimal unitary bialgebra of weight λ on a set X (Theorem 4.5). As an application, we obtain that the undecorated planar rooted forests is the free cocycle infinitesimal unitary bialgebra of weight λ on the empty set (Corollary 4.7).

Notation. Throughout this paper, let $\boldsymbol{k}$ be a unitary commutative ring unless the contrary is specified, which will be the base ring of all modules, algebras, coalgebras, bialgebras, tensor products, as well as linear maps. By an algebra we mean an associative algebra (possibly without unit) and by a coalgebra we mean a coassociative coalgebra (possibly without counit). We use the Sweedler notation:

$$\Delta(a) = \sum_{(a)} a_{(1)} \otimes a_{(2)}.$$

For a set Y, denote by $M(Y)$ and $S(Y)$ the free monoid and semigroup on Y, respectively. For an algebra A, $A \otimes A$ is viewed as an (A, A)-bimodule in the standard way,

$$a \cdot (b \otimes c) := ab \otimes c \quad \text{and} \quad (b \otimes c) \cdot a := b \otimes ca, \tag{5}$$

where $a, b, c \in A$.

2. Weighted infinitesimal unitary bialgebras and examples

In this section, we recall the concept of a weighted infinitesimal unitary bialgebra [Gao and Zhang 2018; Ogievetsky and Popov 2010], which generalize simultaneously the one introduced by Joni and Rota [1979] and the one initiated by Loday and Ronco [2006]. Based on the mixture of Equations (1) and (2) into Equation (4) by Ogievetsky and Popov [2010], we propose:

Definition 2.1 [Gao and Zhang 2018]. Let λ be a given element of $\boldsymbol{k}$. An *infinitesimal bialgebra* (abbreviated *ϵ-bialgebra*) *of weight* λ is a triple (A, m, Δ) consisting of an algebra (A, m) (possibly without a unit) and a coalgebra (A, Δ) (possibly without a counit) that satisfies

(6) $$\Delta(ab) = a \cdot \Delta(b) + \Delta(a) \cdot b + \lambda(a \otimes b) \quad \text{for } a, b \in A.$$

If, further, $(A, m, 1)$ is a unitary algebra, then the quadruple $(A, m, 1, \Delta)$ is called an *infinitesimal unitary bialgebra of weight* λ.

Definition 2.2 [Gao and Zhang 2018]. Let A and B be two ϵ-bialgebras of weight λ. A map $\phi : A \to B$ is called an *infinitesimal bialgebra morphism* if ϕ is an algebra morphism and a coalgebra morphism.

We shall use the infix notation ϵ- interchangeably with the adjective "infinitesimal" throughout the rest of this paper.

Remark 2.3. (a) Let $(A, m, 1, \Delta)$ be an ϵ-bialgebra of weight λ. Then $\Delta(1) = -\lambda(1 \otimes 1)$, as

$$\Delta(1) = \Delta(1 \cdot 1) = 1 \cdot \Delta(1) + \Delta(1) \cdot 1 + \lambda(1 \otimes 1) = 2\Delta(1) + \lambda(1 \otimes 1).$$

(b) The ϵ-bialgebra introduced by Joni and Rota [1979] is the ϵ-bialgebra of weight zero, and the ϵ-bialgebra originated from Loday and Ronco [2006] is the ϵ-bialgebra of weight -1.

(c) Twenty years after Joni and Rota [1979], Aguiar [2000] introduced the concept of an ϵ-Hopf algebra and pointed out that there is no nonzero ϵ-bialgebra which is both unitary and counitary when $\lambda = 0$. Indeed, it follows the counicity that

$$1 \otimes 1_{\boldsymbol{k}} = (\mathrm{id} \otimes \epsilon)\Delta(1) = 0$$

and so $1 = 0$.

(d) Let (A, μ, Δ) be an ϵ-unitary bialgebra of weight λ. Denote by

(7) $$\rhd : A \otimes A \to A, \quad a \otimes b \mapsto a \rhd b := \sum_{(b)} b_{(1)} a b_{(2)},$$

where $b_{(1)}$ and $b_{(2)}$ are from the Sweedler notation $\Delta(b) = \sum_{(b)} b_{(1)} \otimes b_{(2)}$. Then A equipped with the $\rhd$ in (7) is a pre-Lie algebra [Gao and Zhang 2018].

Some well-known algebras possess weighted infinitesimal bialgebraic structures, via constructions of suitable coproducts.

Example 2.4. Here are some examples of weighted ϵ-bialgebras.

(a) Any algebra (A, m) is an ϵ-bialgebra of weight zero when the coproduct is taken to be $\Delta = 0$.

(b) [Aguiar 2000, Example 2.3.2]. A quiver $Q = (Q_0, Q_1, s, t)$ is a quadruple consisting of a set Q_0 of vertices, a set Q_1 of arrows, and two maps $s, t : Q_1 \to Q_0$ which associate each arrow $a \in Q_1$ to its source $s(a) \in Q_0$ and its target $t(a) \in Q_0$. The path algebra $\boldsymbol{k}Q$ can be turned into an ϵ-unitary bialgebra of weight zero with the coproduct Δ given by

$$\Delta(a_1 \cdots a_n) := \begin{cases} 0 & \text{if } n = 0, \\ s(a_1) \otimes t(a_1) & \text{if } n = 1, \\ s(a_1) \otimes a_2 \cdots a_n + a_1 \cdots a_{n-1} \otimes t(a_n) & \\ \qquad + \sum_{i=1}^{n-2} a_1 \cdots a_i \otimes a_{i+2} \cdots a_n & \text{if } n \geq 2, \end{cases}$$

where $a_1 \cdots a_n$ is a path in $\boldsymbol{k}Q$. Here we use the convention that $a_1 \cdots a_n \in Q_0$ when $n = 0$.

(c) [Foissy 2008, Section 1.4]. Let $(A, m, 1, \Delta_c, \epsilon, c)$ be a braided bialgebra with $A = \boldsymbol{k} \oplus \ker \epsilon$ and the braiding $c : A \otimes A \to A \otimes A$ given by

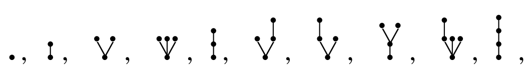
$$c : \begin{cases} 1 \otimes 1 \mapsto 1 \otimes 1, \\ a \otimes 1 \mapsto 1 \otimes a, \\ 1 \otimes b \mapsto b \otimes 1, \\ a \otimes b \mapsto 0, & \text{where } a, b \in \ker \epsilon. \end{cases}$$

Then $(A, m, 1, \Delta_c)$ is an ϵ-unitary bialgebra of weight -1.

3. Weighted infinitesimal unitary bialgebras of decorated planar rooted forests

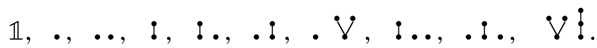
In this section, we first show a general way to decorate planar rooted forests that generalizes the constructions of decorated rooted forests introduced and studied in [Foissy 2002a; Guo 2009; Stanley 1986]. Using a weighted 1-cocycle condition, we then define a coproduct on the space of new decorated planar rooted forests to equip it with a coalgebraic structure, with an eye toward constructing a weighted infinitesimal unitary bialgebra on it.

New decorated planar rooted forests. A *rooted tree* is a finite graph, connected and without cycles, with a distinguished vertex called the *root*. A *planar rooted tree* is a rooted tree with a fixed embedding into the plane. The first few planar rooted trees are listed below:



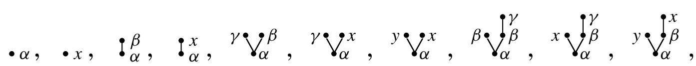
where the root of a tree is on the bottom. Let $\mathcal{T}$ denote the set of planar rooted trees and $M(\mathcal{T})$ the free monoid generated by $\mathcal{T}$ with the concatenation product, denoted by m_{RT} and usually suppressed. The empty tree in $M(\mathcal{T})$ is denoted by $\mathbb{1}$. A *planar rooted forest* is a noncommutative concatenation of planar rooted trees, denoted by $F = T_1 \cdots T_n$ with $T_1, \ldots, T_n \in \mathcal{T}$. Here we use the convention that $F = \mathbb{1}$ when

$n = 0$. The first few planar rooted forests are listed below:



Let Ω be a nonempty set, and let X be a set whose elements are not in the set Ω. For the nonempty set $X \sqcup \Omega$, let $\mathcal{T}(X \sqcup \Omega)$ (resp. $\mathcal{F}(X \sqcup \Omega) := M(\mathcal{T}(X \sqcup \Omega))$) denote the set of planar rooted trees (resp. forests) whose vertices (leaf vertices and internal vertices) are decorated by elements of $X \sqcup \Omega$. Define $H_{\mathrm{RT}}(X \sqcup \Omega) := \boldsymbol{k}\mathcal{F}(X \sqcup \Omega)$ to be the free $\boldsymbol{k}$-module spanned by $\mathcal{F}(X \sqcup \Omega)$.

Let $\mathcal{T}(X, \Omega)$ (resp. $\mathcal{F}(X, \Omega)$) denote the subset of $\mathcal{T}(X \sqcup \Omega)$ (resp. $\mathcal{F}(X \sqcup \Omega)$) consisting of vertex decorated planar rooted trees (resp. forests) whose internal vertices are decorated by elements of Ω exclusively and leaf vertices are decorated by elements of $X \sqcup \Omega$. In other words, all internal vertices, as well as possibly some of the leaf vertices, are decorated by Ω. The only vertex of the tree $\bullet$ is taken to be a leaf vertex. The following are some decorated planar rooted trees in $\mathcal{T}(X, \Omega)$:



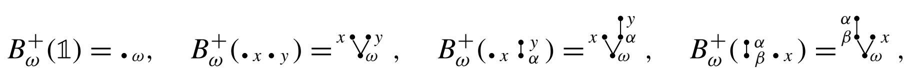
with $\alpha, \beta, \gamma \in \Omega$ and $x, y \in X$. Define

$$H_{\mathrm{RT}}(X, \Omega) := \boldsymbol{k}\mathcal{F}(X, \Omega) = \boldsymbol{k}M(\mathcal{T}(X, \Omega))$$

to be the free $\boldsymbol{k}$-module spanned by $\mathcal{F}(X, \Omega)$. For each $\omega \in \Omega$, define

$$B^+_\omega : H_{\mathrm{RT}}(X, \Omega) \to H_{\mathrm{RT}}(X, \Omega)$$

to be the linear grafting operation by taking $\mathbb{1}$ to $\bullet_\omega$ and sending a rooted forest in $H_{\mathrm{RT}}(X, \Omega)$ to its grafting with the new root decorated by ω. For example,



where $\alpha, \beta, \omega \in \Omega$ and $x, y \in X$. Note that $H_{\mathrm{RT}}(X, \Omega)$ is closed under the concatenation m_{RT}.

Remark 3.1. Here are some special cases of our decorated planar rooted forests.

(a) If $X = \varnothing$ and Ω is a singleton set, then all decorated planar rooted forests in $\mathcal{F}(X, \Omega)$ have the same decoration, which is the object studied in the well-known Foissy–Holtkamp Hopf algebra — the noncommutative version of the Connes–Kreimer Hopf algebra [Foissy 2002a; Holtkamp 2003].

(b) If $X = \varnothing$, then $\mathcal{F}(X, \Omega)$ was studied by Foissy [2002a; 2002b], in which a decorated noncommutative version of the Connes–Kreimer Hopf algebra was constructed.

(c) If Ω is a singleton set, then $\mathcal{F}(X, \Omega)$ was introduced and studied in [Zhang et al. 2016] to construct a cocycle Hopf algebra on decorated planar rooted forests.

(d) The rooted forests in $\mathcal{F}(X, \Omega)$ with leaf vertices decorated by elements of X and internal vertices decorated by elements of Ω were introduced in [Guo 2009]. However, this decoration can't deal with the unity and the algebraic structures on this decorated rooted forests are all nonunitary. The distinction between unitary and nonunitary for $\mathcal{F}(X, \Omega)$ is more significant than for an associative algebra, because of the involvement of the grafting operation.

The following are two basic definitions that will be used in the remainder of the paper. See [Gao and Zhang 2018; Guo 2009] for detailed discussions. For $F = T_1 \cdots T_n \in \mathcal{F}(X, \Omega)$ with $n \geq 0$ and $T_1, \ldots, T_n \in \mathcal{T}(X, \Omega)$, we define $\mathrm{bre}(F) := n$ to be the *breadth* of F. Here we use the convention that $\mathrm{bre}(\mathbb{1}) = 0$ when $n = 0$. In order to define the depth of a decorated planar rooted forests, we build a recursive structure on $\mathcal{F}(X, \Omega)$. Define $\bullet_X := \{\bullet_x \mid x \in X\}$ and set

$$\mathcal{F}_0 := M(\bullet_X) = S(\bullet_X) \sqcup \{\mathbb{1}\},$$

where $M(\bullet_X)$ (resp. $S(\bullet_X)$) is the submonoid (resp. subsemigroup) of $\mathcal{F}(X, \Omega)$ generated by $\bullet_X$. Here we are abusing notion slightly since $M(\bullet_X)$ (resp. $S(\bullet_X)$) is also isomorphic to the free monoid (resp. semigroup) generated by $\bullet_X$. Suppose that $\mathcal{F}_n$ has been defined for an $n \geq 0$, then define

$$\mathcal{F}_{n+1} := M\big(\bullet_X \sqcup \big(\textstyle\bigsqcup_{\omega \in \Omega} B^+_\omega(\mathcal{F}_n)\big)\big).$$

Thus we obtain $\mathcal{F}_n \subseteq \mathcal{F}_{n+1}$ and can define

$$\mathcal{F}(X, \Omega) := \varinjlim \mathcal{F}_n = \bigcup_{n=0}^{\infty} \mathcal{F}_n. \tag{8}$$

Now elements $F \in \mathcal{F}_n \setminus \mathcal{F}_{n-1}$ are said to have *depth* n, denoted by $\mathrm{dep}(F) = n$. For example,

$$\mathrm{dep}(\mathbb{1}) = \mathrm{dep}(\bullet_x) = 0, \quad \mathrm{dep}(\bullet_\omega) = \mathrm{dep}(B^+_\omega(\mathbb{1})) = 1,$$
$$\mathrm{dep}(\,\vdots^{y}_{\omega}) = \mathrm{dep}(B^+_\omega(\bullet_y)) = 1, \quad \mathrm{dep}(\bullet_x \vdots^{y}_{\omega}) = \mathrm{dep}(\bullet_x B^+_\omega(\bullet_y)) = 1,$$
$$\mathrm{dep}({}^{\alpha}\!\vee^{x}_{\omega}) = \mathrm{dep}(B^+_\omega(B^+_\alpha(\mathbb{1})\bullet_x)) = 2,$$

where $\alpha, \omega \in \Omega$ and $x, y \in X$.

Cartier–Quillen cohomology. Given an algebra A and a bimodule M over A. Let $H^*(A, M)$ denote the *Hochschild cohomology* of A with coefficients in M which was defined from a complex with maps $A^{\otimes n} \to M$ as cochains, see [Loday 1992] for more details. Let (C, Δ) be a coalgebra and (B, δ_G, δ_D) be a bicomodule over C.

The *Cartier–Quillen cohomology* of C with coefficients in B is a dual notation of the Hochschild cohomology. Explicitly, it is a cohomology of the complex $\mathrm{Hom}_{\boldsymbol{k}}(B, C^{\otimes n})$ with the maps $b_n : \mathrm{Hom}_{\boldsymbol{k}}(B, C^{\otimes n}) \to \mathrm{Hom}_{\boldsymbol{k}}(B, C^{\otimes (n+1)})$ given by

$$b_n(L) = (\mathrm{id} \otimes L) \circ \delta_G + \sum_{i=1}^{n} (-1)^i (\mathrm{id}_C^{\otimes (i-1)} \otimes \Delta \otimes \mathrm{id}_C^{\otimes (n-i)}) L + (-1)^{n+1} (L \otimes \mathrm{id}) \circ \delta_D,$$

where $L : B \to C^{\otimes n}$. In particular, a linear map $L : B \to C$ is the 1-*cocycle* for this cohomology precisely when it satisfies the following condition:

$$\Delta \circ L = (L \otimes \mathrm{id}) \circ \delta_D + (\mathrm{id} \otimes L) \circ \delta_G,$$

see [Foissy 2013; Moerdijk 2001] for more details. Let e be a *group-like element of weight* λ of C, that is, $\Delta(e) = \lambda(e \otimes e)$. We consider the bicomodule (C, Δ, δ_D) with $\delta_D(x) = \lambda(x \otimes e)$ for any $x \in C$. Then the 1-cocycle L is a linear endomorphism of C satisfying

$$\Delta \circ L(x) = L(x) \otimes \lambda e + (\mathrm{id} \otimes L) \circ \Delta(x) \quad \text{for } x \in C. \tag{9}$$

We call Equation (9) the *1-cocycle condition of weight* λ.

Remark 3.2. (a) The group-like elements in infinitesimal unitary bialgebras always exist. Indeed, the unit of an infinitesimal unitary bialgebra is a group-like element of weight $-\lambda$.

(b) When $L = B^+$ and $\lambda = 1$, the weighted 1-cocycle condition in Equation (9) is

$$\Delta_{\mathrm{RT}}(F) = \Delta_{\mathrm{RT}} B^+(\bar{F}) = F \otimes \mathbb{1} + (\mathrm{id} \otimes B^+) \Delta_{\mathrm{RT}}(\bar{F}) \quad \text{for } F = B^+(\bar{F}) \in \mathcal{F}, \tag{10}$$

which is the usual 1-cocycle condition employed in [Connes and Kreimer 1998; Foissy 2013; Zhang et al. 2016]. Here the empty tree $\mathbb{1}$ is the unique group-like element in the Connes–Kreimer Hopf algebra.

Weighted infinitesimal unitary bialgebras on decorated planar rooted forests. In this subsection, we shall equip a weighted infinitesimal unitary bialgebraic structure on decorated planar rooted forests.

Let us define a new coproduct Δ_ϵ on $H_{\mathrm{RT}}(X, \Omega)$ by induction on depth. By linearity, we only need to define $\Delta_\epsilon(F)$ for basis elements $F \in \mathcal{F}(X, \Omega)$. For the initial step of $\mathrm{dep}(F) = 0$, we define

$$\Delta_\epsilon(F) := \begin{cases} -\lambda(\mathbb{1} \otimes \mathbb{1}) & \text{if } F = \mathbb{1}, \\ \bullet_x \otimes \bullet_x & \text{if } F = \bullet_x \text{ for some } x \in X, \\ \bullet_{x_1} \cdot \Delta_\epsilon(\bullet_{x_2} \cdots \bullet_{x_m}) + \Delta_\epsilon(\bullet_{x_1}) \cdot (\bullet_{x_2} \cdots \bullet_{x_m}) & \\ \qquad + \lambda \bullet_{x_1} \otimes \bullet_{x_2} \cdots \bullet_{x_m} & \text{if } F = \bullet_{x_1} \cdots \bullet_{x_m} \text{ with } m \geq 2. \end{cases} \tag{11}$$

Here in the third case, the definition of Δ_ϵ reduces to induction on breadth and the dot action is defined in Equation (5).

For the induction step of $\mathrm{dep}(F) \geq 1$, we reduce the definition to the induction on breadth. If $\mathrm{bre}(F) = 1$, we write $F = B_\omega^+(\bar{F})$ for some $\omega \in \Omega$ and $\bar{F} \in \mathcal{F}(X, \Omega)$, and define

$$\Delta_\epsilon(F) = \Delta_\epsilon B_\omega^+(\bar{F}) := F \otimes (-\lambda \mathbb{1}) + (\mathrm{id} \otimes B_\omega^+)\Delta_\epsilon(\bar{F}). \tag{12}$$

In other words

$$\Delta_\epsilon B_\omega^+ = B_\omega^+ \otimes (-\lambda \mathbb{1}) + (\mathrm{id} \otimes B_\omega^+)\Delta_\epsilon. \tag{13}$$

If $\mathrm{bre}(F) \geq 2$, we write $F = T_1 T_2 \cdots T_m$ with $m \geq 2$ and $T_1, \ldots, T_m \in \mathcal{T}(X, \Omega)$, and define

$$\Delta_\epsilon(F) = T_1 \cdot \Delta_\epsilon(T_2 \cdots T_m) + \Delta_\epsilon(T_1) \cdot (T_2 \cdots T_m) + \lambda T_1 \otimes T_2 \cdots T_m. \tag{14}$$

Remark 3.3. By Remark 2.3(a), the empty tree $\mathbb{1} \in H_{\mathrm{RT}}(X, \Omega)$ is a group-like element of weight $-\lambda$, and so Equation (13) is the 1-cocycle condition of weight $-\lambda$.

Example 3.4. Let $x, y \in X$ and $\alpha, \beta, \gamma \in \Omega$. Then

$$\begin{aligned}
\Delta_\epsilon(\bullet_\alpha) &= \Delta_\epsilon(B_\alpha^+(\mathbb{1})) = -\lambda(\mathbb{1} \otimes \bullet_\alpha + \bullet_\alpha \otimes \mathbb{1}),\\
\Delta_\epsilon(\ell_\alpha^x) &= \Delta_\epsilon(B_\alpha^+(\bullet_x)) = -\lambda(\ell_\alpha^x \otimes \mathbb{1}) + \bullet_x \otimes \ell_\alpha^x,\\
\Delta_\epsilon(\ell_\alpha^\beta) &= \Delta_\epsilon(B_\alpha^+(\bullet_\beta)) = -\lambda(\mathbb{1} \otimes \ell_\alpha^\beta + \bullet_\beta \otimes \bullet_\alpha + \ell_\alpha^\beta \otimes \mathbb{1}),\\
\Delta_\epsilon(\bullet_\gamma \bullet_y) &= -\lambda(\mathbb{1} \otimes \bullet_\gamma \bullet_y) + \bullet_\gamma \bullet_y \otimes \bullet_y,\\
\Delta_\epsilon(\ell_\alpha^x \bullet_y) &= \ell_\alpha^x \bullet_y \otimes \bullet_y + \bullet_x \otimes \ell_\alpha^x \bullet_y,\\
\Delta_\epsilon(\bullet_x \ell_\beta^\alpha) &= -\lambda(\bullet_x \ell_\beta^\alpha \otimes \mathbb{1} + \bullet_x \bullet_\alpha \otimes \bullet_\beta) + \bullet_x \otimes \bullet_x \ell_\beta^\alpha,\\
\Delta_\epsilon({}^{\beta}\!\vee_\alpha^{x}) &= \Delta_\epsilon(B_\alpha^+(\bullet_\beta \bullet_x)) = -\lambda(\mathbb{1} \otimes {}^{\beta}\!\vee_\alpha^{x} + {}^{\beta}\!\vee_\alpha^{x} \otimes \mathbb{1}) + \bullet_\beta \bullet_x \otimes \ell_\alpha^x.
\end{aligned}$$

To show $(H_{\mathrm{RT}}(X, \Omega), \Delta_\epsilon)$ is a coalgebra, we need the following two lemmas.

Lemma 3.5. *Let $\bullet_{x_1} \cdots \bullet_{x_m} \in H_{\mathrm{RT}}(X, \Omega)$ with $m \geq 1$ and $x_1, \ldots, x_m \in X$. Then*

$$\Delta_\epsilon(\bullet_{x_1} \cdots \bullet_{x_m}) = \sum_{i=1}^{m} \bullet_{x_1} \cdots \bullet_{x_i} \otimes \bullet_{x_i} \cdots \bullet_{x_m} + \lambda \sum_{i=1}^{m-1} \bullet_{x_1} \cdots \bullet_{x_i} \otimes \bullet_{x_{i+1}} \cdots \bullet_{x_m}.$$

Proof. We prove this result by induction on $m \geq 1$. For the initial step of $m = 1$, we have

$$\Delta_\epsilon(\bullet_{x_1}) = \bullet_{x_1} \otimes \bullet_{x_1},$$

and the result is true trivially. For the induction step of $m \geq 2$, we get

$$
\begin{aligned}
&\Delta_\epsilon(\bullet_{x_1}\cdots\bullet_{x_m})\\
&= \bullet_{x_1}\cdot\Delta_\epsilon(\bullet_{x_2}\cdots\bullet_{x_m}) + \Delta_\epsilon(\bullet_{x_1})\cdot(\bullet_{x_2}\cdots\bullet_{x_m}) + \lambda\,\bullet_{x_1}\otimes\bullet_{x_2}\cdots\bullet_{x_m} && \text{(by (11))}\\
&= \bullet_{x_1}\cdot\Delta_\epsilon(\bullet_{x_2}\cdots\bullet_{x_m}) + (\bullet_{x_1}\otimes\bullet_{x_1})\cdot(\bullet_{x_2}\cdots\bullet_{x_m}) + \lambda\,\bullet_{x_1}\otimes\bullet_{x_2}\cdots\bullet_{x_m} && \text{(by (11))}\\
&= \bullet_{x_1}\cdot\Delta_\epsilon(\bullet_{x_2}\cdots\bullet_{x_m}) + \bullet_{x_1}\otimes\bullet_{x_1}\bullet_{x_2}\cdots\bullet_{x_m} + \lambda\,\bullet_{x_1}\otimes\bullet_{x_2}\cdots\bullet_{x_m} && \text{(by (5))}\\
&= \bullet_{x_1}\cdot\Big(\sum_{i=2}^{m}\bullet_{x_2}\cdots\bullet_{x_i}\otimes\bullet_{x_i}\cdots\bullet_{x_m} + \lambda\sum_{i=2}^{m-1}\bullet_{x_2}\cdots\bullet_{x_i}\otimes\bullet_{x_{i+1}}\cdots\bullet_{x_m}\Big) + \bullet_{x_1}\otimes\bullet_{x_1}\bullet_{x_2}\cdots\bullet_{x_m}\\
&\qquad + \lambda\,\bullet_{x_1}\otimes\bullet_{x_2}\cdots\bullet_{x_m} && \text{(by the induction hypothesis)}\\
&= \sum_{i=2}^{m}\bullet_{x_1}\cdots\bullet_{x_i}\otimes\bullet_{x_i}\cdots\bullet_{x_m} + \bullet_{x_1}\otimes\bullet_{x_1}\cdots\bullet_{x_m}\\
&\qquad + \lambda\sum_{i=2}^{m-1}\bullet_{x_1}\cdots\bullet_{x_i}\otimes\bullet_{x_{i+1}}\cdots\bullet_{x_m} + \lambda\,\bullet_{x_1}\otimes\bullet_{x_2}\cdots\bullet_{x_m}\\
&= \sum_{i=1}^{m}\bullet_{x_1}\cdots\bullet_{x_i}\otimes\bullet_{x_i}\cdots\bullet_{x_m} + \lambda\sum_{i=1}^{m-1}\bullet_{x_1}\cdots\bullet_{x_i}\otimes\bullet_{x_{i+1}}\cdots\bullet_{x_m},
\end{aligned}
$$

as required. □

Lemma 3.6. *Let $F_1, F_2 \in H_{\mathrm{RT}}(X, \Omega)$. Then*

$$\Delta_\epsilon(F_1F_2) = F_1\cdot\Delta_\epsilon(F_2) + \Delta_\epsilon(F_1)\cdot F_2 + \lambda(F_1\otimes F_2).$$

Proof. It suffices to consider basis elements $F_1, F_2 \in \mathcal{F}(X, \Omega)$ by linearity. We have two cases to consider.

Case 1. $\mathrm{bre}(F_1) = 0$ or $\mathrm{bre}(F_2) = 0$. In this case, without loss of generality, letting $\mathrm{bre}(F_1) = 0$, then $F_1 = \mathbb{1}$ and by Equation (11),

$$
\begin{aligned}
\Delta_\epsilon(F_1F_2) = \Delta_\epsilon(\mathbb{1}F_2) &= \Delta_\epsilon(F_2) - \lambda(\mathbb{1}\otimes F_2) + \lambda(\mathbb{1}\otimes F_2)\\
&= \Delta_\epsilon(F_2) - \lambda(\mathbb{1}\otimes\mathbb{1})\cdot F_2 + \lambda(\mathbb{1}\otimes F_2)\\
&= \Delta_\epsilon(F_2) + \Delta_\epsilon(\mathbb{1})\cdot F_2 + \lambda(\mathbb{1}\otimes F_2)\\
&= \mathbb{1}\cdot\Delta_\epsilon(F_2) + \Delta_\epsilon(\mathbb{1})\cdot F_2 + \lambda(\mathbb{1}\otimes F_2)\\
&= F_1\cdot\Delta_\epsilon(F_2) + \Delta_\epsilon(F_1)\cdot F_2 + \lambda(F_1\otimes F_2).
\end{aligned}
$$

Case 2. $\mathrm{bre}(F_1) \geq 1$ and $\mathrm{bre}(F_2) \geq 1$. In this case, we prove the result by induction on the sum of breadths $\mathrm{bre}(F_1) + \mathrm{bre}(F_2) \geq 2$. For the initial step of

$$\mathrm{bre}(F_1) + \mathrm{bre}(F_2) = 2,$$

we have $F_1 = T_1$ and $F_2 = T_2$ for some decorated planar rooted trees $T_1, T_2 \in \mathcal{T}(X, \Omega)$. By Equation (14),

$$\begin{aligned}\Delta_\epsilon(F_1F_2) = \Delta_\epsilon(T_1T_2) &= T_1 \cdot \Delta_\epsilon(T_2) + \Delta_\epsilon(T_1) \cdot T_2 + \lambda(T_1 \otimes T_2)\\ &= F_1 \cdot \Delta_\epsilon(F_2) + \Delta_\epsilon(F_1) \cdot F_2 + \lambda(F_1 \otimes F_2).\end{aligned}$$

For the induction step of $\mathrm{bre}(F_1) + \mathrm{bre}(F_2) \geq 3$, without loss of generality, we may suppose $\mathrm{bre}(F_2) \geq \mathrm{bre}(F_1) \geq 1$. If $\mathrm{bre}(F_1) = 1$ and $\mathrm{bre}(F_2) \geq 2$, we may write $F_1 = T_1$ for some decorated planar rooted trees $T_1 \in \mathcal{T}(X, \Omega)$. By Equation (14),

$$\begin{aligned}\Delta_\epsilon(F_1F_2) = \Delta_\epsilon(T_1F_2) &= T_1 \cdot \Delta_\epsilon(F_2) + \Delta_\epsilon(T_1) \cdot F_2 + \lambda(T_1 \otimes F_2)\\ &= F_1 \cdot \Delta_\epsilon(F_2) + \Delta_\epsilon(F_1) \cdot F_2 + \lambda(F_1 \otimes F_2).\end{aligned}$$

If $\mathrm{bre}(F_1) \geq 2$, we can write $F_1 = T_1{F_1}'$ with $\mathrm{bre}(T_1) = 1$ and $\mathrm{bre}({F_1}') = \mathrm{bre}(F_1) - 1$. Then

$$\begin{aligned}
&\Delta_\epsilon(F_1F_2)\\
&= \Delta_\epsilon(T_1{F_1}'F_2)\\
&= T_1 \cdot \Delta_\epsilon({F_1}'F_2) + \Delta_\epsilon(T_1) \cdot ({F_1}'F_2) + \lambda(T_1 \otimes {F_1}'F_2) && \text{(by (14))}\\
&= T_1 \cdot \big({F_1}' \cdot \Delta_\epsilon(F_2) + \Delta_\epsilon({F_1}') \cdot F_2 + \lambda({F_1}' \otimes F_2)\big)\\
&\qquad + \Delta_\epsilon(T_1) \cdot ({F_1}'F_2) + \lambda(T_1 \otimes {F_1}'F_2) && \text{(by the induction hypothesis)}\\
&= (T_1{F_1}') \cdot \Delta_\epsilon(F_2) + T_1 \cdot \Delta_\epsilon({F_1}') \cdot F_2 + \lambda(T_1{F_1}' \otimes F_2) + \Delta_\epsilon(T_1) \cdot ({F_1}'F_2)\\
&\qquad + \lambda(T_1 \otimes {F_1}'F_2)\\
&= (T_1{F_1}') \cdot \Delta_\epsilon(F_2) + \big(T_1 \cdot \Delta_\epsilon({F_1}') + \Delta_\epsilon(T_1) \cdot {F_1}' + \lambda(T_1 \otimes {F_1}')\big) \cdot F_2 + \lambda(T_1{F_1}' \otimes F_2)\\
&= (T_1{F_1}') \cdot \Delta_\epsilon(F_2) + \Delta_\epsilon(T_1{F_1}') \cdot F_2 + \lambda(T_1{F_1}' \otimes F_2)\\
&= F_1 \cdot \Delta_\epsilon(F_2) + \Delta_\epsilon(F_1) \cdot F_2 + \lambda(F_1 \otimes F_2) && \text{(by the induction hypothesis).} \quad \square
\end{aligned}$$

The following lemma shows that $H_{\mathrm{RT}}(X, \Omega)$ is closed under the coproduct Δ_ϵ.

Lemma 3.7. *For $F \in H_{\mathrm{RT}}(X, \Omega)$,*

$$\Delta_\epsilon(F) \in H_{\mathrm{RT}}(X, \Omega) \otimes H_{\mathrm{RT}}(X, \Omega). \tag{15}$$

Proof. We prove the result by induction on $\mathrm{dep}(F) \geq 0$ for basis elements $F \in \mathcal{F}(X, \Omega)$. For the initial step of $\mathrm{dep}(F) = 0$, we have $F = \bullet_{x_1} \cdots \bullet_{x_m}$ for some $m \geq 0$, with the convention that $F = 𝟙$ when $m = 0$. If $m = 0$, then

$$\Delta_\epsilon(F) = \Delta_\epsilon(𝟙) = -\lambda(𝟙 \otimes 𝟙) \in H_{\mathrm{RT}}(X, \Omega) \otimes H_{\mathrm{RT}}(X, \Omega).$$

If $m \geq 1$, then by Lemma 3.5,

$$\begin{aligned}\Delta_\epsilon(F) &= \Delta_\epsilon(\bullet_{x_1} \dots \bullet_{x_m})\\ &= \sum_{i=1}^{m} \bullet_{x_1} \cdots \bullet_{x_i} \otimes \bullet_{x_i} \cdots \bullet_{x_m} + \lambda \sum_{i=1}^{m-1} \bullet_{x_1} \cdots \bullet_{x_i} \otimes \bullet_{x_{i+1}} \cdots \bullet_{x_m}\\ &\qquad \in H_{\mathrm{RT}}(X, \Omega) \otimes H_{\mathrm{RT}}(X, \Omega).\end{aligned}$$

Suppose that Equation (15) holds for $\operatorname{dep}(F) \leq n$ for an $n \geq 0$ and consider the case of $\operatorname{dep}(F) = n + 1$. For this case, we apply the induction on breadth $\operatorname{bre}(F)$. Since $\operatorname{dep}(F) = n + 1 \geq 1$, we get $F \neq \mathbb{1}$ and $\operatorname{bre}(F) \geq 1$. If $\operatorname{bre}(F) = 1$, since $\operatorname{dep}(F) \geq 1$, we have $F = B_\omega^+(\bar{F})$ for some $\omega \in \Omega$ and $\bar{F} \in H_{\mathrm{RT}}(X, \Omega)$. By Equation (12), we have

$$\Delta_\epsilon(F) = \Delta_\epsilon(B_\omega^+(\bar{F})) = F \otimes (-\lambda \mathbb{1}) + (\mathrm{id} \otimes B_\omega^+)\Delta_\epsilon(\bar{F}).$$

By the induction hypothesis on $\operatorname{dep}(F)$,

$$\begin{aligned}\Delta_\epsilon(\bar{F}) &\in H_{\mathrm{RT}}(X, \Omega) \otimes H_{\mathrm{RT}}(X, \Omega),\\ \text{and so} \quad (\mathrm{id} \otimes B_\omega^+)\Delta_\epsilon(\bar{F}) &\in H_{\mathrm{RT}}(X, \Omega) \otimes H_{\mathrm{RT}}(X, \Omega).\end{aligned}$$

Moreover, $-\lambda(F \otimes \mathbb{1}) \in H_{\mathrm{RT}}(X, \Omega) \otimes H_{\mathrm{RT}}(X, \Omega)$ follows from $F \in H_{\mathrm{RT}}(X, \Omega)$. Hence

$$F \otimes (-\lambda \mathbb{1}) + (\mathrm{id} \otimes B_\omega^+)\Delta_\epsilon(\bar{F}) \in H_{\mathrm{RT}}(X, \Omega) \otimes H_{\mathrm{RT}}(X, \Omega).$$

Assume that Equation (15) holds for $\operatorname{dep}(F) = n + 1$ and $\operatorname{bre}(F) \leq m$, in addition to $\operatorname{dep}(F) \leq n$ by the first induction hypothesis, and consider the case of $\operatorname{dep}(F) = n + 1$ and $\operatorname{bre}(F) = m + 1 \geq 2$. Then we may write $F = T_1 T_2 \cdots T_{m+1}$ for some $T_1, \dots, T_{m+1} \in \mathcal{T}(X, \Omega)$ and so by Equation (14)

$$\begin{aligned}\Delta_\epsilon(F) &= \Delta_\epsilon(T_1 T_2 \cdots T_{m+1})\\ &= T_1 \cdot \Delta_\epsilon(T_2 \cdots T_{m+1}) + \Delta_\epsilon(T_1) \cdot (T_2 \cdots T_{m+1}) + \lambda(T_1 \otimes T_2 \cdots T_{m+1}).\end{aligned}$$

By the induction hypothesis on breadth, we have

$$\begin{aligned}\Delta_\epsilon(T_2 \cdots T_{m+1}) &\in H_{\mathrm{RT}}(X, \Omega) \otimes H_{\mathrm{RT}}(X, \Omega),\\ \text{and} \quad \Delta_\epsilon(T_i) &\in H_{\mathrm{RT}}(X, \Omega) \otimes H_{\mathrm{RT}}(X, \Omega),\end{aligned}$$

whence by Equation (5),

$$\begin{aligned}T_1 \cdot \Delta_\epsilon(T_2 \cdots T_{m+1}) &\in H_{\mathrm{RT}}(X, \Omega) \otimes H_{\mathrm{RT}}(X, \Omega),\\ \text{and} \quad \Delta_\epsilon(T_1) \cdot (T_2 \cdots T_{m+1}) &\in H_{\mathrm{RT}}(X, \Omega) \otimes H_{\mathrm{RT}}(X, \Omega).\end{aligned}$$

Thus

$$\Delta_\epsilon(F) = \Delta_\epsilon(T_1 T_2 \cdots T_{m+1}) \in H_{\mathrm{RT}}(X, \Omega) \otimes H_{\mathrm{RT}}(X, \Omega).$$

This completes the induction on the breadth and hence the induction on the depth. □

We now state our first main result in this subsection.

Theorem 3.8. *The pair* $(H_{\mathrm{RT}}(X,\Omega),\Delta_\epsilon)$ *is a coalgebra* (without counit).

Proof. By Lemma 3.7, we only need to verify the coassociative law

$$(\mathrm{id}\otimes\Delta_\epsilon)\Delta_\epsilon(F)=(\Delta_\epsilon\otimes\mathrm{id})\Delta_\epsilon(F)\quad\text{for } F\in\mathcal{F}(X,\Omega), \tag{16}$$

which will be proved by induction on $\operatorname{dep}(F)\geq 0$. For the initial step of $\operatorname{dep}(F)=0$, we have $F=\bullet_{x_1}\bullet_{x_2}\cdots\bullet_{x_m}$ for some $m\geq 0$, with the convention that $F=\mathbb{1}$ if $m=0$. When $m=0$, we have

$$\begin{aligned}(\mathrm{id}\otimes\Delta_\epsilon)\Delta_\epsilon(F)&=(\mathrm{id}\otimes\Delta_\epsilon)\Delta_\epsilon(\mathbb{1})=-\lambda\mathbb{1}\otimes\Delta_\epsilon(\mathbb{1})=\lambda^2(\mathbb{1}\otimes\mathbb{1}\otimes\mathbb{1})\\&=-\lambda\Delta_\epsilon(\mathbb{1})\otimes\mathbb{1}=(\Delta_\epsilon\otimes\mathrm{id})\Delta_\epsilon(\mathbb{1}).\end{aligned}$$

When $m\geq 1$, on the one hand,

$$\begin{aligned}
&(\mathrm{id}\otimes\Delta_\epsilon)\Delta_\epsilon(\bullet_{x_1}\bullet_{x_2}\cdots\bullet_{x_m})\\
&=(\mathrm{id}\otimes\Delta_\epsilon)\Bigg(\sum_{i=1}^{m}\bullet_{x_1}\cdots\bullet_{x_i}\otimes\bullet_{x_i}\cdots\bullet_{x_m}+\lambda\sum_{i=1}^{m-1}\bullet_{x_1}\cdots\bullet_{x_i}\otimes\bullet_{x_{i+1}}\cdots\bullet_{x_m}\Bigg)\\
&\hspace{22em}\text{(by Lemma 3.5)}\\
&=\sum_{i=1}^{m}\bullet_{x_1}\cdots\bullet_{x_i}\otimes\Delta_\epsilon(\bullet_{x_i}\cdots\bullet_{x_m})+\lambda\sum_{i=1}^{m-1}\bullet_{x_1}\cdots\bullet_{x_i}\otimes\Delta_\epsilon(\bullet_{x_{i+1}}\cdots\bullet_{x_m})\\
&=\sum_{i=1}^{m}\bullet_{x_1}\cdots\bullet_{x_i}\otimes\Bigg(\sum_{j=i}^{m}\bullet_{x_i}\cdots\bullet_{x_j}\otimes\bullet_{x_j}\cdots\bullet_{x_m}+\lambda\sum_{j=i}^{m-1}\bullet_{x_i}\cdots\bullet_{x_j}\otimes\bullet_{x_{j+1}}\cdots\bullet_{x_m}\Bigg)\\
&\quad+\lambda\sum_{i=1}^{m-1}\bullet_{x_1}\cdots\bullet_{x_i}\otimes\Bigg(\sum_{j=i+1}^{m}\bullet_{x_{i+1}}\cdots\bullet_{x_j}\otimes\bullet_{x_j}\cdots\bullet_{x_m}+\lambda\sum_{j=i+1}^{m-1}\bullet_{x_{i+1}}\cdots\bullet_{x_j}\otimes\bullet_{x_{j+1}}\cdots\bullet_{x_m}\Bigg)\\
&=\sum_{i=1}^{m}\sum_{j=i}^{m}\bullet_{x_1}\cdots\bullet_{x_i}\otimes\bullet_{x_i}\cdots\bullet_{x_j}\otimes\bullet_{x_j}\cdots\bullet_{x_m}\\
&\qquad+\lambda\sum_{i=1}^{m}\sum_{j=i}^{m-1}\bullet_{x_1}\cdots\bullet_{x_i}\otimes\bullet_{x_i}\cdots\bullet_{x_j}\otimes\bullet_{x_{j+1}}\cdots\bullet_{x_m}\\
&\qquad\quad+\lambda\sum_{i=1}^{m-1}\sum_{j=i+1}^{m}\bullet_{x_1}\cdots\bullet_{x_i}\otimes\bullet_{x_{i+1}}\cdots\bullet_{x_j}\otimes\bullet_{x_j}\cdots\bullet_{x_m}\\
&\qquad\qquad+\lambda^2\sum_{i=1}^{m-1}\sum_{j=i+1}^{m-1}\bullet_{x_1}\cdots\bullet_{x_i}\otimes\bullet_{x_{i+1}}\cdots\bullet_{x_j}\otimes\bullet_{x_{j+1}}\cdots\bullet_{x_m}
\end{aligned}$$

$$
\begin{aligned}
&= \sum_{i=1}^{m}\sum_{j=i}^{m} \bullet_{x_1}\cdots\bullet_{x_i}\otimes\bullet_{x_i}\cdots\bullet_{x_j}\otimes\bullet_{x_j}\cdots\bullet_{x_m} \\
&\qquad + \lambda\sum_{i=1}^{m}\sum_{j=i}^{m-1} \bullet_{x_1}\cdots\bullet_{x_i}\otimes\bullet_{x_i}\cdots\bullet_{x_j}\otimes\bullet_{x_{j+1}}\cdots\bullet_{x_m} \\
&\qquad\qquad + \lambda\sum_{i=1}^{m-1}\sum_{j=i+1}^{m} \bullet_{x_1}\cdots\bullet_{x_i}\otimes\bullet_{x_{i+1}}\cdots\bullet_{x_j}\otimes\bullet_{x_j}\cdots\bullet_{x_m} \\
&\qquad\qquad\qquad + \lambda^2\sum_{i=1}^{m-2}\sum_{j=i+1}^{m-1} \bullet_{x_1}\cdots\bullet_{x_i}\otimes\bullet_{x_{i+1}}\cdots\bullet_{x_j}\otimes\bullet_{x_{j+1}}\cdots\bullet_{x_m}
\end{aligned}
$$

On the other hand,

$$
\begin{aligned}
&(\Delta_\epsilon\otimes \mathrm{id})\Delta_\epsilon(\bullet_{x_1}\bullet_{x_2}\cdots\bullet_{x_m}) \\
&= (\Delta_\epsilon\otimes \mathrm{id})\left(\sum_{i=1}^{m} \bullet_{x_1}\cdots\bullet_{x_i}\otimes\bullet_{x_i}\cdots\bullet_{x_m} + \lambda\sum_{i=1}^{m-1} \bullet_{x_1}\cdots\bullet_{x_i}\otimes\bullet_{x_{i+1}}\cdots\bullet_{x_m}\right) \\
&\hspace{28em}\text{(by Lemma 3.5)} \\
&= \sum_{i=1}^{m} \Delta_\epsilon(\bullet_{x_1}\cdots\bullet_{x_i})\otimes\bullet_{x_i}\cdots\bullet_{x_m} + \lambda\sum_{i=1}^{m-1} \Delta_\epsilon(\bullet_{x_1}\cdots\bullet_{x_i})\otimes\bullet_{x_{i+1}}\cdots\bullet_{x_m} \\
&= \sum_{i=1}^{m}\left(\sum_{j=1}^{i} \bullet_{x_1}\cdots\bullet_{x_j}\otimes\bullet_{x_j}\cdots\bullet_{x_i} + \lambda\sum_{j=1}^{i-1} \bullet_{x_1}\cdots\bullet_{x_j}\otimes\bullet_{x_{j+1}}\cdots\bullet_{x_i}\right)\otimes\bullet_{x_i}\cdots\bullet_{x_m} \\
&\quad + \lambda\sum_{i=1}^{m-1}\left(\sum_{j=1}^{i} \bullet_{x_1}\cdots\bullet_{x_j}\otimes\bullet_{x_j}\cdots\bullet_{x_i} + \lambda\sum_{j=1}^{i-1} \bullet_{x_1}\cdots\bullet_{x_j}\otimes\bullet_{x_{j+1}}\cdots\bullet_{x_i}\right)\otimes\bullet_{x_{i+1}}\cdots\bullet_{x_m} \\
&= \sum_{i=1}^{m}\sum_{j=1}^{i} \bullet_{x_1}\cdots\bullet_{x_j}\otimes\bullet_{x_j}\cdots\bullet_{x_i}\otimes\bullet_{x_i}\cdots\bullet_{x_m} \\
&\qquad + \lambda\sum_{i=1}^{m}\sum_{j=1}^{i-1} \bullet_{x_1}\cdots\bullet_{x_j}\otimes\bullet_{x_{j+1}}\cdots\bullet_{x_i}\otimes\bullet_{x_i}\cdots\bullet_{x_m} \\
&\qquad\qquad + \lambda\sum_{i=1}^{m-1}\sum_{j=1}^{i} \bullet_{x_1}\cdots\bullet_{x_j}\otimes\bullet_{x_j}\cdots\bullet_{x_i}\otimes\bullet_{x_{i+1}}\cdots\bullet_{x_m} \\
&\qquad\qquad\qquad + \lambda^2\sum_{i=1}^{m-1}\sum_{j=1}^{i-1} \bullet_{x_1}\cdots\bullet_{x_j}\otimes\bullet_{x_{j+1}}\cdots\bullet_{x_i}\otimes\bullet_{x_{i+1}}\cdots\bullet_{x_m} \\
&= \sum_{i=1}^{m}\sum_{j=1}^{i} \bullet_{x_1}\cdots\bullet_{x_j}\otimes\bullet_{x_j}\cdots\bullet_{x_i}\otimes\bullet_{x_i}\cdots\bullet_{x_m} \\
&\qquad + \lambda\sum_{i=2}^{m}\sum_{j=1}^{i-1} \bullet_{x_1}\cdots\bullet_{x_j}\otimes\bullet_{x_{j+1}}\cdots\bullet_{x_i}\otimes\bullet_{x_i}\cdots\bullet_{x_m}
\end{aligned}
$$

$$+\lambda\sum_{i=1}^{m-1}\sum_{j=1}^{i}\bullet_{x_1}\cdots\bullet_{x_j}\otimes\bullet_{x_j}\cdots\bullet_{x_i}\otimes\bullet_{x_{i+1}}\cdots\bullet_{x_m}$$
$$+\lambda^2\sum_{i=2}^{m-1}\sum_{j=1}^{i-1}\bullet_{x_1}\cdots\bullet_{x_j}\otimes\bullet_{x_{j+1}}\cdots\bullet_{x_i}\otimes\bullet_{x_{i+1}}\cdots\bullet_{x_m}$$
$$=\sum_{j=1}^{m}\sum_{i=j}^{m}\bullet_{x_1}\cdots\bullet_{x_j}\otimes\bullet_{x_j}\cdots\bullet_{x_i}\otimes\bullet_{x_i}\cdots\bullet_{x_m}$$
$$+\lambda\sum_{j=1}^{m-1}\sum_{i=j+1}^{m}\bullet_{x_1}\cdots\bullet_{x_j}\otimes\bullet_{x_{j+1}}\cdots\bullet_{x_i}\otimes\bullet_{x_i}\cdots\bullet_{x_m}$$
$$+\lambda\sum_{j=1}^{m-1}\sum_{i=j}^{m-1}\bullet_{x_1}\cdots\bullet_{x_j}\otimes\bullet_{x_j}\cdots\bullet_{x_i}\otimes\bullet_{x_{i+1}}\cdots\bullet_{x_m}$$
$$+\lambda^2\sum_{j=1}^{m-2}\sum_{i=j+1}^{m-1}\bullet_{x_1}\cdots\bullet_{x_j}\otimes\bullet_{x_{j+1}}\cdots\bullet_{x_i}\otimes\bullet_{x_{i+1}}\cdots\bullet_{x_m}$$
$$=\sum_{i=1}^{m}\sum_{j=i}^{m}\bullet_{x_1}\cdots\bullet_{x_i}\otimes\bullet_{x_i}\cdots\bullet_{x_j}\otimes\bullet_{x_j}\cdots\bullet_{x_m}$$
$$+\lambda\sum_{i=1}^{m-1}\sum_{j=i+1}^{m}\bullet_{x_1}\cdots\bullet_{x_i}\otimes\bullet_{x_{i+1}}\cdots\bullet_{x_j}\otimes\bullet_{x_j}\cdots\bullet_{x_m}$$
$$+\lambda\sum_{i=1}^{m}\sum_{j=i}^{m-1}\bullet_{x_1}\cdots\bullet_{x_i}\otimes\bullet_{x_i}\cdots\bullet_{x_j}\otimes\bullet_{x_{j+1}}\cdots\bullet_{x_m}$$
$$+\lambda^2\sum_{i=1}^{m-2}\sum_{j=i+1}^{m-1}\bullet_{x_1}\cdots\bullet_{x_i}\otimes\bullet_{x_{i+1}}\cdots\bullet_{x_j}\otimes\bullet_{x_{j+1}}\cdots\bullet_{x_m}$$
(by exchanging the index of i and j).

Thus

$$(\mathrm{id}\otimes\Delta_\epsilon)\Delta_\epsilon(\bullet_{x_1}\bullet_{x_2}\cdots\bullet_{x_m})=(\Delta_\epsilon\otimes\mathrm{id})\Delta_\epsilon(\bullet_{x_1}\bullet_{x_2}\cdots\bullet_{x_m}).$$

Suppose that Equation (16) holds for $\mathrm{dep}(F)\le n$ for an $n\ge 0$ and consider the case of $\mathrm{dep}(F)=n+1$. We now apply the induction on breadth. Since $\mathrm{dep}(F)=n+1\ge 1$, we have $F\ne\mathbb{1}$ and $\mathrm{bre}(F)\ge 1$. If $\mathrm{bre}(F)=1$, then we may write $F=B^+_\omega(\bar F)$ for some $\bar F\in\mathcal{F}(X,\Omega)$ and $\omega\in\Omega$. Hence

$$\begin{aligned}&(\mathrm{id}\otimes\Delta_\epsilon)\Delta_\epsilon(F)\\&=(\mathrm{id}\otimes\Delta_\epsilon)\Delta_\epsilon(B^+_\omega(\bar F))\\&=(\mathrm{id}\otimes\Delta_\epsilon)\big(F\otimes(-\lambda\mathbb{1})+(\mathrm{id}\otimes B^+_\omega)\Delta_\epsilon(\bar F)\big) &&\text{(by (12))}\\&=-\lambda F\otimes\Delta_\epsilon(\mathbb{1})+(\mathrm{id}\otimes(\Delta_\epsilon B^+_\omega))\Delta_\epsilon(\bar F)\\&=\lambda^2F\otimes\mathbb{1}\otimes\mathbb{1}+(\mathrm{id}\otimes(\Delta_\epsilon B^+_\omega))\Delta_\epsilon(\bar F) &&\text{(by (11))}\end{aligned}$$

$$
\begin{aligned}
&= \lambda^2 F \otimes \mathbb{1} \otimes \mathbb{1} + \big(\mathrm{id} \otimes \big(B_\omega^+ \otimes (-\lambda\mathbb{1}) + (\mathrm{id} \otimes B_\omega^+)\Delta_\epsilon\big)\big)\Delta_\epsilon(\bar{F}) && \text{(by (13))}\\
&= \lambda^2 F \otimes \mathbb{1} \otimes \mathbb{1} + \big(\mathrm{id} \otimes B_\omega^+ \otimes (-\lambda\mathbb{1}) + (\mathrm{id} \otimes \mathrm{id} \otimes B_\omega^+)(\mathrm{id} \otimes \Delta_\epsilon)\big)\Delta_\epsilon(\bar{F})\\
&= \lambda^2 F \otimes \mathbb{1} \otimes \mathbb{1} + \big((\mathrm{id} \otimes B_\omega^+)\Delta_\epsilon(\bar{F})\big) \otimes (-\lambda\mathbb{1}) + (\mathrm{id} \otimes \mathrm{id} \otimes B_\omega^+)(\mathrm{id} \otimes \Delta_\epsilon)\Delta_\epsilon(\bar{F})\\
&= \lambda^2 F \otimes \mathbb{1} \otimes \mathbb{1} + \big((\mathrm{id} \otimes B_\omega^+)\Delta_\epsilon(\bar{F})\big) \otimes (-\lambda\mathbb{1}) + (\mathrm{id} \otimes \mathrm{id} \otimes B_\omega^+)(\Delta_\epsilon \otimes \mathrm{id})\Delta_\epsilon(\bar{F})\\
& && \text{(by the induction hypothesis)}\\
&= \lambda^2 F \otimes \mathbb{1} \otimes \mathbb{1} + \big((\mathrm{id} \otimes B_\omega^+)\Delta_\epsilon(\bar{F})\big) \otimes (-\lambda\mathbb{1}) + (\Delta_\epsilon \otimes B_\omega^+)\Delta_\epsilon(\bar{F})\\
&= \big(F \otimes (-\lambda\mathbb{1}) + (\mathrm{id} \otimes B_\omega^+)\Delta_\epsilon(\bar{F})\big) \otimes (-\lambda\mathbb{1}) + (\Delta_\epsilon \otimes B_\omega^+)\Delta_\epsilon(\bar{F})\\
&= \Delta_\epsilon(F) \otimes (-\lambda\mathbb{1}) + (\Delta_\epsilon \otimes B_\omega^+)\Delta_\epsilon(\bar{F}) && \text{(by (12))}\\
&= (\Delta_\epsilon \otimes \mathrm{id})\big(F \otimes (-\lambda\mathbb{1}) + (\mathrm{id} \otimes B_\omega^+)\Delta_\epsilon(\bar{F})\big)\\
&= (\Delta_\epsilon \otimes \mathrm{id})\Delta_\epsilon(F) && \text{(by (12)).}
\end{aligned}
$$

Assume that Equation (16) holds for $\mathrm{dep}(F) = n+1$ and $\mathrm{bre}(F) \le m$, in addition to $\mathrm{dep}(F) \le n$ by the first induction hypothesis. Consider the case when $\mathrm{dep}(F) = n+1$ and $\mathrm{bre}(F) = m+1 \ge 2$. Then $F = F_1F_2$ for some $F_1, F_2 \in \mathcal{F}(X, \Omega)$ with $0 < \mathrm{bre}(F_1), \mathrm{bre}(F_2) < \mathrm{bre}(F)$. Using the Sweedler notation, we may write

$$\Delta_\epsilon(F_1) = \sum_{(F_1)} F_{1(1)} \otimes F_{1(2)} \quad \text{and} \quad \Delta_\epsilon(F_2) = \sum_{(F_2)} F_{2(1)} \otimes F_{2(2)}.$$

Then

$$
\begin{aligned}
&(\mathrm{id} \otimes \Delta_\epsilon)\Delta_\epsilon(F_1F_2)\\
&= (\mathrm{id} \otimes \Delta_\epsilon)(F_1 \cdot \Delta_\epsilon(F_2) + \Delta_\epsilon(F_1) \cdot F_2 + \lambda(F_1 \otimes F_2)) && \text{(by Lemma 3.6)}\\
&= (\mathrm{id} \otimes \Delta_\epsilon)\Bigg(\sum_{(F_2)} F_1F_{2(1)} \otimes F_{2(2)} + \sum_{(F_1)} F_{1(1)} \otimes F_{1(2)}F_2 + \lambda(F_1 \otimes F_2)\Bigg) && \text{(by (5))}\\
&= \sum_{(F_2)} F_1F_{2(1)} \otimes \Delta_\epsilon(F_{2(2)}) + \sum_{(F_1)} F_{1(1)} \otimes \Delta_\epsilon(F_{1(2)}F_2) + \lambda(F_1 \otimes \Delta_\epsilon(F_2))\\
&= \sum_{(F_2)} F_1F_{2(1)} \otimes \Delta_\epsilon(F_{2(2)})\\
&\qquad + \sum_{(F_1)} F_{1(1)} \otimes \big(F_{1(2)} \cdot \Delta_\epsilon(F_2) + \Delta_\epsilon(F_{1(2)}) \cdot F_2 + \lambda(F_{1(2)} \otimes F_2)\big)\\
&\qquad\qquad + \lambda(F_1 \otimes \Delta_\epsilon(F_2)) \quad \text{(by Lemma 3.6)}\\
&= \sum_{(F_2)} F_1F_{2(1)} \otimes \Bigg(\sum_{(F_{2(2)})} F_{2(2)(1)} \otimes F_{2(2)(2)}\Bigg) + \sum_{(F_1)} F_{1(1)} \otimes \Bigg(\sum_{(F_2)} F_{1(2)}F_{2(1)} \otimes F_{2(2)}\Bigg)\\
&\qquad + \sum_{(F_1)} F_{1(1)} \otimes \Bigg(\sum_{(F_{1(2)})} F_{1(2)(1)} \otimes F_{1(2)(2)}F_2\Bigg) + \lambda \sum_{(F_1)} F_{1(1)} \otimes F_{1(2)} \otimes F_2\\
&\qquad\qquad + \lambda \sum_{(F_2)} F_1 \otimes F_{2(1)} \otimes F_{2(2)} \quad \text{(by the Sweedler notation and (5))}
\end{aligned}
$$

$$= \sum_{(F_2)} \sum_{(F_{2(2)})} F_1 F_{2(1)} \otimes F_{2(2)(1)} \otimes F_{2(2)(2)} + \sum_{(F_1)} \sum_{(F_2)} F_{1(1)} \otimes F_{1(2)} F_{2(1)} \otimes F_{2(2)} + \sum_{(F_1)} \sum_{(F_{1(2)})} F_{1(1)} \otimes F_{1(2)(1)} \otimes F_{1(2)(2)} F_2 + \lambda \sum_{(F_1)} F_{1(1)} \otimes F_{1(2)} \otimes F_2 + \lambda \sum_{(F_2)} F_1 \otimes F_{2(1)} \otimes F_{2(2)}.$$

Similarly, we have

$$(\Delta_\epsilon \otimes \mathrm{id})\Delta_\epsilon(F_1 F_2) = \sum_{(F_2)} \sum_{(F_{2(1)})} F_1 F_{2(1)(1)} \otimes F_{2(1)(2)} \otimes F_{2(2)} + \sum_{(F_1)} \sum_{(F_2)} F_{1(1)} \otimes F_{1(2)} F_{2(1)} \otimes F_{2(2)} + \sum_{(F_1)} \sum_{(F_{1(1)})} F_{1(1)(1)} \otimes F_{1(1)(2)} \otimes F_{1(2)} F_2 + \lambda \sum_{(F_1)} F_{1(1)} \otimes F_{1(2)} \otimes F_2 + \lambda \sum_{(F_2)} F_1 \otimes F_{2(1)} \otimes F_{2(2)}.$$

By the induction hypothesis, we have

$$(\mathrm{id} \otimes \Delta_\epsilon)\Delta_\epsilon(F_1) = \sum_{(F_1)} \sum_{(F_{1(2)})} F_{1(1)} \otimes F_{1(2)(1)} \otimes F_{1(2)(2)} = (\Delta_\epsilon \otimes \mathrm{id})\Delta_\epsilon(F_1) = \sum_{(F_1)} \sum_{(F_{1(1)})} F_{1(1)(1)} \otimes F_{1(1)(2)} \otimes F_{1(2)}$$

and

$$(\mathrm{id} \otimes \Delta_\epsilon)\Delta_\epsilon(F_2) = \sum_{(F_2)} \sum_{(F_{2(2)})} F_{2(1)} \otimes F_{2(2)(1)} \otimes F_{2(2)(2)} = (\Delta_\epsilon \otimes \mathrm{id})\Delta_\epsilon(F_2) = \sum_{(F_2)} \sum_{(F_{2(1)})} F_{2(1)(1)} \otimes F_{2(1)(2)} \otimes F_{2(2)}.$$

Thus

$$(\mathrm{id} \otimes \Delta_\epsilon)\Delta_\epsilon(F_1 F_2) = (\Delta_\epsilon \otimes \mathrm{id})\Delta_\epsilon(F_1 F_2).$$

This completes the induction on the breadth and hence the induction on the depth. □

Now we arrive at our second main result in this subsection.

Theorem 3.9. *The quadruple* $(H_{\mathrm{RT}}(X, \Omega), m_{\mathrm{RT}}, \mathbb{1}, \Delta_\epsilon)$ *is an* ϵ*-unitary bialgebra of weight* λ.

Proof. Note that the triple $(H_{\mathrm{RT}}(X, \Omega), m_{\mathrm{RT}}, \mathbb{1})$ is a unitary algebra. Then the result follows from Lemma 3.6 and Theorem 3.8. □

4. Free Ω-cocycle infinitesimal unitary bialgebras

In this section, we conceptualize the combination of operated algebras and weighted infinitesimal unitary bialgebras, and show that $H_{\mathrm{RT}}(X, \Omega)$ is a free object in such category. Let us start with the following concepts.

Definition 4.1 [Guo 2009, Section 1.2]. Let Ω be a nonempty set.

(a) An Ω-*operated monoid* is a monoid M together with a set of operators $P_\omega : M \to M,\ \omega \in \Omega$.

(b) An Ω-*operated algebra* is an algebra A together with a set of linear operators $P_\omega : A \to A,\ \omega \in \Omega$.

Definition 4.2 [Gao and Zhang 2018, Definition 3.17]. Let λ be an element of $\boldsymbol{k}$.

(a) An Ω-*operated* ϵ-*bialgebra of weight* λ is an ϵ-bialgebra H of weight λ together with a set of linear operators $P_\omega : H \to H$, $\omega \in \Omega$.

(b) Let $(H, \{P_\omega \mid \omega \in \Omega\})$ and $(H', \{P'_\omega \mid \omega \in \Omega\})$ be two Ω-operated ϵ-bialgebras of weight λ. A linear map $\phi : H \to H'$ is called an Ω-*operated* ϵ-*bialgebra morphism* if ϕ is a morphism of ϵ-bialgebras of weight λ and $\phi \circ P_\omega = P'_\omega \circ \phi$ for $\omega \in \Omega$.

By Remark 2.3(a), the unit of an infinitesimal unitary bialgebra is a group-like element of weight $-\lambda$. Involving a weighted 1-cocycle condition, we then propose

Definition 4.3. (a) An Ω-*cocycle* ϵ-*unitary bialgebra of weight* λ is an Ω-operated ϵ-unitary bialgebra $(H, m, 1, \Delta, \{P_\omega \mid \omega \in \Omega\})$ of weight λ satisfying the weighted 1-cocycle condition:

$$\Delta P_\omega = P_\omega \otimes (-\lambda 1) + (\mathrm{id} \otimes P_\omega)\Delta \quad \text{for all } \omega \in \Omega. \tag{17}$$

(b) The *free* Ω-*cocycle* ϵ-*unitary bialgebra of weight* λ *on a set* X is an Ω-cocycle ϵ-unitary bialgebra $(H_X, m_X, 1_X, \Delta_X, \{P_\omega \mid \omega \in \Omega\})$ of weight λ together with a set map $j_X : X \to H_X$ with the property that, for any Ω-cocycle ϵ-unitary bialgebra $(H, m, 1, \Delta, \{P'_\omega \mid \omega \in \Omega\})$ of weight λ and any set map $f : X \to H$ whose images are *group-like* (that is, $\Delta(f(x)) = f(x) \otimes f(x)$ for $x \in X$), there is a unique morphism $\bar{f} : H_X \to H$ of Ω-operated ϵ-unitary bialgebras such that $\bar{f} \circ j_X = f$.

Remark 4.4. Note the subtle difference between the weighted cocycle condition (17) and the ϵ-cocycle condition in [Gao and Zhang 2018, Definition 3.17]:

$$\Delta P_\omega = \mathrm{id} \otimes 1 + (\mathrm{id} \otimes P_\omega)\Delta \quad \text{for all } \omega \in \Omega.$$

The following results generalizes the universal properties which were studied in [Connes and Kreimer 1998; Foissy 2013; Guo 2009; Moerdijk 2001; Zhang et al.

2016]. Recall from Equation (8) that

$$\mathcal{F}(X, \Omega) = \varinjlim \mathcal{F}_n = \bigcup_{n=0}^{\infty} \mathcal{F}_n.$$

Theorem 4.5. *Let $j_X : X \hookrightarrow \mathcal{F}(X, \Omega)$, $x \mapsto \bullet_x$ be the natural embedding and m_{RT} the concatenation product.*

(a) *The quadruple $(\mathcal{F}(X, \Omega),\ m_{\mathrm{RT}},\ \mathbb{1},\ \{B_\omega^+ \mid \omega \in \Omega\})$ together with the j_X is the free Ω-operated monoid on X.*

(b) *The quadruple $(H_{\mathrm{RT}}(X, \Omega),\ m_{\mathrm{RT}},\ \mathbb{1},\ \{B_\omega^+ \mid \omega \in \Omega\})$ together with the j_X is the free Ω-operated unitary algebra on X.*

(c) *The quintuple $(H_{\mathrm{RT}}(X, \Omega),\ m_{\mathrm{RT}},\ \mathbb{1},\ \Delta_\epsilon,\ \{B_\omega^+ \mid \omega \in \Omega\})$ together with the j_X is the free Ω-cocycle ϵ-unitary bialgebra of weight λ on X.*

Proof. (a) We only need to verify that $(\mathcal{F}(X, \Omega),\ \{B_\omega^+ \mid \omega \in \Omega\})$ satisfies the universal property. Let $(S, \{P_\omega \mid \omega \in \Omega\})$ be a given Ω-operated monoid and $f : X \to S$ a given set map. We will use induction on n to construct a unique sequence of monoid homomorphisms

$$\bar{f}_n : \mathcal{F}_n \to S, n \geq 0.$$

For the initial step of $n = 0$, by the universal property of the free monoid $M(\bullet_X)$, the map $\bullet_X \to S$, $\bullet_x \mapsto f(x)$ extends to a unique monoid homomorphism $\bar{f}_0 : M(\bullet_X) \to S$. Assume that $\bar{f}_k : \mathcal{F}_k \to S$ has been defined for a $k \geq 0$ and define the set map

$$\bar{f}_{k+1} : \bullet_X \sqcup \big(\textstyle\bigsqcup_{\omega\in\Omega} B_\omega^+(\mathcal{F}_k)\big) \to S, \quad \bullet_x \mapsto f(x), \quad B_\omega^+(\bar{F}) \mapsto P_\omega(\bar{f}_k(\bar{F})),$$

where $x \in X$, $\omega \in \Omega$ and $\bar{F} \in \mathcal{F}_k$. Again by the universal property of the free monoid $M\big(\bullet_X \sqcup \bigsqcup_{\omega\in\Omega} B_\omega^+(\mathcal{F}_k)\big)$, $\bar{f}_{k+1}$ is extended to a unique monoid homomorphism

$$\bar{f}_{k+1} : \mathcal{F}_{k+1} = M\big(\bullet_X \sqcup \big(\textstyle\bigsqcup_{\omega\in\Omega} B_\omega^+(\mathcal{F}_k)\big)\big) \to S.$$

Define

$$\bar{f} := \varinjlim \bar{f}_n : \mathcal{F}(X, \Omega) \to S.$$

Then by the above construction, $\bar{f}$ is the required homomorphism of Ω-operated monoids and the unique one such that $\bar{f} \circ j_X = f$.

(b) It directly follows from Item (a).

(c) By Theorem 3.9, $(H_{\mathrm{RT}}(X, \Omega),\ m_{\mathrm{RT}},\ \mathbb{1},\ \Delta_\epsilon)$ is an ϵ-unitary bialgebra of weight λ. Moreover by Equation (12), $(H_{\mathrm{RT}}(X, \Omega),\ m_{\mathrm{RT}},\ \mathbb{1},\ \Delta_\epsilon,\ \{B_\omega^+ \mid \omega \in \Omega\})$ is an Ω-cocycle ϵ-unitary bialgebra of weight λ.

For the freeness, let $(H, m, 1, \Delta, \{P_\omega \mid \omega \in \Omega\})$ be an Ω-cocycle ϵ-unitary bialgebra of weight λ and $f : X \to H$ a set map such that

$$\Delta(f(x)) = f(x) \otimes f(x) \quad \text{for all } x \in X.$$

In particular, $(H, m, 1, \{P_\omega \mid \omega \in \Omega\})$ is an Ω-operated unitary algebra. By Item (b), there exists a unique Ω-operated unitary algebra morphism $\bar{f} : H_{\mathrm{RT}}(X, \Omega) \to H$ such that $\bar{f} \circ j_X = f$. It remains to check the compatibility of the coproducts Δ and Δ_ϵ for which we verify

$$\Delta \bar{f}(F) = (\bar{f} \otimes \bar{f})\Delta_\epsilon(F) \quad \text{for all } F \in \mathcal{F}(X, \Omega), \tag{18}$$

by induction on the depth $\mathrm{dep}(F) \geq 0$. For the initial step of $\mathrm{dep}(F) = 0$, we have $F = \bullet_{x_1} \cdots \bullet_{x_m}$ for some $m \geq 0$, with the convention that $F = \mathbb{1}$ when $m = 0$. If $m = 0$, then by Remark 2.3(a) and Equation (11),

$$\begin{aligned}\Delta \bar{f}(F) &= \Delta \bar{f}(\mathbb{1}) = \Delta(1) = -\lambda(1 \otimes 1) = -\lambda \bar{f}(\mathbb{1}) \otimes \bar{f}(\mathbb{1}) = (\bar{f} \otimes \bar{f})(-\lambda \mathbb{1} \otimes \mathbb{1}) \\ &= (\bar{f} \otimes \bar{f})\Delta_\epsilon(\mathbb{1}).\end{aligned}$$

If $m \geq 1$, then

$$\begin{aligned}
&\Delta \bar{f}(\bullet_{x_1} \cdots \bullet_{x_m}) \\
&= \Delta\big(\bar{f}(\bullet_{x_1}) \cdots \bar{f}(\bullet_{x_m})\big) \\
&= \sum_{i=1}^{m} \big(\bar{f}(\bullet_{x_1}) \cdots \bar{f}(\bullet_{x_{i-1}})\big) \cdot \Delta(\bar{f}(\bullet_{x_i})) \cdot \big(\bar{f}(\bullet_{x_{i+1}}) \cdots \bar{f}(\bullet_{x_m})\big) \\
&\qquad + \lambda \sum_{i=1}^{m-1} \bar{f}(\bullet_{x_1}) \cdots \bar{f}(\bullet_{x_i}) \otimes \bar{f}(\bullet_{x_{i+1}}) \cdots \bar{f}(\bullet_{x_m}) \quad \text{(by (6))} \\
&= \sum_{i=1}^{m} \big(\bar{f}(\bullet_{x_1}) \cdots \bar{f}(\bullet_{x_{i-1}})\big) \cdot \big(\bar{f}(\bullet_{x_i}) \otimes \bar{f}(\bullet_{x_i})\big) \cdot \big(\bar{f}(\bullet_{x_{i+1}}) \cdots \bar{f}(\bullet_{x_m})\big) \\
&\qquad + \lambda \sum_{i=1}^{m-1} \bar{f}(\bullet_{x_1}) \cdots \bar{f}(\bullet_{x_i}) \otimes \bar{f}(\bullet_{x_{i+1}}) \cdots \bar{f}(\bullet_{x_m}) \\
&\qquad \big(\text{by } \Delta(\bar{f}(\bullet_{x_i})) = \Delta(f(x_i)) = f(x_i) \otimes f(x_i) = \bar{f}(x_i) \otimes \bar{f}(x_i)\big) \\
&= \sum_{i=1}^{m} \bar{f}(\bullet_{x_1}) \cdot \cdots \bar{f}(\bullet_{x_i}) \otimes \bar{f}(\bullet_{x_i}) \cdots \bar{f}(\bullet_{x_m}) \\
&\qquad + \lambda \sum_{i=1}^{m-1} \bar{f}(\bullet_{x_1}) \cdots \bar{f}(\bullet_{x_i}) \otimes \bar{f}(\bullet_{x_{i+1}}) \cdots \bar{f}(\bullet_{x_m}) \\
&= \sum_{i=1}^{m} \bar{f}(\bullet_{x_1} \cdot \cdots \bullet_{x_i}) \otimes \bar{f}(\bullet_{x_i} \cdots \bullet_{x_m}) + \lambda \sum_{i=1}^{m-1} \bar{f}(\bullet_{x_1} \cdots \bullet_{x_i}) \otimes \bar{f}(\bullet_{x_{i+1}} \cdots \bullet_{x_m}) \\
&\qquad \text{(by } \bar{f} \text{ being a unitary algebra morphism)}
\end{aligned}$$

$$= (\bar{f} \otimes \bar{f})\Big(\sum_{i=1}^{m} \bullet_{x_1} \cdots \bullet_{x_i} \otimes \bullet_{x_i} \cdots \bullet_{x_m} + \lambda \sum_{i=1}^{m-1} \bullet_{x_1} \cdots \bullet_{x_i} \otimes \bullet_{x_{i+1}} \cdots \bullet_{x_m}\Big)$$
$$= (\bar{f} \otimes \bar{f})\Delta_\epsilon(\bullet_{x_1} \cdots \bullet_{x_m}) \qquad \text{(by Lemma 3.5).}$$

Suppose Equation (18) holds for $\mathrm{dep}(F) \le n$ for an $n \ge 0$ and consider the case of $\mathrm{dep}(F) = n + 1$. For this case we apply the induction on the breadth $\mathrm{bre}(F)$. Since $\mathrm{dep}(F) = n+1 \ge 1$, we have $F \ne \mathbb{1}$ and $\mathrm{bre}(F) \ge 1$. If $\mathrm{bre}(F) = 1$, we have $F = B^+_\omega(\bar{F})$ for some $\bar{F} \in \mathcal{F}(X, \Omega)$ and $\omega \in \Omega$. Then

$$\begin{aligned}
\Delta \bar{f}(F) &= \Delta \bar{f}(B^+_\omega(\bar{F})) = \Delta P_\omega(\bar{f}(\bar{F})) \\
&\qquad \text{(by } \bar{f} \text{ being an operated unitary algebra morphism)} \\
&= P_\omega(\bar{f}(\bar{F})) \otimes (-\lambda 1) + (\mathrm{id} \otimes P_\omega)\Delta(\bar{f}(\bar{F})) \qquad \text{(by (17))} \\
&= P_\omega(\bar{f}(\bar{F})) \otimes (-\lambda 1) + (\mathrm{id} \otimes P_\omega)(\bar{f} \otimes \bar{f})\Delta_\epsilon(\bar{F}) \\
&\qquad \text{(by the induction hypothesis on } \mathrm{dep}(F)) \\
&= P_\omega(\bar{f}(\bar{F})) \otimes (-\lambda 1) + (\bar{f} \otimes P_\omega \bar{f})\Delta_\epsilon(\bar{F}) \\
&= \bar{f}(B^+_\omega(\bar{F})) \otimes (-\lambda 1) + (\bar{f} \otimes \bar{f} B^+_\omega)\Delta_\epsilon(\bar{F}) \\
&\qquad \text{(by } \bar{f} \text{ being an operated unitary algebra morphism)} \\
&= (\bar{f} \otimes \bar{f})\big(B^+_\omega(\bar{F}) \otimes (-\lambda \mathbb{1}) + (\mathrm{id} \otimes B^+_\omega)\Delta_\epsilon(\bar{F})\big) \\
&= (\bar{f} \otimes \bar{f})\Delta_\epsilon(B^+_\omega(\bar{F})) \qquad \text{(by (12))} \\
&= (\bar{f} \otimes \bar{f})\Delta_\epsilon(F).
\end{aligned}$$

Assume that Equation (18) holds for $\mathrm{dep}(F) = n + 1$ and $\mathrm{bre}(F) \le m$, in addition to $\mathrm{dep}(F) \le n$ by the first induction hypothesis, and consider the case when $\mathrm{dep}(F) = n + 1$ and $\mathrm{bre}(F) = m + 1 \ge 2$. Then we can write $F = F_1 F_2$ for some $F_1, F_2 \in \mathcal{F}(X, \Omega)$ with $0 < \mathrm{bre}(F_1), \mathrm{bre}(F_2) < m + 1$. Using the Sweedler notation, we can write

$$\Delta_\epsilon(F_1) = \sum_{(F_1)} F_{1(1)} \otimes F_{1(2)} \quad \text{and} \quad \Delta_\epsilon(F_2) = \sum_{(F_2)} F_{2(1)} \otimes F_{2(2)}.$$

By the induction hypothesis on the breadth, we have

$$\Delta(\bar{f}(F_1)) = (\bar{f} \otimes \bar{f})\Delta_\epsilon(F_1) = \sum_{(F_1)} \bar{f}(F_{1(1)}) \otimes \bar{f}(F_{1(2)}),$$
$$\Delta(\bar{f}(F_2)) = (\bar{f} \otimes \bar{f})\Delta_\epsilon(F_2) = \sum_{(F_2)} \bar{f}(F_{2(1)}) \otimes \bar{f}(F_{2(2)}).$$

Thus

$$\begin{aligned}
\Delta \bar{f}(F) &= \Delta \bar{f}(F_1 F_2) = \Delta(\bar{f}(F_1)\bar{f}(F_2)) \\
&= \bar{f}(F_1) \cdot \Delta(\bar{f}(F_2)) + \Delta(\bar{f}(F_1)) \cdot \bar{f}(F_2) + \lambda \bar{f}(F_1) \otimes \bar{f}(F_2) \qquad \text{(by (6))}
\end{aligned}$$

$$
\begin{aligned}
&= \bar{f}(F_1)\cdot\Big(\sum_{(F_2)}\bar{f}(F_{2(1)})\otimes\bar{f}(F_{2(2)})\Big)+\Big(\sum_{(F_1)}\bar{f}(F_{1(1)})\otimes\bar{f}(F_{1(2)})\Big)\\
&\qquad\qquad\cdot\bar{f}(F_2)+\lambda\bar{f}(F_1)\otimes\bar{f}(F_2)\\
&= \sum_{(F_2)}\bar{f}(F_1)\bar{f}(F_{2(1)})\otimes\bar{f}(F_{2(2)})+\sum_{(F_1)}\bar{f}(F_{1(1)})\otimes\bar{f}(F_{1(2)})\bar{f}(F_2)\\
&\qquad\qquad+\lambda\bar{f}(F_1)\otimes\bar{f}(F_2)\quad\text{(by (5))}\\
&= \sum_{(F_2)}\bar{f}(F_1F_{2(1)})\otimes\bar{f}(F_{2(2)})+\sum_{(F_1)}\bar{f}(F_{1(1)})\otimes\bar{f}(F_{1(2)}F_2)\\
&\qquad\qquad+\lambda\bar{f}(F_1)\otimes\bar{f}(F_2)\\
&= (\bar{f}\otimes\bar{f})\Big(\sum_{(F_2)}F_1F_{2(1)}\otimes F_{2(2)}\Big)+(\bar{f}\otimes\bar{f})\Big(\sum_{(F_1)}F_{1(1)}\otimes F_{1(2)}F_2\Big)\\
&\qquad\qquad+(\bar{f}\otimes\bar{f})(\lambda F_1\otimes F_2)\\
&= (\bar{f}\otimes\bar{f})\Big(\sum_{(F_2)}F_1F_{2(1)}\otimes F_{2(2)}+\sum_{(F_1)}F_{1(1)}\otimes F_{1(2)}F_2+\lambda F_1\otimes F_2\Big)\\
&= (\bar{f}\otimes\bar{f})\Big(F_1\cdot\sum_{(F_2)}F_{2(1)}\otimes F_{2(2)}+\Big(\sum_{(F_1)}F_{1(1)}\otimes F_{1(2)}\Big)\cdot F_2+\lambda F_1\otimes F_2\Big)\\
&\qquad\qquad\text{(by (5))}\\
&= (\bar{f}\otimes\bar{f})\big(F_1\cdot\Delta_\epsilon(F_2)+\Delta_\epsilon(F_1)\cdot F_2+\lambda(F_1\otimes F_2)\big)\\
&= (\bar{f}\otimes\bar{f})\Delta_\epsilon(F_1F_2)\qquad\text{(by Lemma 3.6)}\\
&= (\bar{f}\otimes\bar{f})\Delta_\epsilon(F).
\end{aligned}
$$

This completes the induction on the breadth and hence the induction on the depth. □

Let $X=\varnothing$. Then we obtain a freeness of $H_{\mathrm{RT}}(\varnothing,\Omega)$, which is the infinitesimal version of decorated noncommutative Connes–Kreimer Hopf algebra by Remark 3.1(b).

Corollary 4.6. *The quintuple* $(H_{\mathrm{RT}}(\varnothing,\Omega),\ m_{\mathrm{RT}},\ \mathbb{1},\ \Delta_\epsilon,\ \{B^+_\omega \mid \omega\in\Omega\})$ *is the free* Ω*-cocycle* ϵ*-unitary bialgebra of weight* λ *on the empty set, that is, the initial object in the category of* Ω*-cocycle* ϵ*-unitary bialgebras of weight* λ.

Proof. It follows from Theorem 4.5(c) by taking $X=\varnothing$. □

Taking Ω to be singleton in Corollary 4.6, all vertices of planar rooted forests have the same decoration. In other words, in this case planar rooted forests have no decorations and that are precisely the one in the classical noncommutative Connes–Kreimer Hopf algebra, introduced by Foissy [2002a] and Holtkamp [2003].

Corollary 4.7. *Let* $\mathcal{F}$ *be the set of planar rooted forests without decorations. Then the quintuple* $(\boldsymbol{k}\mathcal{F},\ m_{\mathrm{RT}},\ \mathbb{1},\ \Delta_\epsilon,\ B^+)$ *is the free cocycle* ϵ*-unitary bialgebra of weight* λ *on the empty set, that is, the initial object in the category of* Ω*-cocycle* ϵ*-unitary bialgebras of weight* λ.

Proof. It follows from Corollary 4.6 by taking Ω to be a singleton set. □

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