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CERTIFYING INCOMPRESSIBILITY OF NONINJECTIVE SURFACES WITH SCL

DANNY CALEGARI

Cooper and Manning (2011) and Louder (2011) gave examples of maps of surface groups to PSL(2, $\mathbb{C}$) which are not injective, but are incompressible (i.e., no simple loop is in the kernel). We construct more examples with very simple *certificates* for their incompressibility arising from the theory of stable commutator length.

The purpose of this note is to give examples of maps of closed surface groups to PSL(2, $\mathbb{C}$) which are not π_1-injective, but are geometrically incompressible, in the sense that no simple loop in the surface is in the kernel (in the sequel we use the word "incompressible" as shorthand for "geometrically incompressible"). The examples are very explicit, and the images can be taken to be all loxodromic. The significance of such examples is that they shed light on the simple loop conjecture, which says that any noninjective map from a closed oriented surface to a 3-manifold should be compressible.

Examples of such maps were first shown to exist in [Cooper and Manning 2011], by a representation variety argument, thereby answering a question of Minsky [2000] (also see [Bowditch 1998]). More sophisticated examples were then found by Louder [2011]; he even found examples with the property that the minimal self-crossing number of a loop in the kernel can be taken to be arbitrarily large. Louder's strategy is to exhibit an explicit finitely presented group (a limit group) which admits noninjective incompressible surface maps, and then to observe that such a group can be embedded as an all-loxodromic subgroup of PSL(2, $\mathbb{C}$).

It is easy to produce examples of noninjective surface groups. What is hard is to certify that they are incompressible. The main point of our construction, and the main novelty and interest of this paper, is to show that stable commutator length (and its cousin Gromov–Thurston norm) can be used to certify incompressibility.

Our examples are closely related to Louder's examples, although our certificates are quite different. So another purpose of this note is to advertise the use of stable

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commutator length as a tool to get at the kind of information that is relevant in certain contexts in the theory of limit groups.

We move back and forward between (fundamental) groups and spaces in the usual way. We assume the reader is familiar with stable commutator length, and Gromov–Thurston norms in dimension 2. Standard references are [Calegari 2009; Gromov 1982; Thurston 1986]. Computations are done with the program `scallop`, available from [Calegari and Walker 2011].

Recall that if X is a $K(\pi, 1)$, the *Gromov–Thurston norm* of a class $\alpha \in H_2(X; \mathbb{Z})$ (denoted $\|\alpha\|$) is the infimum of $-\chi(T)/n$ over all closed, oriented surfaces T without spherical components mapping to X and representing $n\alpha$. Our certificates for incompressibility are guaranteed by the following proposition.

Proposition 1 (certificate). *Let X be a $K(\pi, 1)$, and let $\alpha \in H_2(X; \mathbb{Z})$ be represented by a closed oriented surface S with no torus or spherical components. If there is a strict inequality $\|\alpha\| > -\chi(S) - 2$ (where $\|\cdot\|$ denotes Gromov–Thurston norm) then S is (geometrically) incompressible.*

Proof. If S is compressible, then α is represented by the result of compressing S, which is a surface S' with no spherical components, and $-\chi(S') < \|\alpha\|$. But this contradicts the definition of $\|\alpha\|$. □

On the other hand, a closed surface S without torus or spherical components representing α and with $-\chi(S) = \|\alpha\|$ *is* π_1-injective, so to apply our proposition to obtain examples, we must find examples of spaces X and integral homology classes α for which $\|\alpha\|$ is not equal to $-\chi(S)$ for any closed orientable surface S; i.e., for which $\|\alpha\|$ is not in $2\mathbb{Z}$. Such spaces can never be 3-manifolds, by combined results of [Gabai 1983; Thurston 1986], so our methods will never directly find a counterexample to the simple loop conjecture.

The groups we consider are all obtained by amalgamating two simpler groups over a cyclic subgroup. The generator of the cyclic group is homologically trivial in either factor, giving rise to a class in H_2 in the big group. The Gromov–Thurston norm of this class is related to the stable commutator length of the loop in the two factors as follows:

Proposition 2 (amalgamation). *Let G be an amalgamated product $G = J *_{\langle w\rangle} K$ along a cyclic group $\langle w\rangle$ which is generated by a loop w which is homologically trivial on either side. Let $\phi : H_2(G; \mathbb{Z}) \to H_1(\langle w\rangle; \mathbb{Z})$ be the connecting map in the Mayer–Vietoris sequence, and let $H_w \subset H_2(G; \mathbb{Z})$ be the affine subspace mapping to the generator. If w has infinite order in J and K, then*

$$\inf_{\alpha \in H_w} \|\alpha\| = 2(\mathrm{scl}_J(w) + \mathrm{scl}_K(w)).$$

Proof. This is not difficult to see directly from the definition, and it is very similar to the proof of Theorem 3.4 in [Calegari 2008]. However, for the sake of clarity we give an argument. Note by the way that the hypothesis that w is homologically trivial on either side is equivalent to the statement that the inclusion map $H_1(\langle w\rangle;\mathbb{Z}) \to H_1(J;\mathbb{Z}) \oplus H_1(K;\mathbb{Z})$ is the zero map, so ϕ as above is certainly surjective. Moreover, if $H_2(J;\mathbb{Z})$ and $H_2(K;\mathbb{Z})$ are trivial (as will often be the case below), then ϕ is an isomorphism, and H_w consists of a single class α.

It is convenient to geometrize this algebraic picture, so let X_J and X_K be Eilenberg–MacLane spaces for J and K, and let X_G be obtained from X_J and X_K by attaching the two ends of a cylinder C to loops representing the conjugacy classes corresponding to the images of w in either side. Let γ be the core of C. If S is a closed, oriented surface with no sphere components, and $f : S \to X_G$ represents some $n\alpha$ with $\alpha \in H_w$, then we can homotope f so that it meets γ transversely and efficiently — i.e., so that $f^{-1}(\gamma)$ consists of pairwise disjoint essential simple curves in S. If one of these curves maps to γ with degree zero we can compress S and reduce its complexity, so without loss of generality every component maps with nonzero degree. Hence we can cut S into S_J and S_K each mapping to X_J and X_K respectively and with boundary representing some finite cover of w. By definition this shows $\inf_{\alpha\in H_w} \|\alpha\| \ge 2(\mathrm{scl}_J(w) + \mathrm{scl}_K(w))$.

Conversely, given surfaces S_J and S_K mapping to X_J and X_K with boundary representing finite covers of w (or rather its image in each side), we need to construct a suitable S as above. First, we can pass to a cover of each S_J and S_K in such a way that the boundary of each maps to w with positive degree; see, for example, Proposition 2.13 of [Calegari 2009]. Then we can pass to a further finite cover of each so that the set of degrees with which components of ∂S_J and of ∂S_K map over w are the same (with multiplicity); again, see the argument of the proposition just cited. Once this is done we can glue up S_J to S_K with the opposite orientation to build a surface S mapping to X_G which, by construction, represents a multiple of some α in H_w. We therefore obtain $\inf_{\alpha\in H_w} \|\alpha\| \le 2(\mathrm{scl}_J(w) + \mathrm{scl}_K(w))$ and we are done. □

We now show how to use these propositions to produce examples.

Example 1. Start with a free group; for concreteness, let $F = \langle a, b, c\rangle$. Consider a word $w \in F$ of the form $w = [a, b][c, v]$ for some $v \in F$. Associated to this expression of w as a product of two commutators is a genus 2 surface S with one boundary component mapping to a $K(F, 1)$ in such a way that its boundary represents w. This surface is not injective, since the image of its fundamental group is F which has rank 3. Let $G = \langle a, b, c, x, y \mid w = [x, y]\rangle$; i.e., geometrically a $K(G, 1)$ is obtained from a $K(F, 1)$ by attaching the boundary of a once-punctured torus T to w. The surface $R := S \cup T$ has genus 3, and represents the generator of $H_2(G;\mathbb{Z})$. On the other hand, by the Amalgamation Proposition, the Gromov–Thurston norm of this homology class is equal to $2\cdot\mathrm{scl}_{\langle x,y\rangle}([x, y]) + 2\cdot\mathrm{scl}_F(w)$. Since $\mathrm{scl}_{\langle x,y\rangle}([x, y]) = \frac{1}{2}$

(see [Calegari 2009, Example 2.100], for instance), providing $\frac{1}{2} < \mathrm{scl}(w)$ the result is noninjective but incompressible.

The group G can be embedded in $\mathrm{PSL}(2, \mathbb{C})$ by first embedding F as a discrete subgroup, then embedding $\langle x, y \rangle$ in such a way that $[x, y] = w$. By conjugating $\langle x, y \rangle$ by a generic loxodromic element with the same axis as w, we can ensure this example is injective, and it can even be taken to be all loxodromic. This follows in the usual way by a Bass–Serre type argument; a similar argument appears in [Calegari and Dunfield 2006, Lemma 1.5].

Almost any word v will give rise to w with $\mathrm{scl}(w) > \frac{1}{2}$; for example,

$$\mathrm{scl}([a, b][c, aa]) = 1,$$

as can be computed using `scallop`. Experimentally, it appears that if v is chosen to be random of length n, then $\mathrm{scl}(w) \to \frac{3}{2}$ as $n \to \infty$. For example,

$$\mathrm{scl}([a, b][c, bcABBcABCbbcACbcBcbb]) = \tfrac{7}{5}.$$

The closer $\mathrm{scl}(w)$ is to $\frac{3}{2}$, the bigger the index of a cover in which some simple loop compresses. This gives a practical method to produce examples for any given k in which no loop with fewer than k self-crossings is in the kernel.

Example 2. Note that the groups G produced in Example 1 are 1-relator groups, which are very similar to 3-manifold groups in some important ways. A modified construction shows they can in fact be taken to be 1-relator fundamental groups of hyperbolic 4-manifolds. To see this, we consider examples of the form $G = \langle a, b, c, x_1, y_1, \dots, x_g, y_g \mid w = \prod_{i=1}^{g} [x_i, y_i] \rangle$ i.e., we attach a once-punctured surface T_g of genus g, giving rise to a noninjective incompressible surface $R = S \cup T_g$ of genus $g + 2$.

Let $\langle a, b, c \rangle$ act discretely and faithfully, stabilizing a totally geodesic $\mathbb{H}^3$ in $\mathbb{H}^4$. We can arrange for the axis ℓ of w to be disjoint from its translates. Thinking of $\langle x_1, y_1, \dots, x_g, y_g \rangle$ as the fundamental group of a once-punctured surface T_g, we choose a hyperbolic structure on this surface for which ∂T_g is isometric to $\ell / \langle w \rangle$, and make this group act by stabilizing a totally geodesic $\mathbb{H}^2$ in $\mathbb{H}^4$ in such a way that the axis of ∂T_g intersects the $\mathbb{H}^3$ perpendicularly along ℓ. Providing the shortest essential arc in T_g from ∂T_g to itself is sufficiently long (depending on the minimal distance from ℓ to its translates by $\langle a, b, c \rangle$) the resulting group is discrete and faithful. This follows by applying the Klein–Maskit combination theorem, once we ensure that the limit sets of the conjugates of $\langle a, b, c \rangle$ are contained in regions satisfying the ping-pong hypothesis for the action of $\pi_1(T_g)$. This condition can be ensured by taking g big enough and choosing the hyperbolic structure on T_g accordingly; the details are entirely straightforward.

Example 3. Let H be any nonelementary hyperbolic 2-generator group which is torsion free but not free. Let a, b be the generators. Then the once-punctured torus with boundary $[a, b]$ is not injective. As before, let $G = \langle H, x, y \mid [a, b] = [x, y] \rangle$. Then G contains a genus 2 surface representing the amalgamated class in $H_2(G; \mathbb{Z})$, and the norm of this class is $1 + 2 \cdot \mathrm{scl}_H([a, b]) > 0$, so this example is noninjective but incompressible.

As an example, we could take H to be the fundamental group of a closed hyperbolic 3-manifold of Heegaard genus 2, or a 2-bridge knot complement. Such examples have discrete faithful representations into $\mathrm{PSL}(2, \mathbb{C})$.

Example 4. It is easy to produce examples of 2-generator 1-relator groups $H = \langle a, b \mid v \rangle$ in which $\frac{1}{2} - \epsilon < \mathrm{scl}([a, b]) < \frac{1}{2}$ for any ϵ. Such groups are torsion-free if v is not a proper power. Just fix some big integer N and take

$$v = ([a, b]^{\pm N})^{g_1} ([a, b]^{\pm N})^{g_2} \cdots ([a, b]^{\pm N})^{g_m}$$

to be any product of conjugates for which there are as many $+N$'s as $-N$'s. Such an H maps to the Seifert-fibered 3-manifold group

$$\langle a, b, z \mid [a, b]^N = z^{N-1}, [a, z] = [b, z] = 1 \rangle,$$

in which $\mathrm{scl}([a, b]) = (N - 1)/2N$. The only subtle part of this last equality is the lower bound, which is certified by Bavard duality (see [Calegari 2009, Theorem 2.70]) and the existence of a rotation quasimorphism associated to a realization of the fundamental group of the Seifert manifold as a central extension of the fundamental group of a hyperbolic torus orbifold with one orbifold point of order N. Since scl is monotone nonincreasing under homomorphisms, the claim follows.

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GLOBAL WELL-POSEDNESS FOR THE 3D ROTATING NAVIER–STOKES EQUATIONS WITH HIGHLY OSCILLATING INITIAL DATA

QIONGLEI CHEN, CHANGXING MIAO AND ZHIFEI ZHANG

We prove the global well-posedness for the 3D rotating Navier–Stokes equations in the critical functional framework. This result allows us to construct global solutions for a class of highly oscillating initial data.

1. Introduction

In this paper, we study the 3D rotating Navier–Stokes equations

$$\begin{cases} u_t - \nu\Delta u + \Omega e_3 \times u + u\cdot\nabla u + \nabla p = 0,\\ \operatorname{div} u = 0,\\ u(0,x) = u_0(x), \end{cases} \tag{1-1}$$

where ν denotes the viscosity coefficient of the fluid, Ω the speed of rotation, e_3 the unit vector in the x_3 direction and $\Omega e_3 \times u$ the Coriolis force. We refer to [Chemin et al. 2006; Majda 2003; Pedlosky 1987] for its background in geophysical fluid dynamics. If the Coriolis force is neglected, the equations (1-1) become the classical 3D incompressible Navier–Stokes equations

$$\begin{cases} u_t - \nu\Delta u + u\cdot\nabla u + \nabla p = 0,\\ \operatorname{div} u = 0,\\ u(0,x) = u_0(x). \end{cases} \tag{1-2}$$

The global existence of a weak solution of (1-1) can be proved by the classical compactness method, since we still have the energy estimate

$$\|u(t)\|_{L^2}^2 + 2\int_0^t \|\nabla u(s)\|_{L^2}^2\,ds \le \|u_0\|_{L^2}^2.$$

As in 3D Navier–Stokes equations, the uniqueness and regularity of weak solutions are also open problems. Recently, Giga et al. [2006; 2007; 2008] studied the local

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existence of a mild solution for a class of nondecaying initial data which includes a class of almost periodic functions, as well as global existence for small data. On the other hand, when the speed Ω of rotation is fast enough, the global existence of smooth solution was proved in [Babin et al. 1997; 1999; Chemin et al. 2000; 2006].

For the 3D Navier–Stokes equations, Fujita and Kato [1964; Kato 1984] proved the local well-posedness for large initial data and the global well-posedness for small initial data in the homogeneous Sobolev space $\dot{H}^{\frac{1}{2}}$ and the Lebesgue space L^3, respectively. These spaces are all the critical ones, which are relevant to the scaling of the Navier–Stokes equations: if (u, p) solves (1-2), then

$$\big(u_\lambda(t,x), p_\lambda(t,x)\big) := \big(\lambda u(\lambda^2 t, \lambda x), \lambda^2 p(\lambda^2 t, \lambda x)\big) \tag{1-3}$$

is also a solution of (1-2). The so-called *critical space* is the one such that the associated norm is invariant under the scaling of (1-3). Recently, Cannone [1997] (see also [Cannone 1995; 2004; Cannone et al. 1994]) generalized it to Besov spaces with negative index of regularity. More precisely, he showed that if the initial data satisfies

$$\|u_0\|_{\dot{B}^{-1+\frac{3}{p}}_{p,\infty}} \le c, \quad p > 3$$

for some small constant c, then the Navier–Stokes equations (1-2) are globally well-posed. Let us emphasize that this result allows us to construct global solutions for highly oscillating initial data which may have a large norm in $\dot{H}^{\frac{1}{2}}$ or L^3. A typical example is

$$u_0(x) = \sin\frac{x_3}{\varepsilon}\big(-\partial_2\phi(x), \partial_1\phi(x), 0\big)$$

where $\phi \in \mathcal{S}(\mathbb{R}^3)$ and $\varepsilon > 0$ is small enough. We refer to [Chemin and Gallagher 2006; Chemin and Zhang 2007; Chen et al. 2010a] for some relevant results. A natural question is then to prove a theorem of this type for the rotating Navier–Stokes equations.

We know that Kato's method heavily relies on the uniform boundedness of the Stokes semigroup in L^p and global $L^p - L^q$ estimates, but the Stokes–Coriolis semigroup is not uniformly bounded in L^p for $p \neq 2$; see Theorems 5 and 6 in [Dragičević et al. 2006]. Standard techniques allow us to prove these estimates only locally for the Stokes–Coriolis semigroup, hence one can obtain the local existence of mild solution in L^3 by Kato's method. Whether one can extend this solution to a global one for small data in L^3 is a very interesting problem.

Very recently, based on the global $L^p - L^q$ estimates with $q \le 2 \le p$ and $L^q - H^{\frac{1}{2}}$ estimates with $q > 3$ for the Stokes–Coriolis semigroup, Hieber and Shibata [2010] proved the following global result for small data in $H^{\frac{1}{2}}$.

Theorem 1.1. *Let $q > 3$. Then there exists $c > 0$ independent of Ω such that for any $u_0 \in H^{\frac{1}{2}}_\sigma$ with $\|u_0\|_{H^{\frac{1}{2}}} \le c$, the equations* (1-1) *admit a unique mild solution $u \in C\big([0,\infty), H^{\frac{1}{2}}_\sigma\big)$ satisfying*

$$u \in C((0,\infty), L^q) \quad \text{and} \quad \lim_{t\to 0^+} \sup_{0<s<t} s^{\frac{1}{2}-\frac{3}{2q}} \|u(s,\cdot)\|_{L^q} = 0, \tag{1-4}$$

$$\nabla u \in C((0,\infty), L^2) \quad \text{and} \quad \lim_{t\to 0^+} \sup_{0<s<t} s^{\frac{1}{4}} \|\nabla u(s,\cdot)\|_{L^2} = 0.$$

Here $H^{\frac{1}{2}}_\sigma$ denotes the closure of the set $\{u \in C_c^\infty(\mathbb{R}^3)^3, \operatorname{div} u = 0\}$ in the norm of $\|\cdot\|_{H^{\frac{1}{2}}}$.

The goal of this paper is to prove the global existence of a solution of (1-1) for a class of highly oscillating initial velocity. Thus we need to solve the system (1-1) for the initial data in a critical functional framework whose regularity index is negative, for example, $\dot{B}^{-1+\frac{3}{p}}_{p,q}$ for $p > 3$. However, Cannone's proof [1997] doesn't work for our case, since it also relies on the global $L^p - L^q$ estimates for the Stokes semigroup. Indeed, for the Stokes–Coriolis semigroup $\mathcal{G}(t)$, one has

$$\|\mathcal{G}(t)u_0\|_{L^p} \le C_{p,\Omega} t^2 \|u_0\|_{L^p}, \quad \text{if } p \ne 2;$$

see Proposition 2.2 in [Hieber and Shibata 2010]. Then we can infer from the definition of the Besov space that

$$\|\mathcal{G}(t)u_0\|_{\dot{B}^{-1+\frac{3}{p}}_{p,q}} \le C t^2 \|u_0\|_{\dot{B}^{-1+\frac{3}{p}}_{p,q}}.$$

This means that even if the initial data u_0 is small in $\dot{B}^{-1+\frac{3}{p}}_{p,q}$, the linear part of the solution, $\|\mathcal{G}(t)u_0\|_{\dot{B}^{-1+\frac{3}{p}}_{p,q}}$, may become large after some time $t_0 > 0$.

Fortunately, we have the following important observation: if u is an element of L^p with $\operatorname{supp} \hat{u} \in \{\xi : |\xi| \gtrsim \lambda\}$, then

$$\|\mathcal{G}(t)u\|_{L^p} \le C_{p,\Omega} e^{-t\lambda^2} \|u\|_{L^p}$$

for any $p \in [1,\infty]$ and $t \in [0,\infty]$, while for any $u \in L^2$,

$$\|\mathcal{G}(t)u\|_{L^2} \le \|u\|_{L^2}.$$

This motivates us to introduce the hybrid-Besov spaces $\dot{\mathcal{B}}^{\frac{1}{2},\frac{3}{p}-1}_{2,p}$ (see Definition 2.2). Roughly speaking, if $u \in \dot{\mathcal{B}}^{\frac{1}{2},\frac{3}{p}-1}_{2,p}$, the low frequency part of u belongs to $\dot{H}^{\frac{1}{2}}$ and the high frequency part belongs to $\dot{B}^{-1+\frac{3}{p}}_{p,\infty}$. So, $\dot{\mathcal{B}}^{\frac{1}{2},\frac{3}{p}-1}_{2,p}$ is still a critical space. A remarkable property of $\dot{\mathcal{B}}^{\frac{1}{2},\frac{3}{p}-1}_{2,p}$ is that if $p > 3$, then

$$\|u_0(x)\|_{\dot{\mathcal{B}}^{\frac{1}{2},\frac{3}{p}-1}_{2,p}} \le C\varepsilon^{1-\frac{3}{p}},$$

for $u_0(x) = \sin(x_1/\varepsilon)\phi(x)$, with $\phi(x) \in \mathcal{S}(\mathbb{R}^3)$; see Proposition 2.4. That is, the highly oscillating function is still small in the norm of $\dot{\mathcal{B}}^{\frac{1}{2},\frac{3}{p}-1}_{2,p}$.

Definition 1.2. Let $1 \le p \le \infty$, we denote by E_p the space of functions such that

$$E_p = \{u : \operatorname{div} u = 0, \|u\|_{E_p} < +\infty\},$$

where

$$\|u\|_{E_p} := \|u\|_{\widetilde{L}^\infty\left(\mathbb{R}^+;\dot{\mathcal{B}}^{\frac{1}{2},\frac{3}{p}-1}_{2,p}\right)} + \|u\|_{\widetilde{L}^1\left(\mathbb{R}^+;\dot{\mathcal{B}}^{\frac{5}{2},\frac{3}{p}+1}_{2,p}\right)}.$$

Definition 1.3. We denote by $C_*\big([0,\infty);\dot{\mathcal{B}}^{\frac{1}{2},\frac{3}{p}-1}_{2,p}\big)$ the set of functions u such that u is continuous from $(0,\infty)$ to $\dot{\mathcal{B}}^{\frac{1}{2},\frac{3}{p}-1}_{2,p}$, but weakly continuous at $t=0$; i.e.,

$$\lim_{t\to 0+} \sup_{0<s<t} \big\langle u(s,\cdot),\, g(\cdot)\big\rangle = 0 \quad \text{for all } g \in \mathcal{S} \text{ with } \|g\|_{\dot{\mathcal{B}}^{-\frac{1}{2},1-\frac{3}{p}}_{2,p}} \le 1.$$

Our main results are stated as follows.

Theorem 1.4. *Let $p \in [2,4]$. There exists a positive constant c independent of Ω such that if $\|u_0\|_{\dot{\mathcal{B}}^{\frac{1}{2},\frac{3}{p}-1}_{2,p}} \le c$, then there exists a unique solution $u \in E_p$ of* (1-1) *such that*

$$u \in C_*\big([0,\infty);\dot{\mathcal{B}}^{\frac{1}{2},\frac{3}{p}-1}_{2,p}\big).$$

Remark 1.5. Due to the inclusion map

$$H^{\frac{1}{2}} \subseteq \dot{\mathcal{B}}^{\frac{1}{2},\frac{3}{p}-1}_{2,p} \quad \text{for } p \ge 2,$$

Theorem 1.4 is an improvement on Theorem 1.1. The importance of this is that it allows us to construct global solutions of (1-1) for a class of highly oscillating initial velocity u_0, for example,

$$u_0(x) = \sin\Big(\frac{x_3}{\varepsilon}\Big)(-\partial_2\phi(x), \partial_1\phi(x), 0) \tag{1-5}$$

where $\phi \in \mathcal{S}(\mathbb{R}^3)$ and $\varepsilon > 0$ is small enough. This type of data is large in the Sobolev norm; however, it is small in the norms of Besov spaces with negative regularity index.

Remark 1.6. As shown in Section 4.2 of [Cannone 2004], for the classical Navier–Stokes equations (1-2), there exists the following "highly oscillating" initial data: $u_0(x) \in \mathcal{S}'(\mathbb{R}^3)$ is such that $\hat{u}_0(\xi) = 0$ if $|\xi| \le 1/\varepsilon$. Then

$$\|u_0\|_{\dot{H}^{1/2}} \le \varepsilon^{1/2}\|u_0\|_{\dot{H}^1}. \tag{1-6}$$

We point out that examples like (1-5) are not included in such initial data. In fact, if $\operatorname{supp}\hat{\phi}(\xi) \subset \{|\xi| \le 1/2\varepsilon\}$, then the above estimate is satisfied, while if $\hat{\phi}(\xi)$ has no support, it is not sure that (1-6) holds, which implies the norm of $\|u_0\|_{\dot{H}^{1/2}}$ may not be small enough.

Remark 1.7. The inhomogeneous part of the solution has more regularity:

$$u - \mathcal{G}(t)u_0 \in C\big(\mathbb{R}^+; \dot{B}^{\frac{1}{2}}_{2,\infty}\big),$$

which can be proved by following the proof of Proposition 4.1.

If u_0 lies in $\dot{H}^{\frac{1}{2}}$, we can obtain the following global well-posedness result.

Theorem 1.8. *Let $p \in [2, 4]$. There exists a positive constant c independent of Ω such that, if u_0 belongs to $\dot{H}^{\frac{1}{2}}$ with $\|u_0\|_{\dot{\mathcal{B}}^{\frac{1}{2},\frac{3}{p}-1}_{2,p}} \le c$, then there exists a unique global solution of* (1-1) *in $C(\mathbb{R}^+, \dot{H}^{\frac{1}{2}})$.*

Remark 1.9. Since we only impose the smallness condition of the initial data in the norm of $\dot{\mathcal{B}}^{\frac{1}{2},\frac{3}{p}-1}_{2,p}$, this allows us to obtain the global well-posedness of (1-1) for a class of highly oscillating initial velocity u_0. Moreover, the uniqueness holds in the class $C(\mathbb{R}^+, \dot{H}^{\frac{1}{2}})$; i.e., it is unconditional.

The structure of this paper is as follows. In Section 2, we recall some basic facts about Littlewood–Paley theory and the functional spaces. In Section 3, we recall some results concerning the Stokes–Coriolis semigroup's regularizing effect. Section 4 is devoted to the important bilinear estimates. In Section 5, we prove Theorem 1.4 and Theorem 1.8.

2. Littlewood–Paley theory and the function spaces

First of all, we introduce the Littlewood–Paley decomposition. Choose two radial functions $\varphi, \chi \in \mathcal{S}(\mathbb{R}^3)$ supported in $\mathcal{C} = \{\xi \in \mathbb{R}^3, \frac{3}{4} \le |\xi| \le \frac{8}{3}\}$, $\mathcal{B} = \{\xi \in \mathbb{R}^3, |\xi| \le \frac{4}{3}\}$, respectively, such that

$$\sum_{j\in\mathbb{Z}} \varphi(2^{-j}\xi) = 1 \quad \text{for all } \xi \neq 0.$$

For $f \in \mathcal{S}'(\mathbb{R}^3)$, the frequency localization operators Δ_j and S_j $(j \in \mathbb{Z})$ are defined by

$$\Delta_j f = \varphi(2^{-j}D)f, \quad S_j f = \chi(2^{-j}D)f, \quad D = \frac{\nabla_x}{i}.$$

Moreover, we have

$$S_j f = \sum_{k=-\infty}^{j-1} \Delta_k f \quad \text{in } \mathcal{Z}'(\mathbb{R}^3).$$

Here we denote by $\mathcal{Z}'(\mathbb{R}^3)$ the dual space of

$$\mathcal{Z}(\mathbb{R}^3) = \{f \in \mathcal{S}(\mathbb{R}^3) : D^\alpha \hat{f}(0) = 0 \text{ for all multiindices } \alpha \in (\mathbb{N} \cup 0)^3\}.$$

With our choice of φ, it is easy to verify that

$$\Delta_j \Delta_k f = 0 \quad \text{if } |j-k| \geq 2 \quad \text{and} \quad \Delta_j (S_{k-1} f \Delta_k f) = 0 \quad \text{if } |j-k| \geq 5. \tag{2-1}$$

In the sequel, we will constantly use Bony's decomposition [1981]:

$$fg = T_f g + T_g f + R(f,g), \tag{2-2}$$

with

$$T_f g = \sum_{j \in \mathbb{Z}} S_{j-1} f \Delta_j g, \quad R(f,g) = \sum_{j \in \mathbb{Z}} \Delta_j f \widetilde{\Delta}_j g, \quad \widetilde{\Delta}_j g = \sum_{|j'-j| \leq 1} \Delta_{j'} g.$$

Definition 2.1 (homogeneous Besov space). Let $s \in \mathbb{R}$, $1 \leq p, q \leq +\infty$. The homogeneous Besov space $\dot{B}^s_{p,q}$ is defined by

$$\dot{B}^s_{p,q} := \{ f \in \mathscr{Z}'(\mathbb{R}^3) : \|f\|_{\dot{B}^s_{p,q}} < +\infty \},$$

where

$$\|f\|_{\dot{B}^s_{p,q}} := \big\| 2^{ks} \|\Delta_k f\|_{L^p} \big\|_{l^q}.$$

If $p = q = 2$, $\dot{B}^s_{2,2}$ is equivalent to the homogeneous Sobolev space $\dot{H}^s$.

Definition 2.2 (hybrid-Besov space). Let $s, \sigma \in \mathbb{R}$, $1 \leq p \leq +\infty$. The hybrid-Besov space $\dot{\mathscr{B}}^{s,\sigma}_{2,p}$ is defined by

$$\dot{\mathscr{B}}^{s,\sigma}_{2,p} := \{ f \in \mathscr{Z}'(\mathbb{R}^3) : \|f\|_{\dot{\mathscr{B}}^{s,\sigma}_{2,p}} < +\infty \},$$

where

$$\|f\|_{\dot{\mathscr{B}}^{s,\sigma}_{2,p}} := \sup_{2^k \leq \Omega} 2^{ks} \|\Delta_k f\|_{L^2} + \sup_{2^k > \Omega} 2^{k\sigma} \|\Delta_k f\|_{L^p}.$$

The norm of the space $\widetilde{L}^r_T(\dot{\mathscr{B}}^{s,\sigma}_{2,p})$ is defined by

$$\|f\|_{\widetilde{L}^r_T(\dot{\mathscr{B}}^{s,\sigma}_{2,p})} := \sup_{2^k \leq \Omega} 2^{ks} \|\Delta_k f\|_{L^r_T L^2} + \sup_{2^k > \Omega} 2^{k\sigma} \|\Delta_k f\|_{L^r_T L^p}.$$

It is easy to check that $L^r_T(\dot{\mathscr{B}}^{s,\sigma}_{2,p}) \subseteq \widetilde{L}^r_T(\dot{\mathscr{B}}^{s,\sigma}_{2,p})$, where the norm of $L^r_T(\dot{\mathscr{B}}^{s,\sigma}_{2,p})$ is defined by

$$\|f\|_{L^r_T(\dot{\mathscr{B}}^{s,\sigma}_{2,p})} := \big\| \|f(t)\|_{\dot{\mathscr{B}}^{s,\sigma}_{2,p}} \big\|_{L^r_T}.$$

Bernstein's lemma will be repeatedly used throughout this paper:

Lemma 2.3 [Chemin 1995]. *Let $1 \leq p \leq q \leq +\infty$. Then for any $\beta, \gamma \in (\mathbb{N} \cup \{0\})^3$, there exists a constant C independent of f, j such that, for any $f \in L^p$,*

$$\operatorname{supp} \hat{f} \subseteq \{|\xi| \leq A_0 2^j\} \Rightarrow \|\partial^\gamma f\|_{L^q} \leq C 2^{j|\gamma| + jn(\frac{1}{p} - \frac{1}{q})} \|f\|_{L^p},$$

$$\operatorname{supp} \hat{f} \subseteq \{A_1 2^j \leq |\xi| \leq A_2 2^j\} \Rightarrow \|f\|_{L^p} \leq C 2^{-j|\gamma|} \sup_{|\beta| = |\gamma|} \|\partial^\beta f\|_{L^p}.$$

Proposition 2.4. *Let $\phi \in \mathcal{S}(\mathbb{R}^3)$ and $p > 3$. If $\phi_\varepsilon(x) := e^{i\frac{x_1}{\varepsilon}}\phi(x)$, then, for any $0 < \varepsilon \le \Omega^{-1}$,*

$$\|\phi_\varepsilon\|_{\dot{\mathcal{B}}^{\frac{1}{2},\frac{3}{p}-1}_{2,p}} \le C\varepsilon^{1-\frac{3}{p}},$$

where C is a constant independent of ε.

Proof. Let $j_0 \in \mathbb{N}$ be such that $\Omega \le 2^{j_0} \sim \varepsilon^{-1}$. By Lemma 2.3, we have

$$\sup_{j \ge j_0} 2^{(\frac{3}{p}-1)j}\|\Delta_j\phi_\varepsilon\|_{L^p} \le C2^{(\frac{3}{p}-1)j_0} \le C\varepsilon^{1-\frac{3}{p}}.$$

Noting that $e^{i\frac{x_1}{\varepsilon}} = (-i\varepsilon\partial_1)^N e^{i\frac{x_1}{\varepsilon}}$ for any $N \in \mathbb{N}$, we get, by integration by parts,

$$\Delta_j\phi_\varepsilon(x) = (i\varepsilon)^N 2^{3j}\int_{\mathbb{R}^3} e^{i\frac{y_1}{\varepsilon}}\partial_{y_1}^N\big(h(2^j(x-y))\phi(y)\big)\,dy, \quad h(x) := (\mathcal{F}^{-1}\varphi)(x).$$

By the Leibnitz formula, we have

$$|\Delta_j\phi_\varepsilon(x)| \le C\varepsilon^N 2^{3j}\sum_{k=0}^{N} 2^{kj}\int_{\mathbb{R}^3}\big|(\partial_{y_1}^k h)(2^j(x-y))\big|\big|\partial_{y_1}^{N-k}\phi(y)\big|\,dy,$$

from which, along with Young's inequality, we infer that, for $j \ge 0$,

$$\|\Delta_j\phi_\varepsilon\|_{L^q} \le C\varepsilon^N\sum_{k=0}^{N} 2^{kj}2^{3j}\big\|(\partial_{y_1}^k h)(2^j y)\big\|_{L^1}\big\|\partial_{y_1}^{N-k}\phi(y)\big\|_{L^q} \le C\varepsilon^N 2^{jN},$$

and for $j \le 0$,

$$\|\Delta_j\phi_\varepsilon\|_{L^q} \le C\varepsilon^N\sum_{k=0}^{N} 2^{kj}2^{3j}\big\|(\partial_{y_1}^k h)(2^j y)\big\|_{L^q}\big\|\partial_{y_1}^{N-k}\phi(y)\big\|_{L^1} \le C\varepsilon^N 2^{(1-\frac{1}{q})3j}.$$

Thus we have

$$\sup_{\Omega < 2^j < 2^{j_0}} 2^{(\frac{3}{p}-1)j}\|\Delta_j\phi_\varepsilon\|_{L^p} \le C\varepsilon^N 2^{(N-1+\frac{3}{p})j_0} \le C\varepsilon^{1-\frac{3}{p}},$$

$$\sup_{2^j \le \Omega} 2^{\frac{j}{2}}\|\Delta_j\phi_\varepsilon\|_{L^2} \le C\Omega^{\frac{1}{2}}\varepsilon^N \le C\varepsilon^{N-\frac{1}{2}}.$$

Summing up the above estimates yields that

$$\|\phi_\varepsilon\|_{\dot{\mathcal{B}}^{\frac{1}{2},\frac{3}{p}-1}_{2,p}} \le C\varepsilon^{1-\frac{3}{p}}.$$

The proof of Proposition 2.4 is completed. □

3. Regularizing effect of the Stokes–Coriolis semigroup

We consider the linear system

$$\begin{cases} u_t - \nu\Delta u + \Omega e_3 \times u + \nabla p = 0, \\ \operatorname{div} u = 0, \\ u(0,x) = u_0(x). \end{cases} \tag{3-1}$$

From [Giga et al. 2005; Hieber and Shibata 2010, Proposition 2.1], we know that

$$\hat{u}(t,\xi) = \cos\left(\Omega \frac{\xi_3}{|\xi|} t\right) e^{-\nu|\xi|^2 t} I \widehat{u_0}(\xi) + \sin\left(\Omega \frac{\xi_3}{|\xi|} t\right) e^{-\nu|\xi|^2 t} R(\xi) \widehat{u_0}(\xi), \tag{3-2}$$

for $t \geq 0$ and $\xi \in \mathbb{R}^3$, where I is the identity matrix and

$$R(\xi) = \begin{pmatrix} 0 & \xi_3/|\xi| & -\xi_2/|\xi| \\ -\xi_3/|\xi| & 0 & \xi_1/|\xi| \\ \xi_2/|\xi| & -\xi_1/|\xi| & 0 \end{pmatrix}.$$

The Stokes–Coriolis semigroup is explicitly represented by

$$\mathcal{G}(t)f = \big[\cos(\Omega R_3 t) I + \sin(\Omega R_3 t) R\big] e^{\nu t \Delta} f, \quad \text{for } t \geq 0,\ f \in L^p_\sigma, \tag{3-3}$$

where $\widehat{R_3 f}(\xi) := (\xi_3/|\xi|)\hat{f}(\xi)$ for $\xi \neq 0$.

Proposition 3.1 (smoothing effect of the Stokes–Coriolis semigroup). *Let $\mathcal{C}$ be a ring centered at* 0 *in* $\mathbb{R}^3$. *Then there exist positive constants c and C depending only on ν such that if* $\operatorname{supp}\hat{u} \subset \lambda\mathcal{C}$, *then we have*:

(i) *for any* $\lambda > 0$,

$$\|\mathcal{G}(t)u\|_{L^2} \leq Ce^{-c\lambda^2 t}\|u\|_{L^2}; \tag{3-4}$$

(ii) *if* $\lambda \gtrsim \Omega$, *then*, *for any* $1 \leq p \leq \infty$,

$$\|\mathcal{G}(t)u\|_{L^p} \leq Ce^{-c\lambda^2 t}\|u\|_{L^p}. \tag{3-5}$$

Proof. (i) Thanks to (3-2) and the Plancherel theorem, we get

$$\|\mathcal{G}(t)u\|_{L^2} = \big\|\widehat{\mathcal{G}}(t,\xi)\hat{u}(\xi)\big\|_{L^2} \leq C\big\|e^{-\nu|\xi|^2 t}\hat{u}(\xi)\big\|_2 \leq Ce^{-\nu\lambda^2 t}\|u\|_2,$$

where we have used the support property of $\hat{u}(\xi)$.

(ii) Let $\phi \in \mathcal{D}(\mathbb{R}^3 \setminus \{0\})$, which equals 1 near the ring $\mathcal{C}$. Set

$$g(t,x) := (2\pi)^{-3} \int_{\mathbb{R}^3} e^{ix\cdot\xi}\phi(\lambda^{-1}\xi)\widehat{\mathcal{G}}(t,\xi)\,d\xi.$$

To prove (3-5), it suffices to show

$$\|g(x,t)\|_{L^1} \leq Ce^{-c\lambda^2 t}. \tag{3-6}$$

Thanks to (3-3), we infer that

$$\int_{|x|\le\lambda^{-1}}|g(x,t)|dx\le C\int_{|x|\le\lambda^{-1}}\int_{\mathbb{R}^3}\left|\phi(\lambda^{-1}\xi)\right|\left|\widehat{\mathcal{G}}(t,\xi)\right|d\xi\,dx\le Ce^{-c\lambda^2t}. \tag{3-7}$$

Set $L:=x\cdot\nabla_\xi/(i|x|^2)$. Noting that $L(e^{ix\cdot\xi})=e^{ix\cdot\xi}$, we get, using integration by parts,

$$g(x,t)=\int_{\mathbb{R}^3}L^N(e^{ix\cdot\xi})\phi(\lambda^{-1}\xi)\widehat{\mathcal{G}}(t,\xi)\,d\xi=\int_{\mathbb{R}^3}e^{ix\cdot\xi}(L^*)^N\big(\phi(\lambda^{-1}\xi)\widehat{\mathcal{G}}(t,\xi)\big)\,d\xi,$$

where $N\in\mathbb{N}$ is chosen later. Using the Leibnitz formula, it is easy to verify that

$$\left|\partial^\gamma(e^{\pm i\Omega\frac{\xi_3}{|\xi|}t})\right|\le C|\xi|^{-|\gamma|}(1+\Omega t)^{|\gamma|},\quad \left|\partial^\gamma(e^{-\nu|\xi|^2t})\right|\le C|\xi|^{-|\gamma|}e^{-\frac{\nu}{2}|\xi|^2t}.$$

Thus we obtain

$$\begin{aligned}&\left|(L^*)^N\big(\phi(\lambda^{-1}\xi)\widehat{\mathcal{G}}(t,\xi)\big)\right|\\ &\le C|x|^{-N}\sum_{\substack{|\alpha_1|+|\alpha_2|\\+|\alpha_3|=|\alpha|\\|\alpha|\le N}}\lambda^{-N+\alpha}\left|(\nabla^{N-\alpha}\phi)(\lambda^{-1}\xi)\partial^{\alpha_1}\big(e^{\pm i\Omega\frac{\xi_3}{|\xi|}t}\big)\partial^{\alpha_2}\big(e^{-\nu|\xi|^2t}\big)\partial^{\alpha_3}(I+R(\xi))\right|\\ &\le C|\lambda x|^{-N}\sum_{\substack{|\alpha_1|+|\alpha_2|\\+|\alpha_3|=|\alpha|\\|\alpha|\le N}}\lambda^{\alpha}\left|\big(\nabla^{N-\alpha}\phi\big)(\lambda^{-1}\xi)\right||\xi|^{-|\alpha_1|-|\alpha_2|-|\alpha_3|}e^{-\frac{\nu}{2}|\xi|^2t}(1+\Omega t)^{|\alpha_1|}.\end{aligned}$$

Taking $N=4$, for any $\xi\in\{\xi:A^{-1}\lambda\le|\xi|\le A\lambda\}$ and for some constant A depending on the ring $\mathscr{C}$ and $\lambda\gtrsim\Omega$,

$$\left|(L^*)^4\big(\phi(\lambda^{-1}\xi)\widehat{\mathcal{G}}(t,\xi)\big)\right|\le C|\lambda x|^{-4}e^{-\frac{\nu}{4}|\xi|^2t},$$

which implies that

$$\int_{|x|\ge\frac{1}{\lambda}}|g(x,t)|\,dx\le Ce^{-c\lambda^2t}\lambda^3\int_{|x|\ge\frac{1}{\lambda}}|\lambda x|^{-4}\,dx\le Ce^{-c\lambda^2t},$$

which, together with (3-7), gives (3-6). Then the inequality (3-5) is proved. □

The following proposition is a direct consequence of Proposition 3.1.

Proposition 3.2. *Let $s,\sigma\in\mathbb{R}$, and $(p,q)\in[1,\infty]$. Then, for any $u\in\dot{\mathscr{B}}^{s-\frac{2}{q},\sigma-\frac{2}{q}}_{2,p}$, we have*

$$\|\mathcal{G}(t)u\|_{\widetilde{L}^q_T(\dot{\mathscr{B}}^{s,\sigma}_{2,p})}\le C\|u\|_{\dot{\mathscr{B}}^{s-\frac{2}{q},\sigma-\frac{2}{q}}_{2,p}}, \tag{3-8}$$

and for any $f\in\widetilde{L}^1_T\mathscr{B}^{s,\sigma}_{2,p}$, we have

$$\left\|\int_0^t\mathcal{G}(t-\tau)f(\tau)\,d\tau\right\|_{\widetilde{L}^q_T\big(\dot{\mathscr{B}}^{s+\frac{2}{q},\sigma+\frac{2}{q}}_{2,p}\big)}\le C\|f(t)\|_{\widetilde{L}^1_T(\dot{\mathscr{B}}^{s,\sigma}_{2,p})}. \tag{3-9}$$

Proof. Here we only prove (3-9). For any $2^j \geq \Omega$, we get by Proposition 3.1 that

$$\Big\|\Delta_j \int_0^t \mathcal{G}(t-\tau) f(\tau)\,d\tau\Big\|_{L^p} \leq C \int_0^t e^{-c(t-\tau)2^{2j}} \|\Delta_j f(\tau)\|_{L^p}\,d\tau,$$

from which, along with Young's inequality, it follows that

$$\Big\|\Delta_j \int_0^t \mathcal{G}(t-\tau) f(\tau)\,d\tau\Big\|_{L^q_T L^p} \leq C \big\|e^{-ct2^{2j}}\big\|_{L^q_T} \|\Delta_j f(\tau)\|_{L^1_T L^p} \leq C 2^{-\frac{2}{q}j} \|\Delta_j f(\tau)\|_{L^1_T L^p}. \tag{3-10}$$

Similarly, we also have

$$\Big\|\Delta_j \int_0^t \mathcal{G}(t-\tau) f(\tau)\,d\tau\Big\|_{L^q_T L^2} \leq C \big\|e^{-ct2^{2j}}\big\|_{L^q_T} \|\Delta_j f(\tau)\|_{L^1_T L^2} \leq C 2^{-\frac{2}{q}j} \|\Delta_j f(\tau)\|_{L^1_T L^2}.$$

Then the inequality (3-9) follows from (3-10) and (3-11). □

4. Bilinear estimates

We study the continuity of the inhomogeneous term in the space $E_{p,T}$ whose norm is defined by

$$\|u\|_{E_{p,T}} := \|u\|_{\widetilde{L}^\infty\left(0,T;\dot{\mathcal{B}}^{\frac12,\frac3p-1}_{2,p}\right)} + \|u\|_{\widetilde{L}^1\left(0,T;\dot{\mathcal{B}}^{\frac52,\frac3p+1}_{2,p}\right)}.$$

We define

$$B(u,v) := \int_0^t \mathcal{G}(t-\tau)\mathbb{P}\nabla\cdot(u\otimes v)\,d\tau,$$

where $\mathbb{P}$ denotes the Helmholtz projection which is bounded in the L^p space for $1 < p < \infty$.

Proposition 4.1. *Let $p \in [2,4]$. Assume that $u, v \in E_{p,T}$. There exists a constant C independent of Ω, u, v such that, for any $T > 0$,*

$$\|B(u,v)\|_{E_{p,T}} \leq C\|u\|_{E_{p,T}}\|v\|_{E_{p,T}}. \tag{4-1}$$

Proof. Thanks to Proposition 3.2, it suffices to show that

$$\|uv\|_{\widetilde{L}^1_T\dot{\mathcal{B}}^{\frac32,\frac3p}_{2,p}} \leq C\|u\|_{E_{p,T}}\|v\|_{E_{p,T}}. \tag{4-2}$$

From Bony's decomposition (2-2) and (2-1), we have

$$\begin{aligned}\Delta_j(uv) &= \sum_{|k-j|\leq 4}\Delta_j(S_{k-1}u\Delta_k v) + \sum_{|k-j|\leq 4}\Delta_j(S_{k-1}v\Delta_k u) + \sum_{k\geq j-2}\Delta_j(\Delta_k u\widetilde{\Delta}_k v)\\ &=: I_j + II_j + III_j.\end{aligned}$$

Set $J_j := \{(k', k) : |k - j| \le 4, k' \le k - 2\}$. Then for $2^j > \Omega$,

$$\|I_j\|_{L^1_T L^p} \le \sum_{J_j} \|\Delta_j(\Delta_{k'} u \Delta_k v)\|_{L^1_T L^p}$$
$$\le \Big(\sum_{J_{j,ll}} + \sum_{J_{,lh}} + \sum_{J_{j,hh}}\Big) \|\Delta_j(\Delta_{k'} u \Delta_k v)\|_{L^1_T L^p} := I_{j,1} + I_{j,2} + I_{j,3},$$

where

$$J_{j,ll} = \{(k', k) \in J_j : 2^{k'} \le \Omega, 2^k \le \Omega\},$$
$$J_{j,lh} = \{(k', k) \in J_j : 2^{k'} \le \Omega, 2^k > \Omega\},$$
$$J_{j,hh} = \{(k', k) \in J_j : 2^{k'} > \Omega, 2^k > \Omega\}.$$

We get by using Lemma 2.3 that

$$I_{j,1} \le C \sum_{(k',k)\in J_{j,ll}} \|\Delta_{k'} u\|_{L^\infty_T L^\infty} 2^{k(\frac{3}{2}-\frac{3}{p})} \|\Delta_k v\|_{L^1_T L^2}$$
$$\le C \sum_{(k',k)\in J_{j,ll}} 2^{\frac{k'}{2}} \|\Delta_{k'} u\|_{L^\infty_T L^2} 2^{k'} \|\Delta_k v\|_{L^1_T L^2} 2^{k(\frac{3}{2}-\frac{3}{p})}$$
$$\le C \|u\|_{\widetilde{L}^\infty_T \dot{\mathcal{B}}^{\frac{1}{2},\frac{3}{p}-1}_{2,p}} \|v\|_{\widetilde{L}^1_T \dot{\mathcal{B}}^{\frac{5}{2},\frac{3}{p}+1}_{2,p}} \sum_{(k',k)\in J_{j,ll}} 2^{(k'-k)} 2^{-\frac{3}{p}k}$$
$$\le C 2^{-\frac{3}{p}j} \|u\|_{\widetilde{L}^\infty_T \dot{\mathcal{B}}^{\frac{1}{2},\frac{3}{p}-1}_{2,p}} \|v\|_{\widetilde{L}^1_T \dot{\mathcal{B}}^{\frac{5}{2},\frac{3}{p}+1}_{2,p}},$$

where we used in the last inequality the fact that

$$\sum_{(k',k)\in J_{j,ll}} 2^{(k'-k)} 2^{-\frac{3}{p}k} \le \sum_{k'\le k-2} 2^{(k'-k)} \sum_{|k-j|\le 4} 2^{-\frac{3}{p}k} \le C 2^{-\frac{3}{p}j},$$

with C independent of j. Similarly, we have

$$I_{j,2} \le \sum_{(k',k)\in J_{j,lh}} \|\Delta_{k'} u\|_{L^\infty_T L^\infty} \|\Delta_k v\|_{L^1_T L^p}$$
$$\le C \sum_{(k',k)\in J_{j,lh}} 2^{\frac{k'}{2}} \|\Delta_{k'} u\|_{L^\infty_T L^2} 2^{k'} \|\Delta_k v\|_{L^1_T L^p}$$
$$\le C 2^{-\frac{3}{p}j} \|u\|_{\widetilde{L}^\infty_T \dot{\mathcal{B}}^{\frac{1}{2},\frac{3}{p}-1}_{2,p}} \|v\|_{\widetilde{L}^1_T \dot{\mathcal{B}}^{\frac{5}{2},\frac{3}{p}+1}_{2,p}}$$

and

$$\begin{aligned}I_{j,3} &\le \sum_{(k',k)\in J_{j,hh}} \|\Delta_{k'}u\|_{L^\infty_T L^\infty}\|\Delta_k v\|_{L^1_T L^p}\\ &\le C\sum_{(k',k)\in J_{j,hh}} 2^{k'(\frac{3}{p}-1)}\|\Delta_{k'}u\|_{L^\infty_T L^p}2^{k'}\|\Delta_k v\|_{L^1_T L^p}\\ &\le C2^{-\frac{3}{p}j}\|u\|_{\widetilde{L}^\infty_T\dot{\mathscr{B}}^{\frac12,\frac3p-1}_{2,p}}\|v\|_{\widetilde{L}^1_T\dot{\mathscr{B}}^{\frac52,\frac3p+1}_{2,p}}.\end{aligned}$$

On the other hand, for $2^j\le\Omega$, we have

$$\begin{aligned}\|I_j\|_{L^1_T L^2} &\le \sum_{J_j}\|\Delta_j(\Delta_{k'}u\Delta_k v)\|_{L^1_T L^2}\\ &\le \Big(\sum_{J_{j,ll}}+\sum_{J_{j,lh}}+\sum_{J_{j,hh}}\Big)\|\Delta_j(\Delta_{k'}u\Delta_k v)\|_{L^1_T L^2} := I_{j,4}+I_{j,5}+I_{j,6}.\end{aligned}$$

We get by using Lemma 2.3 that

$$\begin{aligned}I_{j,4} &\le C\sum_{(k,k')\in J_{j,ll}} 2^{\frac{k'}{2}}\|\Delta_{k'}u\|_{L^\infty_T L^2}2^{k'}\|\Delta_k v\|_{L^1_T L^2}\\ &\le C2^{-\frac{3j}{2}}\|u\|_{\widetilde{L}^\infty_T\dot{\mathscr{B}}^{\frac12,\frac3p-1}_{2,p}}\|v\|_{\widetilde{L}^1_T\dot{\mathscr{B}}^{\frac52,\frac3p+1}_{2,p}},\end{aligned}$$

and, noting that $p\le 4$,

$$\begin{aligned}I_{j,5} &\le C\sum_{(k,k')\in J_{j,lh}} \|\Delta_{k'}u\|_{L^\infty_T L^{\frac{2p}{p-2}}}\|\Delta_k v\|_{L^1_T L^p}\\ &\le C\sum_{(k,k')\in J_{j,lh}} 2^{\frac{k'}{2}}\|\Delta_{k'}u\|_{L^\infty_T L^2}2^{k'(\frac3p-\frac12)}\|\Delta_k v\|_{L^1_T L^p}\\ &\le C2^{-\frac{3j}{2}}\|u\|_{\widetilde{L}^\infty_T\dot{\mathscr{B}}^{\frac12,\frac3p-1}_{2,p}}\|v\|_{\widetilde{L}^1_T\dot{\mathscr{B}}^{\frac52,\frac3p+1}_{2,p}},\end{aligned}$$

and

$$\begin{aligned}I_{j,6} &\le C\sum_{(k,k')\in J_{j,hh}} \|\Delta_{k'}u\|_{L^\infty_T L^{\frac{2p}{p-2}}}\|\Delta_k v\|_{L^1_T L^p}\\ &\le C\sum_{(k,k')\in J_{j,hh}} 2^{k'(\frac3p-1)}\|\Delta_{k'}u\|_{L^\infty_T L^p}2^{k'(\frac3p-\frac12)}\|\Delta_k v\|_{L^1_T L^p}\\ &\le C2^{-\frac{3j}{2}}\|u\|_{\widetilde{L}^\infty_T\dot{\mathscr{B}}^{\frac12,\frac3p-1}_{2,p}}\|v\|_{\widetilde{L}^1_T\dot{\mathscr{B}}^{\frac52,\frac3p+1}_{2,p}}.\end{aligned}$$

Summing up the estimates for $I_{j,1}$ through $I_{j,6}$ yields that

$$\sup_{2^j>1} 2^{j\frac3p}\|I_j\|_{L^1_T L^p}+\sup_{2^j\le 1} 2^{\frac{3j}{2}}\|I_j\|_{L^1_T L^2}\le C\|u\|_{E_{p,T}}\|v\|_{E_{p,T}}. \tag{4-3}$$

By the same procedure as the one used to derive (4-3), we have

$$\sup_{2^j>1} 2^{j\frac{3}{p}}\|II_j\|_{L^1_TL^p}+\sup_{2^j\le 1}2^{\frac{3j}{2}}\|II_j\|_{L^1_TL^2}\le C\|u\|_{E_{p,T}}\|v\|_{E_{p,T}}. \tag{4-4}$$

Set $K_j:=\{(k,k'):k\ge j-3,|k'-k|\le 1\}$. Then we have

$$III_j=\Big(\sum_{K_{j,ll}}+\sum_{K_{j,lh}}+\sum_{K_{j,hl}}+\sum_{K_{j,hh}}\Big)\Delta_j(\Delta_k u\Delta_{k'}v):=III_{j,1}+III_{j,2}+III_{j,3}+III_{j,4},$$

where

$$\begin{aligned}K_{j,ll}&=\{(k,k')\in K_j:2^k\le\Omega,2^{k'}\le\Omega\},\\ K_{j,lm}&=\{(k,k')\in K_j:2^k\le\Omega,2^{k'}>\Omega\},\\ K_{j,hm}&=\{(k,k')\in K_j:2^k>\Omega,2^{k'}\le\Omega\},\\ K_{j,hh}&=\{(k,k')\in K_j:2^k>\Omega,2^{k'}>\Omega\}.\end{aligned}$$

We get by Lemma 2.3 that

$$\begin{aligned}\|III_{j,1}\|_{L^1_TL^p}&\le C2^{3j(1-\frac{1}{p})}\sum_{(k,k')\in K_{j,ll}}\|\Delta_k u\Delta_{k'}v\|_{L^1_TL^1}\\ &\le C2^{3j(1-\frac{1}{p})}\sum_{(k,k')\in K_{j,ll}}2^{\frac{k}{2}}\|\Delta_k u\|_{L^\infty_TL^2}2^{-\frac{k}{2}}2^{k'\frac{5}{2}}\|\Delta_{k'}v\|_{L^1_TL^2}2^{-k'\frac{5}{2}}\\ &\le C2^{3j(1-\frac{1}{p})}\|u\|_{\widetilde{L}^\infty_T\dot{\mathcal{B}}^{\frac{1}{2},\frac{3}{p}-1}_{2,p}}\|v\|_{\widetilde{L}^1_T\dot{\mathcal{B}}^{\frac{5}{2},\frac{3}{p}+1}_{2,p}}\sum_{(k,k')\in K_{j,ll}}2^{-\frac{k}{2}-\frac{5}{2}k'}\\ &\le C2^{-\frac{3}{p}j}\|u\|_{\widetilde{L}^\infty_T\dot{\mathcal{B}}^{\frac{1}{2},\frac{3}{p}-1}_{2,p}}\|v\|_{\widetilde{L}^1_T\dot{\mathcal{B}}^{\frac{5}{2},\frac{3}{p}+1}_{2,p}}\sum_{k\ge j-3}2^{-3(k-j)}\\ &\le C2^{-\frac{3}{p}j}\|u\|_{E_{p,T}}\|v\|_{E_{p,T}},\end{aligned}$$

and

$$\|III_{j,1}\|_{L^1_TL^2}\le C2^{\frac{3j}{2}}\sum_{(k,k')\in K_{j,ll}}\|\Delta_k u\Delta_{k'}v\|_{L^1_TL^1}\le C2^{-\frac{3j}{2}}\|u\|_{E_{p,T}}\|v\|_{E_{p,T}}.$$

Similarly, we obtain

$$\begin{aligned}&\|III_{j,2}+III_{j,3}\|_{L^1_TL^p}\\ &\quad\le C2^{\frac{3j}{2}}\sum_{(k,k')\in K_{j,lh}\cup K_{j,hl}}\|\Delta_k u\Delta_{k'}v\|_{L^1_TL^{\frac{2p}{2+p}}}\\ &\quad\le C2^{\frac{3j}{2}}\Big(\sum_{K_{j,lh}}\|\Delta_k u\|_{L^\infty_TL^2}\|\Delta_{k'}v\|_{L^1_TL^p}+\sum_{K_{j,hl}}\|\Delta_k u\|_{L^1_TL^p}\|\Delta_{k'}v\|_{L^\infty_TL^2}\Big)\\ &\quad\le C2^{-\frac{3}{p}j}\|u\|_{E,T}\|v\|_{E_{p,T}}\end{aligned}$$

and

$$\|III_{j,2}+III_{j,3}\|_{L^1_TL^2}\le C2^{\frac{3}{p}j}\sum_{(k,k')\in K_{j,lh}\cup K_{j,hl}}\|\Delta_ku\Delta_{k'}v\|_{L^1_TL^{\frac{2p}{2+p}}}$$
$$\le C2^{-\frac{3j}{2}}\|u\|_{E_{p,T}}\|v\|_{E_{p,T}}.$$

Finally, due to $2\le p\le 4$, we have

$$\|III_{j,4}\|_{L^1_TL^p}\le C2^{\frac{3}{p}j}\sum_{(k,k')\in K_{j,hh}}\|\Delta_ku\Delta_{k'}v\|_{L^1_TL^{\frac{p}{2}}}$$
$$\le C2^{\frac{3}{p}j}\sum_{(k,k')\in K_{j,hh}}\|\Delta_ku\|_{L^\infty_TL^p}\|\Delta_{k'}v\|_{L^1_TL^p}$$
$$\le C2^{-\frac{3}{p}j}\|u\|_{E_{p,T}}\|v\|_{E_{p,T}},$$

and

$$\|III_{j,4}\|_{L^1_TL^2}\le C2^{3j(\frac{2}{p}-\frac{1}{2})}\sum_{(k,k')\in K_{j,hh}}\|\Delta_ku\Delta_{k'}v\|_{L^1_TL^{\frac{p}{2}}}\le C2^{-\frac{3j}{2}}\|u\|_{E_{p,T}}\|v\|_{E_{p,T}}.$$

Summing up the estimates of $III_{j,1}$–$III_{j,4}$, we obtain

$$\sup_{2^j>1}2^{\frac{3}{p}j}\|III_j\|_{L^1_TL^p}+\sup_{2^j\le 1}2^{\frac{3j}{2}}\|III_j\|_{L^1_TL^2}\le C\|u\|_{E_{p,T}}\|v\|_{E_{p,T}}. \tag{4-5}$$

Then the inequality (4-2) can be deduced from (4-3)–(4-5). □

In order to prove the uniqueness of the solution in $C(\mathbb{R}^+;\dot H^{\frac12})$, we establish the following new bilinear estimate in the weighted time-space Besov space introduced in [Chen et al. 2008; 2010b].

Proposition 4.2. *Assume that* $u,v\in L^\infty_T(\dot B^{\frac12}_{2,\infty})$. *Then, for any* $T>0$, *we have*

$$\|B(u,v)\|_{L^\infty_T\dot B^{\frac12}_{2,\infty}}\le C\|u\|_{L^\infty_T\dot B^{\frac12}_{2,\infty}}\big\|\omega_{j,T}2^{\frac{j}{2}}\|\Delta_jv\|_{L^\infty_TL^2}\big\|_{l^\infty},$$

where

$$\omega_{j,T}:=\sup_{k\ge j}e_{k,T}2^{\frac12(j-k)},\quad e_{j,T}:=1-e^{-c2^{2j}T}.$$

Remark 4.3. The inequality $e_{j,T}\le\omega_{j,T}$ (top of page 277) is important to the following estimates. On the other hand, due to the fact $\lim_{T\to 0}\omega_{j,T}=0$, it can be proved that if $u\in C([0,T];\dot H^{\frac12})$, then, for any $\varepsilon>0$, one has

$$\big\|\omega_{j,T}2^{\frac{j}{2}}\|\Delta_jv\|_{L^\infty_TL^2}\big\|_{l^\infty}<\varepsilon\quad\text{if } T \text{ is small enough.}$$

This point is important in the proof of uniqueness.

Proof. First we note that $e_{j,T} \le \omega_{j,T}$ for any $j \in \mathbb{Z}$ and that

$$\omega_{j,T} \le 2^{\frac{1}{2}(j-j')}\omega_{j',T} \quad \text{if } j' \le j, \qquad \omega_{j,T} \le 2\omega_{j',T} \quad \text{if } j \le j'. \tag{4-6}$$

We get by Proposition 3.1 that

$$\begin{aligned} \|B(u,v)\|_{\dot{B}^{\frac{1}{2}}_{2,\infty}} &\le \sup_{j\in\mathbb{Z}} 2^{\frac{j}{2}} \int_0^t \left\|\mathcal{G}(t-\tau)\Delta_j \mathbb{P}\nabla\cdot(u\otimes v)\right\|_{L^2} d\tau \\ &\le \sup_{j\in\mathbb{Z}} 2^{\frac{3j}{2}} \left\|e^{-c2^{2j}t}\right\|_{L^1_T} \|\Delta_j(u\otimes v)\|_{L^\infty_T L^2} \\ &\le C\sup_{j\in\mathbb{Z}} 2^{-\frac{j}{2}} e_{j,T}\|\Delta_j(uv)\|_{L^\infty_T L^2}. \end{aligned} \tag{4-7}$$

We use Bony's decomposition to estimate $\|\Delta_j(uv)\|_{L^\infty_T L^2}$. Since $e_{j,T} \le \omega_{j,T}$ and thanks to (4-6), we have

$$\begin{aligned} \sum_{|k-j|\le 4} &\|\Delta_j(S_{k-1}u\Delta_k v)\|_{L^\infty_T L^2} \\ &\le C\|u\|_{L^\infty_T \dot{B}^{\frac{1}{2}}_{2,\infty}} \sum_{|k-j|\le 4} 2^k \|\Delta_k v\|_{L^\infty_T L^2} \\ &\le C\omega_{j,T}^{-1} 2^{\frac{j}{2}} \|u\|_{L^\infty_T \dot{B}^{\frac{1}{2}}_{2,\infty}} \left\|\omega_{k,T} 2^{\frac{k}{2}} \|\Delta_k v\|_{L^\infty_T L^2}\right\|_{l^\infty}, \end{aligned} \tag{4-8}$$

and, again by the same properties of $\omega_{j,T}$,

$$\begin{aligned} \|S_{k-1}v\|_{L^\infty} &\le \sum_{k'\le k-2} \|\Delta_{k'}v\|_{L^2} 2^{\frac{3}{2}k'} \le \left\|\omega_{k',T} 2^{\frac{k'}{2}} \|\Delta_{k'}v\|_{L^\infty_T L^2}\right\|_{l^\infty} \sum_{k'\le k-2} 2^{k'}\omega_{k',T}^{-1} \\ &\le 2^k \omega_{k,T}^{-1} \left\|\omega_{k',T} 2^{\frac{k'}{2}} \|\Delta_{k'}v\|_{L^\infty_T L^2}\right\|_{l^\infty}, \end{aligned}$$

which implies that

$$\begin{aligned} \sum_{|k-j|\le 4} &\|\Delta_j(S_{k-1}v\Delta_k u)\|_{L^\infty_T L^2} \\ &\le 2^{\frac{k}{2}} \omega_{k,T}^{-1} \|u\|_{L^\infty_T \dot{B}^{\frac{1}{2}}_{2,\infty}} \left\|\omega_{k',T} 2^{\frac{k'}{2}} \|\Delta_{k'}v\|_{L^\infty_T L^2}\right\|_{l^\infty}, \end{aligned} \tag{4-9}$$

and for the remainder term,

$$\begin{aligned} \sum_{k\ge j-2} &\left\|\Delta_j(\Delta_k u\widetilde{\Delta}_k v)\right\|_{L^\infty_T L^2} \\ &\le \sum_{k\ge j-2} 2^{\frac{3}{2}j} \left\|\Delta_j(\Delta_k u\widetilde{\Delta}_k v)\right\|_{L^\infty_T L^1} \\ &\le C\sum_{k\ge j-2} 2^{\frac{3}{2}j} \|\Delta_k u\|_{L^\infty_T L^2} \left\|\widetilde{\Delta}_k v\right\|_{L^\infty_T L^2} \\ &\le C\omega_{j,T}^{-1} 2^{\frac{j}{2}} \|u\|_{L^\infty_T \dot{B}^{\frac{1}{2}}_{2,\infty}} \left\|\omega_{k,T} 2^{\frac{k}{2}} \|\Delta_k v\|_{L^\infty_T L^2}\right\|_{l^\infty}. \end{aligned} \tag{4-10}$$

Substituting (4-8)–(4-10) into (4-7) concludes the proof. □

5. Proofs of Theorem 1.4 and Theorem 1.8

The proof of Theorem 1.4 is based on the following classical lemma.

Lemma 5.1 [Cannone 1995]. *Let X be an abstract Banach space and $B : X \times X \to X$ a bilinear operator, $\|\cdot\|$ being the X-norm, such that for any $x_1 \in X$ and $x_2 \in X$, we have*

$$\|B(x_1, x_2)\| \le \eta \|x_1\| \|x_2\|.$$

Then for any $y \in X$ such that

$$4\eta\|y\| < 1,$$

the equation

$$x = y + B(x, x)$$

has a solution x in X. Moreover, this solution x is the only one such that

$$\|x\| \le \frac{1 - \sqrt{1 - 4\eta\|y\|}}{2\eta}.$$

Proof of Theorem 1.4. Using the Stokes–Coriolis semigroup, we rewrite the system (1-1) as the integral form

$$u(x,t) = \mathscr{G}(t)u_0 - \int_0^t \mathscr{G}(t-\tau)\mathbb{P}\nabla\cdot(u \otimes u)\, d\tau := \mathscr{G}(t)u_0 + B(u,u). \tag{5-1}$$

Thanks to Proposition 3.2, we have

$$\|\mathscr{G}(t)u_0\|_{E_p} \le C\|u_0\|_{\dot{\mathscr{B}}^{\frac{1}{2},\frac{3}{p}-1}_{2,p}} \le Cc.$$

Obviously, $B(u, v)$ is bilinear, and we get by Proposition 4.1 that

$$\|B(u,v)\|_{E_p} \le C\|u\|_{E_p}\|v\|_{E_p}.$$

Taking c such that $4C^2c < \frac{3}{4}$, Lemma 5.1 ensures that the equation

$$u = \mathscr{G}(t)u_0 + B(u,u)$$

has a unique solution in the ball $\{u \in E_p : \|u\|_{E_p} \le \frac{1}{4C}\}$. □

Now we prove Theorem 1.8.

Proof of Theorem 1.8. We introduce a Banach space F_p whose norm is defined by

$$\|u\|_{F_p} := \|u\|_{\widetilde{L}^\infty(\mathbb{R}^+;\dot{H}^{\frac{1}{2}})} + \|u\|_{E_p}.$$

<u>Step 1</u>: existence in F_p. We define the map

$$\mathscr{T}u := \mathscr{G}(t)u_0 + B(u,u).$$

Next we prove that, if c is small enough, the map $\mathcal{T}$ has a unique fixed point in the ball

$$B_A := \{u \in F_p : \|u\|_{E_p} \le Ac, \|u\|_{F_p} \le A\|u_0\|_{\dot{H}^{\frac{1}{2}}}\},$$

for some $A > 0$ to be determined later. From Proposition 3.2 and Proposition 4.1, we infer that

$$\|\mathcal{T}u\|_{E_p} \le C\|u_0\|_{\mathcal{B}^{\frac{1}{2},\frac{3}{p}-1}_{2,p}} + C\|u\|^2_{E_p}. \tag{5-2}$$

On the other hand, we get by Proposition 3.1 that

$$\begin{aligned}
\|B(u,u)\|_{\tilde{L}^\infty(\mathbb{R}^+;\dot{H}^{\frac{1}{2}})} &\le \left\| \int_0^t \mathcal{G}(t-\tau)\mathbb{P}\nabla\cdot(u\otimes u)(\tau)\,d\tau \right\|_{\tilde{L}^\infty(\mathbb{R}^+;\dot{H}^{\frac{1}{2}})} \\
&\le C\biggl(\sum_{j\in\mathbb{Z}} 2^j \biggl(\sup_{t\in\mathbb{R}^+}\int_0^t \|\mathcal{G}(t-\tau)\Delta_j\mathbb{P}\nabla\cdot(u\otimes u)(\tau)\|_{L^2}\,d\tau\biggr)^2\biggr)^{\frac{1}{2}} \\
&\le C\left\| 2^{\frac{3}{2}j} \sup_{t\in\mathbb{R}^+}\int_0^t e^{-\tilde{c}2^{2j}t}\|\Delta_j(u\otimes u)\|_{L^2}\,d\tau \right\|_{l^2}.
\end{aligned} \tag{5-3}$$

In the following, we denote by $\{c_j\}_{j\in\mathbb{Z}}$ a sequence in l^2 with norm $\|\{c_j\}\|_{l^2(\mathbb{Z})} \le 1$. We get by Lemma 2.3 that

$$\begin{aligned}
\sup_{t\in\mathbb{R}^+}\int_0^t e^{-\tilde{c}2^{2j}t}\|\Delta_j(T_u u)\|_{L^2}\,d\tau
&\le \|e^{-\tilde{c}2^{2j}t}\|_{L^1(\mathbb{R}^+)} \sum_{|k-j|\le 4} \|\Delta_j(S_{k-1}u\Delta_k u)\|_{L^\infty(\mathbb{R}^+;L^2)} \\
&\le C2^{-2j}\|S_{k-1}u\|_{L^\infty(\mathbb{R}^+;L^\infty)} \sum_{|k-j|\le 4}\|\Delta_k u\|_{L^\infty(\mathbb{R}^+;L^2)} \\
&\le C\|u\|_{\tilde{L}^\infty\left(\mathbb{R}^+;\dot{\mathcal{B}}^{\frac{1}{2},\frac{3}{p}-1}_{2,p}\right)} 2^k 2^{-2j} \sum_{|k-j|\le 4}\|\Delta_k u\|_{L^\infty(\mathbb{R}^+;L^2)} \\
&\le C2^{-\frac{3}{2}j}\|u\|_{E_p} \sum_{|k-j|\le 4} 2^{\frac{(k-j)}{2}} 2^{\frac{k}{2}}\|\Delta_k u\|_{L^\infty(\mathbb{R}^+;L^2)} \\
&\le C2^{-\frac{3}{2}j} c_j \|u\|_{E_p}\|u\|_{\tilde{L}^\infty(\mathbb{R}^+;\dot{H}^{\frac{1}{2}})}.
\end{aligned} \tag{5-4}$$

The remainder term of uv is estimated by

$$
\begin{aligned}
\text{(5-5)} \quad \sup_{t\in\mathbb{R}^+}\int_0^t e^{-\tilde{c}2^{2j}t}\|\Delta_j R(u,u)\|_{L^2}\,d\tau
&\le \big\|e^{-\tilde{c}2^{2j}t}\big\|_{L^\infty(\mathbb{R}^+)}\sum_{k\ge j-2}\big\|\Delta_j(\Delta_k u\widetilde{\Delta}_k u)\big\|_{L^1(\mathbb{R}^+;L^2)}\\
&\le C\sum_{k\ge j-2}\big\|\widetilde{\Delta}_k u\big\|_{L^1(\mathbb{R}^+;L^\infty)}\|\Delta_k u\|_{L^\infty(\mathbb{R}^+;L^2)}\\
&\le C\|u\|_{\widetilde{L}^1\dot{\mathcal{B}}^{\frac{5}{2},\frac{3}{p}+1}_{2,p}}\sum_{k\ge j-2}2^{-k}\|\Delta_k u\|_{L^\infty(\mathbb{R}^+;L^2)}\\
&\le C\|u\|_{E_p}\sum_{k\ge j-2}2^{-\frac{3}{2}k}2^{\frac{1}{2}k}\|\Delta_k u\|_{L^\infty(\mathbb{R}^+;L^2)}\\
&\le C2^{-\frac{3}{2}j}c_j\|u\|_{E_p}\|u\|_{\widetilde{L}^\infty(\mathbb{R}^+;\dot{H}^{\frac{1}{2}})}.
\end{aligned}
$$

Combining (5-4)–(5-5) with (5-3) yields that

$$\|B(u,u)\|_{\widetilde{L}^\infty(\mathbb{R}^+;\dot{H}^{\frac{1}{2}})}\le C\|u\|_{E_p}\|u\|_{\widetilde{L}^\infty(\mathbb{R}^+;\dot{H}^{\frac{1}{2}})}.$$

It is easy to verify that

$$\|\mathcal{G}(t)u_0\|_{\widetilde{L}^\infty_T\dot{H}^{\frac{1}{2}}}\le C\|u_0\|_{\dot{H}^{\frac{1}{2}}}.$$

Consequently by (5-2) and the estimate

$$\|u_0\|_{\dot{\mathcal{B}}^{\frac{1}{2},\frac{3}{p}-1}_{2,p}}\le C\|u_0\|_{\dot{H}^{\frac{1}{2}}}$$

(which follows from Lemma 2.3 and the definition of the Besov space), we obtain

$$\text{(5-6)} \qquad \|\mathcal{T}u\|_{F_p}\le C\|u_0\|_{\dot{H}^{\frac{1}{2}}}+C\|u\|_{E_p}\|u\|_{F_p}.$$

Taking $A=2C$ and $c>0$ such that $2C^2c\le\frac{1}{2}$, it follows from (5-2) and (5-6) that the map $\mathcal{T}$ is a map from B_A to B_A. Similarly, it can be proved that $\mathcal{T}$ is also a contraction in B_A. Thus, the Banach fixed point theorem ensures that the map $\mathcal{T}$ has a unique fixed point in B_A.

Step 2: uniqueness in $C(\mathbb{R}^+;\dot{H}^{\frac{1}{2}})$. Let u_1 and u_2 be two solutions of (1-1) in $C(\mathbb{R}^+;\dot{H}^{\frac{1}{2}})$ with the same initial data u_0. We consider

$$
\begin{aligned}
u_1-u_2 = B\big(u_1-\mathcal{G}(t)u_0,u_1-u_2\big)+B\big(\mathcal{G}(t)u_0,u_1-u_2\big)\\
+B\big(u_1-u_2,u_2-\mathcal{G}(t)u_0\big)+B\big(u_1-u_2,\mathcal{G}(t)u_0\big).
\end{aligned}
$$

Then we get by Proposition 4.2 that

$$\begin{aligned}
(5\text{-}7)\quad & \sup_{t\in[0,T]} \|(u_1-u_2)(t)\|_{\dot B^{\frac12}_{2,\infty}} \\
&\le C \sup_{t\in[0,T]} \|(u_1-u_2)(t)\|_{\dot B^{\frac12}_{2,\infty}} \Big(\big\|\omega_{j,T} 2^{\frac{j}{2}} \|\Delta_j u_0\|_2 \big\|_{l^\infty} \\
&\qquad + \sup_{t\in[0,T]} \|u_1(t)-\mathcal{G}(t)u_0\|_{\dot H^{\frac12}} + \sup_{t\in[0,T]} \|u_2(t)-\mathcal{G}(t)u_0\|_{\dot H^{\frac12}} \Big),
\end{aligned}$$

where we used the fact $\omega_{j,T}\le 1$ so that

$$\big\|\omega_{j,T} 2^{\frac{j}{2}} \|\Delta_j u\|_{L^\infty_T L^2} \big\|_{l^\infty} \le \sup_{t\in[0,T]} \|u(t)\|_{\dot H^{\frac12}}.$$

Noticing that $\omega_{j,0}=0$ and $u_0\in \dot H^{\frac12}$, we have

$$\big\|\omega_{j,T} 2^{\frac{j}{2}} \|\Delta_j u_0\|_2 \big\|_{l^\infty} \le \frac{1}{3C},$$

for T small enough. On the other hand, since $u_1,\, u_2\in C(\mathbb{R}^+;\dot H^{\frac12})$, we also have

$$\sup_{t\in[0,T]} \|u_1-\mathcal{G}(t)u_0\|_{\dot H^{\frac12}} + \sup_{t\in[0,T]} \|u_2-\mathcal{G}(t)u_0\|_{\dot H^{\frac12}} \le \frac{1}{3C},$$

for T small enough. Then (5-7) ensures that $u_1(t)=u_2(t)$ for T small enough. Then, by a standard continuity argument, we conclude that $u_1=u_2$ on $[0,\infty)$. □

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PRESENTING SCHUR SUPERALGEBRAS

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We provide a presentation of the Schur superalgebra and its quantum analogue which generalizes the work of Doty and Giaquinto for Schur algebras. Our results include a basis for these algebras and a presentation using weight idempotents in the spirit of Lusztig's modified quantum groups.

1. Introduction

1.1. ***The Schur algebra.*** The Schur algebra plays a central role in the representation theory of $\mathrm{GL}(n)$ (e.g., see [Deng et al. 2008]). It is also the prototypical example of a quasihereditary algebra [Cline et al. 1988]. And, of course, it is at center stage in Schur–Weyl duality. If V denotes an n-dimensional vector space and $V^{\otimes d}$ denotes the d-fold tensor product of V with itself (all vector spaces and tensor products are over the rational numbers), then there is action of the symmetric group on d letters, Σ_d, on $V^{\otimes d}$ by permuting the tensor factors. With this notation we can define the Schur algebra by

$$S(n,d) = \mathrm{End}_{\Sigma_d}\big(V^{\otimes d}\big).$$

On the other hand the enveloping algebra of the Lie algebra $\mathfrak{gl}(n)$, $U(\mathfrak{gl}(n))$, has a natural action on V and, hence, on $V^{\otimes d}$. We could instead define $S(n,d)$ as the image of the resulting representation $U(\mathfrak{gl}(n)) \to \mathrm{End}_{\mathbb{Q}}(V^{\otimes d})$. Schur–Weyl duality implies these two definitions coincide. Thus the Schur algebra acts as a bridge between representations of $\mathfrak{gl}(n)$ and the symmetric group. The above story generalizes to the quantum setting if we replace the rational numbers with the rational functions in the indeterminate q, the symmetric group by its Iwahori–Hecke algebra, and the enveloping algebra by the quantum group associated to $\mathfrak{gl}(n)$. The resulting algebra is called the q-Schur algebra.

Because of the fundamental importance of the Schur and q-Schur algebras it is desirable to study them from as many perspectives as possible. Building on [Green 1996], Doty and Giaquinto [2002] provided a presentation of the Schur

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algebras by generators and relations. Since the enveloping algebra surjects onto the Schur algebra, the known generators and relations for $U(\mathfrak{gl}(n))$ yield generators and relations for the Schur algebra. But as $U(\mathfrak{gl}(n))$ is infinite dimensional and $S(n,d)$ is finite dimensional, there must be additional relations. Remarkably, Doty and Giaquinto prove that only two more, easy to state, relations are required. As an outcome of their calculations they obtain a basis and a presentation via weight idempotents reminiscent of Lusztig's modified quantum group, $\dot{\mathbf{U}}$. They also prove quantum analogues of all these results.

One notable application of the Doty–Giaquinto presentation, in [Li 2010], is a geometric realization of Schur algebras as a certain ring of constructible functions on generalized Steinberg varieties. We also see that their presentation of the q-Schur algebra is closely related to the geometric construction of the q-Schur algebras and quantum group $\mathbf{U}_q(\mathfrak{gl}(n))$ given by Beilinson, Lusztig, and MacPherson ([Beilinson et al. 1990]; see also [Deng et al. 2008, Part 5]).

1.2. ***The Schur superalgebra.*** There is a $\mathbb{Z}_2$-graded (i.e., "super") analogue of the above setup. Namely, now let $V = V_{\bar{0}} \oplus V_{\bar{1}}$ denote a $\mathbb{Z}_2$-graded vector space with the dimension of $V_{\bar{0}}$ equal to m and the dimension of $V_{\bar{1}}$ equal to n. We define $V^{\otimes d}$ as the d-fold tensor product of V with itself. The symmetric group Σ_d acts on $V^{\otimes d}$ by signed permutation of the tensor factors. The Schur superalgebra is then defined to be

$$S(m|n,d) = \mathrm{End}_{\Sigma_d}\big(V^{\otimes d}\big).$$

On the other hand the enveloping superalgebra of the Lie superalgebra $\mathfrak{gl}(m|n)$, $U(\mathfrak{gl}(m|n))$, has a natural action on V and, hence, on $V^{\otimes d}$. We could instead define $S(m|n,d)$ as the image of the resulting representation $U(\mathfrak{gl}(m|n)) \to \mathrm{End}_{\mathbb{Q}}(V^{\otimes d})$. The super version of Schur–Weyl duality implies these two definitions coincide [Berele and Regev 1987; Sergeev 1984]. Thus the Schur superalgebra acts as a bridge between representations of $\mathfrak{gl}(m|n)$ and the symmetric group. In positive characteristic this connection can be used to prove the Mullineux conjecture [Brundan and Kujawa 2003].

There is also a quantum version of this story. We again replace the rational numbers with the rational functions in the indeterminate q and the symmetric group by its Iwahori–Hecke algebra, and now replace the enveloping algebra by the quantum group associated to $\mathfrak{gl}(m|n)$. Schur–Weyl duality in this setting was established by Moon [2003] and Mitsuhashi [2006]. The resulting algebra is called the q-Schur superalgebra. Du and Rui [2011] have studied the representation theory and combinatorics of the q-Schur superalgebras.

1.3. ***Results.*** In this paper we generalize the results of Doty and Giaquinto to the Schur and q-Schur superalgebras. It should be noted that after obtaining the appropriate analogues of the ingredients used in [Doty and Giaquinto 2002], the final results are proved using the same arguments as in the nonsuper case. The main challenge is to correctly formulate and prove these analogues.

In Theorem 2.3.1 we obtain a presentation for the Schur superalgebra from the standard presentation of the enveloping algebra for $\mathfrak{gl}(m|n)$. We prove we only need to add two additional relations just as in the case of the Schur algebra. We then give an explicit basis for the Schur superalgebra and its integral form in Theorem 2.14.3. Finally, in Theorem 2.15.1 we prove that the Schur superalgebra admits a presentation using weight idempotents in a form reminiscent of Lusztig's modified quantum group.

We also prove the analogous results in the quantum setting. We use the quantum group $\mathbf{U} = U_q(\mathfrak{gl}(m|n))$ as presented by Zhang [1993] and prove in Theorem 3.3.1 that we need to add only two additional relations to the standard presentation of $\mathbf{U}$ to obtain the q-Schur superalgebra. We also provide a basis for the q-Schur superalgebra and an $\mathcal{A} = \mathbb{Z}[q, q^{-1}]$-form in Theorem 3.12.1. Finally, in Theorem 3.13.1 we prove that the q-Schur superalgebra admits a presentation via weight idempotents which is reminiscent of Lusztig's modified quantum group for $\mathfrak{gl}(n)$.

1.4. ***Future directions.*** The results of this paper open the door to a number of interesting avenues of research. Sergeev [1984] and Olshanski [1992], in the nonquantum and quantum cases, respectively, give a Schur–Weyl duality for the type Q Lie superalgebras. It would be interesting to obtain a presentation for the corresponding type Q Schur superalgebras. In a different direction, our presentation of the Schur and q-Schur superalgebras à la Doty–Giaquinto suggests the possibility of geometric constructions for $\mathfrak{gl}(m|n)$ in the spirit of [Beilinson et al. 1990; Li 2010]. In a third direction, in proving the quantum case we obtain the commutator formulas for the divided powers of root vectors and establish the existence of an $\mathcal{A} = \mathbb{Z}[q, q^{-1}]$-form for the quantum group $\mathbf{U}_q(\mathfrak{gl}(m|n))$. Although perhaps not surprising to experts, to our knowledge this has not appeared elsewhere in the literature. The existence of such a form allows one to consider representations at a root of unity and a super analogue of Lusztig's small quantum group as in [Lusztig 1990]. Finally, the existence of a presentation of the q-Schur superalgebra using weight idempotents suggests that Lusztig's modified quantum groups should have a super analogue. Lusztig's modified quantum group is a key ingredient to the categorification of the quantum group associated to $\mathfrak{sl}(n)$ (for example, as explained in [Lauda 2012]). Also see [Mackaay et al. 2010] and references therein for a discussion of categorifications of the q-Schur algebras. The categorification of quantum supergroups is currently an open problem and a super analogue of Lusztig's modified quantum group may be useful.

2. Nonquantum case

In this section all vector spaces will be over the rational numbers, $\mathbb{Q}$.

2.1. ***The Lie superalgebra $\mathfrak{gl}(m|n)$.*** Given a $\mathbb{Z}_2$-graded vector space $V = V_{\bar{0}} \oplus V_{\bar{1}}$ we write $\bar{v} \in \mathbb{Z}_2$ for the degree of a homogeneous element $v \in V$. For short we call v *even* (resp. *odd*) if $\bar{v} = \bar{0}$ (resp. $\bar{v} = \bar{1}$). Let us also introduce the following convenient notation. For fixed nonnegative integers m and n and $1 \le i \le m+n$ we define

$$\bar{i} = \begin{cases} \bar{0}, & \text{if } i \le m; \\ \bar{1}, & \text{if } i \ge m+1. \end{cases} \tag{1}$$

Let $\mathfrak{g} = \mathfrak{g}_{\bar{0}} \oplus \mathfrak{g}_{\bar{1}}$ denote the Lie superalgebra $\mathfrak{gl}(m|n)$. As a vector space $\mathfrak{g}$ is the set of $m+n$ by $m+n$ matrices. For $1 \le i, j \le m+n$ we set $E_{i,j}$ to be the matrix unit with a 1 in i-th row and j-th column. Then the set of matrix units forms a homogeneous basis for $\mathfrak{g}$. The $\mathbb{Z}_2$-grading on $\mathfrak{g}$ is defined by setting $\mathfrak{g}_{\bar{0}}$ to be the span of $E_{i,j}$ where $1 \le i, j \le m$ or $m+1 \le i, j \le m+n$ and $\mathfrak{g}_{\bar{1}}$ to be the span of the $E_{i,j}$ such that $m+1 \le i \le m+n$ and $1 \le j \le n$ or $1 \le i \le m$ and $m+1 \le j \le m+n$. That is, the degree of $E_{i,j}$ is $\bar{i} + \bar{j}$.

The Lie bracket on $\mathfrak{g}$ is given by the supercommutator:

$$[E_{ij}, E_{kl}] = \delta_{jk} E_{il} - (-1)^{\overline{E}_{ij}\overline{E}_{kl}} \delta_{il} E_{kj}. \tag{2}$$

By definition it is bilinear and so it suffices to define it on the basis of matrix units.

We fix $\mathfrak{h}$ to be the Cartan subalgebra of $\mathfrak{g}$ consisting of all diagonal matrices and let $\mathfrak{h}^*$ be its dual. Let $\varepsilon_i : \mathfrak{h} \to \mathbb{Q}$ be the linear map that takes an element of $\mathfrak{h}$ to its i-th diagonal entry. The set $\{\varepsilon_i \mid 1 \le i \le m+n\}$ forms a basis of $\mathfrak{h}^*$ and we define a bilinear form, $(\ ,\ )$, on $\mathfrak{h}^*$ by setting

$$(\varepsilon_i, \varepsilon_j) = (-1)^{\bar{i}} \delta_{ij}. \tag{3}$$

With our choice of Cartan subalgebra the root system of $\mathfrak{g}$ is

$$\Phi = \{\varepsilon_i - \varepsilon_j \mid 1 \le i \ne j \le m+n\}$$

and the matrix unit $E_{i,j}$ spans the $\varepsilon_i - \varepsilon_j$ root space. In particular there is a natural $\mathbb{Z}_2$-grading on Φ given by declaring that the root $\varepsilon_i - \varepsilon_j$ has degree $\overline{E}_{i,j} = \bar{i} + \bar{j}$. We fix the Borel subalgebra of $\mathfrak{g}$ given by taking all upper triangular matrices. Corresponding to this choice of Borel the positive roots are

$$\Phi^+ = \{\varepsilon_i - \varepsilon_j \mid 1 \le i < j \le m+n\}$$

and if we set $\alpha_i = \varepsilon_i - \varepsilon_{i+1}$, then $\{\alpha_1, \dots, \alpha_{m+n-1}\}$ are the simple roots. The simple roots have degree

$$\bar{\alpha}_i = \begin{cases} \bar{0}, & \text{if } i \neq m; \\ \bar{1}, & \text{if } i = m. \end{cases}$$

2.2. ***The Schur superalgebra.*** A $\mathfrak{g}$-(super)module is a $\mathbb{Z}_2$-graded vector space $M = M_{\bar{0}} \oplus M_{\bar{1}}$ which admits an action by $\mathfrak{g}$. The action respects the $\mathbb{Z}_2$-grading in that for any $r, s \in \mathbb{Z}_2$, if $x \in \mathfrak{g}_r$ and $m \in M_s$, then $x.m \in M_{r+s}$. The action also respects the Lie bracket in that for any homogeneous $x, y \in \mathfrak{g}$ and $m \in M$, we have

$$[x, y].m = x.(y.m) - (-1)^{\bar{x} \cdot \bar{y}} y.(x.m).$$

Note that here and elsewhere we give the condition only on homogeneous elements. The general case is obtained by linearity. As all modules will be $\mathbb{Z}_2$-graded, we choose to omit the prefix “super”.

The natural $\mathfrak{g}$-module, V, is the vector space of column vectors of height $m+n$. For $1 \leq i \leq m+n$, let v_i denote the element of V with a 1 in the i-th row and zeros elsewhere. Then the set $\{v_i \mid 1 \leq i \leq m+n\}$ defines a homogeneous basis for V with $\bar{v}_i = \bar{i}$ for $i = 1, \dots, m+n$. The action of $\mathfrak{g}$ on V is given by left multiplication.

We denote universal enveloping superalgebra of $\mathfrak{g}$ by U. It inherits a $\mathbb{Z}_2$-grading from $\mathfrak{g}$ and natural basis given by the PBW theorem for Lie superalgebras [Kac 1977, Section 1.1.3]. As for Lie algebras, a $\mathfrak{g}$-module can naturally be thought of as a U-module and vice versa. In particular, U admits a coproduct and so if M and N are $\mathfrak{g}$-modules, then $M \otimes N$ is again a $\mathfrak{g}$-module.

As it will be important in the calculations which follow, let us make this explicit. The coproduct $U \to U \otimes U$ is given on elements of $\mathfrak{g}$ by $x \mapsto x \otimes 1 + 1 \otimes x$. We use the convention that in any formula in which two homogenous elements have their order reversed, a sign is introduced which is -1 raised to the product of their degrees. Given a homogeneous element $x \in \mathfrak{g}$ and homogeneous $m \in M$ and $n \in N$, then the coproduct along with the sign convention implies that we have

$$x.(m \otimes n) = (x.m) \otimes n + (-1)^{\bar{x} \cdot \bar{m}} m \otimes (x.n).$$

In particular, for $d \geq 1$ we may define the d-fold tensor product of the natural module:

$$V^{\otimes d} := V \otimes V \otimes \cdots \otimes V.$$

Let

$$\rho_d : U \to \operatorname{End}_{\mathbb{Q}}\big(V^{\otimes d}\big)$$

denote the corresponding superalgebra homomorphism. We define the *Schur superalgebra* $S(m|n, d)$ to be the image of ρ_d. In particular, we can and will think of $S(m|n, d)$ as a quotient of U.

Note that the Schur superalgebra can also be defined as follows. There is a signed permutation action of the symmetric group on d letters, Σ_d, on $V^{\otimes d}$. The super analogue of Schur–Weyl duality [Berele and Regev 1987; Sergeev 1984] then shows that

$$S(m|n,d) = \mathrm{End}_{\Sigma_d}\big(V^{\otimes d}\big).$$

2.3. ***A presentation of the Schur superalgebra.*** Our first main result gives the Schur superalgebra by generators and relations. Here and throughout, if A is an associative superalgebra and $x, y \in A$ are homogeneous elements, then we write

$$[x, y] = xy - (-1)^{\bar{x}\cdot\bar{y}} yx.$$

For an element $x \in A$ the map $\operatorname{ad} x : A \to A$ is defined by $\operatorname{ad} x(y) = [x, y]$. Note that the bilinear form used in the following relations is the one introduced in (3).

Theorem 2.3.1. *The Schur superalgebra $S(m|n,d)$ is generated by homogeneous elements*

$$e_1, \dots, e_{m+n-1},\; f_1, \dots, f_{m+n-1},\; H_1, \dots, H_{m+n},$$

where the $\mathbb{Z}_2$-grading is given by setting $\bar{e}_m = \bar{f}_m = \bar{1}$, $\bar{e}_i = \bar{f}_i = \bar{0}$ for $i \neq m$, and $\overline{H}_i = \bar{0}$.

The following is a complete set of relations:

(R1) $[H_i, H_j] = 0$, *where* $1 \le i,\ j \le m+n$;

(R2) $[e_i, f_j] = \delta_{ij}\big(H_i - (-1)^{\bar{e}_i\cdot\bar{f}_j} H_{j+1}\big), \quad 1 \le i,\ j \le m+n-1$;

(R3) $[H_i, e_j] = (-1)^{\bar{i}}(\varepsilon_i, \alpha_j)e_j$ *and* $[H_i, f_j] = -(-1)^{\bar{i}}(\varepsilon_i, \alpha_j) f_j$, *where* $1 \le i \le m+n, \quad 1 \le j \le m+n-1$;

(R4) $[e_m, e_m] = 0, \quad (\operatorname{ad} e_i)^{1+|(\alpha_i,\alpha_j)|} e_j = 0, \quad$ *if* $1 \le i \neq j \le m+n-1$ *and* $i \neq m$, $[e_m, [e_{m-1}, [e_m, e_{m+1}]]] = 0, \quad$ *if* $m, n \ge 2$;

(R5) $[f_m, f_m] = 0, \quad (\operatorname{ad} f_i)^{1+|(\alpha_i,\alpha_j)|} f_j = 0, \quad$ *if* $1 \le i \neq j \le m+n-1$ *and* $i \neq m$, $[f_m, [f_{m-1}, [f_m, f_{m+1}]]] = 0, \quad$ *if* $m, n \ge 2$;

(R6) $H_1 + H_2 + \cdots + H_{m+n} = d$;

(R7) $H_i(H_i - 1)\cdots(H_i - d) = 0, \quad$ *where* $1 \le i \le m+n$.

2.4. ***Strategy and simplifications.*** The basic strategy of the proof of Theorem 2.3.1 is as in [Doty and Giaquinto 2002] and as follows. For short, let us write S for $S(m|n,d)$. Let T be the superalgebra given by the generators and relations in the theorem. The goal is to prove T is isomorphic to S as superalgebras. We first show that relations (R1)–(R7) hold in S. This implies we have a surjective homomorphism $T \to S$. We then prove that the dimension of T is no larger than the dimension of S by exhibiting a spanning set of T with cardinality equal to the dimension of S. See Section 2.14. This immediately implies that the map is an isomorphism and the spanning set is a basis.

Note that the universal enveloping superalgebra U is the superalgebra on the same generators but subject only to the relations (R1)–(R5) (see [Leites and Serganova 1992] or [Zhang 2011]). As $S(m|n,d)$ is a quotient of U via ρ_d it has the same generators but possibly additional relations. The content of Theorem 2.3.1 is that we only need to add relations (R6) and (R7) to obtain a presentation of $S(m|n,d)$.

As it will be helpful in later calculations, let us briefly pause to make explicit the connection between this presentation of U via generators and relations and the one obtained from the matrix realization of $\mathfrak{g}$ given in Section 2.1. If we write $E_{i,j}$ for the ij-matrix unit as in Section 2.1, then the isomorphism between these superalgebras is given on generators by $e_i \mapsto E_{i,i+1}$, $f_i \mapsto E_{i+1,i}$, and $H_i \mapsto E_{i,i}$. We identify these two realizations of U via this map. In particular, there is a canonical embedding $\mathfrak{g} \hookrightarrow U$ and we will identify $\mathfrak{g}$ with its image under this map.

As both S and T are quotients of U they are both generated by the images of generators of U. To lighten notation, we choose to use the same notation for algebra elements which can be viewed in more than one of these algebras. In particular, we write e_i, f_i, and H_i for the generators of U and their images in S and T. We will endeavor to always be clear in which algebra we are working. If the algebra is not explicitly stated, then the calculation holds for all three algebras U, S, and T.

We will also frequently make use of the fact that the inclusion

$$\mathfrak{gl}(m) \oplus \mathfrak{gl}(n) \cong \mathfrak{g}_{\bar{0}} \subseteq \mathfrak{gl}(m|n)$$

induces an inclusion

$$U(\mathfrak{gl}(m) \oplus \mathfrak{gl}(n)) \hookrightarrow U(\mathfrak{gl}(m|n)).$$

Thus any computation involving purely even elements will carry over from [Doty and Giaquinto 2002]. More generally, when calculations are essentially identical to those in that paper we will usually leave them to the reader.

2.5. ***The new relations.*** We now observe that (R6) and (R7) hold in S.

Lemma 2.5.1. *Under the representation $\rho_d : U \to \mathrm{End}(V^{\otimes d})$ the elements $H_1, \dots, H_{m+n}$ in S satisfy the relations* (R6) *and* (R7). *Moreover, the relation* (R7) *is the minimal polynomial of H_i in* $\mathrm{End}_{\mathbb{Q}}(V^{\otimes d})$.

Proof. Since the elements $H_1, \dots, H_{m+n}$ are purely even, this follows from [Doty and Giaquinto 2002, Lemma 4.1]. □

As explained above, this implies the surjection $\rho_d : U \to S$ factors through T and we obtain a surjective superalgebra homomorphism, $T \to S$. To prove that this map is an isomorphism it suffices to show that their dimensions are equal by obtaining an explicit basis for T and, hence, for $S(m|n,d)$. In fact it turns out to be no harder to work over the integers and so we obtain a basis for an integral form, $S(m|n,d)_{\mathbb{Z}}$, of the Schur superalgebra.

2.6. *Divided powers.* Let A denote any of U, S, or T. Recall from Section 2.4 that we identify $\mathfrak{gl}(m|n)$ as a subspace of U. For each $\alpha = \varepsilon_i - \varepsilon_j \in \Phi^+$ we use this identification and write x_α for the image in A of the matrix unit $E_{i,j}$. We call x_α a *root vector*. For $x \in A$ and $k \in \mathbb{Z}_{\geq 0}$, define the *$k$-th divided power of x* to be

$$x^{(k)} = \frac{x^k}{k!}.$$

In particular, we have the divided powers of the root vectors, $x_\alpha^{(r)}$, for all $\alpha \in \Phi$ and $r \geq 0$.

We define

$$\Lambda(m|n) = \{\lambda = (\lambda_1, \dots, \lambda_{m+n}) \mid \lambda_i \in \mathbb{Z}, \lambda_i \geq 0 \text{ for } 1 \leq i \leq m+n\}.$$

Given any tuple of integers λ (e.g., $\lambda \in \Lambda(m|n)$), let $|\lambda|$ denote the sum of those integers. Using this we define

$$\Lambda(m|n,d) = \{\lambda \in \Lambda(m|n) \mid |\lambda| = d\}.$$

For $i = 1, \dots, m+n$ and $k \geq 0$ define an element of A by

$$\binom{H_i}{k} = \frac{H_i(H_i-1)\cdots(H_i-k+1)}{k!},$$

where, by definition,

$$\binom{H_i}{0} = 1.$$

2.7. *The Kostant $\mathbb{Z}$-form.* We now define analogues of the Kostant $\mathbb{Z}$-form. We also take this opportunity to introduce certain subalgebras which will be needed in what follows. Let A denote U, S, or T. Let A^0 denote the subsuperalgebra of A generated by $H_1, \dots, H_{m+n}$. In particular, if A is S or T, then it is clear that A^0 is the image of U^0 respectively, under the quotient map.

The *Kostant $\mathbb{Z}$-form* for A is denoted by $A_{\mathbb{Z}}$ and it is defined to be the subring of A generated by

$$\{e_i^{(k)}, f_i^{(k)} \mid i = 1, \dots, m+n-1, k \geq 0\} \cup \left\{\binom{H_i}{k} \mid i = 1, \dots, m+n, k \geq 0\right\}.$$

Moreover, we set $A_{\mathbb{Z}}^0$ to be the intersection of A^0 with $A_{\mathbb{Z}}$. For A equal to S or T, it is clear that $A_{\mathbb{Z}}$ and $A_{\mathbb{Z}}^0$ are nothing but the image of $U_{\mathbb{Z}}$ and $U_{\mathbb{Z}}^0$, respectively, under the quotient map.

2.8. ***The weight idempotents.*** We begin by investigating the structure of T^0 and $T^0_{\mathbb{Z}}$. For $\lambda = (\lambda_i) \in \Lambda(m|n)$ we define

$$H_\lambda = \prod_{i=1}^{m+n} \binom{H_i}{\lambda_i}.$$

Note that as $H_1, \dots, H_{m+n}$ commute the product can be taken in any order. When $\lambda \in \Lambda(m|n, d)$ it is convenient to set the notation

$$1_\lambda = H_\lambda.$$

Because of part (b) of the following proposition we refer to these elements as *weight idempotents*.

Proposition 2.8.1. *Let I^0 be the ideal of U^0 generated by the elements*

$$H_1 + H_2 + \cdots + H_{m+n} - d \quad \text{and} \quad H_i(H_i - 1)\cdots(H_i - d)$$

for $i = 1, \dots, m+n$. Then

(a) *we have a superalgebra isomorphism $U^0/I^0 \cong T^0$;*

(b) *the set $\{1_\lambda \mid \lambda \in \Lambda(m|n, d)\}$ is a $\mathbb{Q}$-basis for T^0 and a $\mathbb{Z}$-basis for $T^0_{\mathbb{Z}}$. Moreover, they give a set of pairwise orthogonal idempotents which sum to the identity;*

(c) *in T^0 we have $H_\lambda = 0$ for any $\lambda \in \Lambda(m|n)$ such that $|\lambda| > d$.*

Proof. Since the elements $H_1, \dots, H_{m+n}$ are purely even, this follows from [Doty and Giaquinto 2002, Proposition 4.2]. □

Proposition 2.8.2. *Let $1 \le i \le m+n$, $k \in \mathbb{Z}_{\ge 0}$, $\lambda \in \Lambda(m|n, d)$, and $\mu \in \Lambda(m|n)$. We have the following identities in the superalgebra T^0:*

(1) $H_i 1_\lambda = \lambda_i 1_\lambda, \quad \binom{H_i}{k} 1_\lambda = \binom{\lambda_i}{k} 1_\lambda;$

(2) $H_\mu 1_\lambda = \lambda_\mu 1_\lambda, \quad$ *where* $\lambda_\mu = \prod_i \binom{\lambda_i}{\mu_i};$

(3) $H_\mu = \sum_{\lambda \in \Lambda(m|n,d)} \lambda_\mu 1_\lambda.$

Proof. They follow from [Doty and Giaquinto 2002, Proposition 4.3]. □

2.9. ***The root vectors.*** We continue to let A denote any of U, S, or T. Recall from Section 2.6 that for each $\alpha \in \Phi$ we have the root vector $x_\alpha \in A$. In particular, note that x_α is homogeneous and $\bar{x}_\alpha = \bar{\alpha}$, where the grading on roots is as given in Section 2.1. Given $\alpha = \varepsilon_i - \varepsilon_j \in \Phi$, we set

$$H_\alpha = H_i - (-1)^{\bar{x}_\alpha} H_j.$$

Given $\alpha = \varepsilon_i - \varepsilon_j$, $\beta = \varepsilon_k - \varepsilon_l \in \Phi$ such that $\alpha + \beta \in \Phi$, we define

$$c_{\alpha,\beta} = \begin{cases} 1, & \text{if } j = k; \\ -(-1)^{\bar{x}_\alpha \bar{x}_\beta}, & \text{if } i = l. \end{cases} \tag{4}$$

Using this notation, (2) implies the following commutator formula for root vectors in A.

Lemma 2.9.1. *Let $\alpha, \beta \in \Phi$ and say $\alpha = \varepsilon_i - \varepsilon_j$ and $\beta = \varepsilon_k - \varepsilon_l$. We have*

$$[x_\alpha, x_\beta] = \begin{cases} H_\alpha, & \text{if } \alpha + \beta = 0; \\ c_{\alpha,\beta} x_{\alpha+\beta}, & \text{if } \alpha + \beta \in \Phi; \\ 0, & \text{otherwise}. \end{cases}$$

We also note that an easy induction proves that for all $a, b \geq 0$ and $\alpha \in \Phi$ we have

$$x_\alpha^{(a)} x_\alpha^{(b)} = \binom{a+b}{a} x_\alpha^{(a+b)}. \tag{5}$$

2.10. ***Commutation relations between root vectors and weight idempotents.*** We now compute the commutation relations between root vectors and weight idempotents.

Proposition 2.10.1. *For any $\alpha \in \Phi$, $\lambda \in \Lambda(m|n, d)$ we have the commutation formulas*

$$x_\alpha 1_\lambda = \begin{cases} 1_{\lambda+\alpha} x_\alpha, & \text{if } \lambda + \alpha \in \Lambda(m|n, d); \\ 0, & \text{otherwise}, \end{cases}$$

and

$$1_\lambda x_\alpha = \begin{cases} x_\alpha 1_{\lambda-\alpha}, & \text{if } \lambda - \alpha \in \Lambda(m|n, d); \\ 0, & \text{otherwise}. \end{cases}$$

Proof. Although analogous to [Doty and Giaquinto 2002, Proposition 4.5], the proof involves keeping track of signs so we include it. We first note that (2) implies for all $l = 1, \ldots, m+n$ and $\alpha \in \Phi$ we can use the parity function given in (1) and the bilinear form given in (3) to write

$$[H_l, x_\alpha] = (-1)^{\bar{l}} (\varepsilon_l, \alpha) x_\alpha. \tag{6}$$

Now say $\alpha = \varepsilon_i - \varepsilon_j$. Using (6) we obtain

$$x_\alpha 1_\lambda = \Big(\prod_{l\neq i,j}\binom{H_l}{\lambda_l}\Big)\binom{H_i-(-1)^{\bar{i}}(\varepsilon_i,\alpha)}{\lambda_i}\binom{H_j-(-1)^{\bar{j}}(\varepsilon_j,\alpha)}{\lambda_j}x_\alpha$$
$$= \Big(\prod_{l\neq i,j}\binom{H_l}{\lambda_l}\Big)\binom{H_i-(-1)^{\bar{i}}(-1)^{\bar{i}}}{\lambda_i}\binom{H_j-(-1)^{\bar{j}}(-(-1)^{\bar{j}})}{\lambda_j}x_\alpha$$
$$= \Big(\prod_{l\neq i,j}\binom{H_l}{\lambda_l}\Big)\binom{H_i-1}{\lambda_i}\binom{H_j+1}{\lambda_j}x_\alpha.$$

Multiplying on the left by $\dfrac{H_i}{\lambda_i+1}$ and using the fact that $H_i x_\alpha = x_\alpha(H_i+1)$, we get

$$x_\alpha\frac{H_i+1}{\lambda_i+1}1_\lambda = \frac{H_i}{\lambda_i+1}\binom{H_i-1}{\lambda_i}\binom{H_j+1}{\lambda_j}\Big(\prod_{l\neq i,j}\binom{H_l}{\lambda_l}\Big)x_\alpha,$$

which, using Proposition 2.8.2, simplifies to

(7)
$$x_\alpha 1_\lambda = \Big(\binom{H_i}{\lambda_i+1}\binom{H_j+1}{\lambda_j}\prod_{l\neq i,j}\binom{H_l}{\lambda_l}\Big)x_\alpha.$$

If $\lambda_j > 0$, then this can be rewritten as

$$x_\alpha 1_\lambda = \binom{H_i}{\lambda_i+1}\Big(\binom{H_j}{\lambda_j}+\binom{H_j}{\lambda_j-1}\Big)\prod_{l\neq i,j}\binom{H_l}{\lambda_l}x_\alpha.$$

The first summand on the right-hand side of the preceding equality vanishes by Proposition 2.8.1. This proves the first part of the proposition in the case $\lambda_j > 0$. If $\lambda_j = 0$, then (7) can be written as

$$x_\alpha 1_\lambda = \Big(\binom{H_i}{\lambda_i+1}\prod_{l\neq i,j}\binom{H_l}{\lambda_l}\Big)x_\alpha = H_\mu x_\alpha,$$

where $\mu = (\lambda_1,\dots,\lambda_i+1,\dots,\lambda_{j-1},0,\dots,\lambda_{m+n})$. But then $|\mu| = |\lambda|+1 > d$ and hence the right-hand side is zero by Proposition 2.8.1. This proves the first statement. The proof of the second is similar. □

2.11. ***Commutation relations between divided powers of root vectors.*** We now compute the commutation formulas between divided powers of root vectors, but first we make a simplifying observation. If the root vector x_α is odd (i.e., if α is an odd root), then in $\mathfrak{g}$ we have $[x_\alpha, x_\alpha] = 0$. But in U and, hence, in S and T, we have $[x_\alpha, x_\alpha] = 2x_\alpha^2$. Taken together, this implies

$$x_\alpha^2 = 0$$

in U, S, and T for all odd $\alpha \in \Phi$. That is, for odd roots we only need to consider root vectors of divided power one.

Lemma 2.11.1. *Let α, $\beta \in \Phi$ and r, $s \in \mathbb{Z}_{\geq 0}$.*

(1) *If $\bar{x}_\alpha = 0$ and $\bar{x}_\beta = 0$, then*

(8)
$$x_\alpha^{(r)} x_\beta^{(s)} = \begin{cases} x_\beta^{(s)} x_\alpha^{(r)} + \displaystyle\sum_{j=1}^{\min(r,s)} x_\beta^{(s-j)} \binom{H_\alpha - r - s + 2j}{j} x_\alpha^{(r-j)}, & \text{if } \alpha + \beta = 0; \\ x_\beta^{(s)} x_\alpha^{(r)} + \displaystyle\sum_{j=1}^{\min(r,s)} c_{\alpha,\beta}^j x_\beta^{(s-j)} x_{\alpha+\beta}^{(j)} x_\alpha^{(r-j)}, & \text{if } \alpha + \beta \in \Phi; \\ x_\beta^{(s)} x_\alpha^{(r)}, & \text{otherwise}. \end{cases}$$

(2) *If $\bar{x}_\alpha = 0$ and $\bar{x}_\beta = 1$, then*

$$x_\alpha^{(r)} x_\beta^{(1)} = \begin{cases} x_\beta^{(1)} x_\alpha^{(r)} + c_{\alpha,\beta} x_{\alpha+\beta} x_\alpha^{(r-1)}, & \text{if } \alpha + \beta \in \Phi; \\ x_\beta^{(1)} x_\alpha^{(r)}, & \text{if } \alpha + \beta \notin \Phi. \end{cases} \tag{9}$$

(3) *If $\bar{x}_\alpha = 1$ and $\bar{x}_\beta = 0$, then*

$$x_\alpha^{(1)} x_\beta^{(r)} = \begin{cases} x_\beta^{(r)} x_\alpha^{(1)} + c_{\alpha,\beta} x_{\alpha+\beta} x_\beta^{(r-1)}, & \text{if } \alpha + \beta \in \Phi; \\ x_\beta^{(r)} x_\alpha^{(1)}, & \text{if } \alpha + \beta \notin \Phi. \end{cases} \tag{10}$$

(4) *If $\bar{x}_\alpha = 1$ and $\bar{x}_\beta = 1$, then*

$$x_\alpha^{(1)} x_\beta^{(1)} = \begin{cases} -x_\beta^{(1)} x_\alpha^{(1)} + H_\alpha, & \text{if } \alpha + \beta = 0; \\ -x_\beta^{(1)} x_\alpha^{(1)} + x_{\alpha+\beta}, & \text{if } \alpha + \beta \in \Phi; \\ -x_\beta^{(1)} x_\alpha^{(1)}, & \text{otherwise}. \end{cases} \tag{11}$$

Proof. As (8) involves purely even root vectors, it follows from the classical case (see [Doty and Giaquinto 2002, Equations (5.11a)–(5.11c)]). Equations (9) and (10) are verified by a straightforward induction on r. Equation (11) follows directly from Lemma 2.9.1. □

2.12. *Kostant monomials and content functions.* Any product in A of nonzero elements of the form

$$x_\alpha^{(r)}, \quad \binom{H_i}{s}, \tag{12}$$

taken in any order and for any $r, s \in \mathbb{Z}_{\geq 0}$, $\alpha \in \Phi$, $1 \leq i \leq m+n$, will be called a *Kostant monomial*. Note that by [Kujawa 2006, Lemma 2.1] the set of Kostant monomials span $U_\mathbb{Z}$ and, hence, $T_\mathbb{Z}$ and $S_\mathbb{Z}$. The goal is to find a subset of Kostant monomials which will provide a basis for $T_\mathbb{Z}$.

We now introduce the content function on Kostant monomials. They will be used as a bookkeeping device in the proof of Proposition 2.14.1. It is defined just as in the classical case [Doty and Giaquinto 2002, Section 2].

The *content function*

$$\chi : \{\text{Kostant monomials}\} \to \bigoplus_{i=1}^{m+n} \mathbb{Z}\varepsilon_i \tag{13}$$

is defined as follows. We first define it on the elements in (12). If $\alpha = \varepsilon_i - \varepsilon_j \in \Phi$ and $r \geq 1$, then

$$\chi(x_\alpha^{(r)}) = r\varepsilon_{\max(i,j)}.$$

If $i = 1, \dots, m+n$ and $r \geq 1$, then

$$\chi\left(\binom{H_i}{r}\right) = 0.$$

We then extend this definition by declaring $\chi(XY) = \chi(X) + \chi(Y)$ whenever X, Y are Kostant monomials.

We also define a *left content function*, χ_L, and *right content function*, χ_R, on the elements given in (12) by

$$\chi_L(x_\alpha^{(r)}) = r\varepsilon_i, \quad \chi_R(x_\alpha^{(r)}) = r\varepsilon_j, \quad \chi_L\left(\binom{H_i}{s}\right) = \chi_R\left(\binom{H_i}{s}\right) = 0.$$

They are defined on general Kostant monomials using the rules $\chi_L(XY) = \chi_L(X) + \chi_L(Y)$ and $\chi_R(XY) = \chi_R(X) + \chi_R(Y)$ for any Kostant monomials X and Y.

In what follows we view elements in the image of the content functions as elements of $\Lambda(m|n)$ via the map

$$\sum_{i=1}^{m+n} a_i\varepsilon_i \mapsto (a_1, \dots, a_{m+n}). \tag{14}$$

2.13. ***A lemma on content functions.*** To label the elements of our basis for the Schur superalgebra, we need to define the following set of tuples of nonnegative integers indexed by the positive roots of $\mathfrak{g}$:

(15)

$$P(m|n) = \left\{A = (A(\alpha))_{\alpha\in\Phi^+} \mid A(\alpha) \in \mathbb{Z}_{\geq 0} \text{ if } \bar{\alpha} = \bar{0} \text{ and } A(\alpha) \in \{0, 1\} \text{ if } \bar{\alpha} = \bar{1}\right\}.$$

Fix an order on Φ^+. For $A = (A(\alpha)) \in P(m|n)$ we define

$$e_A = \prod_{\alpha\in\Phi^+} x_\alpha^{(A(\alpha))}, \quad f_A = \prod_{\alpha\in\Phi^+} x_{-\alpha}^{(A(\alpha))},$$

where the products defining e_A and f_A are taken according to the fixed order on Φ^+.

The last ingredient we need is the following partial order on $\Lambda(m|n)$. It is defined by declaring for $\lambda = (\lambda_i)$, $\mu = (\mu_i)$ in $\Lambda(m|n)$ that

$$\lambda \preceq \mu \tag{16}$$

if and only if $\lambda_i \leq \mu_i$ for $i = 1, \dots, m+n$.

Lemma 2.13.1. *For $A = (A(\alpha)),\ C = (C(\alpha)) \in P(m|n)$, $\lambda \in \Lambda(m|n)$ we have*

$$\chi(e_A 1_\lambda f_C) \preceq \lambda \quad \textit{if and only if} \quad \chi_L(1_{\lambda'} e_A f_C) \preceq \lambda'$$
$$\textit{if and only if} \quad \chi_R(e_A f_C 1_{\lambda''}) \preceq \lambda'',$$

where

$$\lambda' := \lambda + \sum_{\alpha \in \Phi^+} A(\alpha)\alpha, \quad \lambda'' := \lambda + \sum_{\alpha \in \Phi^+} C(\alpha)\alpha.$$

Proof. As our content functions are defined just as in [Doty and Giaquinto 2002], the proof of Lemma 5.1 there applies verbatim. □

2.14. ***A basis for the Schur superalgebra.*** Let us define the set

$$Y = \bigcup_{\substack{\lambda \in \Lambda(m|n,d) \\ A,C \in P(m|n)}} \{ e_A 1_\lambda f_C \mid \chi(e_A f_C) \preceq \lambda \}.$$

Note that we have the following alternate descriptions of Y. Following from Proposition 2.10.1 we have

$$e_A 1_\lambda f_C = 1_{\lambda'} e_A f_C = e_A f_C 1_{\lambda''},$$

where λ' and λ'' are as above. Using this and Lemma 2.13.1 we can characterize Y as

$$Y = \bigcup_{\substack{\lambda' \in \Lambda(m|n,d) \\ A,C \in P(m|n)}} \{ 1_{\lambda'} e_A f_C \mid \chi_L(e_A f_C) \preceq \lambda' \} = \bigcup_{\substack{\lambda'' \in \Lambda(m|n,d) \\ A,C \in P(m|n)}} \{ e_A f_C 1_{\lambda''} \mid \chi_R(e_A f_C) \preceq \lambda'' \}.$$

Finally we are prepared to give a basis for T.

Proposition 2.14.1. *The set Y spans the $\mathbb{Z}$-superalgebra $T_\mathbb{Z}$.*

Proof. The proof is exactly parallel to the proof of [Doty and Giaquinto 2002, Proposition 5.2]. Namely, as discussed in Section 2.12, the Kostant monomials span $T_\mathbb{Z}$. From Proposition 2.8.1 we in fact know that $T_\mathbb{Z}$ is spanned by Kostant monomials consisting of products of divided powers of root vectors and weight idempotents. Given such a Kostant monomial, we may use Proposition 2.10.1 to move all weight idempotents to the right-hand side of the Kostant monomial. Thus it suffices to show that Kostant monomials consisting of products of divided powers of root vectors can be written as an integral linear combination of elements in Y. This is done by inducting on the degree and content of the monomial using the commutation formulas. As our content formula and commutation formulas are of the same form as in [Doty and Giaquinto 2002], the inductive argument used there applies here without change. The only difference appears when we use the commutation formulas given in Lemma 2.11.1. Extra signs appear but all coefficients remain integral and this is all that is needed for the proof.

We also need that for all $s, t \in \mathbb{Z}_{\geq 0}$, the term $\binom{H_\alpha - t}{s}$ in (8) belongs to $T^0_{\mathbb{Z}}$. As these elements are purely even this follows from the remark after [ibid., (5.11)]. It can also be verified directly by an inductive argument using the identity

$$\binom{H_\alpha - 1}{s} = \binom{H_\alpha}{s} - \binom{H_\alpha - 1}{s-1}. \qquad \square$$

Lemma 2.14.2. *The cardinality of the set Y is equal to the dimension of the Schur superalgebra.*

Proof. By [Donkin 2001, Section 2.3] the dimension of the Schur superalgebra is equal to the number of monomials of total degree d in the free supercommutative superalgebra in $m^2 + n^2$ even variables and $2mn$ odd variables. Equivalently, the dimension of S is the same as the number of monomials in $m^2 + n^2 - 1$ even variables and $2mn$ odd variables of total degree not exceeding d. From this it is immediate that the dimension of S is the same as the cardinality of the set

$$P = \{e_A H_B f_C \mid B = (B_i) \in \Lambda(m|n);\ B_1 = 0;\ A, C \in P(m|n), |A| + |B| + |C| \leq d\}.$$

Thus to prove the lemma it suffices to give a bijection between P and Y. Define the map $P \to Y$ by

$$e_A H_B f_C \mapsto e_A 1_\lambda f_C,$$

where $\lambda = (d - |A| - |B| - |C|)\varepsilon_1 + B + \chi(e_A f_C)$. The inverse map is given by

$$e_A 1_\lambda f_C \mapsto e_A H_B f_C,$$

where $B = \lambda - \chi(e_A f_C) - \lambda_1 \varepsilon_1$. This completes the proof of the lemma. $\square$

As T surjects onto $S(m|n, d)$, it immediately follows from the previous two results that Y is a basis for the Schur superalgebra and its integral form and that T and S are isomorphic. Therefore we have proven Theorem 2.3.1 and the following result.

Theorem 2.14.3. *The set*

$$Y = \bigcup_{\lambda \in \Lambda(m|n,d)} \{e_A 1_\lambda f_C \mid A, C \in P(m|n), \chi(e_A f_C) \preceq \lambda\}$$

is a $\mathbb{Q}$-basis for $S(m|n, d)$ and a $\mathbb{Z}$-basis for $S(m|n, d)_{\mathbb{Z}}$.

Finally, we note that there is another basis similar to Y in which the e and f monomials are interchanged (see [Doty and Giaquinto 2002, Theorem 2.3] where the analogous basis is denoted Y_{-}).

2.15. ***A weight idempotent presentation.*** We also have an alternate presentation of the Schur superalgebra using weight idempotents.

Theorem 2.15.1. *The Schur superalgebra $S(m|n,d)$ is generated by the homogeneous elements*

$$e_1, \dots, e_{m+n-1},\ f_1, \dots, f_{m+n-1},\ 1_\lambda,$$

where λ runs over the set $\Lambda(m|n,d)$ and the $\mathbb{Z}_2$-grading is given by setting $\bar{e}_m = \bar{f}_m = \bar{1}$, $\bar{e}_i = \bar{f}_i = \bar{0}$ for $i \neq m$, and $\bar{1}_\lambda = \bar{0}$ for all $\lambda \in \Lambda(m|n,d)$.

The following is a complete set of relations:

(R1′) $1_\lambda 1_\mu = \delta_{\lambda,\mu} 1_\lambda, \quad \sum_{\lambda \in \Lambda(m|n,d)} 1_\lambda = 1;$

(R2′) $e_i 1_\lambda = \begin{cases} 1_{\lambda+\alpha_i} e_i, & \textit{if } \lambda+\alpha_i \in \Lambda(m|n,d); \\ 0, & \textit{otherwise}; \end{cases}$

(R2″) $f_i 1_\lambda = \begin{cases} 1_{\lambda-\alpha_i} f_i, & \textit{if } \lambda-\alpha_i \in \Lambda(m|n,d); \\ 0, & \textit{otherwise}; \end{cases}$

(R2‴) $1_\lambda e_i = \begin{cases} e_i 1_{\lambda-\alpha_i}, & \textit{if } \lambda-\alpha_i \in \Lambda(m|n,d); \\ 0, & \textit{otherwise}; \end{cases}$

(R2⁗) $1_\lambda f_i = \begin{cases} f_i 1_{\lambda+\alpha_i}, & \textit{if } \lambda+\alpha_i \in \Lambda(m|n,d); \\ 0, & \textit{otherwise}; \end{cases}$

(R3′) $[e_i, f_j] = \delta_{i,j} \sum_{\lambda \in \Lambda(m|n,d)} \big(\lambda_j - (-1)^{\bar{e}_i \cdot \bar{f}_j} \lambda_{j+1}\big) 1_\lambda;$

and relations (R4) *and* (R5) *given in Theorem 2.3.1.*

The proof of Theorem 2.15.1 is identical to the analogous [Doty and Giaquinto 2002, Theorem 2.4] so we omit it.

3. Quantum case

The ground field is now the field of rational functions in the indeterminate q, $\mathbb{Q}(q)$. In this section all vector spaces will be defined over $\mathbb{Q}(q)$.

3.1. ***The quantum supergroup for $\mathfrak{gl}(m|n)$.*** We have analogous results in the quantum setting. The enveloping superalgebra U is replaced by the quantized enveloping superalgebra $\mathbf{U} = U_q(\mathfrak{gl}(m|n))$ defined in [Zhang 1993; De Wit 2003][1].

[1] There are errors in [Zhang 1993] which are corrected in [De Wit 2003].

By definition **U** is given by generators and relations as follows. The generators are

$$E_1, \ldots, E_{m+n-1},\ F_1, \ldots, F_{m+n-1},\ K_1^{\pm 1}, \ldots, K_{m+n}^{\pm 1}.$$

The $\mathbb{Z}_2$-grading on **U** is given by setting $\overline{E}_m = \overline{F}_m = \bar{1}$, $\overline{E}_a = \overline{F}_a = \bar{0}$ for $a \neq m$, and $\overline{K}_a^{\pm 1} = \bar{0}$. These generators are subject to relations (Q1)–(Q5) in Theorem 3.3.1.

3.2. ***The q-Schur superalgebra.*** To define the q-Schur superalgebra, $S_q(m|n, d)$, we need to introduce the analogue of the natural representation for **U**. Set **V** to be the $(m+n)$-dimensional vector space with fixed basis $v_1, \ldots, v_{m+n}$. A $\mathbb{Z}_2$-grading on **V** is given by setting $\overline{v}_a = \overline{a}$, where we use the notation introduced in (1). Before proceeding we set a convenient notation. For $a = 1, \ldots, m+n$ we define

$$q_a = q^{(-1)^{\overline{a}}}. \tag{17}$$

The analogue of the natural representation, $\rho : \mathbf{U} \to \mathrm{End}_{\mathbb{Q}(q)}(\mathbf{V})$, is defined by

$$\begin{aligned} \rho(K_a)v_b &= q^{(\varepsilon_a, \varepsilon_b)} v_b = q_a^{\delta_{a,b}} v_b, \\ \rho(E_a)v_b &= \delta_{a+1,b} v_a, \\ \rho(F_a)v_b &= \delta_{a,b} v_{a+1}. \end{aligned} \tag{18}$$

The bilinear form used above is as in (3). It is a direct calculation to verify that this defines a representation of **U**.

We define a comultiplication on **U** given on generators by

$$\begin{aligned} \Delta(E_a) &= E_a \otimes K_a^{-1} K_{a+1} + 1 \otimes E_a, \\ \Delta(F_a) &= F_a \otimes 1 + K_a K_{a+1}^{-1} \otimes F_a, \\ \Delta(K_a) &= K_a \otimes K_a. \end{aligned} \tag{19}$$

Using this comultiplication and the sign convention discussed in Section 2.2 we then have an action of **U** for any $d \geq 1$ on the d-fold tensor product of the natural module,

$$\mathbf{V}^{\otimes d} := \mathbf{V} \otimes \mathbf{V} \otimes \cdots \otimes \mathbf{V}.$$

That is, we obtain a superalgebra homomorphism

$$\rho_d : \mathbf{U} \to \mathrm{End}_{\mathbb{Q}(q)}\big(\mathbf{V}^{\otimes d}\big). \tag{20}$$

We define the *q-Schur superalgebra* $S_q(m|n, d)$ to be the image of ρ_d. In particular, we can and will view it as a quotient of the superalgebra **U** and so a set of generators of **U** gives a set of generators for $S_q(m|n, d)$ which are subject to possibly additional relations.

3.3. ***A presentation of the q-Schur superalgebra.*** We first introduce the quantum analogue of root vectors so as to more easily state the relations for the q-Schur superalgebra. For $1 \le a \ne b \le m+n$ we define the root vector $E_{a,b}$ recursively as follows. For $a = 1, \dots, m+n-1$ we set

$$E_{a,a+1} := E_a \quad \text{and} \quad E_{a+1,a} := F_a.$$

If $|a-b| > 1$, then $E_{a,b}$ is defined by setting

$$E_{a,b} = \begin{cases} E_{a,c}E_{c,b} - q_c E_{c,b}E_{a,c}, & \text{if } a > b; \\ E_{a,c}E_{c,b} - q_c^{-1} E_{c,b}E_{a,c}, & \text{if } a < b. \end{cases} \tag{21}$$

where c can be taken to be an arbitrary index strictly between a and b. It is straightforward to see that $E_{a,b}$ is independent of the choice of c. It is also straightforward to see that $E_{a,b}$ is homogeneous and of degree $\overline{\varepsilon_a - \varepsilon_b}$.

We can now give a presentation for $S_q(m|n,d)$. Note that the bilinear form used in the following relations is defined in (3) and the notation q_a is as defined in (17).

Theorem 3.3.1. *The q-Schur superalgebra $S_q(m|n,d)$ is generated by the homogeneous elements*

$$E_1, \dots, E_{m+n-1}, \; F_1, \dots, F_{m+n-1}, \; K_1^{\pm 1}, \dots, K_{m+n}^{\pm 1}.$$

The $\mathbb{Z}_2$-grading is given by setting $\overline{E}_m = \overline{F}_m = \bar{1}$, $\overline{E}_a = \overline{F}_a = \bar{0}$ for $a \ne m$, and $\overline{K}_a^{\pm 1} = \bar{0}$. These elements are subject to the following relations:

(Q1) *for $M, N \in \{\pm 1\}$ and $1 \le a, b \le m+n$,*

$$K_a^M K_b^N = K_b^N K_a^M \quad \textit{and} \quad K_a K_a^{-1} = K_a^{-1} K_a = 1;$$

(Q2) *for $1 \le a \le m+n$ and $1 \le b \le m+n-1$,*

$$K_a E_{b,b+1} = q^{(\varepsilon_a;\alpha_b)} E_{b,b+1} K_a = q_a^{(\delta_{a,b}-\delta_{a,b+1})} E_{b,b+1} K_a,$$
$$K_a E_{b+1,b} = q^{(\varepsilon_a,-\alpha_b)} E_{b+1,b} K_a = q_a^{(\delta_{a,b+1}-\delta_{a,b})} E_{b+1,b} K_a;$$

(Q3) *for $1 \le a, b \le m+n-1$,*

$$[E_{a,a+1}, E_{b+1,b}] = \delta_{a,b} \frac{K_a K_{a+1}^{-1} - K_a^{-1} K_{a+1}}{q_a - q_a^{-1}},$$

and for $|a-b| > 1$, we have the commutations

$$E_{a+1,a} E_{b+1,b} = E_{b+1,b} E_{a+1,a} \quad \textit{and} \quad E_{a,a+1} E_{b,b+1} = E_{b,b+1} E_{a,a+1};$$

(Q4) $E_{m,m+1}^2 = E_{m+1,m}^2 = 0$;

(Q5) *if neither m nor n is* 1, *we have the following $U_q(\mathfrak{gl}(m|n))$ Serre relations. For $a \ne m$, we have*

(a) $E_{a+1,a}E_{a+2,a} = q_a E_{a+2,a}E_{a+1,a}, \quad 1 \le a \le m+n-2,$
(b) $E_{a,a+1}E_{a,a+2} = q_a E_{a,a+2}E_{a,a+1}, \quad 1 \le a \le m+n-2,$
(c) $E_{a+1,a-1}E_{a+1,a} = q_a E_{a+1,a}E_{a+1,a-1}, \quad 2 \le a \le m+n,$
(d) $E_{a-1,a+1}E_{a,a+1} = q_a E_{a,a+1}E_{a-1,a+1}, \quad 2 \le a \le m+n.$

For $a = m$, *we have*

$$[E_{m+1,m}, E_{m+2,m-1}] = [E_{m,m+1}, E_{m-1,m+2}] = 0.$$

If either $m = 1$ *or* $n = 1$, *then these relations are omitted*;

(Q6) $K_1K_2\cdots K_m K_{m+1}^{-1}K_{m+2}^{-1}\cdots K_{m+n}^{-1} = q^d$;

(Q7) $(K_a - 1)(K_a - q_a)(K_a - q_a^2)\cdots(K_a - q_a^d) = 0,$ *for all* $1 \le a \le m+n$.

3.4. ***Strategy and simplifications.*** As in the nonquantum case, the approach of [Doty and Giaquinto 2002] applies in our setting once the correct definitions and calculations are established. Namely, let $\mathbf{T}$ be the algebra defined by the generators and relations of Theorem 3.3.1. The basic line of argument is the same as before: we prove that relations (Q1) through (Q7) hold in $\mathbf{S} = S_q(m|n, d)$ and so we have a surjective map $\mathbf{T} \to \mathbf{S}$ induced by the map ρ_d given in (20). We then show this map is an isomorphism by showing via a series of calculations that the dimension of $\mathbf{T}$ is no more than the dimension of $\mathbf{S}$. As it is no more difficult, we actually prove a slightly stronger result by working with a $\mathbb{Z}[q, q^{-1}]$-form.

As before we lighten the reading by using the same notation for elements of $\mathbf{U}$ and their images in the quotients $\mathbf{T}$ and $\mathbf{S}$. We will make it clear in which algebra we are working whenever it is important to do so. Furthermore, we can again make use of the fact that the quantum group associated to $\mathfrak{g}_{\bar{0}}$ is a subalgebra of $\mathbf{U}$ (as the subalgebra generated by E_a, F_a ($a \ne m$) and $K_1^{\pm 1}, \dots, K_{m+n}^{\pm 1}$) and so calculations on purely even elements follow from the analogous results in the nonsuper setting.

3.5. ***The new relations.*** We first prove that relations (Q6) and (Q7) hold in $\mathbf{S} = S_q(m|n, d)$ and, hence, the surjection $\rho_d : \mathbf{U} \to \mathbf{S}$ factors through $\mathbf{T}$.

Lemma 3.5.1. *Under the representation* $\rho_d : \mathbf{U} \to \mathrm{End}(\mathbf{V}^{\otimes d})$, *the images of the* K_a *satisfy the relations* (Q6) *and* (Q7). *Moreover*, *the relation* (Q7) *is the minimal polynomial of the image of* K_a *in* $\mathrm{End}(\mathbf{V}^{\otimes d})$.

Proof. Using the action of $\mathbf{U}$ on $\mathbf{V}$ given in (18) and on $\mathbf{V}^{\otimes d}$ via the comultiplication (19) and the sign convention discussed in Section 2.2, the argument is as in the nonquantum case except that the calculations are done multiplicatively. We point out that there is one subtlety (and it is the reason why our relations differ slightly from the analogous ones from [Doty and Giaquinto 2002, Lemma 8.1]). Namely, the action of K_a when $a > m$ is the inverse of what might be expected. □

3.6. *Divided powers and weight idempotents.* Let **A** denote **U**, **T**, or **S**. We now define various elements of **A** which are analogous to those defined in the nonquantum setting.

We first introduce notation for the quantum integers. Given $n \in \mathbb{Z}_{\geq 0}$, let

$$[n] = \frac{q^n - q^{-n}}{q - q^{-1}} \quad \text{and} \quad [n]! = [n] \cdot [n-1] \cdots [2] \cdot [1].$$

It is helpful for calculations to note that $[n]$ is unchanged by the substitution $q \mapsto q^{-1}$ and, in particular, under the substitution $q \mapsto q_a$.

Given $x \in \mathbf{A}$ and $k \in \mathbb{Z}_{\geq 0}$, we define the *$k$-th divided power of x* by

$$x^{(k)} = \frac{x^k}{[k]!}.$$

In particular, the root vectors introduced in Section 3.3 have divided powers, $E_{a,b}^{(r)}$, for all $1 \leq a \neq b \leq m+n$ and $r \geq 0$.

If $1 \leq a, b \leq m+n$, then we set

$$K_{a,b} = K_a K_b^{-1}.$$

For $t \in \mathbb{Z}_{\geq 0}$ and $c \in \mathbb{Z}$, we use the q_a notation given in (17) and set

$$\begin{bmatrix} K_a; c \\ t \end{bmatrix} = \prod_{s=1}^{t} \frac{K_a q_a^{c-s+1} - K_a^{-1} q_a^{-c+s-1}}{q_a^s - q_a^{-s}},$$
$$\begin{bmatrix} K_{a,b}; c \\ t \end{bmatrix} = \prod_{s=1}^{t} \frac{K_{a,b} q_a^{c-s+1} - K_{a,b}^{-1} q_a^{-c+s-1}}{q_a^s - q_a^{-s}}.$$

For short, we write

$$\begin{bmatrix} K_a \\ t \end{bmatrix} = \begin{bmatrix} K_a; 0 \\ t \end{bmatrix}.$$

For $\lambda = (\lambda_a) \in \Lambda(m|n)$, we write

$$K_\lambda = \prod_{a=1}^{m+n} \begin{bmatrix} K_a \\ \lambda_a \end{bmatrix}.$$

As the K_a commute, the product can be taken in any order. For $\lambda \in \Lambda(m|n, d)$ we introduce the shorthand

$$1_\lambda := K_\lambda$$

and because of Proposition 3.6.1(b) we call these *weight idempotents*.

We define $\mathbf{A}^0$ as the subalgebra of $\mathbf{A}$ generated by

$$K_a^{\pm 1} \quad \text{and} \quad \begin{bmatrix} K_a \\ t \end{bmatrix}$$

for all $a = 1, \dots, m+n$, $t \in \mathbb{Z}_{\geq 0}$. We define $\mathbf{A}^0_{\mathscr{A}}$ to be the $\mathscr{A} = \mathbb{Z}[q, q^{-1}]$-subalgebra of $\mathbf{A}^0$ generated by

$$K_a^{\pm 1} \quad \text{and} \quad \begin{bmatrix} K_a \\ t \end{bmatrix}$$

for all $a = 1, \dots, m+n$, $t \geq 0$. If $\mathbf{A}$ equals $\mathbf{T}$ or $\mathbf{S}$, then it is clear that $\mathbf{A}^0$ and $\mathbf{A}^0_{\mathscr{A}}$ is the image of $\mathbf{U}^0$ and $\mathbf{U}^0_{\mathscr{A}}$, respectively, under the quotient map.

Now we investigate the structure of $\mathbf{T}^0$ and $\mathbf{T}^0_{\mathscr{A}}$. In the following proposition we continue our use of the notation q_a introduced in (17).

Proposition 3.6.1. *Define* $\mathbf{I}^0$ *to be the ideal of* $\mathbf{U}^0$ *generated by*

$$K_1 K_2 \cdots K_m K_{m+1}^{-1} \cdots K_{m+n}^{-1} - q^d \quad \textit{and} \quad (K_a - 1)(K_a - q_a) \cdots (K_a - q_a^d)$$

for $a = 1, \dots, m+n$. *Then*:

(a) *We have a superalgebra isomorphism* $\mathbf{U}^0/\mathbf{I}^0 \cong \mathbf{T}^0$.

(b) *The set* $\{1_\lambda \mid \lambda \in \Lambda(m|n, d)\}$ *is a* $\mathbb{Q}(q)$*-basis for* $\mathbf{T}^0$ *and a* $\mathbb{Z}[q, q^{-1}]$*-basis for* $\mathbf{T}^0_{\mathscr{A}}$. *Moreover, they give a set of pairwise orthogonal idempotents which sum to the identity.*

(c) $K_\mu = 0$ *for any* $\mu \in \Lambda(m|n)$ *such that* $|\mu| > d$.

Proof. As these elements are purely even, the proof of [Doty and Giaquinto 2002, Proposition 8.2] applies if we keep in mind the slight difference in K_a when $a > m$ and that we should replace each v in their argument by q_a. □

To state the next result we need to introduce the Gaussian binomial coefficient. For $z \in \mathbb{Z}$, and $t \in \mathbb{Z}_{\geq 0}$, define

$$\begin{bmatrix} z \\ t \end{bmatrix} = \prod_{s=1}^{t} \frac{q^{z-s+1} - q^{-z+s-1}}{q^s - q^{-s}}. \tag{22}$$

In the equations which follow one might expect q_a to appear in the binomial coefficients. However, the binomial coefficient is invariant under the map $q \mapsto q^{-1}$ so this dependency is avoided.

Proposition 3.6.2. *Let* $1 \leq a \leq m+n$, $t \in \mathbb{Z}_{\geq 0}$, $c \in \mathbb{Z}$, $\lambda \in \Lambda(m|n, d)$, *and* $\mu \in \Lambda(m|n)$. *We have the following identities in the superalgebra* T^0:

(a) $K_a^{\pm 1} 1_\lambda = q_a^{\pm \lambda_a} 1_\lambda, \quad \begin{bmatrix} K_a; c \\ t \end{bmatrix} 1_\lambda = \begin{bmatrix} \lambda_a + c \\ t \end{bmatrix} 1_\lambda;$

(b) $K_\mu 1_\lambda = \lambda_\mu 1_\lambda$, *where* $\lambda_\mu = \prod_a \begin{bmatrix} \lambda_a \\ \mu_a \end{bmatrix}$;

(c) $K_\mu = \sum_{\lambda \in \Lambda(m|n,d)} \lambda_\mu 1_\lambda$.

Proof. As the elements are purely even, the argument from the proof of [Doty and Giaquinto 2002, Proposition 8.3] carries over if we replace v by q_a. □

3.7. *Commutation relations between root vectors and weight idempotents.* Recall that in Section 3.3 we defined root vectors $E_{a,b} \in \mathbf{U}$ for every $1 \leq a \neq b \leq m+n$. As is our convention, we also write $E_{a,b}$ for their image in $\mathbf{T}$ and $\mathbf{S}$. We now compute the commutation relations between root vectors and weight idempotents.

Proposition 3.7.1. *For any* $\lambda \in \Lambda(m|n,d)$, *and* $\alpha = \varepsilon_b - \varepsilon_c \in \Phi$, *we have the commutation formulas*

$$E_{b,c} 1_\lambda = \begin{cases} 1_{\lambda+\alpha} E_{b,c}, & \text{if } \lambda + \alpha \in \Lambda(m|n,d); \\ 0, & \text{otherwise}, \end{cases}$$

$$1_\lambda E_{b,c} = \begin{cases} E_{b,c} 1_{\lambda-\alpha}, & \text{if } \lambda - \alpha \in \Lambda(m|n,d); \\ 0, & \text{otherwise}. \end{cases}$$

Proof. The following identities are derived by direct computation:

(23) $$\begin{bmatrix} K_a;0 \\ 1 \end{bmatrix} \begin{bmatrix} K_a;-1 \\ \lambda_a \end{bmatrix} = \begin{bmatrix} \lambda_a + 1 \\ 1 \end{bmatrix} \begin{bmatrix} K_a;0 \\ \lambda_a + 1 \end{bmatrix},$$

(24) $$\begin{bmatrix} K_a;1 \\ \lambda_a \end{bmatrix} = q_a^{\lambda_a} \begin{bmatrix} K_a \\ \lambda_a \end{bmatrix} + q_a^{\lambda_a - 1} K_a^{-1} \begin{bmatrix} K_a \\ \lambda_a - 1 \end{bmatrix}.$$

From the defining relation (Q2), we can see that K_a and $E_{b,c}$ commute if $a \neq b$ and $a \neq c$. Moreover,

$$K_b E_{b,c} = q_b E_{b,c} K_b.$$

This implies

(25) $$E_{b,c} \begin{bmatrix} K_b \\ \lambda_b \end{bmatrix} = \begin{bmatrix} K_b;-1 \\ \lambda_b \end{bmatrix} E_{b,c}.$$

We also have

$$K_c E_{b,c} = q_c^{-1} E_{b,c} K_c,$$

which implies

(26) $$E_{b,c} \begin{bmatrix} K_c \\ \lambda_c \end{bmatrix} = \begin{bmatrix} K_c;1 \\ \lambda_c \end{bmatrix} E_{b,c}.$$

Then, for $\lambda \in \Lambda(m|n, d)$, and $b \neq c$, we have

$$E_{b,c} 1_\lambda = \begin{bmatrix} K_b; -1 \\ \lambda_b \end{bmatrix} \begin{bmatrix} K_c; 1 \\ \lambda_c \end{bmatrix} \prod_{l \neq b,c} \begin{bmatrix} K_l \\ \lambda_l \end{bmatrix} E_{b,c}.$$

Multiply both sides of the preceding equality by $\left[\begin{smallmatrix} K_b \\ \lambda_b \end{smallmatrix}\right]$ and use (23) to simplify the right-hand side and (25), (26) to simplify the left-hand side. The result is

$$E_{b,c} \begin{bmatrix} K_b; 1 \\ \lambda_b \end{bmatrix} 1_\lambda = \begin{bmatrix} \lambda_b + 1 \\ 1 \end{bmatrix} \begin{bmatrix} K_b \\ \lambda_b + 1 \end{bmatrix} \begin{bmatrix} K_c; 1 \\ \lambda_c \end{bmatrix} \prod_{l \neq b,c} \begin{bmatrix} K_l \\ \lambda_l \end{bmatrix} E_{b,c}.$$

Assuming $\lambda_c \geq 1$ and using (24), we get

$$E_{b,c} 1_\lambda = \begin{bmatrix} \lambda_b + 1 \\ 1 \end{bmatrix} \begin{bmatrix} K_b \\ \lambda_b + 1 \end{bmatrix} \left(q_c^{\lambda_c} \begin{bmatrix} K_c \\ \lambda_c \end{bmatrix} + q_c^{\lambda_c - 1} K_c^{-1} \begin{bmatrix} K_c \\ \lambda_c - 1 \end{bmatrix} \right) \prod_{l \neq b,c} \begin{bmatrix} K_l \\ \lambda_l \end{bmatrix} E_{b,c}.$$

Thus, when $\lambda_c \geq 1$ we can multiply through in the above expression and apply Proposition 3.6.1(c) to see that the first summand must be zero. The above equality simplifies to

$$E_{b,c} 1_\lambda = q_c^{\lambda_c - 1} K_c^{-1} 1_{\lambda+\alpha} E_{b,c}.$$

Now, by Proposition 3.6.2(a), K_c^{-1} acts on $1_{\lambda+\alpha}$ as $q_c^{-(\lambda_c - 1)}$. Thus we obtain the equality in the first part of the proposition in the case $\lambda_c \geq 1$.

If $\lambda_c = 0$, then the right-hand side is zero by Proposition 3.6.1(c). This proves the first part of the proposition. The proof of the second part is similar. □

3.8. ***Commutation formulas between divided powers of root vectors.*** We will need to know how divided powers of root vectors commute with each other. To obtain this we use the *PBW-commutator lemma* presented in [De Wit 2003]. We first consider the case when both root vectors correspond to positive roots[2]:

$$(27) \quad E_{a,b} E_{c,d} = \begin{cases} (-1)^{\overline{E}_{a,b} \overline{E}_{c,d}} E_{c,d} E_{a,b}, & (b < c \text{ or } c < a < b < d); \\ (-1)^{\overline{E}_{a,b} \overline{E}_{c,d}} q_b E_{c,d} E_{a,b}, & (a < c < b = d); \\ (-1)^{\overline{E}_{a,b} \overline{E}_{c,d}} q_a E_{c,d} E_{a,b}, & (a = c < b < d); \\ E_{a,d} + q_c^{-1} E_{c,d} E_{a,b}, & (b = c); \\ (-1)^{\overline{E}_{a,b} \overline{E}_{c,d}} E_{c,d} E_{a,b} + (q_b - q_b^{-1}) E_{a,d} E_{c,b}, & \\ & (a < c < b < d). \end{cases}$$

Before stating the result, we first observe that we can make the following assumptions. First, since the case when both root vectors have divided power one is handled by (27), we may assume that at least one of the powers is greater than one. Second,

[2]Note that there is a typographic error in [De Wit 2003, 20(b)] and that we have chosen to write signs in an equivalent but more symmetric fashion.

if $\varepsilon_a - \varepsilon_b$ is an odd root, then by [De Wit 2003, Section IV] we have $E_{a,b}^2 = 0$. That is, just as in the nonquantum case we may assume the odd root vectors have divided power at most one. Therefore, in what follows if the power of a root vector is one, then it may be even or odd; but if the power is greater than one, then we are implicitly assuming the root vector is even. In particular, the combination of these two assumptions means that in each formula below at least one root vector is even and, hence, our formulas do not involve extra signs due to the $\mathbb{Z}_2$-grading.

Under the above assumptions lengthy but elementary inductive arguments using (27) imply the following commutator formulas for the divided powers of root vectors associated to positive roots. In these relations and the ones that follow we use the q_a notation introduced in (17) and the Gaussian binomials introduced in (22). The relations given here are analogous to those obtained in [Xi 1999] for the quantum groups of simple Lie algebras.

Proposition 3.8.1. *Let $E_{a,b}$ and $E_{c,d}$ be two root vectors with $a < b$ and $c < d$, and let $M, N \geq 1$ satisfying the assumptions given above. We then have the following commutation formulas.*

(1) *If $b < c$ or $c < a < b < d$, then*
$$E_{a,b}^{(M)} E_{c,d}^{(N)} = E_{c,d}^{(N)} E_{a,b}^{(M)}.$$
(2) *If $a = c < b < d$ or $a < c < b = d$, then*
$$E_{a,b}^{(M)} E_{c,d}^{(N)} = q_b^{MN} E_{c,d}^{(N)} E_{a,b}^{(M)}.$$
(3) *If $a < b = c < d$, then*
$$E_{a,b}^{(M)} E_{c,d}^{(N)} = \sum_{t=0}^{\min(M,N)} q_b^{-(N-t)(M-t)} E_{c,d}^{(N-t)} E_{a,d}^{(t)} E_{a,b}^{(M-t)}.$$
(4) *If $a < c < b < d$, then*
$$E_{a,b}^{(M)} E_{c,d}^{(N)} = \sum_{t=0}^{\min(M,N)} q_b^{\frac{t(t-1)}{2}} (q_b - q_b^{-1})^t [t]! E_{c,b}^{(t)} E_{c,d}^{(N-t)} E_{a,b}^{(M-t)} E_{a,d}^{(t)}.$$

We note that from these commutator formulas we can derive a second set by solving for $E_{c,d}^{(N)} E_{a,b}^{(M)}$ and then interchanging (a, b) and (c, d). Taken together with the formulas given in the proposition these give a complete set of commutator formulas for divided powers of positive root vectors. That this is a complete set of formulas can easily be seen by considering the various possibilities for the subscripts (cf. [Doty and Giaquinto 2002, Section 9]).

There is a similar set of commutator formulas for divided powers of negative root vectors. They can be derived directly using the analogous results from [De Wit 2003]. Alternatively, $\mathbf{U}$ admits an antiautomorphism given by $E_a \mapsto F_a$, $F_a \mapsto E_a$, and $K_a \mapsto K_a^{-1}$. Applying this map to the commutator relations for positive root vectors yields the commutator relations among negative root vectors.

3.9. ***More commutation formulas.*** Finally we give the commutation formulas between a positive and a negative root vector. Let us assume $a < b$ and $c < d$. Then from [De Wit 2003] we have the following:

$$E_{a,b}E_{d,c} = \begin{cases} (-1)^{\bar{E}_{a,b}\bar{E}_{d,c}} E_{d,c}E_{a,b}, & (b \le c \text{ or } c < a < b < d); \\ (-1)^{\bar{E}_{a,b}\bar{E}_{d,c}} E_{d,c}E_{a,b} + K_{c,b}E_{a,c}, & (a < c < b = d); \\ (-1)^{\bar{E}_{a,b}\bar{E}_{d,c}} E_{d,c}E_{a,b} - (-1)^{\bar{E}_{a,b}\bar{E}_{d,c}} K_{a,b}E_{d,b}, & (a = c < b < d); \\ (-1)^{\bar{E}_{a,b}\bar{E}_{d,c}} E_{d,c}E_{a,b} + (q_a - q_a^{-1})^{-1}(K_{a,b} - K_{a,b}^{-1}), & (a = c \text{ and } b = d); \\ (-1)^{\bar{E}_{a,b}\bar{E}_{d,c}} E_{d,c}E_{a,b} - (q_b - q_b^{-1})K_{c,b}E_{a,c}E_{d,b}, & (a < c < b < d). \end{cases} \tag{28}$$

With elementary inductive arguments, this yields the next result. The assumptions on divided powers of root vectors stated before Proposition 3.8.1 apply here as well.

Proposition 3.9.1. *Let $E_{a,b}$ and $E_{d,c}$ be two root vectors with $a < b$ and $c < d$, and let $M, N \ge 1$. We then have the following commutation formulas.*

(1) *If $b \le c$ or $c < a < b < d$, then*

$$E_{a,b}^{(M)} E_{d,c}^{(N)} = E_{d,c}^{(N)} E_{a,b}^{(M)}.$$

(2) *If $a < c < b = d$, then*

$$E_{a,b}^{(M)} E_{d,c}^{(N)} = \sum_{t=0}^{\min(M,N)} q_b^{-t(N-t)} E_{d,c}^{(N-t)} K_{c,d}^t E_{a,b}^{(M-t)} E_{a,c}^{(t)}.$$

(3) *If $a = c < b < d$, then*

$$E_{a,b}^{(M)} E_{d,c}^{(N)} = \sum_{t=0}^{\min(M,N)} (-1)^t q_b^{-t(M-1-t)} E_{d,b}^{(t)} E_{d,c}^{(N-t)} K_{a,b}^t E_{a,b}^{(M-t)}.$$

(4) *If $a < b$, then*

$$E_{a,b}^{(M)} E_{b,a}^{(N)} = \sum_{t=0}^{\min(M,N)} E_{b,a}^{(N-t)} \begin{bmatrix} K_{a,b}; 2t - M - N \\ t \end{bmatrix} E_{a,b}^{(M-t)}.$$

(5) *If $a < c < b < d$, then*

$$E_{a,b}^{(M)} E_{d,c}^{(N)} = \sum_{t=0}^{\min(M,N)} (-1)^t q_b^{-t(2N-3t-1)/2} (q_b - q_b^{-1})^t [t]! E_{d,c}^{(N-t)} E_{d,b}^{(t)} K_{c,b}^t E_{a,b}^{(M-t)} E_{a,c}^{(t)}.$$

We can use the antiautomorphism on $\mathbf{U}$ defined in the previous section along with simple calculations to derive additional identities (compare [Doty and Giaquinto 2002, Section 9]). In this way we obtain a complete set of commutation relations involving a positive root vector to the left of a negative root vector. There are similar commutation formulas for the case of a negative root vector followed by a positive root vector. These can be obtained from the above formulas by solving for the term $E_{d,c}^{(N)} E_{a,b}^{(M)}$. The new formulas will be of a similar form.

Taking all possible formulas we obtain the commutation formulas for divided powers of root vectors. The interested reader can derive the complete set.

3.10. ***An $\mathscr{A}$-form for* U.** Recall that Lusztig defined an $\mathscr{A} = \mathbb{Z}[q, q^{-1}]$-form for $U_q(\mathfrak{g})$ whenever $\mathfrak{g}$ is a semisimple Lie algebra. We define an analogous $\mathscr{A}$-form for $\mathbf{U}$. Let $\mathbf{U}_{\mathscr{A}}$ denote the $\mathscr{A}$-subsuperalgebra of $\mathbf{U}$ generated by

$$\left\{ E_{a,b}^{(M)}, K_a^{\pm 1}, \begin{bmatrix} K_a \\ t \end{bmatrix} \;\middle|\; 1 \le a \neq b \le m+n, M, t \in \mathbb{Z}_{\ge 0} \right\}.$$

Fix an order on the root system Φ^+ and let $P(m|n)$ be as in (15). For $A = (A(\alpha)) \in P(m|n)$, we define

$$E_A = \prod_{\alpha = \varepsilon_a - \varepsilon_b \in \Phi^+} E_{a,b}^{(A(\alpha))}, \quad F_A = \prod_{\alpha = \varepsilon_a - \varepsilon_b \in \Phi^+} E_{b,a}^{(A(\alpha))},$$

where the product is taken according to the fixed order on Φ^+.

There is a known basis for the analogously defined $\mathscr{A}$-form for $\mathbf{U}_q(\mathfrak{g}_{\bar{0}})$ following from Lusztig's basis for $\mathbf{U}_q(\mathfrak{sl}(n))$ [Lusztig 1990, Theorem 4.5] (see also [Xi 1999]). Using this basis and the quantum commutator formulas given in the previous section it follows that $\mathbf{U}_{\mathscr{A}}$ has an $\mathscr{A}$-basis given by the set

(29)
$$\left\{ E_A \prod_{a=1}^{m+n} \left(K_a^{\sigma_a} \begin{bmatrix} K_a \\ \mu_a \end{bmatrix} \right) F_C \;\middle|\; A, C \in P(m|n), \sigma_1, \dots, \sigma_{m+n} \in \{0, 1\}, \mu \in \Lambda(m|n) \right\}.$$

In particular this gives a basis for $\mathbf{U}$ after extending scalars (compare with [Zhang 1993, Proposition 1]).

If $\mathbf{A}$ is $\mathbf{S}$ or $\mathbf{T}$, then we define $\mathbf{A}_{\mathscr{A}}$ to be the image of $\mathbf{U}_{\mathscr{A}}$ under the quotient map. In particular $\mathbf{A}_{\mathscr{A}}$ is a $\mathbb{Z}[q, q^{-1}]$-subsuperalgebra of $\mathbf{A}$ and (the image under the quotient map of) the set given in (29) spans $\mathbf{A}_{\mathscr{A}}$. For short we call $S_q(m|n, d)_{\mathscr{A}}$ the *integral q-Schur superalgebra*.

3.11. ***Quantum Kostant monomials and content functions.*** We now define the quantum analogue of the Kostant monomials. Any finite product of nonzero elements of the form

$$E_{a,b}^{(M)}, \quad K_a^{\pm 1}, \quad \begin{bmatrix} K_a \\ t \end{bmatrix},$$

where $1 \le a \ne b \le m+n$ and $M, t \in \mathbb{Z}_{\ge 0}$, will be called a *Kostant monomial*.

We also define content functions as before. Namely, the content function

$$\chi : \{\text{Kostant monomials}\} \to \bigoplus_{i=1}^{m+n} \mathbb{Z}\varepsilon_i \tag{30}$$

is given on generators by declaring for $\alpha = \varepsilon_a - \varepsilon_b \in \Phi$, $M, N \in \mathbb{N}$, and $t \in \mathbb{Z}_{\ge 0}$ that

$$\chi(E_{a,b}^{(M)}) = M\varepsilon_{\max(a,b)}, \quad \chi(K_a) = \chi(K_a^{-1}) = \chi\left(\begin{bmatrix} K_a \\ t \end{bmatrix}\right) = 0.$$

For general monomials we again use the formula $\chi(XY) = \chi(X) + \chi(Y)$ whenever X, Y are Kostant monomials.

We also define the left content, χ_L, and right content, χ_R, by declaring on generators that

$$\chi_L(E_{a,b}^{(M)}) = M\varepsilon_a, \qquad \chi_L(K_a) = \chi_L(K_a^{-1}) = \chi_L\left(\begin{bmatrix} K_a \\ t \end{bmatrix}\right) = 0,$$
$$\chi_R(E_{a,b}^{(M)}) = M\varepsilon_b, \qquad \chi_R(K_a) = \chi_R(K_a^{-1}) = \chi_R\left(\begin{bmatrix} K_a \\ t \end{bmatrix}\right) = 0,$$

and again using the rule $\chi_L(XY) = \chi_L(X) + \chi_R(Y)$ (similarly for χ_R) whenever X and Y are Kostant monomials. We again use (14) to view outputs of the content functions as elements of $\Lambda(m|n)$.

3.12. ***A basis for the q-Schur superalgebra.*** We can now state the quantum analogue of Theorem 2.14.3.

Theorem 3.12.1. *The integral q-Schur superalgebra is the $\mathcal{A}$-subalgebra of*

$$S_q(m|n, d)$$

generated by

$$E_a^{(M)}, \quad F_a^{(M)}, \quad \begin{bmatrix} K_b \\ t \end{bmatrix},$$

where $1 \le a \le m+n-1$, $1 \le b \le m+n$, and $M \in \mathbb{Z}_{\ge 0}$. Moreover, the set

$$\mathbf{Y} = \bigcup_{\lambda \in \Lambda(m|n,d)} \{E_A 1_\lambda F_C \mid A, C \in P(m|n), \chi(E_A F_C) \preceq \lambda\}$$

forms a $\mathbb{Q}(q)$-basis of $S_q(m|n, d)$ and an $\mathcal{A}$-basis of $S_q(m|n, d)_{\mathcal{A}}$.

We remark that, as in Section 2.14, the set $\mathbf{Y}$ has alternate descriptions using the left and right content functions. Applying the antiautomorphism of $\mathbf{U}$ yields a similar basis in which the positions of the E and F terms are swapped; that is, the analogue of $\mathbf{Y}_-$ in [Doty and Giaquinto 2002].

Proposition 3.12.2. *The set* $\mathbf{Y}$ *spans the superalgebra* $\mathbf{T}$.

Proof. The proof is exactly analogous to the proof of Proposition 2.14.1 and the proof of [Doty and Giaquinto 2002, Proposition 9.1]. One again argues by induction on degree and content using the above commutation formulas to write an arbitrary Kostant monomial as a $\mathbb{Z}[q,q^{-1}]$-linear combination of elements of $\mathbf{Y}$. The coefficients in our commutation formulas are slightly different, but they are still elements of $\mathbb{Z}[q,q^{-1}]$ and so this does not affect the substance of the argument. □

Lemma 3.12.3. *The cardinality of the set* $\mathbf{Y}$ *is equal to the dimension of* $\mathbf{S} = S_q(m|n,d)$.

Proof. It is known that the dimension of $S_q(m|n,d)$ over $\mathbb{Q}(q)$ equals the dimension of $S(m|n,d)$ over $\mathbb{Q}$. This is established, for example, in the proof of [Mitsuhashi 2006, Proposition 4.3]. This can also be seen as an outcome of [Du and Rui 2011, Theorem 9.7]. The result then follows by the proof of Lemma 2.14.2. □

Theorems 3.3.1 and 3.12.1 now follow as in the nonquantum case.

3.13. ***A weight idempotent presentation.*** We also have a quantum analogue of Theorem 2.15.1 which gives the q-Schur superalgebra by generators and relations using the weight idempotents.

Theorem 3.13.1. *The q-Schur superalgebra $S_q(m|n,d)$ is generated by the homogeneous elements*

$$E_1,\dots,E_{m+n-1},\ F_1,\dots,F_{m+n-1},\ 1_\lambda,$$

where λ runs over the set $\Lambda(m|n,d)$. The $\mathbb{Z}_2$-grading is given by setting $\overline{E}_m = \overline{F}_m = \bar{1}$, $\overline{E}_a = \overline{F}_a = \bar{0}$ for $a \neq m$, and $\overline{1}_\lambda = \bar{0}$ for all $\lambda \in \Lambda(m|n,d)$.

These generators are subject only to the relations:

(Q1′) $\quad 1_\lambda 1_\mu = \delta_{\lambda,\mu} 1_\lambda, \quad \sum_{\lambda\in\Lambda(m|n,d)} 1_\lambda = 1;$

(Q2′) $\quad E_a 1_\lambda = \begin{cases} 1_{\lambda+\alpha_a} E_a, & \textit{if } \lambda+\alpha_a \in \Lambda(m|n,d); \\ 0, & \textit{otherwise}; \end{cases}$

(Q2″) $\quad F_a 1_\lambda = \begin{cases} 1_{\lambda-\alpha_a} F_a, & \textit{if } \lambda-\alpha_a \in \Lambda(m|n,d); \\ 0, & \textit{otherwise}; \end{cases}$

(Q2‴) $1_\lambda E_a = \begin{cases} E_a 1_{\lambda-\alpha_a}, & \textit{if } \lambda-\alpha_a \in \Lambda(m|n,d); \\ 0, & \textit{otherwise}; \end{cases}$

(Q2⁗) $1_\lambda F_a = \begin{cases} F_a 1_{\lambda+\alpha_a}, & \textit{if } \lambda+\alpha_a \in \Lambda(m|n,d); \\ 0, & \textit{otherwise}; \end{cases}$

(Q3′) $[E_a, F_b] = \delta_{a,b} \sum_{\lambda\in\Lambda(m|n,d)} \big[\lambda_b - (-1)^{\overline{E}_a \overline{F}_b}\lambda_{b+1}\big] 1_\lambda;$

and relations (Q4) *and* (Q5) *given in Theorem 3.3.1.*

Theorem 3.13.1 is proven just as in the nonquantum case and as in the proof of [Doty and Giaquinto 2002, Theorem 3.4].

4. The q-Schur superalgebra as an endomorphism superalgebra

4.1. ***Quantum Schur–Weyl duality.*** There is a natural signed action of the Iwahori–Hecke algebra associated to the symmetric group on d letters, $\mathbf{H}_q = \mathbf{H}_q(\Sigma_d)$, on $\mathbf{V}^{\otimes d}$. Mitsuhashi [2006] defines the q-Schur superalgebra as the superalgebra

$$\widetilde{\mathbf{S}} := \widetilde{\mathbf{S}}(m|n,d) = \mathrm{End}_{\mathbf{H}_q}\big(\mathbf{V}^{\otimes d}\big).$$

The main result of [Mitsuhashi 2006] is to establish a Schur–Weyl duality between this endomorphism algebra and the Iwahori–Hecke algebra. However, it is not immediately obvious the q-Schur superalgebra defined in this paper as a quotient of $\mathbf{U}$ coincides with the one used there. We now reconcile this difference.

Recall that we have a fixed homogeneous basis $v_1, \dots, v_{m+n}$ for $\mathbf{V}$ and this defines a homogeneous basis $\{v_{i_1} \otimes \cdots \otimes v_{i_d} \mid 1 \le i_1, \dots, i_d \le m+n\}$ for $\mathbf{V}^{\otimes d}$. Define a map $\sigma_d : \mathbf{V}^{\otimes d} \to \mathbf{V}^{\otimes d}$ by

$$\sigma_d(v_{i_1} \otimes \cdots \otimes v_{i_d}) = (-1)^{\bar{v}_{i_1}+\cdots+\bar{v}_{i_d}} v_{i_1} \otimes \cdots \otimes v_{i_d}.$$

It is easily seen that σ_d commutes with the action of $\mathbf{H}_q$ on $\mathbf{V}^{\otimes d}$ defined in [Mitsuhashi 2006].

Let $\mathbf{U}^\sigma$ denote the quantum group associated to $\mathfrak{gl}(m|n)$ in [Benkart et al. 2000; Mitsuhashi 2006]. This algebra is generated by elements $e_1, \dots, e_{m+n-1}$, $f_1, \dots, f_{m+n-1}$, and q^h (where h ranges over the elements of the dual weight lattice), along with an element denoted by σ. For each $d \ge 1$, denote by

$$\tilde{\rho}_d : \mathbf{U}^\sigma \to \mathrm{End}_{\mathbb{Q}(q)}\big(\mathbf{V}^{\otimes d}\big)$$

the homomorphism given in Equation (3.2) of [Mitsuhashi 2006]. Theorem 4.4 of the same reference states that $\widetilde{\mathbf{S}} = \tilde{\rho}_d(\mathbf{U}^\sigma)$. For short we write $\mathbf{S}$ for the q-Schur superalgebra defined in Section 3.2 as a quotient of $\mathbf{U}$. We claim that $\widetilde{\mathbf{S}} = \mathbf{S}$. When $d = 1$, it is straightforward to see that the action of the generators e_a, f_a, q^h, coincide with the action of our E_a, F_a, and $K_a^{\pm 1}$. More generally, this remains true for $d \geq 1$ once we take into account the fact that the difference in the coproducts is exactly explained by the fact that we use the sign convention whereas Mitsuhashi does not but instead introduces the element σ (which acts on $\mathbf{V}^{\otimes d}$ by σ_d).

Thus $\mathbf{S} \subseteq \widetilde{\mathbf{S}}$. It only remains to account for the extra generator σ in $\mathbf{U}^{\sigma}$. That is, since σ acts on $\mathbf{V}^{\otimes d}$ by the map σ_d, we need to show that σ_d lies in $\mathbf{S}$. The next lemma shows that it lies in the image of ρ_d and, hence, in $\mathbf{S}$.

Lemma 4.1.1. *For each $d \geq 1$, there exists $x_d \in \mathbf{U}$ so that $\rho_d(x_d) = \sigma_d$.*

Proof. It suffices to construct an element of $\mathbf{U}$ whose action on our basis for $\mathbf{V}^{\otimes d}$ coincides with the action of σ_d. We build this element up in several steps. First, for $0 \leq s \leq d$ and $1 \leq a \leq m+n$ we use the notation given in (17) and (1) to define $\omega_{s,a} \in \mathbf{U}$ by

$$\omega_{s,a} = \frac{(K_a - 1)(K_a - q_a) \cdots (K_a - q_a^{s-1}) \times (K_a - q_a^s + (-1)^{s \cdot \overline{a}})(K_a - q_a^{s+1}) \cdots (K_a - q_a^d)}{(q_a^s - 1)(q_a^s - q_a) \cdots (q_a^s - q_a^{s-1})(q_a^s - q_a^{s+1}) \cdots (q_a^s - q_a^d)}. \tag{31}$$

Given $1 \leq a \leq m+n$ we define a function,

$$r_a : \{v_{i_1} \otimes \cdots \otimes v_{i_d} \mid 1 \leq i_1, \ldots, i_d \leq m+n\} \to \{0, 1, \ldots, d\},$$

which counts the occurrences of v_a in $v_{i_1} \otimes \cdots \otimes v_{i_d}$. That is, it is defined by

$$r_a = r_a(v_{i_1} \otimes \cdots \otimes v_{i_d}) = |\{t = 1, \ldots, d \mid i_t = a\}|.$$

Then by a direct calculation (cf. the calculation used to prove relation (Q7) in Lemma 3.5.1),

$$\omega_{s,a}(v_{i_1} \otimes v_{i_2} \otimes \cdots \otimes v_{i_d}) = \begin{cases} (-1)^{r_a \cdot \overline{a}}(v_{i_1} \otimes v_{i_2} \otimes \cdots \otimes v_{i_d}), & \text{if } s = r_a; \\ 0, & \text{if } s \neq r_a. \end{cases}$$

Now, for $1 \leq a \leq m+n$ define $\Omega_a \in \mathbf{U}$ by $\Omega_a = \sum_{s=0}^{d} \omega_{s,a}$. It then follows that for any basis vector $v_{i_1} \otimes \cdots \otimes v_{i_d}$ we have

$$\Omega_a(v_{i_1} \otimes \cdots \otimes v_{i_d}) = (-1)^{r_a \cdot \overline{a}}(v_{i_1} \otimes \cdots \otimes v_{i_d}).$$

Finally we define $\Omega \in \mathbf{U}$ to be the element $\Omega = \prod_{a=1}^{m+n} \Omega_a$. It follows that

$$\begin{aligned} \Omega(v_{i_1} \otimes \cdots \otimes v_{i_d}) &= \left(\prod_{a=1}^{m+n} (-1)^{r_a \cdot \overline{a}} \right)(v_{i_1} \otimes \cdots \otimes v_{i_d}) \\ &= (-1)^{r_1 \cdot \overline{1} + \cdots + r_{m+n} \cdot \overline{m+n}}(v_{i_1} \otimes \cdots \otimes v_{i_d}) \\ &= (-1)^{\overline{v}_{i_1} + \cdots + \overline{v}_{m+n}}(v_{i_1} \otimes \cdots \otimes v_{i_d}) \end{aligned}$$

for every basis element $v_{i_1} \otimes \cdots \otimes v_{i_d}$. That is, as desired, $\Omega \in \mathbf{U}$ acts as σ_d on $\mathbf{V}^{\otimes d}$. □

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CLASSIFYING ZEROS OF TWO-SIDED QUATERNIONIC POLYNOMIALS AND COMPUTING ZEROS OF TWO-SIDED POLYNOMIALS WITH COMPLEX COEFFICIENTS

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We improve the method of Janovská and Opfer for computing the zeros on the surface of a given sphere for a quaternionic two-sided polynomial. We classify the zeros of quaternionic two-sided polynomials into three types — isolated, spherical and circular — and characterize each type. We provide a method to find all quaternion zeros for two-sided polynomials with complex coefficients. We also establish standard formulae for roots of a quadratic two-sided polynomial with complex coefficients, which yields a simpler and more efficient algorithm to produce all zeros in the quadratic case.

1. Introduction

In this paper we will treat *two-sided* quaternionic polynomials, those of the form

$$p(x) := \sum_{j=0}^{n} a_j x^j b_j, \quad x, a_j, b_j \in \mathbb{H}, \quad a_n b_n \neq 0, \tag{1}$$

where $\mathbb{H}$ is the skew field of quaternions. These polynomials include also all *one-sided* polynomials, where all coefficients are located on the left side or the right side of the powers. For a long time, it has been known that one-sided quaternionic polynomials may have two classes of zeros: isolated zeros and spherical zeros (see for instance [Pogorui and Shapiro 2004; Topuridze 2003]), while a method to compute all zeros of such polynomials was developed in [Janovská and Opfer 2010b] and a more efficient means was found in [Feng and Zhao 2011].

A general quaternionic polynomial is a finite sum of terms of the form

$$t_j(x) := a_{0j} \cdot x \cdot a_{1j} \cdots a_{j-1,j} \cdot x \cdot a_{jj}, \quad x, a_{0j}, a_{1j}, \ldots, a_{jj} \in \mathbb{H}, \; j \geq 0. \tag{2}$$

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Such a term is called a *monomial of degree* j. The polynomial $p(z)$ in (1) is only a very special type of a general quaternionic polynomial. There are relatively few results on two-sided quaternionic polynomials; we list some that are relevant to our study.

In [De Leo et al. 2006], the authors gave an example of a two-sided polynomial and Opfer [2009] obtained that a general quaternionic polynomial of degree n has at least one zero provided the polynomial has only one monomial of degree n. More recently, for a quaternionic two-sided polynomial of type (1), Janovská and Opfer [2010a] showed that there may be five classes of zeros according to the five possible ranks of a certain real (4×4) matrix, and they provided a method to find the zeros in a given equivalence class.

This paper is organized as follows. In Section 2, by improving the method of [Janovská and Opfer 2010a], we classify the zeros of quaternionic two-sided polynomials into three types — isolated zeros, spherical zeros and circular zeros — and characterize each type of zero. In Section 3, we provide a method to compute all quaternion zeros of a two-sided polynomial with complex coefficients. In Section 4, for a quadratic two-sided polynomial with complex coefficients, we further establish the standard formulae for roots, so that a simpler and more efficient algorithm is given to produce all zeros for a quadratic two-sided polynomial with complex coefficients.

We will now give a short introduction to the quaternionic algebra. By $\mathbb{R}$, $\mathbb{C}$ we denote the fields of real and complex numbers, respectively, and by $\mathbb{N}$ the set of natural numbers. In the skew field $\mathbb{H}$ of quaternions, any element has the form

$$q = a_0 + a_1\boldsymbol{i} + a_2\boldsymbol{j} + a_3\boldsymbol{k} = (a_0 + a_1\boldsymbol{i}) + (a_2 + a_3\boldsymbol{i})\boldsymbol{j}, \tag{3}$$

where $\boldsymbol{i}$, $\boldsymbol{j}$, $\boldsymbol{k}$ satisfy

$$\boldsymbol{i}^2 = \boldsymbol{j}^2 = \boldsymbol{k}^2 = -1, \quad \boldsymbol{ij} = -\boldsymbol{ji} = \boldsymbol{k}, \quad \boldsymbol{jk} = -\boldsymbol{kj} = \boldsymbol{i}, \quad \boldsymbol{ki} = -\boldsymbol{ik} = \boldsymbol{j};$$

the product is extended to $\mathbb{H}$ by $\mathbb{R}$-bilinearity. We call a_0 the *real part* of the quaternion q in (3), also written $\Re q$, while $q - \Re q = a_1\boldsymbol{i} + a_2\boldsymbol{j} + a_3\boldsymbol{k}$ is called the *imaginary part* and denoted by $\Im q$. The *modulus* $|q|$ of q is

$$|q| = \sqrt{a_0^2 + a_1^2 + a_2^2 + a_3^2}.$$

The *conjugate* of q, denoted by $\bar{q}$, is defined by $\bar{q} = a_0 - a_1\boldsymbol{i} - a_2\boldsymbol{j} - a_3\boldsymbol{k}$.

Two quaternions q_1, q_2 are called *equivalent*, denoted by $q_1 \sim q_2$, if there is an $h \in \mathbb{H}\backslash\{0\}$ such that $q_1 = hq_2h^{-1}$. The set $[q] = \{hqh^{-1} : h \in \mathbb{H}\backslash\{0\}\}$ will be called the *equivalence class* of q or, for short, the *class* of q. Indeed "$\sim$" defines an equivalence relation on $\mathbb{H}$. So each quaternion is located in one and only one equivalence class. It is well known that

$$q_1 \sim q_2 \iff \Re q_1 = \Re q_2 \text{ and } |q_1| = |q_2|,$$

that is, $[q] = \{u \in \mathbb{H} : \Re u = \Re q, |u| = |q|\}$, which can be regarded as the surface of a ball in $\mathbb{R}^3 = \mathbb{R}\boldsymbol{i} + \mathbb{R}\boldsymbol{j} + \mathbb{R}\boldsymbol{k}$ if q is not real. It is easy to see that $[q] = \{q\}$ if q is real and $[q]$ contains infinitely many elements if q is not real. In the case that q is not real, the only two complex numbers contained in $[q]$ are ξ and $\bar{\xi}$, where $\xi = \Re q + \sqrt{|q|^2 - (\Re q)^2}\,\boldsymbol{i}$. Here we are calling a quaternion *complex* if it is of the form $a_0 + a_i\boldsymbol{i}$, with $a_0, a_i \in \mathbb{R}$.

There is a very useful tool to study the quaternion algebra, which is the so-called *derived matrix* (appeared in [Feng 2010])

The *derived mapping* $\sigma : \mathbb{H}^{n\times n} \to \mathbb{C}^{2n\times 2n}$ from the set of $n \times n$ quaternionic matrices into the set of $2n \times 2n$ complex matrices is defined by

$$A = A_1 + A_2\,\boldsymbol{j} \mapsto \sigma(A) = \begin{pmatrix} A_1 & A_2 \\ -\overline{A}_2 & \overline{A}_1 \end{pmatrix}, \tag{4}$$

where $A_1, A_2 \in \mathbb{C}^{n\times n}$. This mapping is injective, and obviously preserves addition and multiplication of matrices. We call $\sigma(A)$ the *derived matrix* of A (or, following [Zhang 1997], the *complex adjoint matrix* of A). We will be interested in the case where $n = 1$.

To conclude this introduction, we mention that it was Niven [1941; 1942] who made first steps in generalizing the fundamental theorem of algebra to the quaternionic situation. Since then many attempts have been made to compute roots of a quaternionic polynomial [Serôdio et al. 2001; Serôdio and Siu 2001; Pumplün and Walcher 2002; De Leo et al. 2006; Gentili and Stoppato 2008; Gentili and Struppa 2008; Gentili et al. 2008], most of which have focused on one-sided polynomials. In [Lam 2001, Section 16] and [Wang et al. 2009b] there are several general results on polynomials (of the one-sided type) over division rings. There are also a lot of recent studies on quaternionic matrices, for example [Farid et al. 2011; Wang et al. 2009a]. A large bibliography on quaternions can be found in [Gsponer and Hurni 2008].

2. Classifying zeros of two-sided quaternionic polynomials

To investigate the zeros of the polynomial in (1), we can assume (by left and right division, respectively) that $a_n = 1$ and $b_n = 1$, that is, the polynomial is monic:

$$p(x) := x^n + a_{n-1}x^{n-1}b_{n-1} + \cdots + a_1xb_1 + a_0, \quad x, a_i, b_j \in \mathbb{H}. \tag{5}$$

Let ξ be a fixed complex number. In this section, we shall give a classification of the zeros of $p(x)$, which improves the results in [Janovská and Opfer 2010a].

Furthermore, we give a clear description of the structure of each class of zeros for a polynomial $p(x)$ whose coefficients are complex.

From [Pogorui and Shapiro 2004], we know that all powers x^k, $k \in \mathbb{N}$, of a quaternion x have the form $x^k = \alpha_k x + \beta_k$, where α_k, β_k are real numbers. In order to determine the numbers α_k, β_k, Janovská and Opfer [2010b] gave two approaches. One is via the iteration

$$\begin{cases} \alpha_0 = 0, \quad \beta_0 = 1, \\ \alpha_{j+1} = 2\Re x\, \alpha_j + \beta_j, \\ \beta_{j+1} = -|x|^2 \alpha_j, \;\; j = 0, 1, \dots . \end{cases} \tag{6}$$

The other one relies on the formula

$$\begin{cases} \alpha_j = \Im(u_1^j)/\sqrt{|x|^2 - (\Re x)^2}, \\ \beta_0 = 1, \;\; \beta_{j+1} = -|x|^2 \alpha_j, \;\; j = 0, 1, \dots , \end{cases} \tag{7}$$

where u_1 is the complex solution of $u^2 - 2(\Re x)u + |x|^2 = 0$ with positive imaginary part. Formula (7) for α_j is of course easier to program than the iteration (6). However, since a power is involved, an economic use of (7) would also require an iteration.

For convenience of later use, we will first give a self-closed formula for α_k and β_k to improve the above formulas, that is, we give the following lemma, by which we can determine the real numbers α_k, β_k directly.

Lemma 2.1. *Suppose z is a quaternion, k is a natural number. Let*

$$\xi = \Re z + \sqrt{|z|^2 - (\Re z)^2}\, \boldsymbol{i}.$$

Then $z^k = \alpha_k z + \beta_k$, where

$$\alpha_k = \frac{\xi^k - \bar{\xi}^k}{\xi - \bar{\xi}} \in \mathbb{R}, \qquad \beta_k = |\xi|^2 \cdot \frac{\bar{\xi}^{k-1} - \xi^{k-1}}{\xi - \bar{\xi}} \in \mathbb{R}.$$

Remark 2.2. In this lemma, we set

$$\frac{\xi^k - \bar{\xi}^k}{\xi - \bar{\xi}} = 1 \quad \text{and} \quad \frac{\bar{\xi}^{k-1} - \xi^{k-1}}{\xi - \bar{\xi}} = 0$$

for $k = 1$, while

$$\frac{\xi^k - \bar{\xi}^k}{\xi - \bar{\xi}} = \xi^{k-1} + \xi^{k-2}\bar{\xi} + \cdots + \bar{\xi}^{k-1}, \qquad \frac{\bar{\xi}^{k-1} - \xi^{k-1}}{\xi - \bar{\xi}} = -(\xi^{k-2} + \xi^{k-3}\bar{\xi} + \cdots + \bar{\xi}^{k-2})$$

for $k > 1$ if ξ is real. Actually ξ is a complex number contained in $[z]$.

Proof. Since $\Re z = \Re \xi$ and $|z| = |\xi|$, we see that $z \in [\xi]$. Let

$$g(t) = t^2 - (\xi + \bar{\xi})t + |\xi|^2.$$

Then $g(t)$ is a polynomial with real coefficients, that annihilates each element of $[\xi]$. Note that the polynomial t^k can be expressed as $t^k = h(t)g(t) + \alpha_k t + \beta_k$, where α_k and β_k are real constants, $h(t) \in \mathbb{R}[t]$. Consequently, we have

$$\begin{cases} \alpha_k \xi + \beta_k = \xi^k, \\ \alpha_k \bar{\xi} + \beta_k = \bar{\xi}^k. \end{cases} \tag{8}$$

If $\xi - \bar{\xi} = 0$, then ξ is a real number and $z = \xi$. A straightforward verification shows the statement of the lemma for this case. Now suppose $\xi - \bar{\xi} \neq 0$. By (8),

$$\alpha_k = \frac{\xi^k - \bar{\xi}^k}{\xi - \bar{\xi}}, \qquad \beta_k = \frac{\xi\bar{\xi}^k - \bar{\xi}\xi^k}{\xi - \bar{\xi}} = |\xi|^2 \cdot \frac{\bar{\xi}^{k-1} - \xi^{k-1}}{\xi - \bar{\xi}}.$$

Since $q^k = h(q)g(q) + \alpha_k q + \beta_k = \alpha_k q + \beta_k$ for all $q \in [\xi]$, the proof is complete. □

With Lemma 2.1 in hand, we now introduce the method to find all zeros in the sphere $[\xi]$ for $p(x)$ where ξ is a fixed complex (so $\Re\xi$ is fixed).

Now for the fixed complex number ξ, and for any $z \in [\xi]$, $p(z)$ can be represented by

$$\begin{aligned} p(z) &= (\alpha_n z + \beta_n) + a_{n-1}(\alpha_{n-1} z + \beta_{n-1}) b_{n-1} + \cdots + a_1(\alpha_1 z + \beta_1) b_1 + a_0 \\ &= (\alpha_n z + a_{n-1}\alpha_{n-1} z b_{n-1} + \cdots + a_1 \alpha_1 z b_1) + (\beta_n + \cdots + a_1 \beta_1 b_1 + a_0) \\ &= A(z) + B, \end{aligned}$$

where

$$\begin{aligned} A(z) &= \alpha_n z + \alpha_{n-1} a_{n-1} z b_{n-1} + \cdots + \alpha_1 a_1 z b_1, \\ B &= \beta_n + \beta_{n-1} a_{n-1} b_{n-1} + \cdots + a_1 \beta_1 b_1 + a_0 \in \mathbb{H}. \end{aligned}$$

It is clear that the coefficients α_j, β_j ($j = 1, \ldots, n$) are given in Lemma 2.1. So, solving the equation $p(z) = 0$ in $[\xi]$ is equivalent to finding the solutions in the sphere surface $[\xi]$ of the following equation:

$$A(z) = -B. \tag{9}$$

Let $z = \Re\xi + x_1 \boldsymbol{i} + x_2 \boldsymbol{j} + x_3 \boldsymbol{k}$, $x_1, x_2, x_3 \in \mathbb{R}$. Regard z as the vector

$$\begin{pmatrix} \Re\xi \\ x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

and regard the surface of the sphere $[\xi]$ as

$$\Sigma = \left\{ \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} : x_1^2 + x_2^2 + x_3^2 = |\xi|^2 - (\Re\xi)^2,\ x_1, x_2, x_3 \in \mathbb{R} \right\}.$$

Unfolding the left side of (9) leads to the following linear system consisting of four equations in three variables,

$$M\begin{pmatrix}x_1\\x_2\\x_3\end{pmatrix}=\begin{pmatrix}e_0\\e_1\\e_2\\e_3\end{pmatrix}, \tag{10}$$

where M is a known real 4×3 matrix, e_0, e_1, e_2, and e_3 are known real numbers. Suppose S is the solution set of the linear system (10). Then the set of zeros of $p(x)$ contained in $[\xi]$ is

$$\left\{\begin{pmatrix}\Re\xi\\ s\end{pmatrix} : s\in S\cap\Sigma\right\}.$$

If (10) has no solution, that is, $S=\varnothing$, then $[\xi]$ contains no zero of $p(x)$.

When (10) has a solution, its solution set can be represented by $\mathcal{N}+X_0$, where $\mathcal{N}$ is the solution space of the system of homogeneous linear equations $MX=0$, while X_0 is a particular solution of (10). Now we analyze the set $\mathcal{N}+X_0$ as follows.

If $\dim\mathcal{N}=0$, then (10) has only one solution X_0, so $[\xi]$ contains at most one zero of $p(x)$.

If $\dim\mathcal{N}=1$, then S becomes a straight line in the three-dimensional $\{x_1, x_2, x_3\}$-space. So $[\xi]$ contains no zero of $p(x)$ when S is separated from the sphere $[\xi]$, $[\xi]$ contains only one zero when S is tangent to the sphere $[\xi]$, and $[\xi]$ contains two zeros if the straight line S pierces the sphere $[\xi]$.

If $\dim\mathcal{N}=2$, S is a plane in the three-dimensional $\{x_1, x_2, x_3\}$-space, there are three possible position relationships between the plane and the sphere: separated, tangent and intersected. Then $[\xi]$ contains no zero of $p(x)$ for the separated situation, contains only one zeros for the tangent situation. With respect to the intersected situation, the intersection of the plane and the sphere is a circular curve, so the zeros of $p(x)$ contained in $[\xi]$ form a circle in the three-dimensional $\{x_1, x_2, x_3\}$-space.

Finally, if $\dim\mathcal{N}=3$, then $S=\mathbb{R}^3$, and each point in $[\xi]$ is a zero of $p(x)$.

To sum up the above arguments, we have obtained:

Theorem 2.3. *Let $p(x)$ be as in* (5), *and let ξ be a complex number. If $Z_{[\xi]}(p)$ is the set of zeros of $p(x)$ contained in $[\xi]$ and $|Z_{[\xi]}(p)|$ is its cardinality, we have the following possibilities*:

- $|Z_{[\xi]}(p)|\le 2$.
- $Z_{[\xi]}(p)$ *is a circle on the surface of the sphere* $[\xi]$.
- $Z_{[\xi]}(p)=[\xi]$.

Definition 2.4. Let $p(x)$ be as in (5), and let z_0 be a zero of $p(x)$. If z_0 is not real and $Z_{[z_0]}(p)=[z_0]$, we say that z_0 *generates a spherical zero*, or simply that it is a spherical zero. If z_0 is real or $|Z_{[z_0]}(p)|\le 2$, it is called an isolated zero. If z_0 is not real and has the property that $Z_{[z_0]}(p)$ is a circle on the sphere $[z_0]$, we say that z_0 *generates a circular zero*, or is a circular zero.

Thus Theorem 2.3 classifies the zeros of quaternionic two-sided polynomials into three types: isolated zeros, spherical zeros and circular zeros.

Now we apply Theorem 2.3 to two-sided polynomials with complex coefficients.

Theorem 2.5. *Let* $p(x) := x^n + a_{n-1}x^{n-1}b_{n-1} + \cdots + a_1 x b_1 + a_0$, *where all the* a_i, b_i $(i = 0, 1, \ldots, n-1)$ *are complex numbers. Let* ξ *be a complex number with* $Z_{[\xi]}(p) \neq \varnothing$. *We have the following possibilities*:

- $Z_{[\xi]}(p) \subseteq \{\xi, \bar{\xi}\}$.
- $Z_{[\xi]}(p) = \{z_1 + z_2 \boldsymbol{j} : z_1 \in \mathbb{C}$ *fixed*, $z_2 \in \mathbb{C},\ |z_2|^2 = |\xi|^2 - |z_1|^2 > 0\}$.
- $Z_{[\xi]}(p) = [\xi]$.

Proof. If all a_i, b_i are complex, in (9) we set

$$\begin{aligned} &p_n = \alpha_n, \quad p_{n-1} = \alpha_{n-1}a_{n-1}, \quad \ldots, \quad p_1 = \alpha_1 a_1, \\ &q_n = 1, \quad q_{n-1} = b_{n-1}, \quad \ldots, \quad q_1 = b_1, \quad q_0 = -B. \end{aligned}$$

Then all p_i, q_i are known complex numbers. Writing the point z in $[\xi]$ as

$$z = z_1 + z_2 \boldsymbol{j}, \quad z_1, z_2 \in \mathbb{C},$$

and using the derived mapping, we can write (9) as

$$\begin{pmatrix} p_n & \\ & \bar{p}_n \end{pmatrix} \begin{pmatrix} z_1 & z_2 \\ -\bar{z}_2 & \bar{z}_1 \end{pmatrix} \begin{pmatrix} q_n & \\ & \bar{q}_n \end{pmatrix} + \cdots + \begin{pmatrix} p_1 & \\ & \bar{p}_1 \end{pmatrix} \begin{pmatrix} z_1 & z_2 \\ -\bar{z}_2 & \bar{z}_1 \end{pmatrix} \begin{pmatrix} q_1 & \\ & \bar{q}_1 \end{pmatrix} = \begin{pmatrix} q_0 & \\ & \bar{q}_0 \end{pmatrix},$$

which is equivalent to

$$\Big(\sum_{i=1}^{n} p_i q_i\Big) z_1 = q_0, \quad \Big(\sum_{i=1}^{n} p_i \bar{q}_i\Big) z_2 = 0. \tag{11}$$

Since $Z_{[\xi]}(p) \neq \varnothing$, (11) is consistent.

If $\sum_{i=1}^{n} p_i \bar{q}_i = 0$ and $\sum_{i=1}^{n} p_i q_i \neq 0$, then

$$z_1 = \frac{q_0}{\sum_{i=1}^{n} p_i q_i}, \quad \text{and} \quad |z_2|^2 = |\xi|^2 - \left| \frac{q_0}{\sum_{i=1}^{n} p_i q_i} \right|^2.$$

When

$$|\xi|^2 - \left| \frac{q_0}{\sum_{i=1}^{n} p_i q_i} \right|^2 > 0,$$

the zeros of $p(x)$ contained in $[\xi]$ are circular zeros, and

$$Z_{[\xi]}(p) = \left\{ \frac{q_0}{\sum_{i=1}^{n} p_i q_i} + z_2 \boldsymbol{j} : z_2 \in \mathbb{C}, |z_2|^2 = |\xi|^2 - \left| \frac{q_0}{\sum_{i=1}^{n} p_i q_i} \right|^2 \right\}.$$

Otherwise,

$$Z_{[\xi]}(p) = \left\{ \frac{q_0}{\sum_{i=1}^{n} p_i q_i} \right\} \subseteq \{\xi, \bar{\xi}\}.$$

If $\sum_{i=1}^{n} p_i \bar{q}_i = 0$ and $\sum_{i=1}^{n} p_i q_i = 0$, then $q_0 = 0$ and each point in $[\xi]$ is a zero of $p(x)$. So it is a spherical zero, that is, $Z_{[\xi]}(p) = [\xi]$.

Finally, if $\sum_{i=1}^{n} p_i \bar{q}_i \neq 0$, then $z_2 = 0$ and $z = z_1 + z_2 \boldsymbol{j} = z_1$, which has at most two values in $[\xi]$: ξ and $\bar{\xi}$. □

Janovská and Opfer [2010a] classified the zeros of quaternionic two-sided polynomials $p(x)$ into five classes according to the five possible ranks of a real (4×4) matrix obtained from the coefficients of $p(x)$. In their notation, type 0 and type 1 solutions are isolated solutions, a type 2 solution can be an isolated solution or a circular solution, a type 3 solution is a circular solution or a spherical solution, while a type 4 solution is a spherical solution.

We can understand Theorem 2.3 from the view of point of geometry as follows. The set of isolated zeros in $[\xi]$ is of dimension 0, the set of circular zeros in $[\xi]$ is of dimension 1 because they form a circular line, and the set of spherical zeros in $[\xi]$ is of dimension 2 because these zeros form a surface of a ball.

Remark 2.6. (a) Since one-sided polynomials, as in (5), belong to the class we are considering, isolated zeros and spherical zeros in fact occur (actually these two types are the only solutions; see [Feng and Zhao 2011; Janovská and Opfer 2010b]). From the study of the quadratic case in Section 4 of this paper, we shall see that the polynomial $p(x) = x^2 + \boldsymbol{i} x \boldsymbol{i} + 2$ has circular zeros and two conjugate isolated zeros.

(b) From Theorem 2.5 we see that, for a two-sided polynomial $p(x)$ with complex coefficients, an isolated zero (if exists) of $p(x)$ should be a complex number, and the equivalence class $[z]$ for an arbitrary circular zero z (if it exists) should contain no complex roots of $p(x)$. These facts will be used in the sequel.

3. Finding all zeros of quaternionic two-sided polynomials with complex coefficients

Consider a quaternionic two-sided polynomial with complex coefficients:

$$p(x) := x^n + a_{n-1} x^{n-1} b_{n-1} + \cdots + a_1 x b_1 + a_0, \quad x \in \mathbb{H},\ a_i, b_j \in \mathbb{C}. \tag{12}$$

We will find a method to compute all the zeros of $p(x)$. We introduce the notation

$$\widetilde{p}(x) := x^n + a_{n-1} b_{n-1} x^{n-1} + \cdots + a_1 b_1 x + a_0,$$
$$\overline{\widetilde{p}}(x) := x^n + \bar{a}_{n-1} \bar{b}_{n-1} x^{n-1} + \cdots + \bar{a}_1 \bar{b}_1 x + \bar{a}_0,$$
$$\overleftarrow{p}(x) := x^n + a_{n-1} \bar{b}_{n-1} x^{n-1} + \cdots + a_1 \bar{b}_1 x + a_0.$$

Theorem 3.1 (characterization of spherical zeros). *Let ξ be a complex number. Then each point of $[\xi]$ is a zero of $p(x)$ if and only if*

$$\widetilde{p}(\xi) = \widetilde{p}(\bar{\xi}) = 0 \quad \textit{and} \quad \overleftarrow{p}(\xi) = \overleftarrow{p}(\bar{\xi}).$$

Proof. For any $z \in [\xi]$, we can write z as $z = q\xi q^{-1}$ for some $q = z_1 + z_2\boldsymbol{j}$ with $z_1, z_2 \in \mathbb{C}$, and $|z_1|^2 + |z_2|^2 = 1$. Then $p(z) = 0$ is equivalent to

$$q\xi^n q^{-1} + a_{n-1}q\xi^{n-1}q^{-1}b_{n-1} + \cdots + a_1 q\xi q^{-1}b_1 + a_0 = 0.$$

By the derived mapping, we get

$$\begin{aligned}
&\begin{pmatrix} z_1 & z_2 \\ -\bar{z}_2 & \bar{z}_1 \end{pmatrix}\begin{pmatrix} \xi^n & \\ & \bar{\xi}^n \end{pmatrix}\begin{pmatrix} \bar{z}_1 & -z_2 \\ \bar{z}_2 & z_1 \end{pmatrix} \\
&\quad + \begin{pmatrix} a_{n-1} & \\ & \bar{a}_{n-1} \end{pmatrix}\begin{pmatrix} z_1 & z_2 \\ -\bar{z}_2 & \bar{z}_1 \end{pmatrix}\begin{pmatrix} \xi^{n-1} & \\ & \bar{\xi}^{n-1} \end{pmatrix}\begin{pmatrix} \bar{z}_1 & -z_2 \\ \bar{z}_2 & z_1 \end{pmatrix}\begin{pmatrix} b_{n-1} & \\ & \bar{b}_{n-1} \end{pmatrix} + \cdots \\
&\qquad + \begin{pmatrix} a_1 & \\ & \bar{a}_1 \end{pmatrix}\begin{pmatrix} z_1 & z_2 \\ -\bar{z}_2 & \bar{z}_1 \end{pmatrix}\begin{pmatrix} \xi & \\ & \bar{\xi} \end{pmatrix}\begin{pmatrix} \bar{z}_1 & -z_2 \\ \bar{z}_2 & z_1 \end{pmatrix}\begin{pmatrix} b_1 & \\ & \bar{b}_1 \end{pmatrix} + \begin{pmatrix} a_0 & \\ & \bar{a}_0 \end{pmatrix} = 0,
\end{aligned}$$

which is equivalent to the system of the following two equations:

$$|z_1|^2(\widetilde{p}(\xi) - a_0) + |z_2|^2(\widetilde{p}(\bar{\xi}) - a_0) + a_0 = 0, \tag{13}$$

$$z_1 z_2(\overleftarrow{p}(\bar{\xi}) - \overleftarrow{p}(\xi)) = 0. \tag{14}$$

The above argument will be also used in later proofs.

$\Rightarrow$) Suppose each point of $[\xi]$ is a zero of $p(x)$. Then (13) and (14) hold for any $z_1, z_2 \in \mathbb{C}$ with $|z_1|^2 + |z_2^2| = 1$. Note that (13) can also be written as

$$|z_1|^2(\widetilde{p}(\xi) - \widetilde{p}(\bar{\xi})) + \widetilde{p}(\bar{\xi}) = 0. \tag{15}$$

The equalities (15) and (14) hold for arbitrary complex z_1, z_2 with $|z_1|^2 + |z_2|^2 = 1$, yielding that $\widetilde{p}(\xi) - \widetilde{p}(\bar{\xi}) = 0$, $\widetilde{p}(\bar{\xi}) = 0$, and $\overleftarrow{p}(\bar{\xi}) - \overleftarrow{p}(\xi) = 0$. The rest follow easily for this direction.

$\Leftarrow$) Obvious. □

Theorem 3.2 (characterization of isolated zeros). *Let T be the set of nonreal, isolated zeros of $p(x)$. Then*

$$T = \{\xi \in \mathbb{C} : \widetilde{p}(\xi) = 0, \overleftarrow{p}(\xi) \neq \overleftarrow{p}(\bar{\xi})\} \cup \{\xi \in \mathbb{C} : \widetilde{p}(\xi) = 0, \widetilde{p}(\bar{\xi}) \neq 0\};$$

the set of all isolated zeros of $p(x)$ is $\{$the real roots of $\widetilde{p}(x)\} \cup T$.

Proof. By Remark 2.6, we see that the set of isolated zeros of $p(x)$ is contained in $\{\xi \in \mathbb{C} : \widetilde{p}(\xi) = 0\}$. Let ξ be a nonreal complex root of $\widetilde{p}$. If $\overleftarrow{p}(\xi) = \overleftarrow{p}(\bar{\xi})$ and

$\widetilde{p}(\bar{\xi}) = 0$, then ξ becomes a spherical zero from Theorem 3.1. Hence,

$$T = \{\xi \in \mathbb{C} : \widetilde{p}(\xi) = 0,\ \overleftarrow{p}(\xi) \neq \overleftarrow{p}(\bar{\xi})\} \cup \{\xi \in \mathbb{C} : \widetilde{p}(\xi) = 0,\ \widetilde{p}(\bar{\xi}) \neq 0\},$$

and the set of all isolated zeros of $p(x)$ is {the real roots of $\widetilde{p}$} $\cup\, T$. □

Theorem 3.3 (characterization of circular zeros). *Let ξ be a given complex number. Then $[\xi]$ contains a circular zero of $p(x)$ if and only if*

$$\widetilde{p}(\xi)\overline{\widetilde{p}}(\xi) < 0 \quad \textit{and} \quad \overleftarrow{p}(\xi) = \overleftarrow{p}(\bar{\xi}). \tag{16}$$

Moreover, if $[\xi]$ contains a circular zero of $p(x)$, then

$$(\Im\xi)^2\left(1 - \frac{\widetilde{p}(\bar{\xi}) + \widetilde{p}(\xi)}{\widetilde{p}(\bar{\xi}) - \widetilde{p}(\xi)}\right)^2 > 0$$

and the set of circular zeros in $[\xi]$ is

$$\left\{\Re\xi + \frac{\widetilde{p}(\bar{\xi}) + \widetilde{p}(\xi)}{\widetilde{p}(\bar{\xi}) - \widetilde{p}(\xi)}\Im\xi\boldsymbol{i} + z_2\boldsymbol{j} : z_2 \in \mathbb{C},\ |z_2|^2 = (\Im\xi)^2\left(1 - \frac{\widetilde{p}(\bar{\xi}) + \widetilde{p}(\xi)}{\widetilde{p}(\bar{\xi}) - \widetilde{p}(\xi)}\right)^2\right\}.$$

Proof. $\Rightarrow$) Suppose $[\xi]$ contains a circular zero of $p(x)$. By Theorem 2.5, the circular zeros in $[\xi]$ contain no complex zeros of p. Using the first part of the proof in Theorem 3.1, we know that there exist z_1, $z_2 \in \mathbb{C}$ with $z_1z_2 \neq 0$ and $|z_1|^2 + |z_2|^2 = 1$, such that $z = (z_1 + z_2\boldsymbol{j})\xi(z_1 + z_2\boldsymbol{j})^{-1}$ is a zero of $p(x)$. So (13) and (14) hold for this z, which yield $|z_1|^2\widetilde{p}(\xi) + |z_2|^2\widetilde{p}(\bar{\xi}) = 0$ and $\overleftarrow{p}(\xi) = \overleftarrow{p}(\bar{\xi})$. From $|z_1|^2\widetilde{p}(\xi) + |z_2|^2\widetilde{p}(\bar{\xi}) = 0$, we have

$$|z_1|^2\widetilde{p}(\xi)\overline{\widetilde{p}}(\xi) = -|z_2|^2\widetilde{p}(\bar{\xi})\overline{\widetilde{p}}(\xi) = -|z_2|^2|\overline{\widetilde{p}}(\xi)|^2 < 0,$$

that is $\widetilde{p}(\xi)\overline{\widetilde{p}}(\xi) < 0$, as desired.

$\Leftarrow$) Note that $\widetilde{p}(\xi)\overline{\widetilde{p}}(\xi) < 0$ implies $\Im\xi \neq 0$ and $|\overline{\widetilde{p}}(\xi)|^2 - \widetilde{p}(\xi)\overline{\widetilde{p}}(\xi) > 0$. Let $z_1, z_2 \in \mathbb{C}$ be given by

$$|z_1|^2 = \frac{|\overline{\widetilde{p}}(\xi)|^2}{|\overline{\widetilde{p}}(\xi)|^2 - \widetilde{p}(\xi)\overline{\widetilde{p}}(\xi)}, \qquad |z_2|^2 = 1 - |z_1|^2. \tag{17}$$

Then $z_1z_2 \neq 0$, $|z_1|^2 + |z_2|^2 = 1$ and it is easy to verify that (13) and (14) hold simultaneously. So $(z_1 + z_2\boldsymbol{j})\xi(z_1 + z_2\boldsymbol{j})^{-1}$ is a zero of $p(x)$. From

$$\begin{aligned}(z_1 + z_2\boldsymbol{j})\xi(z_1 + z_2\boldsymbol{j})^{-1} &= |z_1|^2\xi + |z_2|^2\bar{\xi} - 2z_1z_2\Im\xi\,\boldsymbol{j} \\ &= \Re\xi + (2|z_1|^2 - 1)(\Im\xi)\boldsymbol{i} - 2z_1z_2\Im\xi\,\boldsymbol{j},\end{aligned} \tag{18}$$

we see that $[\xi]$ contains a noncomplex zero of $p(x)$. The inequality $\widetilde{p}(\xi)\overline{\widetilde{p}}(\xi) < 0$ also implies $\widetilde{p}(\xi) \neq 0$, so from Theorem 3.1 we know $[\xi]$ contains no spherical zeros of $p(x)$. Now combining with Theorem 2.5 we see $[\xi]$ contains a circular zero of $p(x)$. The proof of this direction is completed.

Finally, if $[\xi]$ contains a circular zero, let z_1 and z_2 be defined by (17). Then

$$(2|z_1|^2-1)\Im\xi = \frac{\widetilde{p}(\bar{\xi})+\widetilde{p}(\xi)}{\widetilde{p}(\bar{\xi})-\widetilde{p}(\xi)}\,\Im\xi,$$

$$\frac{\widetilde{p}(\bar{\xi})+\widetilde{p}(\xi)}{\widetilde{p}(\bar{\xi})-\widetilde{p}(\xi)}-1 = \frac{2\widetilde{p}(\xi)}{\widetilde{p}(\bar{\xi})-\widetilde{p}(\xi)} = \frac{2\widetilde{p}(\xi)\overline{\widetilde{p}}(\xi)}{(\widetilde{p}(\bar{\xi})-\widetilde{p}(\xi))\overline{\widetilde{p}}(\xi)} < 0.$$

Therefore,

$$r := (\Im\xi)^2\left(1-\frac{\widetilde{p}(\bar{\xi})+\widetilde{p}(\xi)}{\widetilde{p}(\bar{\xi})-\widetilde{p}(\xi)}\right)^2 > 0$$

and by Theorem 2.5 and (18), the set of circular zeros in $[\xi]$ is

$$\left\{\Re\xi+\frac{\widetilde{p}(\bar{\xi})+\widetilde{p}(\xi)}{\widetilde{p}(\bar{\xi})-\widetilde{p}(\xi)}\,\Im\xi\boldsymbol{i}+z\boldsymbol{j} : z\in\mathbb{C},\ |z|^2=r\right\}. \qquad \square$$

From Theorems 3.1 and 3.2 we have actually given a method to find all isolated zeros and spherical zeros:

Let the complex solution set of $\widetilde{p}(x)=0$ be

$$\{\xi_1,\dots,\xi_s,\eta_1,\dots,\eta_k,\zeta_1,\bar{\zeta}_1,\dots,\zeta_l,\bar{\zeta}_l,\zeta_{l+1},\bar{\zeta}_{l+1},\dots,\zeta_t,\bar{\zeta}_t\},$$

where $\xi_1,\dots,\xi_s$ are distinct real numbers, $\eta_1,\dots,\eta_k,\zeta_1,\dots,\zeta_t$ are distinct nonreal complex numbers (each $\bar{\eta}_i$ is no longer a root of $\widetilde{p}(x)$), $\overleftarrow{p}(\zeta_i)\neq\overleftarrow{p}(\bar{\zeta}_i)$ for $i=1,\dots,l$ and $\overleftarrow{p}(\zeta_i)=\overleftarrow{p}(\bar{\zeta}_i)$ for $i=l+1,\dots,t$. Then the set of all spherical zeros of $p(x)$ is

$$[\zeta_{l+1}]\cup\cdots\cup[\zeta_t],$$

and the set of all isolated zeros of $p(x)$ is

$$\{\xi_1,\dots,\xi_s,\eta_1,\dots,\eta_k,\zeta_1,\bar{\zeta}_1,\dots,\zeta_l,\bar{\zeta}_l\}.$$

Next we consider how to find all circular zeros of $p(x)$. From Theorem 3.3 we need only to find all complex numbers ξ with $[\xi]$ containing a circular zero of $p(x)$. First we give a necessary condition for $p(x)$ to have a circular zero.

Proposition 3.4. *Let $p(x)$ be a two-sided polynomial of the form of* (12). *If $p(x)$ has a circular zero*, *then*

$$\begin{pmatrix}1\\ a_{n-1}b_{n-1}\\ \vdots\\ a_1b_1\end{pmatrix}\neq\begin{pmatrix}1\\ a_{n-1}\bar{b}_{n-1}\\ \vdots\\ a_1\bar{b}_1\end{pmatrix}\neq\begin{pmatrix}1\\ \bar{a}_{n-1}\bar{b}_{n-1}\\ \vdots\\ \bar{a}_1\bar{b}_1\end{pmatrix};$$

that is, *$p(x)$ cannot be essentially written as a one-sided polynomial.*

Proof. Suppose contrarily

$$\begin{pmatrix} 1 \\ a_{n-1}b_{n-1} \\ \vdots \\ a_1 b_1 \end{pmatrix} = \begin{pmatrix} 1 \\ a_{n-1}\bar{b}_{n-1} \\ \vdots \\ a_1 \bar{b}_1 \end{pmatrix}.$$

Then $\widetilde{p}(x) = \overleftarrow{p}(x)$. Let ξ be a complex number and $[\xi]$ contain a circular zero of $p(x)$. Then by Theorem 3.3 we have

$$\widetilde{p}(\xi) = \overleftarrow{p}(\xi) = \overleftarrow{p}(\bar{\xi}) = \widetilde{p}(\bar{\xi}) \quad \text{and} \quad \widetilde{p}(\xi)\overline{\widetilde{p}}(\xi) = \widetilde{p}(\xi)\overline{\widetilde{p}(\bar{\xi})} = |\widetilde{p}(\xi)|^2 \geq 0,$$

a contradiction to $\widetilde{p}(\xi)\overline{\widetilde{p}}(\xi) < 0$. The proof for the other inequality is similar. □

Lemma 3.5 [Zhang 1998, Theorem 3.16]. *Let $f = a_n(x)y^n + \cdots + a_1(x)y + a_0(x)$ and $g = b_m(x)y^m + \cdots + b_1(x)y + b_0(x) \in \mathbb{C}[x, y]$, where $a_i(x), b_j(x) \in \mathbb{C}[x]$ $(i = 0, \ldots, n,\ j = 0, 1, \ldots, m)$ with $a_n(x)b_m(x) \neq 0$. Let $R(f, g; x)$ be the resultant of f and g of order $m+n$, given by*

$$\begin{vmatrix} a_n(x) & a_{n-1}(x) & \ldots & \ldots & \ldots & a_0(x) & & & \\ & a_n(x) & a_{n-1}(x) & \ldots & \ldots & \ldots & a_0(x) & & \\ & & \ddots & & & & & \ddots & \\ & & & a_n(x) & a_{n-1}(x) & \ldots & \ldots & \ldots & a_0(x) \\ b_m(x) & b_{m-1}(x) & \ldots & \ldots & b_0(x) & & & & \\ & b_m(x) & b_{m-1}(x) & \ldots & \ldots & b_0(x) & & & \\ & & \ddots & & & & \ddots & & \\ & & & \ddots & & & & \ddots & \\ & & & & b_m(x) & b_{m-1}(x) & \ldots & \ldots & b_0(x) \end{vmatrix}$$

where $a_n(x), \ldots, a_1(x), a_0(x)$ are located in the first m rows, and the coefficients $b_m(x), \ldots, b_1(x), b_0(x)$ are located in the lower n rows. Then a complex x_0 is a zero of $R(f, g; x)$ if and only if the system

$$\begin{cases} f(x_0, y) = 0 \\ g(x_0, y) = 0 \end{cases}$$

has a solution $y_0 \in \mathbb{C}$ or the system

$$\begin{cases} a_n(x_0) = 0 \\ b_m(x_0) = 0 \end{cases}$$

holds.

Now suppose $[\xi]$ contains a circular zero of $p(x)$, where ξ is a given complex number. Then by Theorem 3.3 we have $\overleftarrow{p}(\xi) = \overleftarrow{p}(\bar{\xi})$ and $\widetilde{p}(\xi)\overline{\widetilde{p}}(\xi) < 0$. The later inequality implies the imaginary part of $\widetilde{p}(\xi)\overline{\widetilde{p}}(\xi)$ is 0.

Set $a_0 = c_0 + d_0\boldsymbol{i}$, where c_0, d_0 are the real part and imaginary part of a_0, respectively. Also set $(\xi^n, \xi^{n-1}, \cdots, \xi^2, \xi) = \alpha + \beta\boldsymbol{i}$ and

$$\begin{pmatrix} 1 \\ a_{n-1}b_{n-1} \\ \vdots \\ a_1b_1 \end{pmatrix} = U + V\boldsymbol{i},$$

where α, β are both real row vectors (real $1 \times n$ matrices), U and V are both real column vectors (real $n \times 1$ matrices). It is easy to see the first component of U is 1 while the first component of V is 0. From $\overleftarrow{p}(\xi) = \overleftarrow{p}(\bar{\xi})$ we get

$$\beta \begin{pmatrix} 1 \\ a_{n-1}\bar{b}_{n-1} \\ \vdots \\ a_1\bar{b}_1 \end{pmatrix} = 0. \tag{19}$$

And note that the imaginary part of $\widetilde{p}(\xi)\overline{\widetilde{p}}(\xi)$ is 0, so we get

$$\beta U\alpha U + \beta V\alpha V + c_0\beta U + d_0\beta V = 0. \tag{20}$$

Let $\xi = u + y\boldsymbol{i}$ with $u, y \in \mathbb{R}$. Remark 2.6(b) ensures that $y \neq 0$. Then

$$\xi^n = u^n + C_n^1 u^{n-1}(y\boldsymbol{i}) + \cdots + C_n^{n-1} u(y\boldsymbol{i})^{n-1} + (y\boldsymbol{i})^n.$$

When n is even, we have

$$\begin{cases} \Re\xi^n = u^n - C_n^2 u^{n-2}y^2 + \cdots + y^n(-1)^{\frac{n}{2}}, \\ \Im\xi^n = C_n^1 u^{n-1}y + \cdots + C_n^{n-1} uy^{n-1}(-1)^{\frac{n-2}{2}}, \end{cases}$$

and when n is odd we have

$$\begin{cases} \Re\xi^n = u^n - C_n^2 u^{n-2}y^2 + \cdots + C_n^{n-1} uy^{n-1}(-1)^{\frac{n-1}{2}}, \\ \Im\xi^n = C_n^1 u^{n-1}y + \cdots + C_n^{n-2} u^2y^{n-2}(-1)^{\frac{n-3}{2}} + y^n(-1)^{\frac{n-1}{2}}. \end{cases}$$

For convenience we take n to be an odd number, $n = 2k + 1$ since it is similar for the case that n is even. In this case (19) becomes

$$\left(C_n^1 u^{n-1}y + \cdots + C_n^{n-2} u^2y^{n-2}(-1)^{\frac{n-3}{2}} + y^n(-1)^{\frac{n-1}{2}}, \ldots, y\right) \cdot \begin{pmatrix} 1 \\ a_{n-1}\bar{b}_{n-1} \\ \vdots \\ a_1\bar{b}_1 \end{pmatrix} = 0. \tag{21}$$

Since $y \neq 0$, we can write this as

$$(22)\qquad \left(C_n^1 u^{n-1} + \cdots + C_n^{n-2} u^2 y^{n-3} (-1)^{\frac{n-3}{2}} + y^{n-1}(-1)^{\frac{n-1}{2}}, \ldots, 1\right) \cdot \begin{pmatrix} 1 \\ a_{n-1}\bar{b}_{n-1} \\ \vdots \\ a_1 \bar{b}_1 \end{pmatrix} = 0.$$

It is easy to see that (22) can be rewritten as

$$(23)\qquad z^k + d_1(u) z^{k-1} + \cdots + d_{k-1}(u) z + d_k(u) = 0,$$

where $z := y^2$, $k = \frac{n-1}{2}$, $d_1(u), \ldots, d_k(u) \in \mathbb{C}[u]$, $\deg d_k(u) = 2k$ (implying that $d_k(u) \neq 0$).

We treat (20) in a similar manner. Note that $y \neq 0$, the first component of U is 1 and the first component of V is 0, then we obtain from (20) the following equation:

$$(24)\qquad h_1(u) z^{2k} + h_2(u) z^{2k-1} + \cdots + h_n(u) = 0,$$

where $z := y^2$, $k = \frac{n-1}{2}$, $h_1(u), \ldots, h_n(u) \in \mathbb{C}[u]$, $\deg h_n(u) = 2n - 1$.

Up to now, we have shown that, if $[\xi]$ contains a circular zero of $p(x)$, then the real part and imaginary part of ξ must satisfy (23) and (24). Let

$$f := z^k + d_1(u) z^{k-1} + \cdots + d_{k-1}(u) z + d_k(u),$$
$$g := h_1(u) z^{2k} + h_2(u) z^{2k-1} + \cdots + h_n(u).$$

We denote by R_p the resultant of f and g. Then

$$R_p = \begin{vmatrix} 1 & d_1(u) & \ldots & \ldots & \ldots & d_k(u) & & & \\ & 1 & d_1(u) & \ldots & \ldots & \ldots & d_k(u) & & \\ & & \ddots & & & & & \ddots & \\ & & & 1 & d_1(u) & \ldots & \ldots & \ldots & d_k(u) \\ h_1(u) & h_2(u) & \ldots & \ldots & h_n(u) & & & & \\ & h_1(u) & h_2(u) & \ldots & \ldots & h_n(u) & & & \\ & & \ddots & & & & \ddots & & \\ & & & \ddots & & & & \ddots & \\ & & & & h_1(u) & h_2(u) & \ldots & \ldots & h_n(u) \end{vmatrix},$$

which is a polynomial in the variable u with complex coefficients. Let $x_1, \ldots, x_s$ be the real roots of R_p (if R_p has no real root, then $p(x)$ has no circular zero, by Lemma 3.5). Then substitute x_l for u in (23) to get corresponding nonzero solutions for y. In this way we get at most finitely many complex numbers $x_l + y_{lj}\boldsymbol{i}$, where y_{lj} is the real solution of

$$(y^2)^k + d_1(x_l)(y^2)^{k-1} + \cdots + d_{k-1}(x_l)y^2 + d_k(x_l) = 0,$$

$l = 1, \ldots, s$, $j = 1, \ldots, n_l$. (If such a y_{lj} does not exist, this also shows $p(x)$ has no circular zeros.) Now if $[\xi]$ contains a circular zero, then from Lemma 3.5 we know ξ must be equal to some $x_l + y_{lj}\boldsymbol{i}$. Therefore, for the finitely many complex numbers $x_l + y_{lj}\boldsymbol{i}$ ($l = 1, \ldots, s$, $j = 1, \ldots, n_l$), using Theorem 3.3 we can find all circular zeros of $p(x)$.

This method for finding circular zeros will be valid so long as the resultant R_p is not the zero polynomial. Since we have excluded the cases

$$\begin{pmatrix} 1 \\ a_{n-1}b_{n-1} \\ \vdots \\ a_1b_1 \end{pmatrix} = \begin{pmatrix} 1 \\ a_{n-1}\bar{b}_{n-1} \\ \vdots \\ a_1\bar{b}_1 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 1 \\ a_{n-1}\bar{b}_{n-1} \\ \vdots \\ a_1\bar{b}_1 \end{pmatrix} = \begin{pmatrix} 1 \\ \bar{a}_{n-1}\bar{b}_{n-1} \\ \vdots \\ \bar{a}_1\bar{b}_1 \end{pmatrix}$$

(Proposition 3.4 ensures that $p(x)$ has no circular zeros under such circumstances), generally speaking the resultant R_p obtained at the moment cannot vanish. We have done a lot of tests, and have never discovered a two-sided polynomial $p(x)$ of form (12) with the conditions in Proposition 3.4 such that $R_p = 0$.

Example 3.6. Find all zeros of $p(z) = z^3 - \boldsymbol{i}z^2\boldsymbol{i} - \boldsymbol{i}z\boldsymbol{i} + 1$ in $\mathbb{H}$.

Solution. $\widetilde{p}(z) = z^3 + z^2 + z + 1$, $\overleftarrow{p}(z) = z^3 - z^2 - z + 1$. The complex roots of $\widetilde{p}(z)$ are $-1, \boldsymbol{i}, -\boldsymbol{i}$. $\overleftarrow{p}(\boldsymbol{i}) = 2 - 2\boldsymbol{i}$, $\overleftarrow{p}(\bar{\boldsymbol{i}}) = 2 + 2\boldsymbol{i}$. Thus, p has no spherical zero, and the set of isolated zeros is $\{-1, \boldsymbol{i}, -\boldsymbol{i}\}$.

Now we seek the circular zeros. We have

$$U = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad V = 0, \quad c_0 = 1, \quad d_0 = 0,$$

$$\alpha = (x^3 - 3xy^2, x^2 - y^2, x), \quad \beta = (3x^2y - y^3, 2xy, y),$$

In this case, (24) and (23) become

$$(25) \quad (3x+1)t^2 - (10x^3+10x^2+6x+2)t + (3x^5+5x^4+6x^3+6x^2+3x+1) = 0,$$

$$(26) \qquad t + (-3x^2 + 2x + 1) = 0,$$

where $t := y^2$. The resultant R_p is

$$R_p = \begin{vmatrix} 1 & -3x^2+2x+1 & 0 \\ 0 & 1 & -3x^2+2x+1 \\ 3x+1 & -(10x^3+10x^2+6x+2) & 3x^5+5x^4+6x^3+6x^2+3x+1 \end{vmatrix}$$
$$= -32x^4 + 32x^2 + 20x + 4.$$

The real roots of R_p are (from MATLAB)

$$x_1 = -0.500000000000000, \quad x_2 = 1.255773570847266,$$

and from (26) we get the positive roots

$$y_{x_1} = 0.866025403784440, \quad y_{x_2} = 1.104243923243840$$

and their opposites We investigate the complex numbers

$$\xi_1 = x_1 + y_{x_1}\boldsymbol{i}, \quad \xi_2 = \bar{\xi}_1, \quad \xi_3 = x_2 + y_{x_2}\boldsymbol{i}, \quad \xi_4 = \bar{\xi}_3.$$

For ξ_1, we have $\widetilde{p}(\xi_1) = 1$, $\widetilde{p}(\xi_1)\overline{\widetilde{p}}(\xi_1) = 1 > 0$. So, $[\xi_1]$ $(= [\xi_2])$ contains no circular zeros of p.

Since $\widetilde{p}(\xi_3) = 7.7552\boldsymbol{i}$, $\widetilde{p}(\xi_3)\overline{\widetilde{p}}(\xi_3) < 0$, and $\overleftarrow{p}(\xi_3) = \overleftarrow{p}(\bar{\xi}_3)$, then $[\xi_3]$ $(= [\xi_4])$ contains a circular zero of p, and the set of circular zeros of p is

$$\Upsilon = \{1.255773570847266 + z\boldsymbol{j} : z \in \mathbb{C}, |z|^2 = (1.104243923243840)^2\}.$$

Hence the zero set of p is $\{-1, \boldsymbol{i}, -\boldsymbol{i}\} \cup \Upsilon$.

4. Formulae of zeros for quadratic two-sided polynomials with complex coefficients

In this section we concentrate on the case where p is quadratic with complex coefficients. We establish formulae for finding its spherical, circular and isolated zeros, and spell out a simple and efficient algorithm to find all zeros. So let

$$p(x) := x^2 + (a + b\boldsymbol{i})x(c + d\boldsymbol{i}) + (e + f\boldsymbol{i}), \tag{27}$$

where a, b, c, d, e, f are real numbers. In the notation introduced at the beginning of Section 3, we then have

$$\widetilde{p}(x) := x^2 + (a + b\boldsymbol{i})(c + d\boldsymbol{i})x + (e + f\boldsymbol{i}),$$
$$\overleftarrow{p}(x) := x^2 + (a + b\boldsymbol{i})(c - d\boldsymbol{i})x + (e + f\boldsymbol{i}),$$

Recall that a complex ξ is said to be a spherical zero of $p(x)$ if ξ is nonreal and each point of $[\xi]$ is a zero of $p(x)$.

Theorem 4.1 (existence of spherical zeros). *The polynomial $p(x)$ in* (27) *has a spherical zero if and only if one of the following conditions is met*:

- $b = d = f = 0$ *and* $(ac)^2 < 4e$.
- $a = b = f = 0$ *and* $e > 0$.
- $c = d = f = 0$ *and* $e > 0$.

Furthermore, *in this case the set of all zeros of $p(x)$ is*

$$\left[\frac{-ac + \sqrt{4e - (ac)^2}\,\boldsymbol{i}}{2}\right]. \tag{28}$$

Proof. $\Leftarrow$) When one of the conditions is met, $p(x)$ becomes $x^2+axc+e$, which is a real polynomial. So each nonreal zero of $p(x)$ is a spherical zero. In this case the complex roots of $\widetilde{p}$ are

$$\frac{-ac+\sqrt{4e-(ac)^2}\,\boldsymbol{i}}{2}, \qquad \frac{-ac-\sqrt{4e-(ac)^2}\,\boldsymbol{i}}{2}.$$

By the method provided in Section 3 to find all spherical zeros and isolated zeros, we conclude that the set of all zeros of $p(x)$ is given by (28).

$\Rightarrow$) Suppose the complex ξ is a spherical zero of $p(x)$. Then by Theorem 3.1 we have $\widetilde{p}(\xi)=\widetilde{p}(\bar{\xi})=0$ and $\overleftarrow{p}(\xi)=\overleftarrow{p}(\bar{\xi})$. Consequently, $\widetilde{p}$ should be a polynomial with real coefficients, from which we get

$$f=0, \quad ad=-bc, \tag{29}$$

and $\widetilde{p}(x)=x^2+(ac-bd)x+e$. This forces ξ to equal one of the two conjugate numbers

$$\frac{(bd-ac)\pm\sqrt{4e-(ac-bd)^2}\,\boldsymbol{i}}{2},$$

where $(ac-bd)^2<4e$. We may assume that

$$\xi=\frac{(bd-ac)+\sqrt{4e-(ac-bd)^2}\,\boldsymbol{i}}{2}. \tag{30}$$

Since $\overleftarrow{p}(\xi)=\overleftarrow{p}(\bar{\xi})$, we have

$$\xi^2+\big((ac+bd)+(bc-ad)\boldsymbol{i}\big)\xi=\bar{\xi}^2+\big((ac+bd)+(bc-ad)\boldsymbol{i}\big)\bar{\xi}.$$

Substituting (30), simplifying and comparing real and imaginary parts, we obtain

$$((bd-ac)+(ac+bd))\sqrt{4e-(ac-bd)^2}=0, \quad (bc-ad)\sqrt{4e-(ac-bd)^2}=0,$$

which yields

$$bd=0, \quad bc=ad. \tag{31}$$

From (29) and (31) it is easy to see $a=b=f=0$, or $c=d=f=0$, or $b=d=f=0$. If $a=b=f=0$ or $c=d=f=0$, then from $(ac-bd)^2<4e$ we find $e>0$. If $b=d=f=0$, then by $(ac-bd)^2<4e$ we get $(ac)^2<4e$. $\square$

Corollary 4.2. *Let $p(x)$ be a polynomial of the form in* (27). *Then $p(x)$ has a spherical zero if and only if $p(x)$ can be written as $p(x)=x^2+rx+s$, where r, s are real numbers with $r^2-4s<0$. Moreover, in this case, the set of zeros of $p(x)$ is*

$$\left[\frac{-r+\sqrt{4s-r^2}\boldsymbol{i}}{2}\right].$$

Theorem 4.3 (existence of circular zeros). *The polynomial* $p(x)$ *in* (27) *has a circular zero if and only if* $bd \neq 0$, $ad = bc$, *and*

$$\tag{32} \tfrac{3}{4}\left((ac)^2+2(bc)^2+(bd)^2\right)+e-\frac{a}{b}f > \left(\frac{f-(ac+bd)bc}{2bd}\right)^2.$$

Moreover, *in this case the set of all circular zeros of* $p(x)$ *is*

$$\tag{33} \left\{-\frac{ac+bd}{2}+\frac{f-(ac+bd)bc}{2bd}\,\boldsymbol{i}+z\,\boldsymbol{j} : z\in\mathbb{C},\ |z|^2=\Delta-\left(\frac{f-(ac+bd)bc}{2bd}\right)^2\right\},$$

where

$$\Delta := \tfrac{3}{4}((ac)^2+2(bc)^2+(bd)^2)+e-\tfrac{a}{b}f.$$

Proof. $\Rightarrow$) Let $[\xi]$ contain a circular zero of $p(x)$, where ξ is a complex number. Then $[\xi]$ contains no complex zeros of $p(x)$ (see Remark 2.6), and ξ satisfies (17). From Proposition 3.4 we see that $bd \neq 0$.

Let $\xi = u + y\boldsymbol{i}$ where $u, y \in \mathbb{R}$ with $y \neq 0$. From the second equation in (17) we deduce that $u = -(ac+bd)/2$ and $ad = bc$.

Now from Theorem 3.3 we may assume $p(x)$ has a solution $x = u + w\boldsymbol{i} + v\boldsymbol{j}$ with $u, w, v \in \mathbb{R}$ and $v \neq 0$. Substitute x in $p(x)$ with $u + w\boldsymbol{i} + v\boldsymbol{j}$. Then we get

$$\tag{34} u^2-w^2-v^2+acu-bcw-bdu-adw+e=0,$$

$$\tag{35} 2uw+bcu+acw+adu-bdw+f=0.$$

From (34) it follows that $u^2+(ac-bd)u-w^2-2bcw+e=v^2>0$. So,

$$\tag{36} u^2+(ac-bd)u-2bcw+e>w^2.$$

From (35) we have $w = (f-(ac+bd)bc)/2bd$. Substituting this value in (36) yields (32). And in this case it's easy to see by Theorem 2.5 that the set of circular zeros in $[\xi]$ is as given in (33), since

$$u=-\frac{ac+bd}{2},\quad w=\frac{f-(ac+bd)bc}{2bd},$$

$$v^2=u^2+(ac-bd)u-w^2-2bcw+e=\Delta-\left(\frac{f-(ac+bd)bc}{2bd}\right)^2,$$

and $x = u + w\boldsymbol{i} + v\boldsymbol{j}$ is a circular zero of p.

$\Leftarrow$) When the conditions $bd \neq 0$, $ad = bc$, and (32) are satisfied, we can verify directly that each element of the set in (33) is a zero of $p(x)$. Note that (33) has infinitely many elements, and Theorem 4.1 implies that $p(x)$ has no spherical zeros, since $bd \neq 0$. Again by Theorem 2.5 we know that $p(x)$ has a circular zero. □

Next we give a consequence of Theorems 4.1 and 4.3.

Corollary 4.4. (1) *The polynomial* $x^2 + r(t + \boldsymbol{i})x(t + \boldsymbol{i}) + e$, *where* $r, t, e \in \mathbb{R}$, *has a circular zero if and only if* $r \neq 0$ *and* $4e/r^2 + t^4 + 5t^2 + 3 - t^6 > 0$.

(2) *No quadratic polynomial with two-sided complex coefficients can have a spherical zero and a circular zero simultaneously.*

From Theorem 2.5 we know that the set of isolated zeros of $p(x)$ is contained in the nonempty set $\{z : z \in \mathbb{C}, \widetilde{p}(z) = 0\}$ in this case. Using Theorem 4.1 and Theorem 4.3 we have:

Theorem 4.5. *The polynomial* $p(x)$ *in* (27) *has an isolated zero if and only if it either has a circular zero, or has no circular zero or spherical zero. In either case, the set of isolated zeros of* $p(x)$ *is* $\{z : z \in \mathbb{C}, \widetilde{p}(z) = 0\}$, *where* $\widetilde{p}$ *is regarded as a complex polynomial* (*so the classical formula can be used*).

Corollary 4.6. *The zeros of* $p(x)$ *are distributed in at most* 3 *equivalence classes, and* $p(x)$ *has finitely many zeros if and only if* $p(x)$ *has neither circular zeros nor spherical zeros.*

Summary of the algorithm to find all zeros of a quadratic two-sided quaternionic polynomial with complex coefficients. Given a polynomial $a_2x^2b_2 + a_1xb_1 + a_0$, with $x \in \mathbb{H}$, $a_i, b_i \in \mathbb{C}$, $a_2b_2 \neq 0$, first divide it by a_2 and b_2, so as to reduce it to the form

$$p(x) := x^2 + (a + b\boldsymbol{i})x(c + d\boldsymbol{i}) + e + f\boldsymbol{i}.$$

Step 1. Test the three conditions of Theorem 4.1. If any of them is met, the set of zeros of p is

$$\left[\frac{-ac + \sqrt{4e - (ac)^2}\,\boldsymbol{i}}{2}\right].$$

Otherwise, go to the next step.

Step 2. Compute the (real and complex) zeros of the polynomial

$$\widetilde{p}(x) := x^2 + (a + b\boldsymbol{i})(c + d\boldsymbol{i})x + e + f\boldsymbol{i}.$$

Denote them by z_1 and z_2. Test the three conditions of Theorem 4.3. If they are all met, the set of zeros of q is the union of $\{z_1, z_2\}$ with the set (33) of the same theorem. Otherwise, the set of zeros of $q(x)$ is $\{z_1, z_2\}$.

Example 4.7. For the polynomial $p(x) := x^2 + \boldsymbol{i}x\boldsymbol{i} + 2$, none of the conditions in Theorem 4.1 is met, so there are no spherical zeros. In Step 2 we get two (conjugate) isolated zeros and a circular zero. The complete set of zeros is

$$\left\{\frac{1+\sqrt{7}\boldsymbol{i}}{2}, \frac{1-\sqrt{7}\boldsymbol{i}}{2}\right\} \cup \left\{-\tfrac{1}{2} + z\boldsymbol{j} : z \in \mathbb{C}, |z|^2 = \tfrac{11}{4}\right\}.$$

The zeros fall into two equivalence classes.

Example 4.8. For $p(x) := x^2 + (1+\boldsymbol{i})x(1+\boldsymbol{i}) + 1$, again there are no spherical zeros. The algorithm (or Corollary 4.4) gives a circular zero, and two (nonconjugate) isolated zeros, so the set of zeros is

$$\big\{(\sqrt{2}-1)\boldsymbol{i},\, -(\sqrt{2}+1)\boldsymbol{i}\big\} \cup \big\{-1-\boldsymbol{i}+z\boldsymbol{j} : z \in \mathbb{C},\, |z|^2 = 3\big\}.$$

The zeros fall into three equivalence classes.

Example 4.9. The polynomial x^2+1 has a spherical zero; hence (by Step 1 or Corollary 4.2) its set of zeros is $[\boldsymbol{i}] = \{a_1\boldsymbol{i} + a_2\boldsymbol{j} + a_3\boldsymbol{k} : a_1^2 + a_2^2 + a_3^2 = 1\}$, forming a single equivalence class.

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COXETER GROUPS, IMAGINARY CONES AND DOMINANCE

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Brink and Howlett [*Math. Ann.* 296:1 (1993), 179–190] have introduced a partial ordering, called *dominance*, on the root systems of Coxeter groups in their proof that all finitely generated Coxeter groups are automatic. Edgar (Ph.D. thesis, 2009), in an investigation of various regularity properties of Coxeter groups, studied a function on the reflections of such groups, called ∞-*height*. Here we show that these two concepts are closely related to each other. We also give applications of dominance to the study of *imaginary cones* of Coxeter groups.

1. Introduction

In this paper we attempt to extend the understanding of a partial ordering (called *dominance*) defined on the root system of an arbitrary Coxeter group. The dominance ordering was introduced in [Brink and Howlett 1993] (where it was used to prove the automaticity of all finitely generated Coxeter groups). Dominance ordering was further studied in [Brink 1998; Krammer 1994; 2009], and it has only been recently examined again, in [Dyer 2012] (in connection with the representation theory of Coxeter groups) and in [Edgar 2009; Fu 2012]. The present paper is a short addition to the last two references, and it could serve as a building block in the general knowledge of dominance ordering and of the combinatorics and geometry of Coxeter groups in general.

More specifically, this paper has the following two objectives: (1) investigating the connection between the dominance ordering on the root system of an arbitrary Coxeter groups W and a specific function (called ∞-*height*) defined on the set of reflections of W; and (2) exploring the applications of the dominance ordering to the *imaginary cone* of W (as defined by Kac).

The paper is organized into three sections. The first introduces background material: root bases, Coxeter data, and root systems are defined in the context of the paper, and some basic properties of Coxeter groups are recalled for later use in the

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paper (most of them can be found in [Howlett 1996]). Here we follow the definition used in [Krammer 1994], which gives a slight variant of the classical notion of root systems, particularly adapted when working with arbitrary (not necessarily crystallographic) Coxeter groups. Furthermore, this framework allows easy passing to reflection subgroups. Indeed, we recall the fundamental property [Dyer 1987, Theorem 1.8] that the reflection subgroups of a Coxeter group are themselves Coxeter groups, and this particular framework allows us to apply all the definitions and properties to the reflection subgroups and not only to the overgroup.

In the second section, the first main theorem (giving the connection between ∞-height and dominance order) is stated and proved. All results are related to an arbitrary Coxeter datum, implying the data of a root system Φ, its associated Coxeter group W, and the set T of all reflections of W (consisting of all the W-conjugates of the Coxeter generators). The main objects of study are:

- The dominance order on Φ (Definition 3.1). Given $x,\ y \in \Phi$, we say x *dominates* y if whenever $w \in W$ such that $wx \in \Phi^-$ then $wy \in \Phi^-$ too (where Φ^- denotes the set of negative roots).
- The ∞-height function on T. This is a variant of the usual (standard) height function of a reflection $t \in T$, namely, the minimal length of an element of W that maps α_t (the unique positive root associated to t) to an element of the root basis. Adhering to the general framework of this paper, our definition of the height function applies to all reflection subgroups of W. It is easy to check (Lemma 3.13) that the height of t is equal to the sum of the heights of t relative to each maximal (with respect to inclusion) dihedral reflection subgroup containing t. The ∞-height of t is then defined as a subsum of this sum, taking into account only those subgroups which are infinite (Definition 3.8).

We then show that these two concepts are closely related in the following way. The canonical bijection $t \leftrightarrow \alpha_t$, between T and Φ^+ (the set of positive roots), restricts to a bijection between (for any $n \in \mathbb{N}$)

- the set T_n of all reflections whose ∞-height is n, and
- the set D_n of all positive roots which strictly dominate exactly n other positive roots.

The proof of this fact (Theorem 3.15) relies on a study of dihedral reflection subgroups. We have previously studied the partition $(D_n)_{n\in\mathbb{N}}$ of Φ^+ in [Fu 2012]; in particular, we showed there that each D_n is finite and we gave an upper bound for its cardinality. Together with Theorem 3.15, this allows us to deduce here some further information on the combinatorics of the T_n's (Corollary 3.23).

The final section explores the relation between the dominance order and the imaginary cone of a Coxeter group. The concept of *imaginary cone* was introduced in [Kac 1990] to study the imaginary roots of Kac–Moody Lie algebras, and was later generalized to Coxeter groups by Hée [1990; 1993] and Dyer [2012]. It is defined as the subset of the dual of the Tits cone (denoted by U^* here) consisting of elements $v \in U^*$ such that $(v, \alpha) > 0$ for only finitely many $\alpha \in \Phi^+$ (where $(\, , \,)$ denotes the bilinear form associated to the Coxeter datum). The main results (Theorem 4.13 and Corollary 4.15) of this section state the following property: whenever $x, y \in \Phi$, then x dominates y if and only if $x - y$ lies in the imaginary cone. One direction of this property was first suggested to us by Howlett [private communication], and it is a special case of a result obtained independently (but earlier) by Dyer. We are deeply indebted to both of them for helpful discussions inspiring us to study the imaginary cone. We would also like to thank the referee of this paper for many valuable suggestions, especially those resulting in Corollary 4.15. To close this section, we include an alternative definition for the imaginary cone in the case where W is finitely generated.

2. Background material

Definition 2.1 [Krammer 1994]. Suppose that V is a vector space over $\mathbb{R}$. Let $(\, , \,)$ be a bilinear form on V and let Δ be a subset of V. Then Δ is called a *root basis* if the following conditions are satisfied:

(C1) $(a, a) = 1$ for all $a \in \Delta$, and for distinct elements $a, b \in \Delta$, either $(a, b) = -\cos(\pi/m_{ab})$ for some integer $m_{ab} = m_{ba} \geq 2$, or else $(a, b) \leq -1$ (in which case we define $m_{ab} = m_{ba} = \infty$).

(C2) $0 \notin \mathrm{PLC}(\Pi)$, where the *the positive linear cone of* a set A is defined by

$$\mathrm{PLC}(A) = \left\{ \sum_{a \in A} \lambda_a a \;\middle|\; \lambda_a \geq 0 \text{ for all } a \in A \text{ and } \lambda_{a'} > 0 \text{ for some } a' \in A \right\}.$$

If Δ is a root basis, then we call the triple $\mathscr{C} = (V, \Delta, (\, , \,))$ a *Coxeter datum*. Throughout this paper we fix a particular Coxeter datum $\mathscr{C}$. We stress that our definition of a root basis is not the most classical one of [Bourbaki 1968] or even [Humphreys 1990]: the root system (see Definition 2.5) arising from our definition of a root basis is not necessarily crystallographic (indeed, the bilinear form can take values less than -1), and the root basis is not assumed to be linearly independent (this allows us to transmit easily the definitions and properties of a Coxeter group to its reflection subgroups; indeed, the requirements in our definition of a root basis of a Coxeter group are identical to those in the characterization of the equivalent of a root basis in any reflection subgroup). Observe that (C1) implies that $a \notin \mathrm{PLC}(\Delta \setminus \{a\})$ if $a \in \Delta$, and (C1) and (C2) together imply that $\{a, b, c\}$ is linearly independent for all distinct $a, b, c \in \Delta$. Note also that (C2) is equivalent to the requirement that zero does not lie in the convex hull of Δ.

For each $a \in \Delta$, define $\rho_a \in \mathrm{GL}(V)$ by the rule $\rho_a x = x - 2(x, a)a$ for all $x \in V$. Observe that ρ_a is a reflection, and $\rho_a a = -a$. We summarize a few useful results:

Proposition 2.2 [Howlett 1996, Lecture 1, propositions on pp. 2–3]. (i) *Suppose that $a, b \in \Delta$ are distinct such that $m_{ab} \neq \infty$. Set $\theta = \pi/m_{ab}$. Then*

$$(\rho_a \rho_b)^i a = \frac{\sin(2i+1)\theta}{\sin\theta} a + \frac{\sin 2i\theta}{\sin\theta} b$$

for each integer i, and in particular, $\rho_a\rho_b$ has order m_{ab} in $\mathrm{GL}(V)$.

(ii) *Suppose that $a, b \in \Delta$ are distinct such that $m_{ab} = \infty$. Set $\theta = \cosh^{-1}(-(a, b))$. Then*

$$(\rho_a \rho_b)^i a = \begin{cases} \dfrac{\sinh(2i+1)\theta}{\sinh\theta} a + \dfrac{\sinh 2i\theta}{\sinh\theta} b & \text{if } \theta \neq 0, \\ (2i+1)a + 2ib & \text{if } \theta = 0, \end{cases}$$

for each integer i, and in particular, $\rho_a\rho_b$ has infinite order in $\mathrm{GL}(V)$. □

Let $G_{\mathscr{C}}$ be the subgroup of $\mathrm{GL}(V)$ generated by $\{\rho_a \mid a \in \Delta\}$. Suppose that (W, S) is a Coxeter system in the sense of [Hiller 1982] or [Humphreys 1990] with $S = \{r_a \mid a \in \Delta\}$ being a set of involutions generating W subject only to the condition that the order of $r_a r_b$ is m_{ab} for all $a, b \in \Delta$ with $m_{ab} \neq \infty$. Then Proposition 2.2 yields that there exists a group homomorphism $\phi_{\mathscr{C}}\colon W \to G_{\mathscr{C}}$ satisfying $\phi_{\mathscr{C}}(r_a) = \rho_a$ for all $a \in \Delta$. This homomorphism, together with the $G_{\mathscr{C}}$-action on V, gives rise to a W-action on V: for each $w \in W$ and $x \in V$, define $wx \in V$ by $wx = \phi_{\mathscr{C}}(w)x$. It can be easily checked that this W-action preserves $(\ ,\ )$. Denote the length function of W with respect to S by ℓ, and call an expression $w = r_1 r_2 \cdots r_n$ (where $w \in W$ and $r_i \in S$) *reduced* if $\ell(w) = n$. The following is a useful result:

Proposition 2.3 [Howlett 1996, Lecture 1, theorem, p. 4]. *Let $G_{\mathscr{C}}$, W, S and ℓ be as above, and let $w \in W$ and $a \in \Delta$. If $\ell(wr_a) \geq \ell(w)$, then $wa \in$* $\mathrm{PLC}(\Delta)$. □

An immediate consequence of the proposition is the following important fact:

Corollary 2.4 [Howlett 1996, Lecture 1, corollary, p. 5]. *Let $G_{\mathscr{C}}$, W, S and $\phi_{\mathscr{C}}$ be as above. Then $\phi_{\mathscr{C}}\colon W \to G_{\mathscr{C}}$ is an isomorphism.* □

In particular, the corollary yields that $(G_{\mathscr{C}}, \{\rho_a \mid a \in \Delta\})$ is a Coxeter system isomorphic to (W, S). We call (W, S) the *abstract Coxeter system* associated to the Coxeter datum $\mathscr{C}$, and we call W a *Coxeter group* of rank #S (where # denotes cardinality).

Definition 2.5. The *root system* of W in V is the set

$$\Phi = \{wa \mid w \in W \text{ and } a \in \Delta\}.$$

The set $\Phi^+ = \Phi \cap \mathrm{PLC}(\Delta)$ is called the set of *positive roots*, and the set $\Phi^- = -\Phi^+$ is called the set of *negative roots*.

From Proposition 2.3 we may readily deduce that:

Proposition 2.6 [Howlett 1996, Lecture 3, corollary on p. 11, proposition on p. 10 and lemma on p. 4]. (i) *Let* $w \in W$ *and* $a \in \Delta$. *Then*

$$\ell(wr_a) = \begin{cases} \ell(w) - 1 & \text{if } wa \in \Phi^-, \\ \ell(w) + 1 & \text{if } wa \in \Phi^+. \end{cases}$$

(ii) $\Phi = \Phi^+ \uplus \Phi^-$, *where* $\uplus$ *denotes disjoint union.*

(iii) W *is finite if and only if* Φ *is finite.* □

Define $T = \bigcup_{w \in W} wSw^{-1}$. We call T the set of *reflections* in W. For each $x \in \Phi$, let $\rho_x \in \mathrm{GL}(V)$ be defined by the rule $\rho_x(v) = v - 2(v, x)x$ for all $v \in V$. Since $x \in \Phi$, it follows that $x = wa$ for some $w \in W$ and $a \in \Delta$. Direct calculations yield that $\rho_x = (\phi_{\mathscr{C}}(w))\rho_a(\phi_{\mathscr{C}}(w))^{-1} \in G_{\mathscr{C}}$. Now let $r_x \in W$ be such that $\phi_{\mathscr{C}}(r_x) = \rho_x$. Then $r_x = wr_a w^{-1} \in T$, and we call r_x the reflection corresponding to x. It is readily checked that $r_x = r_{-x}$ for all $x \in \Phi$ and $T = \{r_x \mid x \in \Phi\}$. For each $t \in T$ we let α_t be the unique positive root with the property that $r_{\alpha_t} = t$. It is also easily checked that there is a bijection $\psi \colon T \to \Phi^+$ given by $\psi(t) = \alpha_t$, and we call ψ the *canonical bijection*.

For each $x \in \Phi^+$, as in [Brink and Howlett 1993], we define the *depth* of x relative to S to be $\min\{\ell(w) \mid w \in W \text{ and } wx \in \Phi^-\}$, and we denote it by $\mathrm{dp}(x)$. The following lemma gives some basic properties of depth:

Lemma 2.7 [Brink and Howlett 1993; Brink 1994; Saunders 1991]. (i) *Let* $\alpha \in \Phi^+$. *Then* $\mathrm{dp}(\alpha) = \frac{1}{2}(\ell(r_\alpha) + 1)$.

(ii) *Let* $r \in S$ *and* $\alpha \in \Phi^+ \setminus \{\alpha_r\}$. *Then*

$$\mathrm{dp}(r\alpha) = \begin{cases} \mathrm{dp}(\alpha) - 1 & \text{if } (\alpha, \alpha_r) > 0, \\ \mathrm{dp}(\alpha) & \text{if } (\alpha, \alpha_r) = 0, \\ \mathrm{dp}(\alpha) + 1 & \text{if } (\alpha, \alpha_r) < 0. \end{cases}$$

Proof. (i) See [Brink 1994, Corollary 2.7]. This is also a special case of [Fu 2010, Lemma 1.3.19].

(ii) See [Brink and Howlett 1993, Lemma 1.7]. □

Remark 2.8. Part (i) of Lemma 2.7 is equivalent to the property that any reflection in a Coxeter group has a palindromic expression which is reduced, and this was indeed noted in [Saunders 1991, Proposition 4.3].

Define functions $N \colon W \to \mathscr{P}(\Phi^+)$ and $\overline{N} \colon W \to \mathscr{P}(T)$ (where $\mathscr{P}$ denotes the power set) by setting

$$N(w) = \{x \in \Phi^+ \mid wx \in \Phi^-\},$$
$$\overline{N}(w) = \{t \in T \mid \ell(wt) < \ell(w)\},$$

for all $w \in W$. We call $\overline{N}$ the *reflection cocycle* of W (sometimes $\overline{N}(w)$ is also called the *right descent set* of w). Standard arguments such as those in [Humphreys 1990, Section 5.6] yield that, for each $w \in W$,

$$\ell(w) = \#N(w) \tag{2-1}$$

and

$$\overline{N}(w) = \{r_x \mid x \in N(w)\}. \tag{2-2}$$

In particular, $N(r_a) = \{a\}$ for $a \in \Delta$. Moreover, $\ell(wv^{-1}) + \ell(v) = \ell(w)$ for some $w, v \in W$ if and only if $N(v) \subseteq N(w)$.

A subgroup W' of W is a *reflection subgroup* of W if it is generated by the reflections contained in it: $W' = \langle W' \cap T\rangle$. For any reflection subgroup W' of W, let

$$S(W') = \{t \in T \mid \overline{N}(t) \cap W' = \{t\}\} \quad \text{and} \quad \Delta(W') = \{x \in \Phi^+ \mid r_x \in S(W')\}.$$

It was shown by Dyer [1990] and Deodhar [1982] that $(W', S(W'))$ forms a Coxeter system:

Theorem 2.9 (Dyer). (i) *Suppose that W' is an arbitrary reflection subgroup of W. Then $(W', S(W'))$ forms a Coxeter system. Moreover, $W' \cap T = \bigcup_{w \in W'} wS(W')w^{-1}$.*

(ii) *Suppose that W' is a reflection subgroup of W, and suppose that $a, b \in \Delta(W')$ are distinct. Then*

$$(a, b) \in \{-\cos(\pi/n) \mid n \in \mathbb{N} \text{ and } n \geq 2\} \cup (-\infty, -1].$$

Conversely, if Δ' is a subset of Φ^+ satisfying the condition that

$$(a, b) \in \{-\cos(\pi/n) \mid n \in \mathbb{N} \text{ and } n \geq 2\} \cup (-\infty, -1]$$

for all $a, b \in \Delta'$ with $a \neq b$, then $\Delta' = \Delta(W')$ for some reflection subgroup W' of W. In fact, $W' = \langle\{r_a \mid a \in \Delta'\}\rangle$.

Proof. (i) See [Dyer 1990, Theorem 3.3].

(ii) See [Dyer 1990, Theorem 4.4]. □

Let $(\ ,\ )'$ be the restriction of $(\ ,\ )$ to the subspace $\operatorname{span}(\Delta(W'))$. Then $\mathscr{C}' = (\operatorname{span}(\Delta(W')), \Delta(W'), (\ ,\ )')$ is a Coxeter datum with $(W', S(W'))$ being the associated abstract Coxeter system. Thus the notion of a root system applies to $\mathscr{C}'$. We let $\Phi(W')$, $\Phi^+(W')$ and $\Phi^-(W')$ be, respectively, the set of roots, positive roots and negative roots for the datum $\mathscr{C}'$. Then $\Phi(W') = W'\Delta(W')$, and Theorem 2.9(i) yields that $\Phi(W') = \{x \in \Phi \mid r_x \in W'\}$. Furthermore, we have $\Phi^+(W') = \Phi(W') \cap \operatorname{PLC}(\Delta(W'))$ and $\Phi^-(W') = -\Phi^+(W')$. We call $S(W')$ the set of *canonical generators* of W', and we call $\Delta(W')$ the set of *canonical roots* of $\Phi(W')$. In this paper a reflection subgroup W' is called a *dihedral reflection subgroup* if $\#S(W')=2$.

A subset Φ' of Φ is called a *root subsystem* if $r_y x \in \Phi'$ whenever x, y are both in Φ'. It is easily seen that there is a bijective correspondence between the set of reflection subgroups W' of W and the set of root subsystems Φ' of Φ: W' uniquely determines the root subsystem $\Phi(W')$, and Φ' uniquely determines the reflection subgroup $\langle\{r_x \mid x \in \Phi'\}\rangle$.

The notion of a length function also applies to the Coxeter system $(W', S(W'))$, and we let $\ell_{(W',S(W'))}\colon W' \to \mathbb{N}$ be the length function for $(W', S(W'))$. If $w \in W'$ and $a \in \Delta(W')$ then applying Proposition 2.6 to the Coxeter datum $\mathscr{C}' = (\operatorname{span}(\Delta(W')), \Delta(W'), (\ ,\ ))$ yields

$$\ell_{(W',S(W'))}(wr_a) = \begin{cases} \ell_{(W',S(W'))}(w)-1 & \text{if } wa \in \Phi^-(W'), \\ \ell_{(W',S(W'))}(w)+1 & \text{if } wa \in \Phi^+(W'). \end{cases} \tag{2-3}$$

Similarly, the notion of a reflection cocycle also applies to the Coxeter system $(W', S(W'))$. Let $\overline{N}_{(W',S(W'))}\colon W \to \mathscr{P}(W' \cap T)$ denote the reflection cocycle for $(W', S(W'))$. Then, for each $w \in W'$,

$$\overline{N}_{(W',S(W'))}(w) = \{t \in W' \cap T \mid \ell_{(W',S(W'))}(wt) < \ell_{(W',S(W'))}(w)\},$$

and we define $N_{(W',S(W'))}(w) = \{x \in \Phi^+(W') \mid wx \in \Phi^-(W')\}$ for each $w \in W'$. It is shown in [Dyer 1987] that $\overline{N}_{(W',S(W'))}(w) = \overline{N}(w) \cap W'$ for an arbitrary reflection subgroup W' of W. Furthermore, it is readily seen that the canonical bijection ψ restricts to a bijection $\psi'\colon T \cap W' \to \Phi^+(W')$ given by $\psi'(t) = \alpha_t$. For $w \in W'$, applying (2-1) to the Coxeter datum $\mathscr{C}' = (\operatorname{span}(\Delta(W'), \Delta(W'), (\ ,\ )')$ yields that

$$\ell_{(W',S(W'))}(w) = \#N_{(W',S(W'))}(w). \tag{2-4}$$

Furthermore, $\ell_{(W',S(W'))}(wv^{-1}) + \ell_{(W',S(W'))}(v) = \ell_{(W',S(W'))}(w)$ for some w, $v \in W'$ precisely when $N_{(W',S(W'))}(v) \subseteq N_{(W',S(W'))}(w)$.

For a Coxeter datum $\mathscr{C} = (V, \Delta, (\ ,\ ))$, since Δ may be linearly dependent, the expression of a root in Φ as a linear combination of elements of Δ may not be unique. Thus the concept of the coefficient of an element of Δ in any given root in Φ is potentially ambiguous. We close this section by specifying a canonical way of expressing a root in Φ as a linear combination of elements from Δ. This canonical expression follows from a standard construction similar to that considered in [Howlett et al. 1997, Proposition 2.9].

Given a Coxeter datum $\mathscr{C} = (V, \Delta, (\ ,\ ))$, let E be a vector space over $\mathbb{R}$ with basis $\Delta_E = \{e_a \mid a \in \Delta\}$ in bijective correspondence with Δ, and let $(\ ,\ )_E$ be the unique bilinear form on E satisfying

$$(e_a, e_b)_E = (a, b) \quad \text{for all } a, b \in \Delta.$$

Then $\mathscr{C}_E = (E, \Delta_E, (\ ,\ )_E)$ is a Coxeter datum. Moreover, $\mathscr{C}_E$ and $\mathscr{C}$ are associated to the same abstract Coxeter system (W, S); indeed, Corollary 2.4 yields that the abstract Coxeter group W is isomorphic to both $G_{\mathscr{C}} = \langle\{\rho_a \mid a \in \Delta\}\rangle$ and $G_{\mathscr{C}_E} = \langle\{\rho_{e_a} \mid a \in \Delta\}\rangle$. Furthermore, W acts faithfully on E via $r_a y = \rho_{e_a} y$ for all $a \in \Delta$ and $y \in E$.

Let $f\colon E \to V$ be the unique linear map satisfying $f(e_a) = a$ for all $a \in \Delta$. It is readily checked that $(f(x), f(y)) = (x, y)_E$ for all x, $y \in E$. Now, for all $a \in \Delta$ and $y \in E$,

$$\begin{aligned} r_a(f(y)) = \rho_a(f(y)) = f(y) - 2(f(y), a)a &= f(y) - 2(f(y), f(e_a))f(e_a) \\ &= f(y - 2(y, e_a)_E e_a) = f(r_a y). \end{aligned}$$

Then it follows that $w(f(y)) = f(wy)$ for all $w \in W$ and all $y \in E$, since W is generated by $\{r_a \mid a \in \Delta\}$. Let Φ_E denote the root system associated to the datum $\mathscr{C}_E$. Standard arguments yield that:

Proposition 2.10 [Fu 2012, Proposition 2.1]. *The restriction of f defines a W-equivariant bijection $\Phi_E \leftrightarrow \Phi$.* □

Since Δ_E is linearly independent, it follows that each root $y \in \Phi_E$ can be written uniquely as $y = \sum_{e_a \in \Delta_E} \lambda_a e_a$; we write $\lambda_a = \operatorname{coeff}_{e_a}(y)$ and call it the *coefficient* of e_a in y. We use this uniqueness together with the W-equivariant bijection $f\colon \Phi_E \leftrightarrow \Phi$ to give a canonical expression of a root in Φ in terms of Δ:

Definition 2.11. Suppose that $x \in \Phi$. For each $a \in \Delta$, define the *canonical coefficient* of a in x, written $\operatorname{coeff}_a(x)$, by requiring that $\operatorname{coeff}_a(x) = \operatorname{coeff}_{e_a}(f^{-1}(x))$. The *support*, written $\operatorname{supp}(x)$, is the set of $a \in \Delta$ with $\operatorname{coeff}_a(x) \neq 0$.

3. Dominance, maximal dihedral reflection subgroups and infinity height

Throughout this section, let W be the abstract Coxeter group associated to the Coxeter datum $\mathscr{C} = (V, \Delta, (\ ,\ ))$, and let Φ and T be the corresponding root system and the set of reflections, respectively. Recently, in [Edgar 2009], a uniquely determined nonnegative integer, called ∞-*height*, was assigned to each reflection in W. (Edgar attributes the concept to Dyer.) Naturally, the set T is then the disjoint union of the sets T_0, T_1, $T_2, \ldots$, where the set T_n consists of all the reflections with ∞-height equal to n.

These T_n were used in [Edgar 2009, Chapter 5] to demonstrate nice regularity properties of W. They gave rise to a family of modules in the generic Iwahori–Hecke algebra associated to W, and in turn, these modules were used by Dyer (unpublished) to prove a weak form of Lusztig's conjecture on the boundedness of the **a**-function. Dyer also showed that if W is of finite rank, then there are finitely many reflections in T_n for each n.

In this section we prove that for an arbitrary reflection $t \in T$ whose ∞-height equals n, the corresponding positive root α_t dominates precisely n other positive roots. This observation will then establish a bijection between the set of all reflections in W with ∞-height equal to n and the set of all positive roots that dominate precisely n other positive roots. Recent results on dominance obtained in [Fu 2012] may then be immediately applied to the T_n's, answering a number of basic questions about these T_n's.

Following [Howlett et al. 1997] and [Björner and Brenti 2005, Section 4.7], we generalize the definition of dominance to the whole of Φ (whereas in [Brink and Howlett 1993] and [Brink 1998], dominance was only defined on Φ^+), and we stress that all the notations are the same as in the previous section.

Definition 3.1. (i) Let W' be a reflection subgroup of W, and let $x, y \in \Phi(W')$. Then we say that x *dominates* y with respect to W' if

$$\{w \in W' \mid wx \in \Phi^-(W')\} \subseteq \{w \in W' \mid wy \in \Phi^-(W')\}.$$

If x dominates y with respect to W' then we write $x \operatorname{dom}_{W'} y$.

(ii) Let W' be a reflection subgroup of W and let $x \in \Phi^+(W')$. Define

$$D_{W'}(x) = \{y \in \Phi^+(W') \mid y \neq x \text{ and } x \operatorname{dom}_{W'} y\}.$$

If $D_{W'}(x) = \varnothing$ we call x *elementary with respect to* W'. For each nonnegative integer n, define

$$D_{W',n} = \{x \in \Phi^+(W') \mid \#D_{W'}(x) = n\}.$$

If $W' = W$, we write $D(x)$ for $D_{W'}(x)$ and D_n for $D_{W',n}$. If $D(x) = \varnothing$ then we call x *elementary*.

It is readily checked that dominance with respect to any reflection subgroup W' of a Coxeter group W is a partial ordering on $\Phi(W')$. The following lemma summarizes some basic properties of dominance:

Lemma 3.2 [Fu 2012, Lemma 3.2]. (i) *Let $x, y \in \Phi^+$ be arbitrary. Then $x \operatorname{dom}_W y$ if and only if $(x, y) \geq 1$ and* $\operatorname{dp}(x) \geq \operatorname{dp}(y)$.

(ii) *Dominance is W-invariant, that is, if $x \operatorname{dom}_W y$ then $wx \operatorname{dom}_W wy$ for all $w \in W$.*

(iii) *Let $x, y \in \Phi$ be such that $x \operatorname{dom}_W y$. Then $-y \operatorname{dom}_W -x$.*

(iv) *Let $x, y \in \Phi$. Then there is dominance between x and y if and only if $(x, y) \geq 1$.* □

Corollary 3.3. *Let x, $y \in \Phi$, and let W' be an arbitrary reflection subgroup containing both r_x and r_y.*

(i) *There is dominance with respect to W' between x and y if and only if $(x, y)' \geq 1$, where $(\, , \,)'$ is the restriction of $(\, , \,)$ to the subspace* $\operatorname{span}(\Delta(W'))$.

(ii) $x \operatorname{dom}_W y$ *if and only if* $x \operatorname{dom}_{W'} y$.

Proof. (i) This follows from Lemma 3.2(iv) applied to the Coxeter group W' and the datum $\mathscr{C}' = (\operatorname{span}(\Delta(W')), \Delta(W'), (\, , \,)')$.

(ii) The desired result is trivially true if $x = y$, so we may assume that $x \neq y$. It is clear that $x \operatorname{dom}_W y$ implies that $x \operatorname{dom}_{W'} y$. Conversely, suppose that $x \operatorname{dom}_{W'} y$. Then (i) yields that $(x, y) = (x, y)' \geq 1$. Thus Lemma 3.2(iv) yields that either $x \operatorname{dom}_W y$, or else $y \operatorname{dom}_W x$. If the latter is the case, then by the first part of the current proof, $y \operatorname{dom}_{W'} x$, and hence it follows that $x = y$ (since dominance with respect to W' is a partial ordering), contradicting our choice of x and y. □

Next is a well-known result whose proof can be found in the remarks immediately before Lemma 2.3 of [Brink and Howlett 1993]:

Lemma 3.4. *There is no nontrivial dominance between positive roots in the root system of a finite Coxeter group.* □

Next we have a technical result which is going to be used repeatedly in the rest of this paper.

Proposition 3.5. *Let α, $\beta \in \Phi^+$ with $(\alpha, \beta) \leq -1$, and let W' be the dihedral reflection subgroup generated by r_α and r_β. Further, we set $\theta = \cosh^{-1}(-(\alpha, \beta))$, and for each $i \in \mathbb{Z}$ adopt the notation*

$$c_i = \begin{cases} \dfrac{\sinh i\theta}{\sinh \theta} & \text{if } \theta \neq 0, \\ i & \text{if } \theta = 0. \end{cases} \tag{3-1}$$

(i) *W' is infinite, and $\Phi(W') = \{c_{i\pm 1}\alpha + c_i\beta \mid i \in \mathbb{Z}\}$.*

(ii) *Suppose that $x, y \in \Phi(W')$. Then $(x, y) \in (-\infty, -1] \cup [1, \infty)$, and in particular, if $x \neq \pm y$ then $\langle \{r_x, r_y\} \rangle$ is an infinite dihedral reflection subgroup. More specifically,*

(a) *If $x = c_{n+1}\alpha + c_n\beta$ and $y = c_{m+1}\alpha + c_m\beta$, then*

$$(x, y) = \begin{cases} \cosh((n-m)\theta) \geq 1 & \text{if } \theta \neq 0, \\ 1 & \text{if } \theta = 0. \end{cases}$$

(b) *If $x = c_{n+1}\alpha + c_n\beta$ and $y = c_{m-1}\alpha + c_m\beta$, then*

$$(x, y) = \begin{cases} -\cosh((n+m)\theta) \leq -1 & \text{if } \theta \neq 0, \\ -1 & \text{if } \theta = 0. \end{cases}$$

(c) *If* $x = c_{n-1}\alpha + c_n\beta$ *and* $y = c_{m+1}\alpha + c_m\beta$, *then*

$$(x, y) = \begin{cases} -\cosh((n+m)\theta) \leq -1 & \text{if } \theta \neq 0, \\ -1 & \text{if } \theta = 0. \end{cases}$$

(d) *If* $x = c_{n-1}\alpha + c_n\beta$ *and* $y = c_{m-1}\alpha + c_m\beta$, *then*

$$(x, y) = \begin{cases} \cosh((n-m)\theta) \geq 1 & \text{if } \theta \neq 0, \\ 1 & \text{if } \theta = 0. \end{cases}$$

(iii) *If* $x \in \Phi^+(W') \setminus \{\alpha, \beta\}$, *then* $D_{W'}(x) \neq \varnothing$.

Proof. (i) Proposition 4.5.4(ii) of [Björner and Brenti 2005] implies that W' is infinite, and the rest of statement follows from direct calculations similar to those in Proposition 2.2.

(ii) This follows from (i) and a direct calculation.

(iii) If $x \in \Phi^+(W') \setminus \{\alpha, \beta\}$, part (i) yields that either $x = c_{n+1}\alpha + c_n\beta$ (for some $n \neq 0$), or else $x = c_{n-1}\alpha + c_n\beta$ (for some $n \neq 1$). Then part (ii) and Corollary 3.3(i) imply that we can find some $y \in \Phi^+(W') \setminus \{x\}$ such that $x \operatorname{dom}_{W'} y$. ☐

The other key object to be studied in this section is the numeric function ∞-*height* on T. As mentioned in the introduction, this function is defined in terms of infinite dihedral reflection subgroups of W, and in order to make a precise definition of this function we need a few technical results on infinite dihedral reflection subgroups. We begin with a well-known one, whose proof we include for completeness.

Proposition 3.6 [Dyer 1991]. *Suppose that* $\alpha, \beta \in \Phi^+$ *are distinct. Let*

$$W' = \langle \{ r_\gamma \mid \gamma \in (\mathbb{R}\alpha + \mathbb{R}\beta) \cap \Phi^+ \} \rangle.$$

Then W' *is a dihedral reflection subgroup of* W.

Proof. Suppose for a contradiction that W' is not dihedral. Then $\#S(W') \geq 3$, and let $x_1, x_2, x_3 \in \Delta(W')$ be distinct. Theorem 2.9(ii) then yields that $(x_i, x_j) \leq 0$ whenever $i, j \in \{1, 2, 3\}$ are different. Clearly x_1, x_2, x_3 are all in the two-dimensional subspace $\mathbb{R}\alpha + \mathbb{R}\beta$, and thus a contradiction would arise if we could show that x_1, x_2, x_3 are linearly independent. Let $c_1, c_2, c_3 \in \mathbb{R}$ be such that $c_1x_1 + c_2x_2 + c_3x_3 = 0$. Since $x_1, x_2, x_3 \in \Phi^+$, and $0 \notin \mathrm{PLC}(\Delta)$, it follows that c_1, c_2, c_3 cannot be all positive or all negative. Renaming x_1, x_2, x_3 if necessary, we have the following three possibilities:

(3-2) $$c_1, c_2 \geq 0 \quad \text{and} \quad c_3 < 0, \quad \text{or}$$

(3-3) $$c_1, c_2 \leq 0 \quad \text{and} \quad c_3 > 0, \quad \text{or}$$

(3-4) $$c_1, c_2, c_3 = 0.$$

If (3-2) is the case then $0 = (c_1x_1 + c_2x_2 + c_3x_3, x_3) < 0$, and if (3-3) is the case then $0 = (c_1x_1 + c_2x_2 + c_3x_3, x_3) > 0$; both are clearly absurd. Hence (3-4) must be the case and x_1, x_2, x_3 are linearly independent, a contradiction, as required. □

Let $\alpha, \beta \in \Phi^+$ be distinct. Let W'' be an arbitrary dihedral reflection subgroup of W containing the dihedral reflection subgroup $\langle\{r_\alpha, r_\beta\}\rangle$. Let x, y be the canonical roots for W''. It can be readily checked that $\mathbb{R}x + \mathbb{R}y = \mathbb{R}\alpha + \mathbb{R}\beta$, and hence $x, y \in (\mathbb{R}\alpha + \mathbb{R}\beta) \cap \Phi^+$. It then follows that $W'' \subseteq \langle\{r_\gamma \mid \gamma \in (\mathbb{R}\alpha + \mathbb{R}\beta) \cap \Phi^+\}\rangle$. This observation, together with Proposition 3.6, readily yields the following well-known result:

Proposition 3.7. *Every dihedral reflection subgroup $\langle\{r_\alpha, r_\beta\}\rangle$ of W (where the elements α and β of Φ^+ are distinct), is contained in a unique maximal dihedral reflection subgroup, namely $\langle\{r_\gamma \mid \gamma \in \Phi^+ \cap (\mathbb{R}\alpha + \mathbb{R}\beta)\}\rangle$.* □

Definition 3.8. (i) Define $\mathcal{M}$ to be the set of all maximal dihedral reflection subgroups of W.

(ii) Define $\mathcal{M}_\infty$ to be the set $\{W' \in \mathcal{M} \mid \#W' = \infty\}$.

(iii) For each $t \in T$, define $\mathcal{M}_t$ to be the set $\{W' \in \mathcal{M} \mid t \in W'\}$.

(iv) Let W' be a reflection subgroup of W, and let $t \in W' \cap T$. Define the *standard height*, $h_{(W',S(W'))}(t)$, of t with respect to the Coxeter system $(W', S(W'))$ to be

$$\min\{\ell_{(W',S(W'))}(w) \mid w \in W',\ w\alpha_t \in \Delta(W')\}.$$

For the standard height of t with respect to the Coxeter system (W, S), we simply write $h(t)$ in place of $h_{(W,S)}(t)$.

Remark 3.9. For arbitrary reflection subgroup W' of W, the depth function naturally applies to $\Phi^+(W')$: if $x \in \Phi^+(W')$, then the *depth* of x relative to $S(W')$ (written $\mathrm{dp}_{(W',S(W'))}(x)$) is defined to be

$$\min\{\ell_{(W',S(W'))}(w) \mid w \in W' \text{ and } wx \in \Phi^-(W')\}.$$

Now, for each $t \in W' \cap T$, it is easily checked that

$$\mathrm{dp}_{(W',S(W'))}(\alpha_t) = h_{(W',S(W'))}(t) + 1,$$

and hence applying Lemma 2.7(i) to the Coxeter system $(W', S(W'))$ yields that

$$h_{(W',S(W'))}(t) = \frac{\ell_{(W',S(W'))}(t) - 1}{2}. \tag{3-5}$$

We include a proof of the next result for completeness:

Lemma 3.10 [Edgar 2009]. *For each $t \in T$, we have*

$$T \setminus \{t\} = \biguplus_{W' \in \mathcal{M}_t} ((W' \cap T) \setminus \{t\}).$$

Proof. It is readily checked that $T \setminus \{t\} = \bigcup_{W' \in \mathcal{M}_t} ((W' \cap T) \setminus \{t\})$, and hence we only need to check that this union is indeed disjoint. Suppose for a contradiction that there are distinct $W_1, W_2 \in \mathcal{M}_t$ with $r \in W_1 \cap W_2$ for some $r \in T \setminus \{t\}$. Then clearly $\langle \{r, t\} \rangle \subseteq W_1$ and $\langle \{r, t\} \rangle \subseteq W_2$, contradicting Proposition 3.7. □

From this and the canonical bijection $\psi \colon T \leftrightarrow \Phi^+$ we immediately get:

Corollary 3.11. $\Phi^+ \setminus \{\alpha\} = \biguplus_{W' \in \mathcal{M}_{r_\alpha}} (\Phi^+(W') \setminus \{\alpha\})$, *for each* $\alpha \in \Phi^+$. □

Remark 3.12. In particular, the corollary implies that for $t \in T$, if $W_1, W_2 \in \mathcal{M}_t$ are distinct, then $\Phi^+(W_1) \cap \Phi^+(W_2) = \{\alpha_t\}$.

Lemma 3.13 [Edgar 2009]. *Let* $t \in T$ *be arbitrary. Then*

$$h(t) = \sum_{W' \in \mathcal{M}_t} h_{(W', S(W'))}(t).$$

Proof. For any reflection $t \in T$, Corollary 3.11 yields that

$$\{\alpha \in \Phi^+ \mid t\alpha \in \Phi^-\} = \{\alpha_t\} \cup \Bigl(\biguplus_{W' \in \mathcal{M}_t} \{\alpha \in \Phi^+(W') \setminus \{\alpha_t\} \mid t\alpha \in \Phi^-\} \Bigr). \tag{3-6}$$

Since $h(t) = \frac{1}{2}(\ell(t) - 1) = \frac{1}{2}(\#N(t) - 1)$, it follows from (3-6) that

$$\begin{aligned} h(t) &= \frac{1}{2}\Bigl(\sum_{W' \in \mathcal{M}_t} \#\{\alpha \in \Phi^+(W') \setminus \{\alpha_t\} \mid t\alpha \in \Phi^-(W')\} \Bigr) \\ &= \sum_{W' \in \mathcal{M}_t} \tfrac{1}{2}\bigl(\ell_{(W', S(W'))}(t) - 1\bigr) \qquad \text{(by (2-4))} \\ &= \sum_{W' \in \mathcal{M}_t} h_{(W', S(W'))}(t) \qquad \text{(by (3-5))}. \end{aligned}$$ □

Definition 3.14 [Edgar 2009]. For $t \in T$, define the ∞-*height* of t to be

$$h^\infty(t) = \sum_{W' \in \mathcal{M}_t \cap \mathcal{M}_\infty} h_{(W', S(W'))}(t),$$

and for each nonnegative integer n, we define

$$T_n = \{t \in T \mid h^\infty(t) = n\}.$$

From this definition it is not clear whether, for a specific nonnegative integer n, there is a reflection $t \in T$ with $h^\infty(t) = n$. It turns out that a number of basic questions like this can be solved with the aid of the results obtained in [Fu 2012] once we prove the following:

Theorem 3.15. *For each nonnegative integer* n, *there is a bijection* $T_n \leftrightarrow D_n$ *given by* $t \leftrightarrow \alpha_t$.

The proof of the theorem will be deferred until we have all the necessary tools.

Proposition 3.16. *Suppose that $t \in T$, and let W' be an infinite dihedral reflection subgroup containing t. If $h_{(W',S(W'))}(t) \geq 1$, then there exists some $x \in \Phi^+(W')$ distinct from α_t and satisfying $\alpha_t \operatorname{dom}_W x$.*

Proof. Observe that the condition $h_{(W',S(W'))}(t) \geq 1$ is equivalent to $\alpha_t \notin \Delta(W')$, and hence the required result follows immediately from Proposition 3.5(iii). □

The following proposition will be a key step to prove Theorem 3.15:

Proposition 3.17. *Let W' be an infinite dihedral reflection subgroup, and let $\Delta(W') = \{\alpha, \beta\}$.*

(i) *There are two disjoint dominance chains in $\Phi(W')$, namely*:

$$\cdots \operatorname{dom}_W\ r_\alpha r_\beta r_\alpha(\beta)\ \operatorname{dom}_W\ r_\alpha r_\beta(\alpha)\ \operatorname{dom}_W r_\alpha(\beta)\ \operatorname{dom}_W\ \alpha \\ \operatorname{dom}_W\ (-\beta)\ \operatorname{dom}_W\ r_\beta(-\alpha)\ \operatorname{dom}_W\ r_\beta r_\alpha(-\beta)\ \operatorname{dom}_W\ \cdots \tag{3-7}$$

and

$$\cdots \operatorname{dom}_W\ r_\beta r_\alpha r_\beta(\alpha)\ \operatorname{dom}_W\ r_\beta r_\alpha(\beta)\ \operatorname{dom}_W\ r_\beta(\alpha)\ \operatorname{dom}_W\ \beta \\ \operatorname{dom}_W (-\alpha)\ \operatorname{dom}_W\ r_\alpha(-\beta)\ \operatorname{dom}_W\ r_\alpha r_\beta(-\alpha)\ \operatorname{dom}_W\ \cdots . \tag{3-8}$$

In particular, each root in $\Phi(W')$ lies in exactly one of these two chains, and the negative of any element of one chain lies in the other. The roots in $\Phi(W')$ dominated by either α or β are all negative.

(ii) *If $x \in \Phi(W')$ then $\#D_{W'}(x) = h_{(W',S(W'))}(r_x)$.*

Proof. (i) Theorem 2.9(ii) and [Björner and Brenti 2005, Proposition 4.5.4 (ii)] yield that $(\alpha, \beta) \leq -1$. Hence it follows from Lemma 3.2(iv) that $\alpha \operatorname{dom}_W -\beta$ and $\beta \operatorname{dom}_W -\alpha$. Then we can immediately verify the existence of the two dominance chains (3-7) and (3-8), and from these two chains the remaining statements in (i) follow readily.

(ii) The required result follows immediately from the definition of $h_{(W',S(W'))}(r_x)$ and the two dominance chains (3-7) and (3-8). □

Proposition 3.18. *Suppose that $x, y \in \Phi^+$ are distinct with $x \operatorname{dom}_W y$, and let W' be a dihedral reflection subgroup containing r_x and r_y. Then $h_{(W',S(W'))}(r_x) \geq 1$.*

Proof. It follows from Corollary 3.3(ii) that $x \operatorname{dom}_{W'} y$, so Lemma 3.4 above yields that W' is an infinite dihedral reflection subgroup. Let $\{\alpha, \beta\} = \Delta(W')$. We know from Proposition 3.17(i) that the roots in $\Phi(W')$ dominated by either α or β are all negative, and since $x \operatorname{dom}_W y \in \Phi^+$, it follows that $x \notin \{\alpha, \beta\}$. Hence by definition $h_{(W',S(W'))}(r_x) \geq 1$. □

From the last two propositions we may deduce the following special case of Theorem 3.15:

Lemma 3.19. *There is a bijection $T_0 \leftrightarrow D_0$ given by $t \leftrightarrow \alpha_t$.*

Proof. Let $t \in T_0$, and suppose for a contradiction that $\alpha_t \notin D_0$. Then there exists $s \in T \setminus \{t\}$ such that $\alpha_t \operatorname{dom}_W \alpha_s$. Let W' be the unique maximal dihedral reflection subgroup of W containing $\langle\{s,t\}\rangle$. Proposition 3.18 yields that $h_{(W',S(W'))}(t) \geq 1$. Since $\alpha_t \operatorname{dom}_{W'} \alpha_s$, it follows from Lemma 3.4 that $W' \in \mathcal{M}_\infty$, and consequently $h^\infty(t) \geq 1$, contradicting the assumption that $t \in T_0$.

Conversely, suppose that $\alpha_t \in D_0$, and suppose for a contradiction that $t \notin T_0$. Then there exists some $W' \in \mathcal{M}_t \cap \mathcal{M}_\infty$ with $h_{(W',S(W'))}(t) \geq 1$. But then Proposition 3.16 yields that $\alpha_t \notin D_0$, producing a contradiction as required. □

Observe that Proposition 3.17(ii) can be equivalently stated as:

Proposition 3.20. *Suppose that $t \in T$, and suppose that W' is an infinite dihedral reflection subgroup containing t. Then*

$$\#D_{W'}(\alpha_t) = h_{(W',S(W'))}(t).$$ □

Proposition 3.21. *Suppose that $t \in T$ is arbitrary. Then*

$$\biguplus_{W' \in \mathcal{M}_t \cap \mathcal{M}_\infty} D_{W'}(\alpha_t) = D(\alpha_t).$$

Proof. First we observe that Remark 3.12 yields that the union of the sets $D_{W'}(\alpha_t)$ over all W' in $\mathcal{M}_t \cap \mathcal{M}_\infty$ is indeed disjoint.

It is clear that $\biguplus_{W' \in \mathcal{M}_t \cap \mathcal{M}_\infty} D_{W'}(\alpha_t) \subseteq D(\alpha_t)$.

Conversely, suppose that $x \in D(\alpha_t)$. Let W' be the unique maximal dihedral reflection subgroup of W containing $\langle\{t, r_x\}\rangle$. Then Corollary 3.3(ii) yields that $\alpha_t \operatorname{dom}_{W'} x$. Finally since there is no nontrivial dominance in any finite Coxeter group, it follows that $W' \in \mathcal{M}_\infty$, as required. □

Now we prove that for any reflection $t \in W$, its ∞-height $h^\infty(t)$ equals the number of positive roots strictly dominated by α_t:

Theorem 3.22. *Let $t \in T$ be arbitrary. Then $h^\infty(t) = \#D(\alpha_t)$.*

Proof. It follows from Proposition 3.20 and Proposition 3.21 that

$$h^\infty(t) = \sum_{W' \in \mathcal{M}_t \cap \mathcal{M}_\infty} h_{(W',S(W'))}(t) = \sum_{W' \in \mathcal{M}_t \cap \mathcal{M}_\infty} \#D_{W'}(\alpha_t) = \#D(\alpha_t).$$ □

Proof of Theorem 3.15. The theorem follows immediately from Theorem 3.22. □

Combining [Fu 2012, Theorem 3.8, Corollary 3.9, and Corollary 3.21] with Theorem 3.15 we may deduce:

Corollary 3.23. (i) *For each positive integer n,*

$$T_n \subseteq \{tt't \mid t \in T_0 \text{ and } t' \in T_m \text{ for some } m \leq n-1\}.$$

(ii) *Suppose that W is an infinite Coxeter group with $\#S < \infty$. Then*

$$0 < \#T_n \leq (\#T_0)^{n+1} - (\#T_0)^n$$

for each positive integer n. □

Remark 3.24. An upper bound for $\#T_0(=\#D_0)$ is given in [Brink and Howlett 1993]; furthermore, for any fixed finitely generated Coxeter group, this number can be explicitly calculated following the methods presented in [Brink 1998].

4. Dominance and imaginary cone

Kac introduced the concept of an *imaginary cone* in the study of the imaginary roots of Kac–Moody Lie algebras. In [Kac 1990, Chapter 5] the imaginary cone of a Kac–Moody Lie algebra was defined to be the positive cone on the positive imaginary roots. The generalization of imaginary cones to arbitrary Coxeter groups was first introduced in [Hée 1990], and subsequently reproduced in [Hée 1993]. This generalization has also been studied in [Dyer 2012] and [Edgar 2009]. In this section we investigate the connections between this generalized imaginary cone and dominance in Coxeter groups; in particular, we show that whenever x and y are roots of a Coxeter group, then $x \operatorname{dom}_W y$ if and only if $x-y$ lies in the imaginary cone of that Coxeter group.

Let (W, S) be the abstract Coxeter system associated to the Coxeter datum $\mathscr{C} = (V, \Delta, (\ ,\ ))$, and let Φ be the corresponding root system. Let X be a vector subspace of V. In this paper, a *cone* is assumed to be a convex cone. For any cone C in X, we define $C^* = \{f \in \operatorname{Hom}(X, \mathbb{R}) \mid f(v) \geq 0 \text{ for all } v \in C\}$ and call C^* the *dual* of C; and for any cone $F \in \operatorname{Hom}(X, \mathbb{R})$, we define $F^* = \{v \in X \mid f(v) \geq 0 \text{ for all } f \in F\}$ and call F^* the *dual* of F. If W acts on X, then $\operatorname{Hom}(X, \mathbb{R})$ bears the *contragredient representation* of W in the following way: if $w \in W$ and $f \in \operatorname{Hom}(X, \mathbb{R})$ then $wf \in \operatorname{Hom}(X, \mathbb{R})$ is given by the rule $(wf)(v) = f(w^{-1}v)$ for all $v \in X$. It is readily checked that for a cone C in X, we have $C \subseteq C^{**}$, and also for any $w \in W$, we have $(wC)^* = wC^*$.

The following is a well-known result whose proof can be found in [Howlett 1996, Lecture 1, Note (c)]:

Lemma 4.1. *Suppose that X is a real vector space of finite dimension, and let C be a cone in X. Then $(C^*)^* = \overline{C}$, where $\overline{C}$ is the topological closure of C in X (with respect to the standard topology on X).* □

Set $P = \operatorname{PLC}(\Delta) \cup \{0\}$. It is clear that P is a cone in V. We define the Tits cone of W in the same way as in Section 5.13 of [Humphreys 1990]:

Definition 4.2. The *Tits cone* of the Coxeter group W is the W-invariant set

$$U = \bigcup_{w \in W} wP^*.$$

It is not obvious from this definition that the Tits cone is indeed a cone; however, this is made clear by the following result:

Proposition 4.3.

$$U = \{f \in \mathrm{Hom}(\mathrm{span}(\Delta), \mathbb{R}) \mid f(x) \geq 0 \textit{ for all but finitely many } x \in \Phi^+\}. \tag{4-1}$$

Proof. Denote the set on the right-hand side of (4-1) by Y, and for each $f \in \mathrm{Hom}(\mathrm{span}(\Delta), \mathbb{R})$ define $\mathrm{Neg}(f)$ by $\mathrm{Neg}(f) = \{x \in \Phi^+ \mid f(x) < 0\}$.

If $f \in U$ then $f = wg$ for some $w \in W$ and $g \in P^*$, and it is readily checked that $\mathrm{Neg}(f) \subseteq N(w^{-1})$. Since $N(w^{-1})$ is a finite set, it follows that $f \in Y$, and hence $U \subseteq Y$. Conversely, suppose that $f \in Y$. If $\mathrm{Neg}(f) = \varnothing$ then $f \in P^* \subseteq U$. Thus we may assume that $\#\mathrm{Neg}(f) > 0$, and proceed by induction. Observe that then there exists some $\alpha \in \Delta$ such that $f(\alpha) < 0$. It is then readily checked that $\#\mathrm{Neg}(r_\alpha f) = \#\mathrm{Neg}(f) - 1$, and hence it follows from the inductive hypothesis that $r_\alpha f \in U$. Since U is W-invariant, it follows that $f \in U$, and hence $Y \subseteq U$. □

Lemma 4.4. *$U^* = \bigcap_{w \in W} w(P^*)^*$. Furthermore, $U^* = \bigcap_{w \in W} wP$ whenever Δ is a finite set.*

Proof. Write
$$\begin{aligned} U^* &= \{v \in V \mid f(v) \geq 0, \text{ for all } f \in U\} \\ &= \{v \in V \mid (w\phi)(v) \geq 0 \text{ for all } \phi \in P^* \text{ and all } w \in W\} \\ &= \{v \in V \mid \phi(w^{-1}v) \geq 0, \text{ for all } \phi \in P^* \text{ and all } w \in W\} \\ &= \bigcap_{w \in W} \{v \in V \mid \phi(w^{-1}v) \geq 0 \text{ for all } \phi \in P^*\} \\ &= \bigcap_{w \in W} \{wv \in V \mid \phi(v) \geq 0 \text{ for all } \phi \in P^*\}. \end{aligned}$$
Thus

$$U^* = \bigcap_{w \in W} \{wv \in V \mid v \in (P^*)^*\}. \tag{4-2}$$

Let $X = \mathrm{span}(\Delta)$. If $\#\Delta$ is finite then it follows from Lemma 4.1 that $(P^*)^* = \overline{P}$. It is clear that P is topologically closed; hence (4-2) yields that $U^* = \bigcap_{w \in W} wP$ when Δ is a finite set. □

Lemma 4.5. *Suppose that $v \in V$ has the property that $(a, v) \leq 0$ for all $a \in \Delta$. Then $wv - v \in P$ for all $w \in W$. Moreover, if $v \in P$ then $v \in U^*$.*

Proof. Use induction on $\ell(w)$. If $\ell(w) = 0$ then there is nothing to prove. If $\ell(w) \geq 1$ then we may write $w = w'r_a$ where $w' \in W$ and $a \in \Delta$ with $\ell(w) = \ell(w') + 1$.

Then Proposition 2.3 yields that $w'a \in \Phi^+ \subseteq P$, and we have

$$wv - v = (w'r_a)v - v = w'(v - 2(v,a)a) - v = (w'v - v) - 2(a,v)w'a.$$

By the inductive hypothesis, $w'v - v \in P$. Since $(a, v) \leq 0$, it follows from the above that $wv - v \in P$.

If $v \in P$ then $wv = (wv - v) + v \in P$ for all $w \in W$, and hence

$$v \in \bigcap_{w \in W} w^{-1} P \subseteq U^*. \qquad \square$$

Proposition 4.6 [Fu 2012, Proposition 3.4]. *Suppose that x, $y \in \Phi$ are distinct with $x \operatorname{dom}_W y$. Let W' be the dihedral reflection subgroup generated by r_x and r_y, and let $\Delta(W') = \{\alpha, \beta\}$. Then there exists some $w \in W'$ such that*

$$\begin{cases} wx = \alpha, \\ wy = -\beta, \end{cases} \quad \textit{or} \quad \begin{cases} wx = \beta, \\ wy = -\alpha. \end{cases}$$

In particular, $(x, y) = -(a, b)$. $\square$

Proposition 4.7. *Suppose that x, $y \in \Phi$ such that $x \operatorname{dom}_W y$. Then $w(x - y) \in$ PLC(Δ) for all $w \in W$, that is, $x - y \in U^*$.*

Proof. The assertion is trivially true if $x = y$, so we may assume that $x \neq y$. Since $x \operatorname{dom}_W y$, Lemma 3.2(iv) yields that $(x, y) \geq 1$. Let W' be the (infinite) dihedral subgroup of W generated by r_x and r_y. Let $S(W') = \{s, t\}$ and $\triangle(W') = \{\alpha_s, \alpha_t\}$. Proposition 4.6 yields that $(\alpha_s, \alpha_t) = -(x, y) \leq -1$. Set c_i as in Proposition 3.5 for each $i \in \mathbb{Z}$. Since $x \operatorname{dom}_W y$, it follows that $(x, y) \geq 1$, and Proposition 3.5(ii) then yields that there exist integers m and n such that

$$\begin{cases} x = c_{n+1}\alpha_s + c_n\alpha_t, \\ y = c_{m+1}\alpha_s + c_m\alpha_t, \end{cases} \quad \text{or} \quad \begin{cases} x = c_{n-1}\alpha_s + c_n\alpha_t, \\ y = c_{m-1}\alpha_s + c_m\alpha_t. \end{cases}$$

Next we shall show that $n > m$. Suppose for a contradiction that $m \geq n$. Then either $x = y$ (when $n = m$) or else there will be a $w \in W'$ such that $wx \in \Phi(W') \cap \Phi^-$ and yet $wy \in \Phi(W') \cap \Phi^+$ (when $n < m$), both contradicting the fact that $x \operatorname{dom}_W y$. Since $c_n > c_m$ whenever $n > m$, it follows that $x - y \in$ PLC(Δ). Given the W-invariance of dominance, for any $w \in W$, repeat the argument with x replaced by wx and y replaced by wy, we may conclude that $w(x - y) \in$ PLC$(\Delta) \subseteq (P^*)^*$. It then follows from Lemma 4.4 that $x - y \in U^*$. $\square$

When $\#\Delta$ is finite, it can be checked that Lemma 4.4 yields that whenever x, $y \in \Phi$ such that $x - y \in U^*$, then $x \operatorname{dom}_W y$. In fact we can remove this finiteness condition and still prove the same result, and to do so we need some special notations and a few extra elementary results. We thank the referee of this paper for prompting us to look in this direction.

Notations 4.8. For a subset I of S we set $\Delta_I = \{x \in \Delta \mid r_x \in I\}$; $V_I = \text{span}(\Delta_I)$; $W_I = \langle I \rangle$; and $P_I = \text{PLC}(\Delta_I) \cup \{0\}$. Furthermore, we set

$$P_I^* = \{f \in \text{Hom}(V_I, \mathbb{R}) \mid f(x) \geq 0 \text{ for all } x \in P_I\};$$
$$P_I^{**} = \{x \in V_I \mid f(x) \geq 0 \text{ for all } f \in P_I^*\}.$$

Then $\mathscr{C}_I = (V_I, \Delta_I, (\ ,\ )_I)$ (where $(\ ,\ )_I$ is the restriction of $(\ ,\ )$ on V_I) is a Coxeter datum with corresponding Coxeter system (W_I, I), and we call W_I the *standard parabolic subgroup* of W corresponding to I. Clearly W_I preserves V_I.

Lemma 4.9. *Suppose that I is a subset of S. Then $P^{**} \cap V_I \subseteq P_I^{**}$.*

Proof. Write $V = V_I \oplus V_I'$, where V_I' is a vector space complement of V_I. Then every $v \in V$ is uniquely written as $v = v_I + v_I'$, where $v_I \in V_I$ and $v_I' \in V_I'$. Every $g \in P_I^*$ gives rise to a $g' \in P^*$ as follows: for any $v \in V$, simply set $g'(v) = g(v_I)$. Now let $x \in P^{**} \cap V_I$ and $f \in P_I^*$ be arbitrary. Then $f(x) = f'(x) \geq 0$, since $f' \in P^*$ and $x \in P^{**}$. Hence $x \in P_I^{**}$, and so $P^{**} \cap V_I \subseteq P_I^{**}$. □

Proposition 4.10. *Let $x, y \in \Phi$. Then $x - y \in U^*$ if and only if $x \operatorname{dom}_W y$.*

Proof. By Proposition 4.7 we only need to prove that when x and y are both roots then $x - y \in U^*$ implies that $x \operatorname{dom}_W y$. The assertion certainly holds if $x = y$, thus we only need to check the case when $x \neq y$.

Since dominance and U^* are both W-invariant, it follows that we only need to prove the following statement: if $x \in \Phi^-$ then $y \in \Phi^-$ too.

Take $I = \{r_\alpha \mid \alpha \in \text{supp}(x) \cup \text{supp}(y)\}$, and note that in particular, I is a finite set. Now in view of Lemma 4.4, Lemma 4.9 and the fact that W_I preserves V_I we have

$$\begin{aligned} x - y \in \Big(\bigcap_{w \in W} wP^{**}\Big) \cap V_I \subseteq \Big(\bigcap_{w \in W_I} wP^{**}\Big) \cap V_I &\subseteq \bigcap_{w \in W_I} w(P^{**} \cap V_I) \\ &\subseteq \bigcap_{w \in W_I} wP_I^{**} = \bigcap_{w \in W_I} wP_I, \end{aligned}$$

where the equality follows from Lemma 4.1, since I is a finite set. Thus $x - y \in P_I$, and this implies, precisely, that $y \in \Phi^-$ whenever $x \in \Phi^-$. □

Next we have a technical result which is a key component of the main theorem of this section.

Proposition 4.11. *Suppose that $x, y \in \Phi$ are distinct with $x \operatorname{dom}_W y$. Then there exists some $w \in W$ such that $wx \in \Phi^+$, $wy \in \Phi^-$ and $(w(x - y), z) \leq 0$ for all $z \in \Phi^+$.*

Proof. Clearly it is enough to show that under such assumptions there exists some $w \in W$ with $wx \in \Phi^+$, $wy \in \Phi^-$ and $(w(x - y), z) \leq 0$ for all $z \in \Delta$.

Let W' be the (infinite) dihedral reflection subgroup of W generated by r_x and r_y, and let $\triangle(W') = \{a_0, b_0\}$. Clearly a_0, $b_0 \in \Phi^+$, and Proposition 4.6 yields that $(a_0, b_0) = -(x, y) \leq -1$; furthermore, there is some $u \in \langle\{r_x, r_y\}\rangle$ such that

$$\begin{cases} u(x) = a_0, \\ u(y) = -b_0, \end{cases} \quad \text{or} \quad \begin{cases} u(x) = b_0, \\ u(y) = -a_0. \end{cases} \tag{4-3}$$

At any rate, $u(x - y) = a_0 + b_0$. Since the W-action preserves (,), it follows that $(a_0, a_0) = 1 = (b_0, b_0)$, and hence $(a_0 + b_0, a_0) \leq 0$ and $(a_0 + b_0, b_0) \leq 0$. However there may exist some $c_1 \in \Delta$ with $(a_0 + b_0, c_1) > 0$. If this is the case, set $a_1 = r_{c_1} a_0$ and $b_1 = r_{c_1} b_0$. Recall that $(d, c_1) \leq 0$ for all $d \in \Delta \setminus \{c_1\}$, so it follows that

$$c_1 \in \operatorname{supp}(a_0) \cup \operatorname{supp}(b_0). \tag{4-4}$$

Since $(a_0 + b_0, c_1) > 0$, whereas $(a_0 + b_0, a_0) \leq 0$ and $(a_0 + b_0, b_0) \leq 0$, it follows that $a_0 \neq c_1$ and $b_0 \neq c_1$. Therefore we see that a_1, $b_1 \in \Phi^+$, and $(a_1, b_1) = (a_0, b_0) \leq -1$. Consequently Theorem 2.9(ii) yields that a_1, b_1 are the canonical roots for the root subsystem $\Phi(\langle\{r_{a_1}, r_{b_1}\}\rangle)$. Since $r_{c_1}(a_0 + b_0) = a_0 + b_0 - 2(a_0 + b_0, c_1)c_1$ and $(a_0 + b_0, c_1) > 0$, it follows that

$$\operatorname{supp}(a_1) \cup \operatorname{supp}(b_1) \subseteq \operatorname{supp}(a_0) \cup \operatorname{supp}(b_0)$$

and

$$\sum_{a \in \Delta} \operatorname{coeff}_a(a_1) + \sum_{a \in \Delta} \operatorname{coeff}_a(b_1) < \sum_{a \in \Delta} \operatorname{coeff}_a(a_0) + \sum_{a \in \Delta} \operatorname{coeff}_a(b_0).$$

Moreover, since $(a_0 + b_0, c_1) > 0$, it follows that at least one of (a_0, c_1) or (b_0, c_1) must be strictly positive. Hence Lemma 2.7 yields that

$$dp(a_1) + dp(b_1) \leq dp(a_0) + dp(b_0).$$

Repeating this process, we can obtain new pairs of positive roots $\{a_2, b_2\}, \dots,$ $\{a_{m-1}, b_{m-1}\}$, $\{a_m, b_m\}$ with

$$\operatorname{supp}(a_m) \cup \operatorname{supp}(b_m) \subseteq \operatorname{supp}(a_{m-1}) \cup \operatorname{supp}(b_{m-1}) \subseteq \cdots \subseteq \operatorname{supp}(a_0) \cup \operatorname{supp}(b_0)$$

and $\operatorname{dp}(a_m) + \operatorname{dp}(b_m) \leq \operatorname{dp}(a_{m-1}) + \operatorname{dp}(b_{m-1}) \leq \cdots \leq \operatorname{dp}(a_0) + \operatorname{dp}(b_0)$, so long as we can find a $c_m \in \Delta$ such that $(a_{m-1} + b_{m-1}, c_m) > 0$. This process only terminates at a pair $\{a_n, b_n\}$ for some n if $(a_n + b_n, z) \leq 0$ for all $z \in \Delta$. Now if we could show that this process terminates at some such $\{a_n, b_n\}$ after a finite number of iterations, then we have in fact found a $w \in W$ given by

$$w = r_{c_n} r_{c_{n-1}} \cdots r_{c_1} u, \quad \text{where } u \text{ is as in (4-3),} \tag{4-5}$$

satisfying

$$(w(x-y),z) = (r_{c_n}\cdots r_{c_1}(a_0+b_0),z) = (a_n+b_n,z) \le 0$$

for all $z \in \Delta$.

Observe that the set of positive roots having depth less than or equal to the specific bound $\mathrm{dp}(a_0)+\mathrm{dp}(b_0)$ and support in the fixed finite subset $\mathrm{supp}(a_0)\cup\mathrm{supp}(b_0)$ of Δ is finite; indeed, Lemma 2.7(ii) implies that there are at most

$$\#(\mathrm{supp}(a_0)\cup\mathrm{supp}(b_0))^{\mathrm{dp}(a_0)+\mathrm{dp}(b_0)}$$

such positive roots. Hence it follows that the possible pairs of positive roots $\{a_i, b_i\}$ obtainable in the process above must be finite too. Since

$$\sum_{a\in\Delta}\mathrm{coeff}_a(a_j)+\sum_{a\in\Delta}\mathrm{coeff}_a(b_j) < \sum_{a\in\Delta}\mathrm{coeff}_a(a_i)+\sum_{a\in\Delta}\mathrm{coeff}_a(b_i)$$

for all $j > i$, it follows that the sequence $\{a_0, b_0\}, \{a_1, b_1\}, \ldots$ must terminate at $\{a_n, b_n\}$ for some finite n, as required.

Finally, keeping w as in (4-5), we see from the construction above that either $wx = a_n \in \Phi^+$ and $wy = -b_n \in \Phi^-$, or $wx = b_n \in \Phi^+$ and $wy = -a_n \in \Phi^-$. □

Definition 4.12. We define the *imaginary cone* Q of W by

$$Q = \{v \in U^* \mid (v,a) \le 0 \text{ for all but finitely many } a \in \Phi^+\}.$$

The following result was obtained independently by Dyer as a consequence of [Dyer 2012, Theorem 6.3], stating that *the imaginary cone of a reflection subgroup is contained in that of the overgroup*.

Theorem 4.13. *Suppose that $x, y \in \Phi$ such that $x \operatorname{dom}_W y$. Then $x - y \in Q$.*

Proof. By Proposition 4.7 we know that $x - y \in U^*$, thus to prove the desired result, we only need to show that $(x-y,z) \le 0$ for all but finitely many $z \in \Phi^+$. Suppose that $z \in \Phi^+$ such that $(x-y,z) > 0$. Let $w \in W$ be as in Proposition 4.11. Then $(w(x-y), wz) > 0$, and by Proposition 4.11 this is possible only if $z \in N(w)$. Since $\#N(w)$ is clearly finite (equal to $\ell(w)$), it follows that indeed $(x-y,z) \le 0$ for all but finitely many $z \in \Phi^+$. □

Remark 4.14. The above theorem is a special case of Dyer's result when the subgroup is dihedral. In fact, Dyer's result, when applied to dihedral reflection subgroups, implies that if x and y are roots with $x \operatorname{dom}_W y$, then $x - cy \in Q$ for an explicit range of $c \in \mathbb{R}$ depending on the value of (x, y). Our formulation was first suggested to us by Howlett and Dyer, and we gratefully acknowledge their help.

Theorem 4.13, combined with Proposition 4.10, immediately implies this:

Corollary 4.15. *Let $x, y \in \Phi$. Then $x - y \in Q$ if and only if $x \operatorname{dom}_W y$.* □

Remark 4.16. By Proposition 4.10 and Corollary 4.15, when $x,\ y \in \Phi$, it is impossible for $x - y$ to be in $U^* \setminus Q$.

Corollary 4.17. *Suppose that $x,\ y \in \Phi$ are distinct. The following are equivalent*:

(i) *Whenever $x \operatorname{dom}_W z \operatorname{dom}_W y$ for some $z \in \Phi$, then either $z = x$ or $z = y$ (thus forming a cover of dominance)*;

(ii) *There exists a $w \in W$ such that $wx \in D_0$ and $wy \in -D_0$.*

Proof. Suppose that (i) is the case. Let w be as in Proposition 4.11 above. First we show that then $wx \in D_0$. Suppose for a contradiction that $wx \notin D_0$, and let $z \in D(wx)$. Then Proposition 4.11 yields that $wy \in \Phi^-$ and $(wy, z) \geq (wx, z) \geq 1$. Hence it is clear that $z \operatorname{dom}_W wy$. But this implies that $x \operatorname{dom}_W w^{-1}z \operatorname{dom}_W y$ with $x \neq w^{-1}z \neq y$, contradicting (i). Therefore $wx \in D_0$, as required. Exchanging the roles of x and $-y$ we may deduce that $wy \in -D_0$.

Suppose that (ii) is the case and suppose for a contradiction that there exists some $z \in \Phi \setminus \{x, y\}$ such that $x \operatorname{dom}_W z \operatorname{dom}_W y$. Let $w \in W$ with $wx \in D_0$ and $wy \in -D_0$. If $wz \in \Phi^+$ then Lemma 3.2(ii) yields that $wx \operatorname{dom}_W wz$, contradicting the fact that $wx \in D_0$. On the other hand, if $wz \in \Phi^-$, then parts (ii) and (iii) of Lemma 3.2 yield that $-wy \operatorname{dom}_W -wz \in \Phi^+$, contradicting the fact that $-wy \in D_0$. □

Observe that applying Corollary 4.17 to arbitrary reflection subgroup W' of W yields the following:

Corollary 4.18. *Suppose that W' is a reflection subgroup of W with x and $y \in \Phi(W')$ being distinct. The following are equivalent*:

(i) *Whenever $x \operatorname{dom}_{W'} z \operatorname{dom}_{W'} y$ for some $z \in \Phi(W')$, then either $z = x$ or $z = y$*;

(ii) *There exists a $w \in W'$ such that $wx \in D_{W',0}$ and $wy \in -D_{W',0}$.* □

Definition 4.19. Suppose that W' is a reflection subgroup of W and $x,\ y \in \Phi(W')$ satisfy both (i) and (ii) of Corollary 4.18. Then we say that the dominance between x and y is *minimal* with respect to W'.

Proposition 4.20. *Suppose that $x,\ y \in \Phi$ are distinct with $x \operatorname{dom}_W y$, and let W' be the dihedral reflection subgroup generated by r_x and r_y. Then the dominance between x and y with respect to W' is minimal.*

Proof. It follows from Corollary 3.3(ii) that $x \operatorname{dom}_{W'} y$, and hence Lemma 3.4 yields that W' is infinite dihedral. Let $\Delta(W') = \{\alpha, \beta\}$. Then Proposition 3.17(i) yields that $D_{W',0} = \{\alpha, \beta\}$.

On the other hand, it follows from Proposition 4.6 that there is some $w \in W'$ such that

$$\begin{cases} wx = a, \\ wy = -b, \end{cases} \quad \text{or} \quad \begin{cases} wx = b, \\ wy = -a; \end{cases}$$

consequently Corollary 4.18 yields that the dominance between x and y with respect to $\langle\{r_x, r_y\}\rangle$ is minimal. □

From this proposition we may deduce:

Proposition 4.21. *Suppose that $x \in \Phi^+$ with $D(x) = \{x_1, x_2 \ldots, x_m\}$. For each $i \in \{1, 2, \ldots, m\}$, set $W_i = \langle\{r_x, r_{x_i}\}\rangle$. Then $W_i \neq W_j$ whenever $i \neq j$.*

Proof. For each $i \in \{1, 2, \ldots, m\}$, set $\{s_i, t_i\} = S(W_i)$. Suppose for a contradiction that $W' = W_i = W_j$ for some $i \neq j$. Then we may write $\{s, t\} = \{s_i, t_i\} = \{s_j, t_j\}$. Corollary 3.3(ii) yields that $x \operatorname{dom}_{W_k} x_k$ for all $k \in \{1, 2, \ldots, m\}$, and since there is no nontrivial dominance in finite Coxeter groups, it follows that $W_1, W_2, \ldots, W_m$ are all infinite dihedral reflection subgroups. Hence it follows from Proposition 4.5.4 of [Björner and Brenti 2005] that $(\alpha_s, \alpha_t) \leq -1$. Set c_n as in Proposition 3.5 for each $n \in \mathbb{Z}$. Since $x \operatorname{dom}_W x_i$ and $x \operatorname{dom}_W x_j$, Proposition 3.5(ii) yields that either

$$\begin{cases} x = c_m\alpha_s + c_{m+1}\alpha_t, \\ x_i = c_{m'}\alpha_s + c_{m'+1}\alpha_t, \\ x_j = c_{m''}\alpha_s + c_{m''+1}\alpha_t, \end{cases} \quad \text{or} \quad \begin{cases} x = c_m\alpha_s + c_{m-1}\alpha_t, \\ x_i = c_{m'}\alpha_s + c_{m'-1}\alpha_t, \\ x_j = c_{m''}\alpha_s + c_{m''-1}\alpha_t, \end{cases}$$

for some distinct integers m, m' and m''. Observe that in either case $(x_i, x_j) \geq 1$, and therefore there will be (nontrivial) dominance between x_i and x_j. Without loss of any generality, we may assume that $x \operatorname{dom}_W x_i \operatorname{dom}_W x_j$. Then

$$x \operatorname{dom}_{W'} x_i \operatorname{dom}_{W'} x_j$$

by Corollary 3.3(ii), contradicting Proposition 4.20. □

We close this paper with an alternative characterization for the imaginary cone Q when $\#\Delta < \infty$.

Proposition 4.22. *If $\#\Delta < \infty$ then*

$$Q = \{wv \mid w \in W \text{ and } v \in P \text{ such that } (v, a) \leq 0 \text{ for all } a \in \Phi^+\}. \tag{4-6}$$

Proof. First we denote the set on the right-hand side of (4-6) by Z, and for each $b \in P$, define $\operatorname{Pos}(b) = \{c \in \Phi^+ \mid (b, c) > 0\}$. Recall that, under the assumption that $\#\Delta < \infty$, Lemma 4.4 yields that

$$Q = \left\{ v \in \bigcap_{w \in W} wP \;\middle|\; (v, a) \leq 0 \text{ for all but finitely many } a \in \Phi^+ \right\}.$$

Let $u \in Q$ be arbitrary. Since $\#\Delta < \infty$, it follows from Lemma 4.4 that $u \in P$. If $\operatorname{Pos}(u) = \varnothing$, then trivially $u \in Z$. Therefore we may assume that $\operatorname{Pos}(u) \neq \varnothing$, and proceed by induction on $\#\operatorname{Pos}(u)$ (this is only possible because $u \in Q$, and so $\#\operatorname{Pos}(u) < \infty$). Let $a \in \Delta$ be chosen such that $(u, a) > 0$. Then it can be readily checked that $\mathrm{Pos}(r_a u) = r_a(\mathrm{Pos}(u) \setminus \{a\})$. Thus the inductive hypothesis yields that $r_a u \in Z$. Clearly Z is W-invariant, and so $u \in Z$, and hence $Q \subseteq Z$.

Conversely, if $x \in Z$, then $x = wv$ for some $w \in W$ and $v \in P$ such that $(v, a) \leq 0$ for all $a \in \Delta$. Lemma 4.5 yields that $v \in U^*$, and since U^* is clearly W-invariant, it follows that $x \in U^*$. Suppose that $y \in \Phi^+$ with $(x, y) > 0$. Since $(x, y) = (wv, y) = (v, w^{-1}y)$, and since $(v, a) \leq 0$ for all $a \in \Phi^+$, it follows that $w^{-1}y \in \Phi^-$ and thus $y \in N(w^{-1})$. The finiteness of the set $N(w^{-1})$ then implies that $x \in Q$, and hence $Z \subseteq Q$. □

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SEMICONTINUITY OF AUTOMORPHISM GROUPS OF STRONGLY PSEUDOCONVEX DOMAINS: THE LOW DIFFERENTIABILITY CASE

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We study the semicontinuity of automorphism groups for perturbations of domains in complex space or in complex manifolds. We provide a new approach to the study of such results for domains having minimal boundary smoothness. The emphasis in this study is on the low differentiability assumption and the new methodology developed accordingly.

1. Introduction

It is a familiar perception of everyday life that symmetry is hard to create, but easy to destroy. To make the crooked straight requires some definite effort, but the slightest change can suffice to make the straight a little crooked and hence not straight at all. This perception is easily substantiated in precise form for geometric objects in Euclidean space. It is natural to ask if something similar might apply for automorphism groups in complex analysis, that is, for the group of biholomorphic self-maps of, say, a bounded domain in complex Euclidean space.

In one complex variable, this idea does not yield much, at least in the topologically trivial case. Since all bounded domains that are topologically equivalent to the unit

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disc are biholomorphic to the unit disc (Riemann mapping theorem, of course), there is not much interest in discussing how the automorphism group varies with the domain: it does not vary at all.

But, in higher dimensions, the idea comes into its own. Domains near the unit ball can have no automorphisms whatever except the identity, and indeed domains with trivial automorphism group are dense in the set of C^∞ strongly pseudoconvex domains in the C^∞ topology (see [Greene and Krantz 1982a] for detailed references to the literature): the proof of this result in fact goes back really to Poincaré, in effect, since it depends essentially only on counting parameters rather than on the details of local invariant theory, at least once one knows that biholomorphic maps extend smoothly to the boundary [Fefferman 1974]. It is also the case that domains near the unit ball have automorphism groups which are isomorphic to a subgroup of the automorphism group of the ball. Indeed, if a domain is C^∞ close enough to the ball, then the domain is either biholomorphic to the ball or its automorphism group is isomorphic to a (closed) subgroup of the unitary group [Greene and Krantz 1982a].

This kind of semicontinuity holds in greater generality [ibid.]. If a C^∞ strongly pseudoconvex domain is not biholomorphic to the ball, then there is a neighborhood of the domain in the C^∞ topology on the set of all C^∞ bounded domains with the property that the automorphism group of every domain in the neighborhood is isomorphic to a subgroup of the automorphism group of the original domain. (The case of the fixed domain being biholomorphic to the ball is as in the previous paragraph.)

The goal of this paper is to explore the possibility of reducing the level of differentiability required for this type of semicontinuity result, both for the fixed domain itself and for the perturbed domains and the topology upon them. We shall show in fact that C^∞ can be reduced to C^2. This is optimal in the sense that C^2 is the natural setting for the discussion of strong pseudoconvexity and is the lowest level of regularity for which the definition is naturally given. (One can, of course, construct somewhat more intricate and to some extent artificial ideas of strong pseudoconvexity wherein the boundary need not have that much regularity, but these will not be explored here.)

It will turn out that the complex analysis results just discussed can in fact best be treated by changing the whole context to manifolds and general group actions. The role of complex analysis becomes simply to guarantee a kind of uniform compactness discussed in Section 2 in detail.

To put this matter in perspective, it is desirable to recall in outline how the semicontinuity results in [Greene and Krantz 1982a] were obtained. The starting point is the use of normal family arguments. In this context, the setup is as follows. Fix a bounded domain Ω_0. Then a sequence of bounded domains Ω_j is considered to converge to Ω_0 if there is a sequence of maps $\Phi_j : \Omega_0 \to \Omega_j$ which converges to the identity in some appropriate topology. Now, in this situation, a sequence of automorphisms $f_j : \Omega_j \to \Omega_j$ always has a subsequence f_{j_k} such that the maps $\Phi_{j_k}^{-1} \circ f_{j_k} \circ \Phi_{j_k}$ converge to some map of Ω_0 to the closure of Ω_0. Here convergence means uniform convergence on compact subsets of Ω_0.

However, it is relatively easy to show, and it is in fact a classical result that, if the limit mapping is in fact interior, i.e., if its image lies in Ω_0 itself, then that limit is an automorphism of Ω_0. (A detailed proof is given in [Krantz 2001].) Thus, in trying to relate the automorphisms of the Ω_j's to those of Ω_0, one is interested in situations where it is guaranteed that the family of maps of the sort described always has "nondegenerate" limits; that is, the limits are necessarily the maps into Ω_0 itself, with no boundary points in the image.

As it happens, every strongly pseudoconvex bounded domain that is not biholomorphic to the ball has a compact automorphism group. This was proved in [Wong 1977] and has been much generalized since, to the point where the result is not only valid for C^2 domains but is localized completely: if a sequence of automorphisms has the property that, for some interior point the sequence of the images of the point converge to a C^2 strongly pseudoconvex boundary point of a domain in a general complex manifold, then the domain is biholomorphic to the ball [Efimov 1995; Gaussier et al. 2002]. This line of thought makes it natural to consider the whole normal families situation for bounded strongly pseudoconvex domains that are not biholomorphic to the ball, which will indeed be the main topic in this paper. However, certain aspects of the situation can be treated with no pseudoconvexity invoked at all. If one simply assumes the relevant kind of nondegeneracy of normal families as a hypothesis, then a semicontinuity result already follows. This matter is treated in Section 2.

It is natural to ask when that nondegeneracy hypothesis is satisfied, that is, under what conditions of a more familiar sort the nondegeneracy condition (stably interior) that is required in Section 2 is sure to hold. As we shall see, it in fact always holds under the hypothesis of C^2 strong pseudoconvexity of the boundary of Ω_0 (Ω_0 not biholomorphic to the ball) and the assumption that the Ω_j converge to Ω_0 in the C^2 topology. How this arises requires some explanation.

The semicontinuity of automorphism groups in the C^2 case will be obtained in this paper again by using curvature invariants to bound the distance of orbits from the boundary stably. But the stability of the asymptotic constancy of holomorphic curvature of the Bergman metric will be obtained without using the Fefferman expansion, thus avoiding the need for a large number of derivatives. Instead, the behavior of the holomorphic sectional curvature of the Bergman metric will be analyzed using the "scaling method," as explained in Section 3. The possibility of using the scaling method depends on noting that the holomorphic sectional curvature can be expressed in terms of a special basis for the Hilbert space of square integrable holomorphic functions (see [Greene and Wu 1979] and [Epstein 1965] for the special basis concept in generality). This means that one can detour around the rather awkward formulas from Riemannian geometry that express the curvature tensor as a whole in terms of the metric and operate instead with more directly accessible aspects of the fundamental Bergman construction.

In the last section of the present paper, a more refined kind of semicontinuity result involving not just isomorphism to a subgroup but isomorphism to a subgroup via diffeomorphism conjugacy will be obtained for strongly pseudoconvex domains with low boundary regularity. For technical reasons, the regularity cannot be quite reduced to the C^2 level which would be all that is needed for the subgroup semicontinuity. This is related to the present Theorem 4.3, a uniform version of Lempert's extension theorem for biholomorphic mappings of bounded domains with $C^{k,\alpha}$ smooth boundaries for every $k \geq 2$. For the conjugacy arguments, the necessary regularity here turns out to be $C^{4,\alpha}$. It may be possible that diffeomorphism conjugacy also applies in the C^2 case, but this result cannot be proved by the methods used here.

It is worth noting that in [Greene and Krantz 1985] we established a version of the semicontinuity theorem for automorphism groups in the context of C^2 convergence. That paper was an important first step in the program we are developing here. The role of holomorphic curvature of the Bergman metric was replaced by the quotient invariant, that is the Carathéodory volume divided by the Kobayashi–Eisenmann volume. But the curvature methods here are of independent interest, and the needed stable uniformity of C^k extension of automorphisms, for low k, is checked here in Theorem 4.3.

2. Normal families and general semicontinuity of groups of mappings

In this section, some very general results will be discussed about groups of diffeomorphisms of open sets in Euclidean spaces. The fundamental idea is that, as far as semicontinuity of the groups is concerned, the noncompact case can be converted to the compact case. This is, more precisely, true as far as semicontinuity in the sense of isomorphism to a subgroup is concerned. We begin with a definition of an appropriate idea of convergence of the open sets. For convenience, and without any particular loss of generality, we restrict our attention to connected open sets, i.e., domains.

Definition 2.1. A sequence Ω_j of connected open sets, or domains, in a Euclidean space $\mathbb{R}^n$, is said to *containment-converge* to a limit domain Ω_0 if, for every compact subset K of Ω_0, K is contained in Ω_j for all sufficiently large j.

Definition 2.2. If the sequence $\{\Omega_j\}$ of domains containment-converges to a domain Ω_0, then a sequence of C^∞ mappings $f_j : \Omega_j \to \mathbb{R}^n$ is said to *converge* C^∞

normally if, for each compact subset K of Ω_0, the mappings f_j and their derivatives of all orders converge uniformly on K.

Note here that the f_j are defined in a neighborhood of K, any compact set K, for all j sufficiently large, so that the desired uniform convergence indeed makes sense.

For our next definition, we recall that there is a metric, to be denoted γ_K, on the set of all C^∞ mappings of a neighborhood of a compact subset K to $\mathbb{R}^n$ such that convergence in this metric is equivalent to convergence of the mappings and their derivatives of all orders uniformly on the compact set K (see [Greene and Krantz 1982b], for example).

Definition 2.3. Suppose that $\{\Omega_j\}$ is a sequence of domains which containment-converges to a domain Ω_0 and also suppose that, for each j, G_j is a group of diffeomorphisms of Ω_j, and that G_0 is a group of diffeomorphisms of Ω_0. We say that the sequence of groups G_j *converges normally* to G_0 if, for each compact subset K of Ω_0 and for each $\epsilon > 0$, there is a $j_{\epsilon,K}$ such that, for each $j > j_{\epsilon,K}$ and each $\phi_j \in G_j$, the mapping $\phi_j|_K$ lies within γ_K-distance ϵ of some element of G_0.

In case one has not domains, but compact manifolds and compact groups, then the situation is as follows:

Lemma 2.4 (from [Ebin 1968]; cf. [Kim 1987] and [Greene et al. 2011]). *If M is a compact manifold and if G_j is a sequence of compact subgroups of the diffeomorphism group of M* [*in the topology determined by the metric γ_M*] *such that G_j converges to the compact subgroup G_0 then*, *for all j sufficiently large*, *G_j is isomorphic to a subgroup of G_0. Moreover*, *the isomorphism can be obtained by conjugation by a diffeomorphism ϕ_j and the ϕ_j can be chosen to converge to the identity* [*again in the topology determined by the metric γ_M*].

This follows from the original result of [Ebin 1968] as follows. Averaging on arbitrary Riemannian metric on M with respect to the action of G gives a Riemannian metric g on M which is G-invariant; i.e., $G \subset \mathrm{Isom}(g)$, where $\mathrm{Isom}(g)$ is the isometry group of g. Averaging g with respect to the action of G_j for each j yields Riemannian metric g_j with $G_j \subset \mathrm{Isom}(g_j)$ for each j. Since the elements of G_j are close to the elements of G by hypothesis, when j is large, it follows easily that the sequence $\{g_j\}$ of metrics converges C^∞ to g. By Ebin's original result, there are, for all j sufficiently large, diffeomorphisms $\phi_j : M \to M$ such that ϕ_j conjugates $\mathrm{Isom}(g_j)$ to a subgroup $\phi_j \circ \beta \circ \phi_j^{-1} \in \mathrm{Isom}(g)$ for all $\beta \in \mathrm{Isom}(g_j)$ of $\mathrm{Isom}(g)$; moreover, the sequence $\{\phi_j\}$ can be taken to converge C^∞ to the identity. Then each ϕ_j conjugates G_j (for j large) to a subgroup $\widehat{G}_j$ of $\mathrm{Isom}(g)$, with $\widehat{G}_j$ C^∞-close to G. By a classical theorem of [Montgomery and Samelson 1943], it follows that $\widehat{G}_j$ is isomorphic to a subgroup of G via conjugation by an element σ_j of $\mathrm{Isom}(g)$, with the σ_j converging to the identity.

This point will arise again in a slightly different form in Section 5, q.v.

Our goal here is to show how to reduce the domain case to the compact manifold situation described in Lemma 2.4. Specifically, we want to prove the following proposition:

Proposition 2.5. *Suppose that* $\{\Omega_j\}$ *is a sequence of bounded domains in* $\mathbb{R}^N$ *which containment-converges to* Ω_0 *in the sense of Definition 2.1 and that, for each* j, G_j *is a compact group of diffeomorphisms of* $\mathrm{cl}(\Omega_j)$ *and that the sequence* $\{G_j\}$ *converges* C^∞ *normally to a compact group* G_0 *of diffeomorphisms of* $\mathrm{cl}(\Omega_0)$ [*convergence in the sense of Definition 2.3*]. *Here, of course,* cl *denotes the closure of the indicated set. Then, for all sufficiently large* j, *the group* G_j *is isomorphic to a subgroup of* G_0.

Proof. The essential tool is to use group-invariant exhaustion functions to find a smoothly bounded subdomain of Ω_0 that is taken to itself by each element of the group G_0 and then to pass to the "double" of these subdomains to form a compact manifold. Then one does a similar construction to nearby G_j-invariant subdomains of Ω_j and thus attains the situation of Ebin's theorem. We now describe this situation in more detail, following the arguments developed in [Greene and Krantz 1982b]:

> **Definition 2.6.** A real-valued function $\rho : \Omega \to \mathbb{R}$ on a domain Ω is said to be an *exhaustion function* if, for every $\alpha \in \mathbb{R}$, the set $\rho^{-1}((-\infty, \alpha])$ is compact — that is, the sublevel sets of ρ are compact.

Exhaustion functions of course always exist on domains and indeed on manifolds in general. One for (not necessarily bounded) domains that frequently occurs in complex analysis is $\max(\|z\|^2, -\log \operatorname{dist}(z, \text{the complement of the domain}))$. Exhaustion functions with special properties play an important role, for instance, in the study of Stein manifolds; these are of course more difficult to construct.

Now suppose that G is a compact group of diffeomorphisms on a domain Ω and suppose that ρ is an exhaustion function on Ω. Then the function $\hat{\rho}$ defined by

$$\hat{\rho}(z) := \int_G \rho(g(z))\, d\lambda(g),$$

where $d\lambda$ is the normalized Haar measure on G, is also an exhaustion function, as one easily sees. This function is G-invariant in the sense that $\hat{\rho}(g(z)) = \hat{\rho}(z)$. Thus its sublevel sets are invariant under the action of G: a given sublevel set is mapped to itself by each element of G.

If ρ is C^∞, then $\hat{\rho}$ is also C^∞. In this case, for all sufficiently large α, except for a set of measure 0, the sublevel set $\hat{\rho}^{-1}(-\infty, \alpha]$ is a compact C^∞ manifold-with-boundary. This follows from Sard's theorem: one need only take α so large that the sublevel set is nonempty and such that α is a regular value for $\hat{\rho}$.

Now we return to the situation of a sequence of compact groups G_j converging in our previous sense to a compact group G_0. As in the general setting above, we choose a C^∞ exhaustion function ρ_0 and average it over G_0 to get a G_0-invariant, C^∞exhaustion function $\hat{\rho}_0$.

Because G_j is defined on Ω_j while $\hat{\rho}_0$ is defined on Ω_0, we cannot average $\hat{\rho}_0$ to make it G_j-invariant. We can, however, perform the averaging on arbitrary compact subsets.

Specifically, choose α as above, so that $\hat{\rho}_0^{-1}(-\infty, \alpha]$ is nonempty and of course is a compact subset of Ω_0. Let L be a compact subset of Ω_0 which contains $\hat{\rho}_0^{-1}(-\infty, \alpha]$ in its interior and let L_1 be a compact subset of Ω_0 that contains L in its interior.

Because the sequence G_j converges to G_0, it follows easily that, for j sufficiently large, the images under G_j of points of L lie in L_1. It then follows in addition that one can average the function ρ_0 over the action of G_j, as in the process of averaging to construct $\hat{\rho}$. Denote this new function on L by $\hat{\rho}_j$. Note that, because the elements of G_j are, for j large, close to those of G_0, the function $\hat{\rho}_j$ is C^∞-close (i.e., γ_L-close) to $\hat{\rho}_0$ on L. In particular, the sublevel set $L_1 \cap \hat{\rho}_j^{-1}(-\infty, \alpha]$ will be, for j sufficiently large, a smooth manifold-with-boundary which is C^∞ close to $\hat{\rho}_0^{-1}(-\infty, \alpha]$.

In particular, if we choose a regular value α for $\hat{\rho}_0$ with the sublevel set $M_0 := \hat{\rho}_0^{-1}(-\infty, \alpha]$ nonempty then, for all j sufficiently large, the sublevel set $M_j := \hat{\rho}_j^{-1}(-\infty, \alpha]$ will be a nonempty C^∞ manifold-with-boundary. Moreover it will be close to $\hat{\rho}_0^{-1}(-\infty, \alpha]$ in the C^∞ sense. Namely, there will be a sequence of diffeomorphisms $\phi_j : M_0 \to M_j$ which converges in the C^∞ sense to the identity on M_0.

More precisely, these diffeomorphisms can be obtained as follows: for j large, $\hat{\rho}_j$ has derivative bounded away from 0 along integral curves of the gradient of $\hat{\rho}$ (gradient relative to an arbitrary Riemannian metric, indeed) near $\hat{\rho}^{-1}(\{\alpha\})$. Motion along the integral curves gives a diffeomorphism of the α-level of $\hat{\rho}$ onto the α-level of $\hat{\rho}_j$. Standard Morse theory then establishes a diffeomorphism of $\hat{\rho}^{-1}([\beta, \alpha])$ onto $\hat{\rho}_j^{-1}([\beta, \alpha])$ for some $\beta < \alpha$ but with β close to α. This diffeomorphism is C^∞ close to the identity and can hence be patched via a partition of unity to the identity diffeomorphism on $\tilde{\rho}^{-1}([\frac{1}{2}(\alpha + \beta), \alpha])$ to give the desired diffeomorphism of $\tilde{\rho}^{-1}((-\infty, \alpha])$ to $\tilde{\rho}_j^{-1}((-\infty, \alpha])$, C^∞ close to the identity.

The next step of the proof is to form the doubles of the invariant subdomains with smooth boundary and extend the compact group actions to them. This will make it possible to apply the lemma above to the present situation.

For this, suppose that Ω is a domain, M a compact subset that is a (nonempty) smooth manifold with boundary and H a compact group of diffeomorphisms of Ω that map M to itself. By the usual averaging process, similar to the construction of the invariant exhaustion functions as already discussed, there is a Riemannian metric

g on Ω for which the elements of H act as isometries; i.e., H is contained in $\mathrm{Isom}(g)$. Now the metric g restricted to M can be modified so as to remain invariant under H while being a product metric at and near the boundary of M (see [Greene and Krantz 1982a] for an early instance of this construction). This modification is obtained by first noting that, if N is the inward unit normal (relative to g) along the boundary ∂M, then there is an $\epsilon > 0$ such that the g-exponential map $E : \partial M \times [0, \epsilon) \to M$ defined by $E(p, s) = \exp_p(sN(p))$ is a diffeomorphism for $|s| < \epsilon$ and moreover $E(p, s)$, $p \in \partial M$, $0 \le s < \epsilon$, is a diffeomorphism of manifolds with boundary onto a neighborhood V of ∂M in M. This is the usual tubular neighborhood construction.

Then one obtains a product metric h on the neighborhood of the boundary as

$$h = ds^2 + dp^2,$$

where dp^2 is the metric on ∂M and we push this metric over via E to the neighborhood V of ∂M in M. This is clearly invariant under H. Then one can extend this metric to all of M in an H-invariant way, by taking a function ϕ on V that depends on s alone and hence is invariant under the H-action. This function is to be 1 in a neighborhood of $s = 0$, and hence as a function on M, is equal to 1 in a neighborhood of ∂M. It is to be equal to 0 when $s > \epsilon/2$. Then $\phi h + (1 - \phi)g$ will be a metric on M as desired: it is smooth on all of M, is invariant under H, and is a product metric near ∂M.

This metric now extends smoothly to be a metric $\widehat{h}$ on the double $\widehat{M}$ of M in an obvious way. The group H acts on $\widehat{M}$ as a subgroup of the isometry group of $\widehat{h}$. This subgroup of the isometry group of $\widehat{h}$ will be denoted by $\widehat{H}$.

Our construction can clearly be taken to be stable with respect to the original H-invariant metric g on M in the sense that, if g_1 is another H-invariant metric on M which is C^∞ close to g, then the corresponding metric $\widehat{h}_1$ on the double $\widehat{M}$ of M will be C^∞ close to $\widehat{h}$.

With these ideas in mind, we return to the convergence situation as before. Namely, we continue to denote by $\widehat{M}_j$ the doubles of the G_j-invariant sublevel sets, and let $\widehat{G}_j$ denote the extension of the G_j. Now, when j is large, there are diffeomorphisms $\beta_j : \widehat{M}_0 \to \widehat{M}_j$ which have the property that the pullback to $\widehat{M}_0$ of the G_j-action on M_j via β_j converges in the sense of Lemma 2.4 above.

In particular, G_j is then isomorphic to a subgroup of G_0, for all sufficiently large j. Note that, as such, these isomorphisms apply not to G_j itself but to the restriction of G_j to M_j. But, since M_j has nonempty interior, the restriction of G_j to be an action on the (G_j-invariant) set M_j is injective: two isometries of a connected manifold which are equal on a nonempty open set are equal. (This follows easily by a standard continuation argument.) Hence the original G_j are indeed isomorphic to a subgroup of G_0 when j is sufficiently large. Thus the proposition is established. $\square$

3. Bergman metric and curvature with C^2 stability near the strongly pseudoconvex boundary

Let $n > 1$ throughout this section. Denote by $\mathcal{D}_n$ the collection of bounded domains in $\mathbb{C}^n$ with C^2 smooth, strongly pseudoconvex boundary, equipped with the C^2 topology via the C^2 topology on defining functions. The goal of this section is to establish the following result, which is Klembeck's theorem [1978] for domains in $\mathcal{D}_n$, with C^2 stability. In the statement below the notation $S_\Omega(p;\xi)$ denotes the holomorphic sectional curvature of the Bergman metric of the domain Ω at p along the holomorphic section generated by the tangent vector ξ.

Theorem 3.1. *Let $\widehat{\Omega} \in \mathcal{D}_n$. Then, for every $\epsilon > 0$, there exist $\delta > 0$ and an open neighborhood $\mathcal{U}$ of $\widehat{\Omega}$ in $\mathcal{D}_n$ such that, whenever $\Omega \in \mathcal{U}$,*

$$\sup\left\{\left|S_\Omega(p;\xi) - \left(-\frac{4}{n+1}\right)\right| : \Omega \in \mathcal{U}, \xi \in \mathbb{C}^n \setminus \{0\}\right\} < \epsilon$$

for any $p \in \Omega$ satisfying $\mathrm{dis}(p, \mathbb{C}^n \setminus \Omega) < \delta$.

We remark, before giving the proof, that this result is crucial in establishing the semicontinuity theorem (Theorem 5.2): if $\widehat{\Omega}$ is not biholomorphic to the unit open ball, there exists $(\hat{p}, \hat{\xi}) \in T\Omega_0 = \Omega_0 \times \mathbb{C}^n$ such that $S_{\widehat{\Omega}}(\hat{p}, \hat{\xi}) \neq -4/(n+1)$ due to Lu Qi-Keng's theorem [Lu 1966; Greene et al. 2011, Theorem 4.2.2]. Now Theorem 3.1 implies that, choosing $\mathcal{U}$ smaller if necessary, this curvature difference continues to hold for every domain $\Omega \in \mathcal{U}$. Consequently, one sees that there exist a constant $\delta > 0$ depending only on $(\hat{p}, \hat{\xi})$ and a neighborhood $\mathcal{U}$ of $\widehat{\Omega}$ in the space of domains such that

$$\mathrm{dis}(\phi(\hat{p}), \mathbb{C}^n \setminus \Omega) > \delta \quad \text{for all } \phi \in \mathrm{Aut}(\Omega)$$

for every $\Omega \in \mathcal{U}$, a crucial point in the proof of Theorem 5.2.

Proof. It suffices to show that the following *cannot* hold:

(†) *there exist $\epsilon_0 > 0$ and $\{\Omega_\nu\} \subset \mathcal{D}_n$ such that $\Omega_\nu \to \widehat{\Omega}$ in the C^2 topology as $\nu \to \infty$ and there exists a sequence $\{p_\nu \in \Omega_\nu\}$ with* $\lim_{\nu\to\infty} \mathrm{dis}(p_\nu, \partial\Omega_\nu) = 0$ *such that*

$$\left|S_{\Omega_\nu}(p_\nu, \xi_\nu) + \frac{4}{n+1}\right| \geq \epsilon_0$$

for every ν.

Since the goal is to show that

$$\lim_{\nu\to\infty}\left|S_{\Omega_\nu}(p_\nu, \xi_\nu) + \frac{4}{n+1}\right| = 0,$$

we may assume without loss of generality that $\lim_{\nu\to\infty} p_\nu$ exists. Denote this limit by $\hat{p}$. Notice that $\hat{p} \in \partial\widehat{\Omega}$.

Let $q_\nu \in \partial\Omega_\nu$ be the closest boundary point of Ω_ν to p_ν for every $\nu = 1, 2, \ldots$. Then consider a sequence $R_\nu : \mathbb{C}^n \to \mathbb{C}^n$ of complex rigid motions (i.e., unitary maps followed by translations) in $\mathbb{C}^n$ and another rigid motion $\widehat{R}$ satisfying

(1) $\widehat{R}(\widehat{p}) = 0$ and $R_\nu(q_\nu) = 0$ for every ν;

(2) $R_\nu(\partial\Omega_\nu)$ for every ν, and $\widehat{R}(\partial\widehat{\Omega})$ are tangent at 0 to the hyperplane defined by $\operatorname{Re} z_1 = 0$;

(3) $\lim_{\nu\to\infty} \|R_\nu - \widehat{R}\|_{C^2} = 0$, where the norm here is the C^2-norm of mappings on an open neighborhood of the closure of $\widehat{\Omega}$ in $\mathbb{C}^n$.

Notice that $R_\nu(\Omega_\nu)$ converges to $\widehat{R}(\widehat{\Omega})$ in the C^2 topology on bounded domains with smooth boundaries. Therefore, without loss of generality, we may also assume the following:

(1′) $0 \in \partial\widehat{\Omega} \cap \left(\bigcap_{\nu=1}^{\infty} \partial\Omega_\nu\right)$;

(2′) $\partial\widehat{\Omega}$ and $\partial\Omega_\nu$ (for every $\nu = 1, 2, \ldots$) share the same outward normal vector $\mathbf{n} = (-1, 0, \ldots, 0)$ at the origin;

(3′) $p_\nu = (r_\nu, 0, \ldots, 0)$ with $r_\nu > 0$ for every ν.

Now we need the following three lemmas for the proof. The first is:

Lemma 3.2 ([Kim and Yu 1996]; cf. [Greene et al. 2011, Chapter 10]). *There exists an open neighborhood U of the origin in $\mathbb{C}^n$ such that*

$$\lim_{\nu\to\infty} \sup_{0\neq\xi\in\mathbb{C}^n} \left| \frac{2 - S_{\Omega_\nu\cap U}(p_\nu;\xi)}{2 - S_{\Omega_\nu}(p_\nu;\xi)} - 1 \right| = 0.$$

The proof of this lemma is a normal families argument.

Notice that this lemma implies: *if* $\lim_{\nu\to\infty} S_{\Omega_\nu\cap U}(p_\nu;\xi)$ *exists, it will coincide with* $\lim_{\nu\to\infty} S_{\Omega_\nu}(p_\nu;\xi)$.

The next two lemmas convert the problem of understanding the boundary asymptotic behavior of the Bergman curvature to that of the stability of the Bergman kernel function in the interior under perturbation of the boundary:

Lemma 3.3 ([Kim and Yu 1996]; cf. [Greene et al. 2011, Chapter 10]). *Let the sequence $\{(p_\nu;\xi_\nu) \in \Omega_\nu \times (\mathbb{C}^n \setminus \{0\})\}$ be chosen as above. Let B^n denote the open unit ball in $\mathbb{C}^n$. Then there exists a sequence of injective holomorphic mappings $\sigma_\nu : \Omega_\nu \cap U \to \mathbb{C}^n$ with the following properties*:

(i) $\sigma_\nu(p_\nu) = 0$ (*the origin of* $\mathbb{C}^n$);

(ii) *for every r with $0 < r < 1$, there exists $N > 0$ such that, for every $\nu > N$,*

$$(1-r)B^n \subset \sigma_\nu(\Omega_\nu \cap U) \subset (1+r)B^n.$$

The third and last lemma toward the proof of Theorem 3.1 is as follows:

Lemma 3.4 ([Ramadanov 1967; Kim and Yu 1996]; cf. [Greene et al. 2011, Chapter 10]). *Let D be a bounded domain in $\mathbb{C}^n$ containing the origin* 0. *Let $\{D_\nu\}$ denote a sequence of bounded domains in $\mathbb{C}^n$ that satisfies the following convergence condition*:

> *given* $\epsilon > 0$, *there exists* $N > 0$ *such that* $(1-\epsilon)D \subset D_\nu \subset (1+\epsilon)D$ *for every* $\nu > N$.

Then, for every compact subset F of D, the sequence of Bergman kernel functions K_{D_ν} of D_ν converges uniformly to the Bergman kernel function K_D of D on $F \times F$.

This is a result of Ramadanov [1967]. Now we return to the proof of Theorem 3.1.

Let q_ν, ξ_ν, $\widehat{\Omega}$, Ω_ν be as above. Let U be an open neighborhood of the origin as in Lemma 3.2. Taking a subsequence, we may assume that $q_\nu \in \Omega_\nu \cap U$ for every ν. Select σ_ν as in Lemma 3.3.

Apply Lemma 3.4 to our setting, with $D_\nu = \sigma_\nu(\Omega_\nu \cap U)$ and $D = B^n$. The conclusion of Lemma 3.4 states that the sequence $K_{D_\nu}(z, \zeta)$ converges uniformly to $K_D(z, \zeta)$ on $F \times F$. This of course implies that the sequence $K_{D_\nu}(z, \bar{\zeta})$ converges to $K_D(z, \bar{\zeta})$. Notice that the functions now involved are holomorphic functions in the z and ζ variables together. Therefore Cauchy estimates imply that $K_{D_\nu}(z, \zeta)$ converges uniformly to $K_D(z, \zeta)$ on $F \times F$ in the C^k sense for any positive integer k. Since the holomorphic sectional curvature of the Bergman metric involves derivatives of the Bergman kernel function up to fourth order, we may conclude that $S_{\sigma_\nu(\Omega_\nu \cap U)}(0; \cdot)$ converges uniformly to $S_{B^n}(0; \cdot)$ on $\{\xi \in \mathbb{C}^n : \|\xi\| = 1\}$. Notice that the latter is the constant function with value $-4/(n+1)$.

Combining this result with the localization lemma (Lemma 3.2), the conversion lemma (Lemma 3.3), and the fact that every biholomorphism is an isometry for the Bergman metric, we see that

$$
\begin{aligned}
-\frac{4}{n+1} &= \lim_{\nu\to\infty} S_{\sigma_\nu(\Omega_\nu\cap U)}(0; d\sigma_\nu|_{q_\nu}(\xi_\nu)) = \lim_{\nu\to\infty} S_{\sigma_\nu(\Omega_\nu\cap U)}(\sigma_\nu(q_\nu); d\sigma_\nu|_{q_\nu}(\xi_\nu)) \\
&= \lim_{\nu\to\infty} S_{\Omega_\nu\cap U}(q_\nu; \xi_\nu) = \lim_{\nu\to\infty} S_{\Omega_\nu}(q_\nu; \xi_\nu).
\end{aligned}
$$

This completes the proof of Theorem 3.1. □

Remark 3.5 (completeness of the Bergman metric). The Bergman metric of a bounded strongly pseudoconvex domain is known to be complete ([Diederich 1973]; for the more general case see [Ohsawa 1981]). Since the scaled limit shown in the proof of Lemma 3.3 is the unit ball, a variation of that proof argument also yields the same conclusion as [Diederich 1973] regarding completeness also (see [Greene et al. 2011, Section 10.1.7]).

4. Stable C^k-extension of automorphisms

The purpose of this section is to establish the stability of the extension theorem for the automorphisms of a bounded strongly pseudoconvex domain under C^k perturbation for finite k.

The result and the techniques involved in the proofs are new. More importantly, the contents of this section (especially Theorem 4.3 on page Theorem 4.3) are essential in creating the necessary "metric double" in the proof of Theorem 5.2.

Convergence of Lempert's representative map. Let X, Y be complex Banach spaces. Let $\phi : U \to Y$ be a map from an open subset U of X into Y. The map ϕ is said to be *differentiable* at $x \in X$, if there exists a bounded linear map $D_x\phi : X \to Y$ such that

$$\left\| \phi(x+h) - \phi(x) - (D_x\phi)(h) \right\|_Y = o(\|h\|_X)$$

as $\|h\|_X \to 0$. Let $L(X, Y)$ denote the set of bounded linear maps from X into Y. It is naturally equipped with the operator norm and hence becomes a Banach space. Then ϕ is said to be C^1 on U if $D_x\phi$ exists for all $x \in U$ and

$$D\phi : x \in U \mapsto D_x\phi \in L(X, Y)$$

is continuous.

It is also well established what it means for ϕ to belong to the class C^k; see, [Mujica 1986], for example. To understand this point, consider the space $L(X \times \cdots \times X, Y)$ of bounded k-linear maps with values in Y. For an $S \in L(X \times \cdots \times X, Y)$, define its norm as follows:

$$\|S\|_k = \sup\left\{ \|S(h_1, \ldots, h_k)\|_Y : \|h_1\|_X \le 1, \ldots, \|h_k\|_X \le 1 \right\}.$$

One more piece of notation is necessary: for a k-linear map S, a $(k-1)$-linear map $[S](h)$ is defined by

$$[S](h)(h_1, \ldots, h_{k-1}) := S(h, h_1, \ldots, h_{k-1}).$$

Now the idea of a map belonging to the class C^k can be defined inductively: the map ϕ is said to be C^k at $x \in X$, for $k = 1, 2, \ldots$, if there exits a bounded k-linear map $D_x^k\phi : \underbrace{X \times \cdots \times X}_{k} \to Y$ such that

$$\left\| D_{x+h}^{k-1}\phi - D_x^{k-1}\phi - [D_x^k\phi](h) \right\|_{k-1} = o(\|h\|_X)$$

as $h \to 0$ and

$$D^k\phi : x \in U \mapsto D_x^k\phi \in L(\underbrace{X \times \cdots \times X}_{k}, Y)$$

is continuous. It is also known that such a $D_x^k\phi$ is symmetric k-linear.

Similarly, we may define the concept of Hölder class. For an α with $0<\alpha\le 1$, a map ϕ is said to belong to the class $C^{k,\alpha}$ if ϕ is C^k and

$$\sup_{\substack{x,y\in U\\ x\neq y}} \frac{\|D_x^k\phi - D_y^k\phi\|_k}{\|x-y\|_X^\alpha} < \infty.$$

Throughout this section, we denote by Δ the open unit disc $\{z\in\mathbb{C} : |z|<1\}$. We shall follow the terminology of [Lempert 1986] closely. Let s be such that $0<s<\alpha$ and set

$$X_n = \{f : \partial\Delta\to\mathbb{C}^n \mid f\in C^{0,s}\},$$

$$Y_n = \{f\in X_n : f \text{ admits a holomorphic continuation to } \mathrm{cl}(\Delta)\},$$

$$Y_n^\perp = \{f\in X_n : f \text{ admits an antiholomorphic continuation to } \mathrm{cl}(\Delta) \text{ with } f(0)=0\}.$$

Notice that $X_n = Y_n\oplus Y_n^\perp$.

Let $\Omega=\Omega_\rho$ be a bounded strictly convex domain defined by the $C^{k+1,\alpha}$ defining function ρ. Then there exists a convex open neighborhood V of $\mathrm{cl}(\Omega)$ such that $\Omega=\Omega_\rho=\{z\in V : \rho(z)<0\}$, where the defining function $\rho : U\to\mathbb{R}$, defined on a convex open set U with $\mathrm{cl}(V)\subset U$, is of class $C^{k+1,\alpha}$ ($k\ge 1$, $0<\alpha<1$) with $d\rho\neq 0$ at any point of $\partial\Omega$. We may further assume without loss of generality that

(1) $\rho : U\to\mathbb{R}$ is compactly supported, and

(2) the real Hessian of ρ is strictly positive at every point of $\partial\Omega$.

Let $\mathcal{N}$ be a $C^{k+1,\alpha}$ neighborhood of ρ chosen so small that every element of $\mathcal{N}$ has its real Hessian strictly positive at every point of V. We may require further that there exists a constant $R'>0$ such that, if η, $\tau\in\mathcal{N}$, then $\|\eta-\tau\|_{C^{k+1,\alpha}(U)}<1$ and $\|\eta\|_{C^{k+1,\alpha}(U)}<R'$.

Let p be a point in Ω and let W a neighborhood of p in Ω such that $W\subset\Omega_\eta$ for all $\eta\in\mathcal{N}$. Define $\Theta : \mathcal{N}\oplus(\mathbb{C}^n\setminus\{0\})\oplus W\to Y_n$ by $\Theta(\eta,\zeta,q)=e_{\eta,\zeta,q}$, where $e_{\eta,\zeta,q}$ is the stationary map (i.e., extremal map) from $\mathrm{cl}(\Delta)$ to $\mathrm{cl}(\Omega_\eta)$ satisfying $e_{\eta,\zeta,q}(0)=q$ and ${e_{\eta,\zeta,q}}'(0)=\mu\zeta$ for some $\mu>0$.

Proposition 4.1. *The map Θ is locally $C^{k,\alpha-s}$ for any $0<s<\alpha$.*

Proof. Let $(\eta,v,q)\in\mathcal{N}\oplus\mathbb{C}^n\setminus\{0\}\oplus\mathcal{W}$. We shall prove that Θ is $C^{k,\alpha-s}$ near (η,v,q). Let $e=e_{\eta,v,q}=(e_1,\dots,e_n) : \mathrm{cl}(\Delta)\to\mathrm{cl}(\Omega_\eta)$ and $\tilde e=(\tilde e_1,\dots,\tilde e_n)$ be the *dual map* of e. (See [Lempert 1981] for the definition of the dual map and its basic properties.) Since $\tilde e$ has no zeros, there exist two components which do not vanish simultaneously by a generic linear change of coordinates. Hence we may assume without loss of generality that $\tilde e_1$ and $\tilde e_2$ do not vanish simultaneously on $\mathrm{cl}(\Delta)$. It is also shown in [Lempert 1981] that $\tilde e$ extends to a $C^{k,\alpha}$ map up to the boundary, and that there exist functions $G_1, G_2 \in C^{k,\alpha}(\mathrm{cl}(\Delta))$ that are holomorphic in Δ and satisfy $\tilde{e}_1 G_1 + \tilde{e}_2 G_2 \equiv 1$. Define the holomorphic matrix H on Δ by

$$H = \begin{pmatrix} e_1' & -\tilde{e}_2 & -G_1\tilde{e}_3 & \cdots & -G_1\tilde{e}_n \\ e_2' & \tilde{e}_2 & -G_2\tilde{e}_3 & \cdots & -G_2\tilde{e}_n \\ e_3' & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ e_n' & 0 & 0 & \cdots & 1 \end{pmatrix}.$$

Notice that $H \in C^{0,s}(\mathrm{cl}(\Delta))$ and $\det(H) \neq 0$ on $\mathrm{cl}(\Delta)$. Set

$$Y_n^{R,U} = \{ f \in Y_n : \|f\|_{C^1(\mathrm{cl}(\Delta))} < R, f(\partial\Delta) \subset U \}$$

and define the map

$$\Phi : \mathcal{N} \oplus \mathbb{C}^n \setminus \{0\} \oplus \mathcal{W} \oplus Y_n^{R,U} \oplus \mathbb{R} \to T \oplus Y_{n-1}^{\perp} \oplus \mathbb{C}^n \oplus \mathbb{C}^n$$

by

$$\Phi(r, v, q, f, \lambda) = \left(r \circ f, \pi\left(\frac{\langle H^t r_z \circ f \rangle}{(H^t r_z \circ f)_1} \right), f(0) - q, f'(0) - \lambda v \right),$$

where

(i) $T = \{ g : \partial\Delta \to \mathbb{R} : g \in C^{0,s} \}$,

(ii) $\pi : Y_{n-1} \to Y_{n-1}^{\perp}$ is defined by $\pi\left(\sum_{-\infty}^{\infty} a_k z^k\right) = \sum_{-\infty}^{-1} a_k z^k$, and

(iii) $(H^t r_z \circ f)_j$ denotes the j-th component of $H^t r_z \circ f$ and $\langle H^t r_z \circ f \rangle = ((H^t r_z \circ f)_2, \ldots, (H^t r_z \circ f)_n)$.

Then $f : \mathrm{cl}(\Delta) \to \mathrm{cl}(\Omega_r)$ is an extremal map satisfying $f(0) = q$, $f'(0) = \lambda v$ if and only if $\Phi(r, v, q, f, \lambda) = 0$. So, according to [Lempert 1986], we only need to prove that Φ is $C^{k,\alpha-s}$. For this purpose define the map $\Psi : \mathcal{N} \oplus Y_n^{R,U} \to T$ by $\Psi(r, f) = r \circ f$. Then we pose the following:

Claim. *Ψ is $C^{k,\alpha-s}$.*

We shall prove this claim by induction on k. We need some notation. For a domain Ω, $k \in \mathbb{Z}^+$, and $0 < \alpha \leq 1$, define

$$\|g\|_{C^{k,\alpha}(\mathrm{cl}(\Omega))} = \sup_{\substack{x \in \mathrm{cl}(\Omega) \\ |\gamma| = 0,1,\ldots,k}} |D^\gamma g(x)| + \sup_{\substack{x, y \in \mathrm{cl}(\Omega) \\ x \neq y, |\gamma| = k}} \frac{|D^\gamma g(x) - D^\gamma g(y)|}{|x - y|^\alpha}.$$

Moreover, $A \lesssim B$ will mean that $A \leq CB$ for some constant C. In turn, $A \lessapprox B$ will mean that $A \to 0$ whenever $B \to 0$.

Let $j \in \{0, \ldots, k\}$. Let $\mathcal{N}_j = \{ r \in C^{j+1,\alpha}(U) : \|r\|_{C^{j+1,\alpha}(U)} < R' \}$. Define $\Psi_j : \mathcal{N}_j \oplus Y_n^{R,U} \to T$ by $\Psi_j(r, f) = r \circ f$. Suppose that, for all $r, \tau \in \mathcal{N}_j$, we have $\|r - \tau\|_{C^{j,\alpha}(U)} < 1$.

In case $j = 0$, it suffices to show that

$$\|\Psi_0(r, f) - \Psi_0(\tau, g)\|_{C^{0,s}(\partial\Delta)} \lesssim \big(\|r-\tau\|_{C^{0,\alpha}(U)} + \|f-g\|_{C^{0,s}(\partial\Delta)}\big)^{\alpha-s}.$$

For $x \in \partial\Delta$,

$$\begin{aligned} |r\circ f(x) - \tau\circ g(x)| &\le |r\circ f(x) - r\circ g(x)| + |r\circ g(x) - \tau\circ g(x)| \\ &\lesssim |f(x)-g(x)|^{\alpha-s} + |(r-\tau)\circ g(x)| \\ &\lesssim \big(\|f-g\|_{C^{0,s}(\partial\Delta)} + \|r-\tau\|_{C^{0,\alpha}(U)}\big)^{\alpha-s}. \end{aligned}$$

For $x, y \in \partial\Delta$, let $\delta(x, y) = r\circ f(x) - \tau\circ g(x) - r\circ f(y) + \tau\circ g(y)$. Then

$$\begin{aligned} |\delta(x, y)| &\le |r\circ f(x) - r\circ g(x)| + |r\circ g(x) - \tau\circ g(x)| \\ &\qquad + |r\circ f(y) - r\circ g(y)| + |r\circ g(y) - \tau\circ g(y)| \\ &\le 2(R')^\alpha |f(x)-g(x)|^\alpha + 2\|r-\tau\|_{C^{0,\alpha}(U)} \\ &\le 2(RR')^\alpha \|f-g\|^\alpha_{C^{0,s}(\partial\Delta)} + 2\|r-\tau\|_{C^{0,\alpha}(U)} \end{aligned}$$

and

$$\begin{aligned} |\delta(x, y)| &\le |r\circ f(x) - r\circ f(y)| + |\tau\circ g(x) - \tau\circ g(y)| \\ &\le R'|f(x)-f(y)|^\alpha + R'|g(x)-g(y)|^\alpha \le 2RR'|x-y|^\alpha. \end{aligned}$$

This implies that

$$|\delta(x, y)| \lesssim \big(\|f-g\|_{C^{0,s}(\partial\Delta)} + \|r-\tau\|_{C^{0,\alpha}(U)}\big)^{\alpha-s}|x-y|^s,$$

which proves the case $j = 0$.

Let $j > 0$. Suppose that $\Psi_j : \mathcal{N}_j \oplus Y_n^{R,U} \to T$ is of class $C^{j,\alpha-s}(U)$. Then, since

$$D_{(r,f)}\Psi_{j+1}(\tau, g) = (r'\circ f)g + \tau\circ f = \Psi_j(r', f)g + \Psi_j(\tau, f),$$

it follows that Ψ_{j+1} is of $C^{j+1,\alpha-s}(U)$. This proves the claim.

Since π is a bounded linear map, the second component of Φ is also of class $C^{k,\alpha-s}(U)$. The proof of the proposition is now complete. □

Next, for $r \in \mathcal{N}$, $q \in W$, consider *Lempert's representation map* at q for the domain Ω_r. We have $L_{r,q} : \mathrm{cl}(\mathbb{B}^n) \to \mathrm{cl}(\Omega_r)$ defined by $L_{r,q}(\zeta) = \Theta(r, \zeta, q)(|\zeta|) = e_{r,\zeta,q}(|\zeta|)$. The following proposition discusses the convergence of these representation maps.

Proposition 4.2. *Let $\rho_j, \rho \in \mathcal{N}$ and $p_j, p \in W$ be such that $\|\rho_j - \rho\|_{C^{k+1,\alpha}(U)} \to 0$, $|p_j - p| \to 0$ as $j \to \infty$. Set the notation $L_j := L_{\rho_j,p_j}$, $L := L_{\rho,p}$ and $\mathbb{B}^n_\delta := \mathbb{B}^n \setminus \{z \in \mathbb{C}^n : |z| < \delta\}$. Then, for $0 < \beta < \alpha$ and $0 < \delta < 1$, Lempert's representation* *maps L_j for Ω_{ρ_j} converge to Lempert's representation map L for Ω_ρ on $\mathbb{B}^n_\delta$ in the $C^{k,\beta}$ norm, as $j \to \infty$.*

Proof. Let $\mathrm{ev}: Y_n \to \mathbb{C}^n$ be defined by $\mathrm{ev}(g) = g(1)$ (here "ev" stands for "evaluation" map). Since $L(\zeta) = \Theta(\rho, \zeta, p)(1) = \mathrm{ev} \circ \Theta(\rho, \zeta, p)$ for $\zeta \in \partial\mathbb{B}^n$, ev is bounded linear. Write $D^\ell = \partial^{m_1+\cdots+m_n}/\partial x_1^{m_1} \cdots \partial x_n^{m_n}$, where $|\ell| = m_1 + \cdots + m_n$. Then

$$D^\ell L(\zeta) = \big(D^{|\ell|}_{(\rho,\zeta,p)}\Theta\big)\big(\underbrace{\vec{x}_1, \ldots, \vec{x}_1}_{m_1}; \ldots; \underbrace{\vec{x}_n, \ldots, \vec{x}_n}_{m_n}\big)(1).$$

So $\|L_j - L\|_{C^{k,\beta}(\partial\mathbb{B}^n)} \to 0$ as $j \to \infty$.

Given $v \in \mathbb{C}^n$, $|v| = 1$, $\xi \in \Delta$, denote by e the extremal map satisfying $e(0) = p$, $e'(0) = \mu v$ for some $\mu > 0$. Then $L(\xi v) = e(\xi|v|) = e(\xi)$. This implies that $L(\xi v)$ is holomorphic with respect to ξ. Now the Poisson integral formula for Δ yields the desired conclusion. □

A simultaneous extension theorem for automorphisms. The next goal is to establish the following theorem, which treats the $C^{k,\beta}$ convergence of sequences of automorphisms. This result is new, and the proof technique is new. It has independent interest.

Theorem 4.3 (uniform extension). *Let Ω_j, Ω be bounded, strongly pseudoconvex domains in $\mathbb{C}^n$ with $C^{k+1,\alpha}$ ($k \in \mathbb{Z}$, $k \geq 2$, $0 < \alpha \leq 1$) boundaries such that Ω_j converges to Ω as $j \to \infty$ in the $C^{k+1,\alpha}$ topology, and with Ω not biholomorphic to the ball. Let a sequence $\{f_j \in \mathrm{Aut}(\Omega_j) : j = 1, 2, \ldots\}$ be given. Then, for any β with $0 < \beta < \alpha$, the sequence f_j (every one of which extends to a $C^{k,\beta}$ diffeomorphism of the closure* $\mathrm{cl}(\Omega_j)$ *by the "sharp extension theorem" of* [Lempert 1986]) *admits a subsequence Ω_{j_ℓ} and $f_{j_\ell} \in \mathrm{Aut}(\Omega_{f_\ell})$ that converges to the $C^{k,\beta}$-diffeomorphism, the extension of $f \in \mathrm{Aut}(\Omega)$, in the $C^{k,\beta}$ topology.*

This indeed is a normal family theorem together with Hölder convergence up to the boundary. Of course precise definitions and terminology are in order, which will be presented here as the exposition progresses.

Definition 4.4. Let Ω_j and Ω be bounded strongly pseudoconvex domains in $\mathbb{C}^n$ with $C^{k,\alpha}$ ($k \in \mathbb{Z}$, $k \geq 2$, $0 < \alpha \leq 1$) boundaries. As $j \to \infty$, the sequence of domains Ω_j is said to *converge to Ω in the $C^{k,\alpha}$ topology*, if there exist an open neighborhood U of $\mathrm{cl}(\Omega)$, $C^{k,\alpha}$ diffeomorphisms $F_j : U \to U$, and a positive integer N such that

- $\mathrm{cl}(\Omega) \Subset U$;
- $\mathrm{cl}(\Omega_j) \Subset U$ for all $j > N$;
- each F_j maps $\mathrm{cl}(\Omega)$ onto $\mathrm{cl}(\Omega_j)$ as a $C^{k,\alpha}$ diffeomorphism; for every $j > N$;
- $\|F_j - \mathrm{id}\|_{C^{k,\alpha}(U)} \to 0$ and $\|F_j^{-1} - \mathrm{id}\|_{C^{k,\alpha}(U)} \to 0$, as $j \to \infty$.

In a similar manner, we say that the sequence of maps $f_j \in C^{k,\alpha}(\Omega_j, \mathbb{C}^m)$ *converges to* $f \in C^{k,\alpha}(\Omega, \mathbb{C}^m)$ *in the* $C^{k,\alpha}$ *sense*, if

$$\lim_{j\to\infty} \|f_j \circ F_j - f\|_{C^{k,\alpha}(\Omega)} = 0.$$

We now present several technical lemmas.

Lemma 4.5. *Let* Ω_j *be a domain in* $\mathbb{R}^{n_j}$ *for each* $j = 1, 2, 3$. *If*

(i) $g, h : \Omega_1 \to \Omega_2$ *are* $C^{k',\alpha'}$ *maps that are injective*,

(ii) $f : \Omega_2 \to \Omega_3$ *is a* $C^{k'',\alpha''}$ *map*, *and*

(iii) (k, α) *is the pair of the positive integer* k *and the real number* α *satisfying* $k + \alpha = \min\{k' + \alpha', k'' + \alpha''\}$ *and* $0 < \alpha \leq 1$,

then

(1) $f \circ g \in C^{k,\alpha}(\Omega_1, \Omega_3)$ *and*

(2) $\|f \circ g - f \circ h\|_{C^{k,\beta}(\Omega_1)} \lessapprox \|g - h\|_{C^{k,\alpha}(\Omega_1)}$ *for any* β *with* $0 < \beta < \alpha$.

Proof. We present the verification of (1) only, as our arguments are mostly straightforward computations and the proof of (2) is similar. The chain rule implies that

$$D^\ell(f\circ g)(x) = \sum (D^m f)(g(x))(D^{m_1} g(x))^{m'_1}(D^{m_2} g(x))^{m'_2} \cdots (D^{m_n} g(x))^{m'_n},$$

where ℓ and m are multiindices and m_j nonnegative integers satisfying $|m| \leq |\ell|$ and $\sum m'_j \leq |\ell|$. (We use the usual multiindex notation here; we omit detailed expressions as they are standard.) Note that

$$\|f\circ g\|_{C^{k,\alpha}} = \sup_{\substack{x\in\Omega_1 \\ 0\leq|\gamma|\leq k}} |D^\gamma(f\circ g)(x)| + \sup_{\substack{x,y\in\Omega_1 \\ x\neq y,\, |\gamma|=k}} \frac{|D^\gamma(f\circ g)(x) - D^\gamma(f\circ g)(y)|}{|x-y|^\alpha}.$$

First, one sees immediately that

$$\sup_{\substack{x\in\Omega_1 \\ |\gamma|=0,1,\ldots,k}} |D^\gamma(f\circ g)(x)| \lesssim \|f\|_{C^{k,\alpha}(\Omega_2)} \sum \|g\|^{m'_1+\cdots+m'_n}_{C^{k,\alpha}(\Omega_1)} < \infty.$$

On the other hand,

$$\begin{aligned}
&|D^\gamma(f\circ g)(x) - D^\gamma(f\circ g)(y)| \\
&\quad = \Big|\sum \{D^m f(g(x)) \cdot (D^{m_1} g(x))^{m'_1} \cdot \cdots \cdot (D^{m_n} g(x))^{m'_n} \\
&\qquad\qquad - D^m f(g(y)) \cdot (D^{m_1} g(y))^{m'_1} \cdot \cdots \cdot (D^{m_n} g(y))^{m'_n}\}\Big|
\end{aligned}$$

$$\begin{aligned}
&\le \sum \Big\{ \big| \big(D^m f(g(x)) - D^m f(g(y))\big) \cdot (D^{m_1} g(x))^{m_1'} \cdot \dots \cdot (D^{m_n} g(x))^{m_n'} \big| \\
&\qquad + \big| \big(D^m f(g(y))\big) \cdot \big((D^{m_1} g(x))^{m_1'} - D^{m_1} g(y))^{m_1'}\big) \\
&\qquad\qquad\qquad\qquad\qquad\qquad \cdot (D^{m_2} g(x))^{m_2'} \cdot \dots \cdot (D^{m_n} g(x))^{m_n'} \big| \\
&\qquad + \cdots \\
&\qquad + \big| \big(D^m f(g(y))\big) \cdot \big(D^{m_1} g(y))^{m_1'}\big) \cdot \dots \cdot \big((D^{m_n} g(x))^{m_n'} - (D^{m_1} g(y))^{m_1'}\big) \big| \Big\} \\
&\lesssim \|f\|_{C^{k,\alpha}(\Omega_2)} (1 + \|g\|^{\alpha}_{C^0(\Omega_1)}) P(\|g\|_{C^{k,\alpha}(\Omega_1)}) |x-y|^{\alpha},
\end{aligned}$$

where P is an appropriate polynomial with $P(0, \dots, 0) = 0$. Hence (1) follows. We omit the proof of (2). □

Lemma 4.6. *Let $k \ge 1$. Assume that Ω_1, Ω_2 are bounded domains in $\mathbb{R}^n$ admitting $C^{k,\alpha}$ diffeomorphisms $f_j, f : \mathrm{cl}(\Omega_1) \to \mathrm{cl}(\Omega_2)$ satisfying $\|f_j - f\|_{C^{k,\alpha}(\mathrm{cl}(\Omega_1))} \to 0$ as $j \to \infty$. If $\lim_{j\to\infty} \sup_{x \in \mathrm{cl}(\Omega_2)} |f_j^{-1}(x) - f^{-1}(x)| = 0$, then*

$$\lim_{j\to\infty} \|f_j^{-1} - f^{-1}\|_{C^{k,\beta}(\mathrm{cl}(\Omega_2))} = 0$$

for any $0 < \beta < \alpha$.

Proof. The inverse function theorem implies that $df_j^{-1}|_{f_j(y)} = (df_j|_y)^{-1}$ and $df^{-1}|_{f(y)} = (df|_y)^{-1}$. Since $\mathrm{cl}(\Omega_1)$ and $\mathrm{cl}(\Omega_2)$ are compact, there exist a constant $C > 0$ and a positive integer N such that $|\det(df|_y)| > C$ and $|\det(df_j|_y)| > C$ for any point $y \in \Omega_1$ and any integer $j > N$. Lemma 4.5 and its proof argument now yield the desired conclusion. □

Lemma 4.7. *Let k be an integer with $k \ge 2$ and α a real number satisfying $0 < \alpha \le 1$. If Ω is a bounded, strongly pseudoconvex domain in $\mathbb{C}^n$, not biholomorphic to the unit open ball, with $C^{k+1,\alpha}$ boundary then, for any β with $0 < \beta < \alpha$, there exist an open neighborhood $\mathcal{U}$ of Ω and a constant C such that $\|f\|_{C^{k,\beta}(\mathrm{cl}(\Omega'))} < C$ for any $\Omega' \in \mathcal{U}$ and any $f \in \mathrm{Aut}(\Omega')$.*

Proof. Assume the contrary. Then there exists a sequence of strongly pseudoconvex domains Ω_j with $C^{k+1,\alpha}$ boundary converging to Ω in the $C^{k+1,\alpha}$ topology and a sequence $f_j \in \mathrm{Aut}(\Omega_j)$ such that

$$\lim_{j\to\infty} \|f_j\|_{C^{k,\beta}(\mathrm{cl}(\Omega_j))} = \infty.$$

Then either

(1) there exists a sequence $\{x_j \in \Omega_j : j = 1, 2, \dots\}$ such that $|D^\gamma f_j(x_j)| \to \infty$ as $j \to \infty$ for some multiindex γ satisfying $0 \le |\gamma| \le k$; or

(2) there exist $x_j, y_j \in \Omega_j$ such that $\big|D^\gamma f_j(x_j) - D^\gamma f_j(y_j)\big| / |x_j - y_j|^\beta$ goes to infinity with j for some multiindex γ with $|\gamma| = k$.

Suppose that (1) holds. Then, since the sequence f_j converges to f in the $C^\infty(K)$ topology on every compact subset K of Ω, it must be the case that $\lim_{j\to\infty} x_j = p \in \partial\Omega$ (taking a subsequence if necessary).

We shall arrive at the desired contradiction to (1) by means of the following three steps:

Step 1. *Adjustments.* Let F_j denote the same diffeomorphism of $\mathrm{cl}(\Omega)$ onto $\mathrm{cl}(\Omega_j)$ as in Definition 4.4. Set $F_j(p) = p_j$, $f_j(p_j) = q_j$, $f(p) = q$. Take the invertible affine $\mathbb{C}$-linear transformations $T, T_j, t, t_j : \mathbb{C}^n \to \mathbb{C}^n$ such that

- $T_j(p_j) = T(p) = t_j(q_j) = t(q) = (0, \ldots, 0)$;
- the outward normal vectors to the boundaries of $T_j(\Omega_j)$, $T(\Omega)$, $t_j(\Omega_j)$ and $t(\Omega)$ at $(0, \ldots, 0)$ are equal to $(1, 0, \ldots, 0)$; and
- $\lim_{j\to\infty} T_j = T$ and $\lim_{j\to\infty} t_j = t$.

Then $T_j(\Omega_j)$ converges to $T(\Omega)$ in the $C^{k+1,\alpha}$ topology, and also $t_j(\Omega_j)$ converges to $t(\Omega)$. Replacing therefore f and f_j, respectively, by $t \circ f \circ T^{-1}$ and $t_j \circ f_j \circ T_j^{-1}$, we may assume that:

- Ω, Ω_j, $\widehat{\Omega}$, $\widehat{\Omega}_j$ are bounded strongly pseudoconvex domains with $C^{k+1,\alpha}$ boundaries such that Ω_j (and $\widehat{\Omega}_j$, respectively) converges to Ω (and to $\widehat{\Omega}$, respectively) in the $C^{k+1,\alpha}$ topology. More precisely, there exist a neighborhood U (and $\widehat{U}$, respectively) of $\mathrm{cl}(\Omega)$ (and of $\mathrm{cl}(\widehat{\Omega})$, respectively) and diffeomorphisms $F_j : \mathrm{cl}(\Omega) \to \mathrm{cl}(\Omega_j)$ and $\widehat{F}_j : \mathrm{cl}(\widehat{\Omega}) \to \mathrm{cl}(\widehat{\Omega}_j)$ such that $F_j(0) = \widehat{F}_j(0) = 0$ and the maps F_j, F_j^{-1}, $\widehat{F}_j$ and $\widehat{F}_j^{-1}$ converge to the identity map in the $C^{k+1,\alpha}$ sense.
- ρ, $\rho_j = \rho \circ F_j^{-1}$, $\widehat{\rho}$, $\widehat{\rho}_j = \widehat{\rho} \circ \widehat{F}_j^{-1}$ are defining functions of Ω, Ω_j, $\widehat{\Omega}$, $\widehat{\Omega}_j$, respectively, such that $\|\rho - \rho_j\|_{C^{k+1,\beta}(U)} \to 0$ and $\|\widehat{\rho} - \widehat{\rho}_j\|_{C^{k+1,\beta}(\widehat{U})} \to 0$ as $j \to \infty$ and
$$
\begin{aligned}
(1, 0, \ldots, 0) &= \left(\frac{\partial\rho}{\partial z_1}(0), \ldots, \frac{\partial\rho}{\partial z_n}(0)\right) = \left(\frac{\partial\rho_j}{\partial z_1}(0), \ldots, \frac{\partial\rho_j}{\partial z_n}(0)\right) \\
&= \left(\frac{\partial\widehat{\rho}}{\partial z_1}(0), \ldots, \frac{\partial\widehat{\rho}}{\partial z_n}(0)\right) = \left(\frac{\partial\widehat{\rho}_j}{\partial z_1}(0), \ldots, \frac{\partial\widehat{\rho}_j}{\partial z_n}(0)\right).
\end{aligned}
$$
- There exist biholomorphisms $f_j : \Omega_j \to \widehat{\Omega}_j$, $f : \Omega \to \widehat{\Omega}$ and a sequence $x_j \in \Omega_j$ converging to $0 \in \partial\Omega$ as $j \to \infty$ such that f_j converges to f uniformly on every compact subset K of Ω while $|D^\ell f_j(x_j)| \to \infty$ as $j \to \infty$ for some multiindex ℓ with $1 \le |\ell| \le k$.

Step 2. *Simultaneous convexification.* This step is directly from [Fornaess 1976]. To the expansion of ρ at 0,

$$\rho(z) = 2\,\mathrm{Re}\, z_1 + \mathrm{Re} \sum \frac{\partial^2 \rho}{\partial z_i z_j}(0) z_i z_j + \frac{1}{2} \sum_{i,j} \frac{\partial^2 \rho}{\partial z_i \bar{z}_j}(0) z_i \bar{z}_j + o(|z|^2),$$

apply the local biholomorphic change $\Upsilon = (w_1, w_2, \ldots, w_n)$ of holomorphic coordinate system at the origin 0 defined by

$$w_i(z) = \begin{cases} 2z_1 + \sum \dfrac{\partial^2 \rho}{\partial z_i z_j}(0) z_i z_j, & i = 1, \\ z_i, & i = 2, \ldots, n. \end{cases}$$

The new defining function (we continue to use ρ, as there is little danger of confusion) takes the form

$$\rho = \mathrm{Re}\, w_1 + \frac{1}{2} \sum_{i,j} \frac{\partial^2 \rho}{\partial w_i \overline{w}_j}(0) w_i \overline{w}_j + \varepsilon(w),$$

where $\varepsilon(w) = o(|w|^2)$. Note that $\Upsilon(\Omega)$ is strictly convex in a small neighborhood of 0. Furthermore, there exists a positive integer N such that $\Upsilon(U' \cap \Omega_j)$ is strictly convex for any $j > N$. Let ρ_j denote $\tilde{\rho}_j \circ \Upsilon$, where $\tilde{\rho}_j$is strictly convex on $V' \cap \Omega_j$ for all $j > N$. Set

$$\tilde{\rho}(z) = \mathrm{Re}\, z_1 + \frac{1}{2} \sum_{i,j} \frac{\partial^2 \rho}{\partial z_i \bar{z}_j}(0) z_i \bar{z}_j + \sigma(z).$$

There exists a positive constant R sufficiently large so that the real Hessian forms of $\tilde{\rho}(z) - |z|^2/(2R) - \mathrm{Re}\, z_1$ and $\tilde{\rho}_j(z) - |z|^2/(2R) - \mathrm{Re}\, z_1$ are positive definite at every $z \in V'$. Choose $h \in C^\infty(\mathbb{R})$ such that

$$\begin{aligned} h(x) &= 0 \quad \text{if} \quad x \geq 1, \\ 0 \leq h(x) &\leq 1 \quad \text{if} \quad 0 \leq x \leq 1, \\ h(x) &= 1 \quad \text{if} \quad x \leq 0. \end{aligned}$$

Taking a larger value for N if necessary, we may have that the real Hessian forms of

$$\mathrm{Re}\, z_1 + \frac{|z|^2}{2R} + \frac{1}{N} h\left(\frac{|z| - \eta}{\eta}\right)\left(\tilde{\rho}(z) - \frac{|z|^2}{2R} - \mathrm{Re}\, z_1\right),$$
$$\mathrm{Re}\, z_1 + \frac{|z|^2}{2R} + \frac{1}{N} h\left(\frac{|z| - \eta}{\eta}\right)\left(\tilde{\rho}_j(z) - \frac{|z|^2}{2R} - \mathrm{Re}\, z_1\right)$$

are both positive definite real Hessian at every point of $V_\delta := \{z \in \mathbb{C}^n : |z| < \delta\} \Subset V'$ whenever η satisfies $0 < \eta < \frac{\delta}{3}$. Take $\eta > 0$ such that $2^{2N+2}\eta < \frac{\delta}{3}$ and set

$$\tau(z) = \operatorname{Re} z_1 + \frac{|z|^2}{2R} + \frac{1}{N}\sum_{m=1}^{N} h\Big(\frac{|z| - 2^{2m}\eta}{2^{2m}\eta}\Big)\Big(\tilde{\rho}(z) - \frac{|z|^2}{2R} - \operatorname{Re} z_1\Big),$$
$$\tau_j(z) = \operatorname{Re} z_1 + \frac{|z|^2}{2R} + \frac{1}{N}\sum_{m=1}^{N} h\Big(\frac{|z| - 2^{2m}\eta}{2^{2m}\eta}\Big)\Big(\tilde{\rho}_j(z) - \frac{|z|^2}{2R} - \operatorname{Re} z_1\Big).$$

We further let $C = \{z \in \mathbb{C}^n : \tau(z) < 0\}$, $C_j = \{z \in \mathbb{C}^n : \tau_j(z) < 0\}$ and $U'' = W^{-1}(V_{\delta/3})$. Then C, C_j are bounded strictly convex domains such that the restricted mappings

$$\Upsilon|_{U''\cap\Omega} : U'' \cap \Omega \to V_{\delta/3} \cap C \quad \text{and} \quad \Upsilon|_{U''\cap\Omega_j} : U'' \cap \Omega_j \to V_{\delta/3} \cap C_j$$

are biholomorphisms, and τ_j converges to τ in the $C^{k+1,\beta}$ norm, for every β, $0 < \beta < \alpha$.

Apply the same process to $\widehat{\Omega}$ and to $\widehat{\Omega}_j$ at 0. Denote by $\widehat{C}, \widehat{C}_j$ the respective strictly convex domains with defining functions $\hat{\tau}, \hat{\tau}_j$ and $\widehat{W} : \widehat{U} \to \widehat{V}$ produced by the same procedures.

Step 3. *Estimates.* Let $\omega \in C \cap V' \cap \big(\bigcap_{j=1}^{\infty} C_j\big)$ be a point that admits an extremal map $e : \mathrm{cl}(\Delta) \to \mathrm{cl}(C)$ satisfying

$$e(0) = \omega, \quad e(1) = 0, \quad \text{and} \quad e(\mathrm{cl}(\Delta)) \subset \mathrm{cl}(C) \cap V'.$$

Let $e'(0) = \mu v$ where $|v| = 1$. Let $L : \mathrm{cl}(\mathbb{B}^n) \to \mathrm{cl}(C)$ ($L_j : \mathrm{cl}(\mathbb{B}^n) \to \mathrm{cl}(C_j)$, respectively) be the Lempert representative map of C (C_j, respectively) at ω. By Proposition 4.2, there exists a $\epsilon > 0$ such that $\lim_{j\to\infty} \|L_j - L\|_{C^{k,\beta}(\mathrm{cl}(\mathbb{B}^n_\varepsilon))} = 0$ for any β with $0 < \beta < \alpha$. Let Γ be a closed cone containing v in $\mathrm{cl}(\mathbb{B}^n)$ so that $L(\Gamma) \subset \mathrm{cl}(C) \cap V_{\delta/3}$ and $L_j(\Gamma) \subset \mathrm{cl}(C_j) \cap V_{\delta/3}$ for all $j > N$. Let

$$\Upsilon^{-1}(\omega) = \zeta, \quad f(\zeta) = \hat{\zeta}, \quad f_j(\zeta) = \hat{\zeta}_j, \quad \widehat{\Upsilon}(\hat{\zeta}) = \hat{\omega}, \quad \widehat{\Upsilon}(\hat{\zeta}_j) = \hat{\omega}_j$$

and let $\widehat{L} : \mathrm{cl}(\mathbb{B}^n) \to \mathrm{cl}(\widehat{C})$ and $\widehat{L}_j : \mathrm{cl}(\mathbb{B}^n) \to \mathrm{cl}(\widehat{C}_j)$, respectively, denote the Lempert representative map of $\widehat{C}$ at the point $\hat{\omega}$ and the Lempert representative map of $\widehat{C}_j$ at the point $\hat{\omega}_j$.

Consider now the composite maps $\widehat{L}^{-1} \circ \widehat{\Upsilon} \circ f \circ \Upsilon^{-1} \circ L : \Gamma \to \mathbb{B}^n$ and $\widehat{L}_j^{-1} \circ \widehat{\Upsilon} \circ f_j \circ \Upsilon^{-1} \circ L_j : \Gamma \to \mathbb{B}^n$. Denote by $h : \mathrm{cl}(D) \to \mathrm{cl}(C)$ the extremal map satisfying $h(0) = \omega$, $h'(0) = \lambda\zeta$, for some $\lambda > 0$, and by $\hat{h} = \widehat{\Upsilon} \circ f \circ \Upsilon^{-1} \circ h : \mathrm{cl}(D) \to \mathrm{cl}(\widehat{C})$ the extremal map satisfying

$$\hat{h}(0) = \hat{\omega}, \quad \hat{h}'(0) = \hat{\lambda}|\zeta| \frac{d(\widehat{\Upsilon} \circ f \circ \Upsilon^{-1})|_\omega(\zeta)}{\big|d(\widehat{\Upsilon} \circ f \circ \Upsilon^{-1}|_\omega(\zeta)\big|}$$

for some $\hat{\lambda}$. Since $\widehat{C}$ is strictly convex and f extends to $\mathrm{cl}(\Omega)$ as a $C^{k,\gamma}$ diffeomorphism for all $\gamma < \alpha$, we have

$$\widehat{W}^{-1} \circ \widehat{L}\left(\frac{|\zeta| d(\widehat{W} \circ f \circ W^{-1})|_{\omega}(\zeta)}{\left| d(\widehat{W} \circ f \circ W^{-1}|_{\omega}(\zeta) \right|} \right) = f \circ W^{-1} \circ L(\zeta).$$

By the same reasoning we also have

$$\widehat{W}_j^{-1} \circ \widehat{L}\left(\frac{|\zeta| d(\widehat{W} \circ f_j \circ W^{-1})|_{\omega}(\zeta)}{\left| d(\widehat{W} \circ f_j \circ W^{-1}|_{\omega}(\zeta) \right|} \right) = f_j \circ W^{-1} \circ L_j(\zeta).$$

Considering the left-hand sides of the preceding identities, for any β, $0 < \beta < \alpha$, we obtain

$$\lim_{j \to \infty} \| f \circ W^{-1} \circ L - f_j \circ W^{-1} \circ L_j \|_{C^{k,\beta}(\Gamma_\varepsilon)} = 0,$$

where $\Gamma_\varepsilon = \Gamma \setminus \{z \in \Gamma : |z| < \varepsilon\}$. Therefore

$$\begin{aligned} \lim_{j \to \infty} & \| f \circ \Upsilon^{-1} \circ L - f \circ F_j^{-1} \circ \Upsilon^{-1} \circ L_j \|_{C^{k,\beta}(\Gamma_\varepsilon)} \\ &= \lim_{j \to \infty} \| f \circ F_j^{-1} \circ \Upsilon^{-1} \circ L_j - f_j \circ \Upsilon^{-1} \circ L_j \|_{C^{k,\beta}(\Gamma_\varepsilon)}. \end{aligned}$$

Hence

$$\begin{aligned} \| f \circ \Upsilon^{-1} & \circ L - f \circ F_j^{-1} \circ \Upsilon^{-1} \circ L_j \|_{C^{k,\beta}(\Gamma_\varepsilon)} \\ &\lessapprox \| \Upsilon^{-1} \circ L - F_j^{-1} \circ \Upsilon^{-1} \circ L_j \|_{C^{k,\beta}(\Gamma_\varepsilon)} \\ &\lesssim \| \Upsilon^{-1} \circ L - \Upsilon^{-1} \circ L_j \|_{C^{k,\beta}(\Gamma_\varepsilon)} + \| \Upsilon^{-1} \circ L_j - F_j^{-1} \circ \Upsilon^{-1} \circ L_j \|_{C^{k,\beta}(\Gamma_\varepsilon)} \\ &\lesssim \| L - L_j \|_{C^{k,\beta}(\Gamma_\varepsilon)} + \| (\mathrm{id} - F_j^{-1}) \Upsilon^{-1} \circ L_j \|_{C^{k,\beta}(\Gamma_\varepsilon)} \to 0 \text{ as } j \to \infty. \end{aligned}$$

On the other hand, by the proof argument of Lemma 4.5, we have

$$\begin{aligned} \| f \circ F_j^{-1} & \circ \Upsilon^{-1} \circ L_j - f_j \circ \Upsilon^{-1} \circ L_j \|_{C^{k,\beta}(\Gamma_\varepsilon)} \\ &= \| (f - f_j \circ F_j) \circ F_j^{-1} \circ \Upsilon^{-1} \circ L_j \|_{C^{k,\beta}(\Gamma_\varepsilon)} \gtrapprox \| (f - f_j \circ F_j) \|_{C^{k,\beta}(\sigma)} \end{aligned}$$

on a sufficiently small neighborhood σ of p. This contradicts (1).

To complete the proof let us now suppose that (2) holds. If $|x_j - y_j| > \kappa$ for some positive constant κ, then

$$\frac{|D^\gamma f_j(x_j) - D^\gamma f_j(y_j)|}{|x_j - y_j|^\beta} < \frac{2C}{\kappa^\beta}$$

holds for some constant C. Without loss of generality, we may assume that $x_j \to p \in \partial\Omega$ and $|x_j - y_j| < \kappa$. Suppose that there exist sequences x_j, $y_j \in \Omega_j$ and a positive constant ν such that $x_j \to 0 \in \partial\Omega$ as $j \to \infty$ and $|x_j - y_j| < \nu$ so that

$$\frac{|D^\ell f_j(x_j) - D^\ell f_j(y_j)|}{|x_j - y_j|^\beta} \to \infty$$

as $j \to \infty$ for some multiindex ℓ where $|\ell| = k$. Repeating Steps 1, 2 and 3 above, we again arrive at a contradiction. Hence the proof of Lemma 4.7 is complete. □

Proof of Theorem 4.3. Throughout the proof, we shall take subsequences from the $\{f_j\}$ several times. But we denote them by the same notation f_j, since there is little danger of any confusion.

By Cauchy estimates and the standard normal family theorem, for any compact subset K of Ω we have

$$\lim_{j\to\infty} \|f_j - f\|_{C^{k,\beta}(K)} = 0.$$

Denote by $K_\eta = \{z \in \Omega \mid \operatorname{dist}(\partial\Omega, z) \geq \eta\}$. Then there exist $N > 0$ and $\eta > 0$ such that $F_j(K) \Subset K_\eta \Subset \Omega$ for all $j > N$. So

$$\|f_j \circ F_j - f\|_{C^{k,\beta}(K)} \leq \|f_j \circ F_j - f_j\|_{C^{k,\beta}(K)} + \|f_j - f\|_{C^{k,\beta}(K)} \to 0$$

as $j \to \infty$ for all $\beta < \alpha$ by the proof of Lemma 4.6.

Let $\lambda > 0$. For $x \in \mathrm{cl}(\Omega) - K_\epsilon$, there exists $y \in K_\epsilon$ such that $|x - y| < \epsilon$. By Lemma 4.7, we have

$$\begin{aligned}\left|D^l(f_j\circ F_j)(x) - D^l f(x)\right| &\leq \left|D^l(f_j\circ F_j)(x) - D^l(f_j\circ F_j)(y)\right| \\ &\quad + \left|D^l(f_j\circ F_j)(y) - D^l f(y)\right| + \left|D^l f(y) - D^l f(x)\right| \\ &\lesssim 2|x-y|^\beta + \epsilon \lesssim 2\epsilon^\beta + \epsilon.\end{aligned}$$

Since

$$\begin{aligned}&\sup_{\substack{x\in\mathrm{cl}(\Omega)\\ 0\leq|\ell|\leq k}} |D^\ell(f_j\circ F_j)(x) - D^\ell f(x)| \\ &\leq \max\left\{\sup_{\substack{x\in K_\epsilon\\ 0\leq|\ell|\leq k}} |D^\ell(f_j\circ F_j)(x) - D^\ell f(x)|, \sup_{\substack{x\in\mathrm{cl}(\Omega)\setminus K_\epsilon\\ 0\leq|\ell|\leq k}} |D^\ell(f_j\circ F_j)(x) - D^\ell f(x)|\right\},\end{aligned}$$

there exist $N > 0$ and ϵ such that, for all $j > N$,

$$\sup_{\substack{x\in\mathrm{cl}(\Omega)\\ 0\leq|\ell|\leq k}} |D^\ell(f_j\circ F_j)(x) - D^\ell f(x)| < \lambda.$$

Let $\delta_\ell(x, y) := \dfrac{|D^\ell(f_j\circ F_j)(x) - D^\ell f(x) - D^\ell(f_j\circ F_j)(y) + D^\ell f(y)|}{|x-y|^\beta}$. Then

$$\sup_{\substack{x,y\in\mathrm{cl}(\Omega)\\ |\ell|=k}} \delta_\ell(x, y) \leq \max\left(\sup_{\substack{x\in\mathrm{cl}(\Omega)\\ y\in K_\epsilon, |\ell|=k}} \delta_\ell(x, y), \sup_{\substack{x,y\in\mathrm{cl}(\Omega)\setminus K_\epsilon\\ |\ell|=k}} \delta_\ell(x, y)\right). \tag{1}$$

Consider the first supremum in the right-hand side of (1). For $x \in \mathrm{cl}(\Omega)$, $y \in K_\epsilon$, there exists $z \in K_\epsilon$ such that $\mathrm{dist}(K_\epsilon, x) = |x - z|$. Therefore we see that

$$\begin{aligned}\delta_\ell(x, y) \le & \frac{|D^\ell(f_j \circ F_j)(x) - D^\ell f(x) - D^\ell(f_j \circ F_j)(z) + D^\ell f(z)|}{|x-y|^\beta} \\ & + \frac{|D^\ell(f_j \circ F_j)(z) - D^\ell f(z) - D^\ell(f_j \circ F_j)(y) + D^\ell f(y)|}{|x-y|^\beta} \\ & \lesssim \delta_\ell(x, z) + \delta_\ell(z, y),\end{aligned}$$

because $|x - y| \ge |x - z|$ and $|y - z| \le |y - x| + |x - z| \le 2|x - y|$. Notice now that, for μ satisfying $\beta + \mu < \alpha$, we have that $\delta_\ell(x, z) \lesssim |x - z|^\mu < \epsilon^\mu$. So

$$\sup_{\substack{x \in \mathrm{cl}(\Omega),\, y \in K_\epsilon \\ |\ell| = k}} \delta_\ell(x, y) < \lambda$$

for any $j > N$. (For this last, one may need to adjust the sizes of N and ϵ.)

Consider now the second supremum in the right-hand side of (1). Let x, $y \in \mathrm{cl}(\Omega) - K_\epsilon$. If $|x - y| < \epsilon$, then for μ satisfying $\beta + \mu < \alpha$, $\delta_\ell(x, y) \lesssim |x - y|^\mu < \epsilon^\mu$. If $|x - y| \ge \epsilon$, let z be a point in K_ϵ satisfying $|x - z| = \mathrm{dist}(K_\epsilon, x)$. Then $\delta_\ell(x, y) \lesssim \delta_\ell(x, z) + \delta_\ell(z, y)$, since $|x - z| < \epsilon < |x - y|$ and $|y - z| < 2|x - y|$. So

$$\sup_{\substack{x, y \in \mathrm{cl}(\Omega) \setminus K_\epsilon \\ |\ell| = k}} \delta_l(x, y) < \lambda.$$

Since $\lambda > 0$ is arbitrary, we see that

$$\lim_{j \to \infty} \sup_{\substack{x, y \in \mathrm{cl}(\Omega) \\ |\ell| = k}} \delta_\ell(x, y) = 0$$

for any $\beta < \alpha$. This completes the proof of Theorem 4.3. □

5. Conjugation by diffeomorphism

For isometries of compact Riemannian manifolds, semicontinuity involves not just that nearby metrics have isometry groups which are isomorphic to subgroups of the unperturbed metric, but that the isomorphisms are obtainable via conjugation by diffeomorphism (cf. [Ebin 1968; Guillemin et al. 2002]). This conjugation by diffeomorphism actually applies in the case of bounded C^∞ strongly pseudoconvex domains as well; see, e.g., [Greene and Krantz 1982b; Greene et al. 2011]. Naturally, the C^∞ hypothesis used in these references is, as usually happens, replaceable by a finite differentiability hypotheses simply by tracing through the arguments and checking how many derivatives are needed.

In this section, the subject will be investigated of the finite differentiability version of the conjugation by diffeomorphism results already shown in the references indicated in the C^∞ case. These results are of active interest because, by this time, quite precise results are known about extension to the boundary with finite smoothness of automorphisms of bounded strongly pseudoconvex domains with boundaries of finite smoothness. In particular, the results of the previous sections give motivation to study the issues discussed in the present section.

In the C^∞ version presented in [Greene and Krantz 1982a] and [Greene et al. 2011], the basic technique was to pass to the double in the topologist's sense of the domain, thus creating a situation to which the compact manifold results could be applied. This technique can still be applied in the present case. The difference is that we need now to keep track of how many derivatives are lost in the passage to the double. For the manifold with boundary itself, no derivatives are lost. It is shown in [Munkres 1963] that a C^k manifold with boundary, $k \geq 1$, has a C^k double that is unique up to C^k diffeomorphism.

In our case Theorem 4.3 allows us to have the $C^{k,\alpha}$ metric double for every $k \geq 2$ and any $0 < \alpha < 1$. But, the need to make the group act on the double requires that the doubling construction be invariant under the group, which actually needs $k \geq 4$. And this will turn out to reduce the guaranteed differentiability of the conjugating diffeomorphism.

To facilitate the discussion, we introduce a definition (similar to one given in Section 2) of the sense in which a sequence of groups of diffeomorphisms might converge to a limit group:

Suppose that M is a compact C^k manifold with boundary, k a positive integer. Suppose that G_0 is a compact Lie group of C^k diffeomorphisms of M and that moreover G_j, $j = 1, 2, \dots$ are a sequence of compact Lie groups of C^k diffeomorphisms. Then we say that the sequence G_j converges to G_0 in the C^k sense if for each $\epsilon > 0$ there is a number j_0 such that, if $j > j_0$ and $g \in G_j$, then there is an element $g_0 \in G_0$ such that the distance from g to g_0 is less than ϵ. Here the distance means relative to any metric on the set of C^k mappings which gives the usual C^k topology on C^k maps from M to M.

In these terms, we can now formulate the general real-differentiable result we shall use in the complex case:

Theorem 5.1. *Suppose that M is a compact C^r manifold with boundary and that $r > 2$ is an integer, that G_0 is a compact Lie group of C^r diffeomorphisms of M, and that G_j, $j = 1, 2, \dots,$ is a sequence of compact groups of C^r diffeomorphisms which converge in the C^r sense to G_0. Then, for all j sufficiently large, there is a C^{r-2} diffeomorphism F_j of M to itself such that $F_j \circ G_j \circ F_j^{-1}$ is a subgroup of G_0, i.e., F_j conjugates the elements of G_j into elements of G_0.*

The proof of this theorem follows almost precisely the pattern of the proof of Theorem 0.1 in [Greene and Krantz 1982a] (cf. [Greene et al. 2011, Theorem 4.4.1]). The only difference is that we must here keep some track of the number of derivatives involved: Ebin's theorem concerned the C^∞ case so that loss of a derivative or two or indeed of any finite number was irrelevant. This is why we need the results of Section 4.

Discussion of the proof of Theorem 5.1. As in Section 2, the essential method is to pass to the double of M and extend the action of the groups to the double. Then one can use Ebin's result in the form presented in [Guillemin et al. 2002], where only C^1 is required for the closeness of the group actions. But here we have to keep track of degrees of differentiability as opposed to the C^∞ situation of Section 2.

The most natural way to form the equivariant double is via metric construction as already explained in Section 2 (cf. [Greene and Krantz 1982a]). As before one takes a metric g on the manifold with boundary that is invariant under the group G. Then one defines charts in neighborhoods of boundary points p using the normal field to the boundary. Specifically, let $N(q)$ be the g-metric normal to the tangent space to the boundary ∂M at the point q in ∂M. Then one defines charts in a neighborhood of points p in the boundary as follows: map $\partial M \times (-\epsilon, \epsilon) \to M$ by $(q,t) \mapsto \exp_q(tN(q))$, where exp is the geodesic exponential map of the Riemannian metric g and $N(q)$ is the inward pointing normal at q. Choosing a chart around p in ∂M then gives a chart in a neighborhood of p in the double of M if we interpret $\exp_q(tN(q))$ to be in the second copy of M when $t < 0$.

In terms of derivative loss, the choice of the normal vector N loses one derivative, since it is an algebraic process using g and the tangent space of the boundary and the latter is not C^r but C^{r-1}. But an additional loss of derivative, so that two derivatives are lost, occurs because the exponential map is defined by the geodesic equation and that equation involves the Christoffel symbols, which involve the first derivative of the metric g. And the metric g has already lost one derivative in the averaging over the action of the group G.

Thus one obtains a G-equivariant construction of the double $\widetilde{M}$ of M and by construction the action of G on M extends to be an action of G on $\widetilde{M}$. This extended group action is C^{r-2}. Associate to the group G a group $\widetilde{G}$ defined to be $G \oplus \mathbb{Z}_2$. Then $\widetilde{G}$ acts on $\widetilde{M}$ in a natural way. Namely, we label the elements of $\widetilde{M}$ by (m,a) where $m \in M$ and $a \in \{0,1\}$ with 0 corresponding to the original of M and 1 corresponding to the second copy of M. Then we let (g,b) acting on (m,a) be

$$(g(m), a+b),$$

where the addition $a+b$ is in $\mathbb{Z}_2$. For example $(\mathrm{id}_G, 1)$ acts on $\widetilde{M}$ as the "flip" map that interchanges the two copies of M.

Note that the fixed point set of $(\mathrm{id}_G, 1)$ is exactly ∂M. And, for any element $g \in G$, the fixed point set of $(g, 1)$ is contained in ∂M, though it need not be all of it, and can indeed be empty if the action of g on ∂M has no fixed point. These observations will be important later.

Now we turn to the explicit situation of Theorem 5.1. We choose a sequence of G_j-invariant C^{r-1} metrics on M, which can clearly be taken to converge in the C^{r-1} sense to a G_0-invariant C^{r-1} metric on M. Passing to the double $\widetilde{M}$ gives a sequence of $\widetilde{G}_j$ group actions on $\widetilde{M}$. We can form a sequence of $\widetilde{G}_j$ invariant metrics by combining, via a partition of unity, a product metric structure near the boundary with the G_j-invariant metric on the interior of M. Namely, as similar to before, let E_j be the exponential map of the metric g_j, $j = 0, 1, 2, \ldots$, acting on the normal bundle of the boundary ∂M of M in M to give maps also to be denoted by $E_j : \partial M \times (-a, a) \to \widetilde{M}$ of the boundary ∂M of M producted with an open interval $(-a, a)$ into $\widetilde{M}$. The size of a can, by the C^{r-2} convergence of the E_j to E_0, be chosen uniformly so that these E_j are diffeomorphisms onto their images in ∂M, which themselves converge in the C^{r-2} sense to the limit C^{r-2} diffeomorphism E_0.

Via this diffeomorphism, we transfer the product metrics on $\partial M \times [0, \epsilon)$, namely $H_j \times dt^2$, to the associated tubular neighborhoods of ∂M in M. This transfer gives a $\widetilde{G}_j$-invariant metric for each j and these metrics converge C^{r-2} to the limit $\widetilde{G}_0$-invariant metric. Now we can combine, using a $\widetilde{G}_j$-equivariant partition of unity, these product metrics with the G_j-invariant metric g_j on M to obtain a $\widetilde{G}_j$-invariant metric on $\widetilde{M}$, to be denoted $\widetilde{g}_j$. This metric is C^{r-2}. And it converges in the C^{r-2} topology to the corresponding $\widetilde{G}_0$-invariant metric $\widetilde{g}_0$ on $\widetilde{M}$. (The G_j-equivariant partition of unity is obtained by taking the partition of unity function to depend on t alone, t as above).

Now we can apply Ebin's theorem, in the form given in [Guillemin et al. 2002] and [Kim 1987], for the C^{r-2} case to get C^{r-2} diffeomorphisms $F_j : \widetilde{M} \to \widetilde{M}$ which conjugate $\widetilde{G}_j$ into a subgroup of $\widetilde{G}_0$. (Here we are reasoning as follows: there is a diffeomorphism that conjugates $\mathrm{Isom}(\widetilde{g}_j)$ into a subgroup of $\mathrm{Isom}(\widetilde{g}_0)$ and hence conjugates $\widetilde{G}_j$ into a subgroup of $\mathrm{Isom}(\widetilde{g}_0)$ and these diffeomorphisms can be taken to converge to the identity map. So the image of $\widetilde{G}_j$ under this conjugation is close to $\widetilde{G}_0$ for large j in the sense of C^{r-2} convergence. By the classical theorem of [Montgomery and Samelson 1943], this conjugation image is in fact itself conjugate in $\mathrm{Isom}(\widetilde{g}_0)$ to a subgroup of G_0 by an element close to the identity. (See, e.g., [Greene et al. 2011, Chapter 4], for more detail.)

Now we need to know that in fact the conjugation image of G_j lies in G_0, not just in $\widetilde{G}_0$. For this, we need only show that the diffeomorphism that is conjugating takes ∂M to itself. This can be deduced as follows: let us denote by $\mathrm{Fix}(\psi)$ the fixed point set of ψ. Then conjugation takes fixed points to fixed points in the sense that $\mathrm{Fix}(f \circ \psi \circ f^{-1}) = f(\mathrm{Fix}(\psi))$. Now consider the case of ψ equal to the flip map which interchanges the two copies of M in $\widetilde{M}$. When f is close to the identity, $f \circ \psi \circ f^{-1}$ has to belong to the part of the group that interchanges the two components. So its fixed point set cannot be larger than ∂M. Thus $f(\partial M)$ lies in ∂M and hence equals ∂M (since f is a diffeomorphism of ∂M onto its image).

This completes the proof of the theorem. □

Note that these considerations of fixed points of the interchange map did not arise in Section 2, since we were concerned there only with isomorphism, not with the existence of a conjugating diffeomorphism of the manifolds with boundary.

The application to the strongly pseudoconvex case now follows:

Theorem 5.2. *Let Ω_0 be a bounded strongly pseudoconvex domain with a $C^{k,\alpha}$ boundary in $\mathbb{C}^n$, not biholomorphic to the unit ball. Then there is a $C^{k,\alpha}$ neighborhood $\mathcal{N}$ of Ω_0 such that, for any $\Omega \in \mathcal{N}$, there is a C^{k-3} diffeomorphism $f : \Omega \to \Omega_0$ with the property that $f \circ \mathrm{Aut}(\Omega) \circ f^{-1} \subset \mathrm{Aut}(\Omega_0)$.*

Theorem 5.2 is derived from Theorem 5.1 by exactly the arguments of [Greene and Krantz 1982a].

In outline, these arguments are as follows: first, the stable estimation of Bergman metric curvature (Theorem 3.1) in Section 3 guarantees that, if $\{\Omega_j\}$ is a sequence of domains converging in $C^{k,\alpha}$ to Ω_0 ($k \geq 4$) with Ω_0 not biholomorphic to the ball, and if $p_0 \in \Omega_0$, then there is a $\delta_p > 0$ such that the distance $\phi_j(p_0)$ to $\mathbb{C}^n - \Omega_j$ is at least δ_p for all $\phi_j \in \mathrm{Aut}(\Omega_j)$ for all j sufficiently large. This in turn makes possible the application of normal families arguments to show that for every sequence $\phi_j \in \mathrm{Aut}(\Omega_j)$, there is a subsequence $\{\phi_{j_k}\}$ which converges uniformly on compact subsets (of Ω_0). The uniformity of boundary behavior established in Section 4 then implies that this subsequence converges uniformly in the C^{k-3} topology on the closure of the domains, where comparison over different domains is via fixed diffeomorphisms of $\Omega_j \to \Omega_j$ for each j, these converging in the C^k topology to the identity. Thus one passes to the situation of Theorem 5.1. For further details, the reader can consult [Greene and Krantz 1982a].

6. Concluding remarks

Semicontinuity of symmetry in the general sense is an idea with deep roots in intuition to the point that it arguably predates formal mathematical thought altogether. In precise form, when all the symmetry groups belong to one fixed (compact) Lie group, it was given definitive formulation in the result of [Montgomery and Samelson 1943]. The situation for isometry groups and automorphism groups is made more delicate because a priori not all the groups are even isomorphic to subgroups of any fixed Lie group. In [Greene and Krantz 1985], ways of dealing with this issue in the automorphism group case were introduced. The results obtained turned out to have some interesting applications, e.g., they played a role in [Bedford and Dadok 1987]. One of the main points of the first part of this paper was that, on account of normal families considerations, in fact this difficulty of the groups not belonging a priori to a fixed larger group is obviated in very general situations. All that is needed is that the groups keep some fixed compact set in the domain (or manifold) within another fixed compact set: this is in effect the stably interior property introduced in Section 2. The remainder of the paper describes how this condition can be guaranteed in the case of C^2 strongly pseudoconvex domains. In view of the great generality of the stably interior property, it is natural to ask whether some similar guarantee of the property might be available for other classes of domains, for example, those of finite type in the sense of D'Angelo. This would seem to be a potentially fruitful topic for further investigation.

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KLEIN FOUR-SUBGROUPS OF LIE ALGEBRA AUTOMORPHISMS

JING-SONG HUANG AND JUN YU

We classify the Klein four-subgroups Γ of $\mathrm{Aut}(\mathfrak{u}_0)$ for each compact simple Lie algebra $\mathfrak{u}_0$ up to conjugation, by calculating the symmetric subgroups $\mathrm{Aut}(\mathfrak{u}_0)^\theta$ and their involution classes. This leads to a new approach to the classification of semisimple symmetric pairs and $\mathbb{Z}_2 \times \mathbb{Z}_2$-symmetric spaces. We also determine the fixed point subgroups $\mathrm{Aut}(\mathfrak{u}_0)^\Gamma$.

1. Introduction

Riemannian symmetric pairs were classified by Élie Cartan (see [Carter 1993], for example) and the more general semisimple symmetric pairs were classified by Marcel Berger [1957]. The algebraic structure of semisimple symmetric spaces is even more interesting for geometric and analytic reasons. Some of the recent works are Ōshima and Sekiguchi's classification [1984] of reduced root systems and Helminck's classification [1988] for algebraic groups. Most recently some new approaches to the classification and the parametrization of semisimple symmetric pairs were given in [Huang 2002] by using admissible quadruplets and in [Chuah and Huang 2010] by using double Vogan diagrams.

In this paper we study semisimple symmetric spaces from a different point of view — by determining the Klein four-subgroups in Lie algebra automorphisms. Let $\mathfrak{u}_0$ be a compact simple Lie algebra and $\mathfrak{g}$ be its complexification. Denote by $\mathrm{Aut}(\mathfrak{u}_0)$ the automorphism group of $\mathfrak{u}_0$. For any involution θ in $\mathrm{Aut}(\mathfrak{u}_0)$, we first determine the centralizer $\mathrm{Aut}(\mathfrak{u}_0)^\theta$ of θ, which is a symmetric subgroup. By understanding the conjugacy classes of involutions in $\mathrm{Aut}(\mathfrak{u}_0)^\theta$, we proceed to classify Klein four-subgroups Γ of $\mathrm{Aut}(\mathfrak{u}_0)$ up to conjugation. This gives a new approach to the classification of commuting pairs of involutive automorphisms of $\mathfrak{u}_0$ or $\mathfrak{g}$. We note that the ordered commuting pairs of involutions correspond to

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Berger's classification of semisimple symmetric pairs.

If Γ is a finite abelian subgroup of the automorphism group of a Lie group G, then the homogeneous space G/H is called a Γ-symmetric space provided that $(G^\Gamma)_0 \subseteq H \subseteq G^\Gamma$; see [Lutz 1981]. In the case of $\Gamma = \mathbb{Z}_2$ this is a symmetric space and in the case of $\Gamma = \mathbb{Z}_k$ it is the k-symmetric space studied in [Wolf and Gray 1968]. In the case of $\Gamma = \mathbb{Z}_2 \times \mathbb{Z}_2$ it is the Klein four-group; $\mathbb{Z}_2 \times \mathbb{Z}_2$-symmetric spaces were studied in [Bahturin and Goze 2008; Kollross 2009]. This paper contains a complete list of all $\mathbb{Z}_2 \times \mathbb{Z}_2$-symmetric pairs and our method is very different from theirs. Finally, we determine the fixed point subgroups $\mathrm{Aut}(\mathfrak{u}_0)^\Gamma$.

2. Preliminaries

2A. ***Complex semisimple Lie algebras and Dynkin diagrams.*** Let $\mathfrak{g}$ be a complex semisimple Lie algebra and $\mathfrak{h}$ a Cartan subalgebra. Then $\mathfrak{g}$ has a root-space decomposition

$$\mathfrak{g} = \mathfrak{h} \oplus \Big(\bigoplus_{\alpha \in \Delta} \mathfrak{g}_\alpha \Big),$$

where $\Delta = \Delta(\mathfrak{g}, \mathfrak{h})$ is the root system of $\mathfrak{g}$ and $\mathfrak{g}_\alpha$ is the root space of the root $\alpha \in \Delta$. Let B be the Killing form on $\mathfrak{g}$. It is a nondegenerate symmetric form. The restriction of B to $\mathfrak{h}$ is also nondegenerate. For any $\lambda \in \mathfrak{h}^*$, let $H_\lambda \in \mathfrak{h}$ be determined by

$$B(H_\lambda, H) = \lambda(H) \quad \text{for all } \ H \in \mathfrak{h}.$$

For any $\lambda, \mu \in \mathfrak{h}^*$, define $\langle \lambda, \mu \rangle := B(H_\lambda, H_\mu)$.

For any root α, we have

$$H_\alpha \in \mathfrak{h}. \tag{1}$$

Define

$$H'_\alpha = \frac{2}{\alpha(H_\alpha)} H_\alpha, \tag{2}$$

which is called a coroot; let

$$0 \neq X_\alpha \in \mathfrak{g}_\alpha \tag{3}$$

be any nonzero vector (recall that $\dim \mathfrak{g}_\alpha = 1$), which is called a root vector of the root α. The notation H_α, H'_α, X_α will be used frequently in this paper.

Note that, for any $\alpha, \beta \in \Delta$,

$$\langle \alpha, \beta \rangle = B(H_\alpha, H_\beta) = \beta(H_\alpha) = \alpha(H_\beta) \in \mathbb{R},$$
$$\langle \alpha, \alpha \rangle = B(H_\alpha, H_\alpha) = \alpha(H_\alpha) \neq 0,$$

and $2\langle \alpha, \beta \rangle / \langle \beta, \beta \rangle \in \mathbb{Z}$. We also note that $\mathrm{span}_{\mathbb{R}}\{\alpha \mid \alpha \in \Delta\} \subset \mathfrak{h}^*$ is a real vector space of dimension equal to $r = \mathrm{rank}\, \mathfrak{g} = \dim_{\mathbb{C}} \mathfrak{h}$; see [Knapp 2002, pp. 140–162].

We set $A_{\alpha,\beta} = 2\langle\alpha, \beta\rangle/\langle\beta, \beta\rangle = \alpha(H'_\beta)$. Then

$$[H'_\alpha, X_\beta] = \beta(H'_\alpha)X_\beta = \frac{2\langle\alpha, \beta\rangle}{\langle\alpha, \alpha\rangle} X_\beta = A_{\beta,\alpha} X_\beta.$$

Choose a lexicography order of $\mathrm{span}_{\mathbb{R}}\{\alpha \mid \alpha \in \Delta\}$ to get a positive system Δ^+ and a simple system Π. Let

$$\Pi = \{\alpha_1, \alpha_2, \ldots, \alpha_r\}. \tag{4}$$

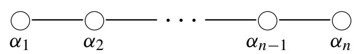
For brevity, we write

$$H_i,\ H'_i \tag{5}$$

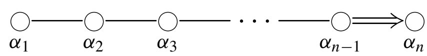
instead of H_{α_i}, H'_{α_i} for a simple root α_i.

Draw $A_{\alpha,\beta}A_{\beta,\alpha}$ edges to connect any two distinct simple roots α and β, and draw an arrow from α to β if $\langle\alpha, \alpha\rangle > \langle\beta, \beta\rangle$; this gives us a graph. This graph is connected if and only if $\mathfrak{g}$ is a simple Lie algebra; in this case it is called the Dynkin diagram of $\mathfrak{g}$. In this paper, we always follow Bourbaki numbering to order the simple roots; see [Bourbaki 2002, pp. 265–300]. The following are all the possible (connected) Dynkin diagrams.[1]

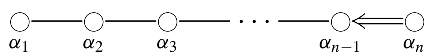
A_n



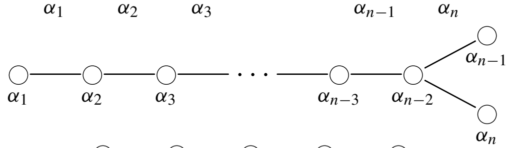
B_n



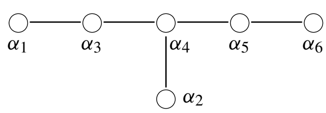
C_n



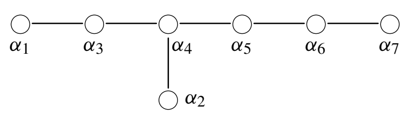
D_n



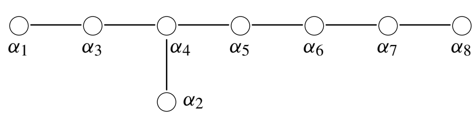
E_6



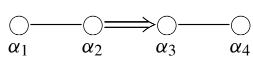
E_7



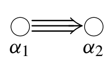
E_8



F_4



G_2



[1] These diagrams are drawn by using a Latex package of Professor Jiu-Kang Yu. We are grateful to him for the kind permission to use this package.

Let $\mathrm{Aut}(\mathfrak{g})$ be the group of all complex linear automorphisms of $\mathfrak{g}$ and $\mathrm{Int}(\mathfrak{g})$ be the subgroup of inner automorphisms. We define

$$\mathrm{Out}(\mathfrak{g}) := \mathrm{Aut}(\mathfrak{g})/\,\mathrm{Int}(\mathfrak{g}).$$

The exponential map $\exp : \mathfrak{g} \to \mathrm{Aut}(\mathfrak{g})$ is given by

$$\exp(X) = \exp(\mathrm{ad}(X)) \quad \text{for all } \; X \in \mathfrak{g} = \mathrm{Lie}(\mathrm{Aut}(\mathfrak{g})).$$

2B. ***A compact real form.*** One can normalize the root vectors $\{X_\alpha, X_{-\alpha}\}$ so that $B(X_\alpha, X_{-\alpha}) = 2/\alpha(H_\alpha)$. Then $[X_\alpha, X_{-\alpha}] = H'_\alpha$. Moreover, one can normalize $\{X_\alpha\}$ appropriately, such that

$$\mathfrak{u}_0 = \mathrm{span}_{\mathbb{R}}\{X_\alpha - X_{-\alpha},\; i(X_\alpha + X_{-\alpha}),\; iH_\alpha : \alpha \in \Delta^+\} \tag{6}$$

is a compact real form of $\mathfrak{g}$ [Knapp 2002, pp. 348–354]. Define

$$\theta(X + iY) := X - iY \quad \text{for all } \; X, Y \in \mathfrak{u}_0.$$

Then θ is a Cartan involution of $\mathfrak{g}$ (as a real semisimple Lie algebra) and $\mathfrak{u}_0 = \mathfrak{g}^\theta$ is a maximal compact subalgebra of $\mathfrak{g}$. Any other compact real form of $\mathfrak{g}$ is conjugate to $\mathfrak{u}_0$. Below, whenever we discuss a compact real form of $\mathfrak{g}$, we always use this compact real form $\mathfrak{u}_0$ in (6).

Let $\mathrm{Aut}(\mathfrak{u}_0)$ be the group of automorphisms of $\mathfrak{u}_0$ and $\mathrm{Int}(\mathfrak{u}_0)$ be the subgroup of inner automorphisms. Any automorphism of $\mathfrak{u}_0$ extends uniquely to a holomorphic automorphism of $\mathfrak{g}$, so $\mathrm{Aut}(\mathfrak{u}_0) \subset \mathrm{Aut}(\mathfrak{g})$. Similarly, $\mathrm{Int}(\mathfrak{u}_0) \subset \mathrm{Int}(\mathfrak{g})$. Define

$$\Theta(f) := \theta f \theta^{-1} \quad \text{for all } \; f \in \mathrm{Aut}(\mathfrak{g}).$$

Then it is a Cartan involution of $\mathrm{Aut}(\mathfrak{g})$ with differential θ. It follows that $\mathrm{Aut}(\mathfrak{u}_0) = \mathrm{Aut}(\mathfrak{g})^\Theta$ and $\mathrm{Int}(\mathfrak{u}_0) = \mathrm{Int}(\mathfrak{g})^\Theta$ are maximal compact subgroups of $\mathrm{Aut}(\mathfrak{g})$ and $\mathrm{Int}(\mathfrak{g})$, respectively. We also have

$$\mathrm{Out}(\mathfrak{u}_0) := \mathrm{Aut}(\mathfrak{u}_0)/\,\mathrm{Int}(\mathfrak{u}_0) \cong \mathrm{Out}(\mathfrak{g}) \cong \mathrm{Aut}(\Pi),$$

where $\mathrm{Aut}(\Pi)$ is the symmetry group of the graph Π consisting of permutations of vertices preserving the multiples of edges and directions of arrows.

2C. ***Notation.*** We denote by $\mathfrak{e}_6$ the compact simple Lie algebra of type $\mathbf{E_6}$. Let E_6 be the connected and simply connected Lie group with Lie algebra $\mathfrak{e}_6$. Let $\mathfrak{e}_6(\mathbb{C})$ and $\mathrm{E}_6(\mathbb{C})$ denote their complexifications. Similar notation will be used for other types.

Let $Z(G)$ and $\mathfrak{z}(\mathfrak{g})$ denote the center of a group G and a Lie algebra $\mathfrak{g}$, respectively, and G_0 denote the connected component of G containing identity element. For Lie groups $H \subset G$, let $Z_G(H)$ denote the centralizer of H in G, and for Lie algebras $\mathfrak{h} \subset \mathfrak{g}$, let $Z_{\mathfrak{g}}(\mathfrak{h})$ denote the centralizer of $\mathfrak{h}$ in $\mathfrak{g}$. Let $N_G(H)$ denote the normalizer of H in G. For any two elements $x, y \in G$, we write $x \sim y$ to mean x, y are conjugate in G, that is, $y = gxg^{-1}$ for some $g \in G$ and $x \sim_H y$ to mean $y = gxg^{-1}$ for some $g \in H$.

In the case of $G = \mathrm{E}_6$ or E_7, let c denote a nontrivial element in $Z(G)$.

In the case of $\mathfrak{u}_0 = \mathfrak{e}_7$, let

$$H'_0 = \frac{H'_2 + H'_5 + H'_7}{2} \in i\mathfrak{e}_7 \subset \mathfrak{e}_7(\mathbb{C}).$$

Let $\mathrm{Pin}(n)$ ($\mathrm{Spin}(n)$) be the Pin (Spin) group in degree n. Write

$$c = e_1 e_2 \cdots e_n \in \mathrm{Pin}(n).$$

Then c is in $\mathrm{Spin}(n)$ if and only if n is even; in this case $c \in Z(\mathrm{Spin}(n))$. If n is odd, then $\mathrm{Spin}(n)$ has a spinor module M of dimension $2^{(n-1)/2}$. If n is even, then $\mathrm{Spin}(n)$ has two spinor modules M_+, M_- of dimension $2^{(n-2)/2}$. We distinguish M_+ and M_- by requiring that c acts on M_+ as the identity when $4 \mid n$ and as multiplication by $-i$ when $4 \mid n-2$ (and thus c acts on M_- as multiplication by -1 and i, respectively, in the same two cases).

We define the matrices

$$J_m = \begin{pmatrix} 0 & I_m \\ -I_m & 0 \end{pmatrix}, \quad I_{p,q} = \begin{pmatrix} -I_p & 0 \\ 0 & I_q \end{pmatrix},$$

$$I'_{p,q} = \begin{pmatrix} -I_p & 0 & 0 & 0 \\ 0 & I_q & 0 & 0 \\ 0 & 0 & -I_p & 0 \\ 0 & 0 & 0 & I_q \end{pmatrix}, \quad J_{p,q} = \begin{pmatrix} 0 & I_p & 0 & 0 \\ -I_p & 0 & 0 & 0 \\ 0 & 0 & 0 & I_q \\ 0 & 0 & -I_q & 0 \end{pmatrix},$$

$$K_p = \begin{pmatrix} 0 & 0 & 0 & I_p \\ 0 & 0 & -I_p & 0 \\ 0 & I_p & 0 & 0 \\ -I_p & 0 & 0 & 0 \end{pmatrix}.$$

and the groups

$$Z_m = \{\lambda I_m \mid \lambda^m = 1\},$$

$$Z' = \{(\epsilon_1, \epsilon_2, \epsilon_3, \epsilon_4) \mid \epsilon_i = \pm 1, \epsilon_1\epsilon_2\epsilon_3\epsilon_4 = 1\},$$

$$\Gamma_{p,q,r,s} = \left\langle \begin{pmatrix} -I_p & 0 & 0 & 0 \\ 0 & -I_q & 0 & 0 \\ 0 & 0 & I_r & 0 \\ 0 & 0 & 0 & I_s \end{pmatrix}, \begin{pmatrix} -I_p & 0 & 0 & 0 \\ 0 & I_q & 0 & 0 \\ 0 & 0 & -I_r & 0 \\ 0 & 0 & 0 & I_s \end{pmatrix} \right\rangle.$$

3. Involutions

The classical compact simple Lie algebras are as follows. For $F = \mathbb{R}, \mathbb{C}, \mathbb{H}$, let $M_n(F)$ be the set of $n \times n$ matrices with entries in F, and

$$\begin{aligned}\mathfrak{so}(n) &= \{X \in M_n(\mathbb{R}) \mid X + X^t = 0\},\\ \mathfrak{su}(n) &= \{X \in M_n(\mathbb{C}) \mid X + X^* = 0, \operatorname{tr} X = 0\},\\ \mathfrak{sp}(n) &= \{X \in M_n(\mathbb{H}) \mid X + X^* = 0\}.\end{aligned}$$

Then $\{\mathfrak{su}(n) : n \geq 3\}$, $\{\mathfrak{so}(2n+1) : n \geq 1\}$, $\{\mathfrak{sp}(n) : n \geq 3\}$, $\{\mathfrak{so}(2n) : n \geq 4\}$ represent all isomorphism classes of compact classical simple Lie algebras.

Let $\mathfrak{u}_0$ be a compact simple Lie algebra and $\mathfrak{g} = (\mathfrak{u}_0) \otimes_{\mathbb{R}} \mathbb{C}$ be its complexification. Note that the conjugacy classes of involutions in $\operatorname{Aut}(\mathfrak{u}_0)$ are in one-to-one correspondence with isomorphism classes of noncompact real forms of $\mathfrak{g}$, and are also in one-to-one correspondence with isomorphism classes of irreducible Riemannian symmetric pairs $(\mathfrak{u}_0, \mathfrak{k}_0)$ of compact type or $(\mathfrak{g}_0, \mathfrak{k}_0)$ of noncompact type; see [Huang 2002; Helminck 1988] and references therein. One direction of this correspondence is as follows: let θ be an involutive automorphism of a compact real simple Lie algebra $\mathfrak{u}_0$, and extend it to a holomorphic automorphism of $\mathfrak{g}$. Let $\mathfrak{k}_0 \subset \mathfrak{u}_0$ and $i\mathfrak{p}_0 \subset \mathfrak{u}_0$ (so $\mathfrak{p}_0 \subset i\mathfrak{u}_0$) be the $+1$, -1 eigenspaces of θ on $\mathfrak{u}_0$, respectively. Let

$$\mathfrak{g}_0 = \mathfrak{k}_0 \oplus \mathfrak{p}_0$$

(this is also the Cartan decomposition of $\mathfrak{g}_0$). Then $\mathfrak{g}_0$ is a real simple Lie algebra (that is, a real form of $\mathfrak{g}$), $(\mathfrak{u}_0, \mathfrak{k}_0)$ is a Riemannian symmetric pair of compact type and $(\mathfrak{g}_0, \mathfrak{k}_0)$ is a Riemannian symmetric pair of noncompact type. The other direction of this correspondence needs a sophisticated argument.

These objects were classified by Élie Cartan in 1926. We list this classification here. Our presentation below is mainly from [Knapp 2002, pp. 408–426; Helgason 2001, pp. 515–518]. In each case, we also define a specific involution in each conjugacy class of involutions in $\operatorname{Aut}(\mathfrak{u}_0)$, which corresponds to a real simple Lie algebra or symmetric space. In the exceptional simple Lie algebras case, these involutions are labeled as σ_1, σ_2, σ_3, σ_4, σ and $\tau = \sigma_3$ (this is used only in the E_6 case). We will use this notation for involutions frequently in the rest of this paper.

The notation **AI–G** is Cartan notation and the notation $\mathfrak{e}_{6,-2}$, etc., is Helgason notation (with a little difference). For a real simple Lie algebra $\mathfrak{g}_0$ with a Cartan decomposition $\mathfrak{g}_0 = \mathfrak{k}_0 \oplus \mathfrak{p}_0$ and whose complexified Lie algebra $\mathfrak{g}$ is an exceptional simple Lie algebra, Helgason [2001, pp. 517–518] made an interesting observation: the isomorphism type of $\mathfrak{g}_0$ is distinguished by the type of $\mathfrak{g}$ (or its compact real form $\mathfrak{u}_0$) and the integer $\dim \mathfrak{k}_0 - \dim \mathfrak{p}_0$. For example, the notation $\mathfrak{e}_{6,-2}$ (written by Helgason as $\mathfrak{e}_{6(2)}$, as he used the integer $\dim \mathfrak{p}_0 - \dim \mathfrak{k}_0$ instead) means the compact real form of the complexified Lie algebra has type $\mathfrak{e}_6$ and $\dim \mathfrak{k}_0 - \dim \mathfrak{p}_0 = -2$.

The elements (coroots) H'_i are defined in (2) and (5).

i) Type **A**. For $\mathfrak{u}_0 = \mathfrak{su}(n)$, $n \geq 3$, $\{\mathrm{Ad}(I_{p,n-p}) \mid 1 \leq p \leq n/2\}$ (type **AIII**), $\{\tau = \text{complex conjugation}\}$ (type **AI**), $\{\tau \circ \mathrm{Ad}(J_{n/2})\}\}$ (type **AII**) represent all conjugacy classes of involutions in $\mathrm{Aut}(\mathfrak{u}_0)$. The corresponding real forms are $\mathfrak{su}(p, n-p)$, $\mathfrak{sl}(n, \mathbb{R})$, $\mathfrak{sl}(\frac{n}{2}, \mathbb{H})$.

ii) Type **B**. For $\mathfrak{u}_0 = \mathfrak{so}(2n+1)$, $n \geq 1$, $\{\mathrm{Ad}(I_{p,2n+1-p}) \mid 1 \leq p \leq n\}$ (type **BI**) represent all conjugacy classes of involutions in $\mathrm{Aut}(\mathfrak{u}_0)$. The corresponding real forms are $\mathfrak{so}(p, 2n+1-p)$.

iii) Type **C**. For $\mathfrak{u}_0 = \mathfrak{sp}(n)$, $n \geq 3$, $\{\mathrm{Ad}(I_{p,n-p}) \mid 1 \leq p \leq n/2\}$ (type **CII**) and $\{\mathrm{Ad}(\mathbf{i}I)\}$ (type **CI**) represent all conjugacy classes of involutions in $\mathrm{Aut}(\mathfrak{u}_0)$. The corresponding real forms are $\mathfrak{sp}(p, n-p)$, $\mathfrak{sp}(n, \mathbb{R})$.

iv) Type **D**. For $\mathfrak{u}_0 = \mathfrak{so}(2n)$, $n \geq 4$, $\{\mathrm{Ad}(I_{p,2n-p}) \mid 1 \leq p \leq n\}$ (type **DI**) and $\{\mathrm{Ad}(J_n)\}$ (type **DIII**) represent all conjugacy classes of involutions in $\mathrm{Aut}(\mathfrak{u}_0)$. The corresponding real forms are $\mathfrak{so}(p, 2n-p)$, $\mathfrak{so}^*(2n, \mathbb{R})$.[2]

v) Type $\mathbf{E_6}$. For $\mathfrak{u}_0 = \mathfrak{e}_6$, let τ be a specific diagram involution defined by

$$\begin{aligned}
&\tau(H_{\alpha_1}) = H_{\alpha_6}, && \tau(H_{\alpha_6}) = H_{\alpha_1}, && \tau(H_{\alpha_3}) = H_{\alpha_5},\\
&\tau(H_{\alpha_5}) = H_{\alpha_3}, && \tau(H_{\alpha_2}) = H_{\alpha_2}, && \tau(H_{\alpha_4}) = H_{\alpha_4},\\
&\tau(X_{\pm\alpha_1}) = X_{\pm\alpha_6}, && \tau(X_{\pm\alpha_6}) = X_{\pm\alpha_1}, && \tau(X_{\pm\alpha_3}) = X_{\pm\alpha_5},\\
&\tau(X_{\pm\alpha_5}) = X_{\pm\alpha_3}, && \tau(X_{\pm\alpha_2}) = X_{\pm\alpha_2}, && \tau(X_{\pm\alpha_4}) = X_{\pm\alpha_4}.
\end{aligned}$$

Let $\sigma_1 = \exp(\pi i H'_2)$, $\sigma_2 = \exp(\pi i (H'_1 + H'_6))$, $\sigma_3 = \tau$, $\sigma_4 = \tau \exp(\pi i H'_2)$. Then σ_1, σ_2, σ_3, σ_4 represent all conjugacy classes of involutions in $\mathrm{Aut}(\mathfrak{u}_0)$, which correspond to Riemannian symmetric pairs of type **EII**, **EIII**, **EIV**, **EI** and the corresponding real forms are $\mathfrak{e}_{6,-2}$, $\mathfrak{e}_{6,14}$, $\mathfrak{e}_{6,26}$, $\mathfrak{e}_{6,-6}$. Also, σ_1, σ_2 are inner automorphisms and σ_3, σ_4 are outer automorphisms.

vi) Type $\mathbf{E_7}$. For $\mathfrak{u}_0 = \mathfrak{e}_7$, let

$$\begin{aligned}
\sigma_1 &= \exp(\pi i H'_2),\\
\sigma_2 &= \exp\left(\pi i \frac{H'_2 + H'_5 + H'_7}{2}\right),\\
\sigma_3 &= \exp\left(\pi i \frac{H'_2 + H'_5 + H'_7 + 2H'_1}{2}\right).
\end{aligned}$$

Then σ_1, σ_2, σ_3 represent all conjugacy classes of involutions in $\mathrm{Aut}(\mathfrak{u}_0)$, which correspond to Riemannian symmetric pairs of type **EVI**, **EVII**, **EV** and the corresponding real forms are $\mathfrak{e}_{7,5}$, $\mathfrak{e}_{7,25}$, $\mathfrak{e}_{7,-7}$.

vii) Type $\mathbf{E_8}$. For $\mathfrak{u}_0 = \mathfrak{e}_8$, let

$$\sigma_1 = \exp(\pi i H'_2), \quad \sigma_2 = \exp(\pi i (H'_2 + H'_1)).$$

[2]When $n = 4$, we have $\mathrm{Ad}(I_{2,6}) \sim \mathrm{Ad}(J_4)$, and $\mathfrak{so}(2, 6) \cong \mathfrak{so}^*(8)$.

Then σ_1, σ_2 represent all conjugacy classes of involutions in $\mathrm{Aut}(\mathfrak{u}_0)$, which correspond to Riemannian symmetric pairs of type **EIX**, **EVIII** and the corresponding real forms are $\mathfrak{e}_{8,24}$, $\mathfrak{e}_{8,-8}$.

viii) Type $\mathbf{F_4}$. For $\mathfrak{u}_0 = \mathfrak{f}_4$, let

$$\sigma_1 = \exp(\pi i H_1'), \quad \sigma_2 = \exp(\pi i H_4').$$

Then σ_1, σ_2 represent all conjugacy classes of involutions in $\mathrm{Aut}(\mathfrak{u}_0)$, which correspond to Riemannian symmetric pairs of type **FI**, **FII** and the corresponding real forms are $\mathfrak{f}_{4,-4}$, $\mathfrak{f}_{4,20}$.

ix) Type $\mathbf{G_2}$. For $\mathfrak{u}_0 = \mathfrak{g}_2$, let $\sigma = \exp(\pi H_1')$, which represents the unique conjugacy class of involutions in $\mathrm{Aut}(\mathfrak{u}_0)$ and corresponds to a Riemannian symmetric pair of type **G** and the corresponding real form is $\mathfrak{g}_{2,-2}$.

4. Centralizer of an automorphism

In this section we prove a property of the centralizer G^x of an element x in a complex or compact Lie group G. First, we recall a theorem of Steinberg [Carter 1993, pp. 93–95].

Proposition 4.1 (Steinberg). *Let G be a connected and simply connected semisimple complex* (*or compact*) *Lie group. Then the centralizer G^x for any $x \in G$ is connected.*

For an element x in a group, we write $o(x)$ for the order of x. The notation

$$\mathrm{Int}(\mathfrak{g})_0^\theta \tag{7}$$

in this paper always means $(\mathrm{Int}(\mathfrak{g})^\theta)_0$, not $(\mathrm{Int}(\mathfrak{g})_0)^\theta$. Similarly for

$$\mathrm{Int}(\mathfrak{u}_0)_0^\theta,\ \mathrm{Aut}(\mathfrak{u}_0)_0^\theta,\ \mathrm{Aut}(\mathfrak{g})_0^\theta. \tag{8}$$

Proposition 4.2. *Let $\mathfrak{g}$ be a complex simple Lie algebra. Suppose that the order of an element $\theta \in \mathrm{Aut}(\mathfrak{g})$ is equal to the order of the coset element $\theta\,\mathrm{Int}(\mathfrak{g})$ in $\mathrm{Out}(\mathfrak{g}) = \mathrm{Aut}(\mathfrak{g})/\mathrm{Int}(\mathfrak{g})$, that is, $o(\theta) = o(\theta\,\mathrm{Int}(\mathfrak{g}))$. Then $Z_{\mathrm{Int}(\mathfrak{g})}(\mathrm{Int}(\mathfrak{g})_0^\theta) = 1$.*

Proof. By the assumption, θ is a diagram automorphism; this means there exists a Cartan subalgebra $\mathfrak{t}$ which is stable under θ and θ maps Δ^+ to itself, where $\Delta = \Delta(\mathfrak{g}, \mathfrak{t})$ and Δ^+ is a positive system. For any $\alpha \in \Delta$, let $\theta(X_\alpha) = a_\alpha X_{\theta\alpha}$ with $a_\alpha \neq 0$.

Let $k = o(\theta) = o(\theta\,\mathrm{Int}(\mathfrak{g}))$. Then, for any $\alpha \in \Delta$,

$$X_\alpha = \theta^k(X_\alpha) = \Bigl(\prod_{0 \le j \le k-1} a_{\theta^j\alpha}\Bigr) X_{\theta^k\alpha}.$$

It follows that

$$\prod_{0 \le j \le k-1} a_{\theta^j\alpha} = 1.$$

Let $L = \mathrm{Int}(\mathfrak{g})_0^\theta$, $\mathfrak{s} = \mathfrak{t}^\theta$, $T = \exp(\mathrm{ad}\,\mathfrak{t})$ and $S = \exp(\mathrm{ad}\,\mathfrak{s})$. It is clear that $S \subset L$.

We first show that $Z_{\mathrm{Int}(\mathfrak{g})}(S) = T$. It is clear that $\mathfrak{t} \subset Z_{\mathfrak{g}}(\mathfrak{s})$. Suppose that $X_\alpha \in Z_{\mathfrak{g}}(\mathfrak{s})$ for some $\alpha \in \Delta^+$. Since $\theta^k = 1$, we have $\sum_{0\le j\le k-1} \theta^j(H) \in \mathfrak{t}^\theta = \mathfrak{s}$ for any $H \in \mathfrak{t}$. Then $\left[\sum_{0\le j\le k-1} \theta^j(H), X_\alpha\right] = 0$.

For any j, we have

$$\begin{aligned}
[\theta^j H, X_\alpha] = \theta^j([H, \theta^{k-j} X_\alpha]) &= \theta^j\Bigg(\Bigg(\prod_{0\le i\le k-j-1} a_{\theta^i\alpha}\Bigg)\cdot((\theta^{k-j}\alpha)H)\cdot X_{\theta^{k-j}\alpha}\Bigg)\\
&= \Bigg(\prod_{0\le i\le k-j-1} a_{\theta^i\alpha}\Bigg)\cdot((\theta^{k-j}\alpha)H)\cdot\Bigg(\prod_{0\le i\le j-1} a_{\theta^{k-j+i}\alpha}\Bigg)X_\alpha\\
&= \Bigg(\prod_{0\le i\le k-1} a_{\theta^i\alpha}\Bigg)\cdot((\theta^{k-j}\alpha)H)\cdot X_\alpha = ((\theta^{k-j}\alpha)H)\cdot X_\alpha.
\end{aligned}$$

Hence $0 = \left[\sum_{0\le j\le k-1} \theta^j(H), X_\alpha\right] = \left(\left(\sum_{0\le j\le k-1}\theta^{k-j}\alpha\right)H\right)\cdot X_\alpha$. This implies

$$\sum_{0\le j\le k-1} \theta^j\alpha = 0,$$

which contradicts that all $\theta^j\alpha$ are positive roots. So $Z_{\mathfrak{g}}(\mathfrak{s}) = \mathfrak{t}$. Since $Z_{\mathrm{Int}(\mathfrak{g})}(S)$ is connected (by Corollary 4.51 of [Knapp 2002, p. 260], which also applies to complex semisimple groups), $Z_{\mathrm{Int}(\mathfrak{g})}(S) = T$.

Now we show that $Z_{\mathrm{Int}(\mathfrak{g})}(L) = 1$. Suppose that $1 \ne \tau \in Z_{\mathrm{Int}(\mathfrak{g})}(L)$. By the above, we have $Z_{\mathrm{Int}(\mathfrak{g})}(L) \subset Z_{\mathrm{Int}(\mathfrak{g})}(S) = T$, then $\tau = \exp(\mathrm{ad}\,H)$ for some $H \in \mathfrak{t}$. For any $\alpha \in \Delta$, $\sum_{0\le j\le k-1} \theta^j(X_\alpha) \in \mathfrak{g}^\theta$ (since $\theta^k = 1$), so

$$\sum_{0\le j\le k-1} \theta^j(X_\alpha) = \tau\Bigg(\sum_{0\le j\le k-1} \theta^j(X_\alpha)\Bigg) = \sum_{0\le j\le k-1} \tau(\theta^j(X_\alpha)) = \sum_{0\le j\le k-1} e^{(\theta^j\alpha)H}\theta^j(X_\alpha).$$

Since each $\theta^j(X_\alpha)$ is of the form $\theta^j(X_\alpha) = b_j X_{\theta^j\alpha}$ for some $b_j \ne 1$, the last equality implies $\tau(X_\alpha) = X_\alpha$ if $\{\theta^j\alpha, 0 \le j \le k-1\}$ are distinct.

Claim 4.3. *Those $\alpha \in \Delta$ with roots in $\{\theta^j\alpha, 0 \le j \le k-1\}$ pairwise different generate Δ (as a root system).*

Since $\tau(X_\alpha) = X_\alpha$ when the elements $\theta^j\alpha$ are distinct for $0 \le j \le k-1$, by Claim 4.3, we have $\tau(X_\alpha) = X_\alpha$ for any $\alpha \in \Delta$. Hence $\tau = 1$, which is to say, $Z_{\mathrm{Int}(\mathfrak{g})}(\mathrm{Int}(\mathfrak{g})_0^\theta) = 1$. □

Proof of Claim 4.3. Note that θ maps Δ^+ to itself, so it maps the simple system $\Pi = \{\alpha_1, \dots, \alpha_r\}$ to itself. We have four cases to consider, that is, $\Delta = \mathrm{A}_n$ ($n \ge 2$), D_n ($n \ge 4$), E_6 and θ is an automorphism of order 2, or $\Delta = \mathrm{D}_4$ and θ is an automorphism of order 3. We give the proof when $\Delta = \mathrm{A}_{2n}$ ($n \ge 1$) and $o(\theta) = 2$. The proof for other cases is similar.

When $\Delta = \mathrm{A}_{2n}$ $(n \geq 1)$ and $o(\theta) = 2$, we have $\theta(\alpha_i) = \alpha_{2n+1-i}$ and $\theta(\alpha_{2n+1-i}) = \alpha_i$ for any i, $1 \leq i \leq n$. For $1 \leq i \leq n$, let

$$\beta_i = \sum_{1 \leq j \leq i} \alpha_j \quad \text{and} \quad \beta_i' = \sum_{1 \leq j \leq i} \alpha_{2n+1-j}.$$

Then $\theta(\pm\beta_i) \neq \pm\beta_i$, $\theta(\pm\beta_i') \neq \pm\beta_i'$ and $\{\pm\beta_i, \pm\beta_i' : 1 \leq i \leq n\}$ generate Δ. □

Corollary 4.4. *Let $\mathfrak{u}_0$ be a compact simple Lie algebra. If $\theta \in \mathrm{Aut}(\mathfrak{u}_0)$ satisfies the condition $o(\theta) = o(\theta\,\mathrm{Int}(\mathfrak{u}_0))$, then $Z_{\mathrm{Int}(\mathfrak{u}_0)}(\mathrm{Int}(\mathfrak{u}_0)_0^\theta) = 1$.*

Corollary 4.4 indicates that if G is a compact (simple) Lie group of adjoint type and x is of minimal possible order among all elements in the connected component containing it, then $(G^x)_0$ is also of adjoint type and the conjugation action of any element $y \in G^x - (G^x)_0$ on $(G^x)_0$ is an outer automorphism.

5. Symmetric subgroups of $\mathrm{Aut}(\mathfrak{u}_0)$

Let $\mathfrak{u}_0$ be a compact simple Lie algebra. For each conjugacy class of involutions in $\mathrm{Aut}(\mathfrak{u}_0)$, we choose a representative θ as in Section 3 and determine the symmetric subgroup $\mathrm{Aut}(\mathfrak{u}_0)^\theta$.

When $\mathfrak{u}_0$ is a classical simple Lie algebra nonisomorphic to $\mathfrak{so}(8)$ or $\mathfrak{u}_0 = \mathfrak{so}(8)$ but $\theta \not\sim \mathrm{Ad}(I_{4,4})$, we can use matrices to represent involutions θ and calculate the corresponding $\mathrm{Aut}(\mathfrak{u}_0)^\theta$. In the case of $\theta = \mathrm{Ad}(I_{4,4}) \in \mathrm{Aut}(\mathfrak{so}(8))$, we have $\theta \sim \exp(\pi i H_2')$. Then

$$\mathrm{Int}(\mathfrak{so}(8))^\theta = (\mathrm{Sp}(1)^4/Z') \rtimes D,$$

where $Z' = \{(\epsilon_1, \epsilon_2, \epsilon_3, \epsilon_4) \mid \epsilon_i = \pm 1, \epsilon_1\epsilon_2\epsilon_3\epsilon_4 = 1\}$, and $D \subset S_4$ is the (unique) normal order four subgroup of S_4 with conjugation action on $(\mathrm{Sp}(1)^4)/Z'$ by permutations. Then we observe that there exists a subgroup of $\mathrm{Aut}(\mathfrak{so}(8))$ that projects isomorphically to $\mathrm{Aut}(\mathfrak{so}(8))/\mathrm{Int}(\mathfrak{so}(8)) \cong S_3$ and is contained in $\mathrm{Aut}(\mathfrak{so}(8))^\theta$. A little more argument shows

$$\mathrm{Aut}(\mathfrak{so}(8))^\theta = (\mathrm{Sp}(1)^4/Z') \rtimes S_4.$$

When $\mathfrak{u}_0$ is an exceptional simple Lie algebra, we first determine the symmetric subalgebra $\mathfrak{k}_0 = \mathfrak{u}_0^\theta$ and the highest weights of the isotropic space $\mathfrak{p}_0 = \mathfrak{u}_0^{-\theta}$ as a $\mathfrak{k}_0$-module. The results are summarized in Table 1. The coroots H_i' are defined in (2) and (5) and the involutions are defined in Section 3.

Since any element of $\mathrm{Aut}(\mathfrak{u}_0)^\theta$ which acts trivially on both $\mathfrak{k}_0$ and $\mathfrak{p}_0$ must be trivial, the isomorphism type of $\mathfrak{k}_0$ and its isotropic module $\mathfrak{p}$ determine $\mathrm{Aut}(\mathfrak{u}_0)_0^\theta$ completely. We may get $\mathrm{Aut}(\mathfrak{u}_0)_0^\theta$ in the following way. Start with a compact connected Lie group H of the form $H = A \times H_s$ with $A = Z(\mathrm{Aut}(\mathfrak{u}_0)_0^\theta)_0$ a connected torus ($A \cong \mathrm{U}(1)^s$ with $s = \dim \mathfrak{z}(\mathfrak{k}_0)$) and H_s a connected and simply connected

	θ	$\mathfrak{k}_0$	$\mathfrak{p}$
EI	$\sigma_4 = \tau \exp(\pi i H_2')$	$\mathfrak{sp}(4)$	V_{ω_4}
EII	$\sigma_1 = \exp(\pi i H_2')$	$\mathfrak{su}(6) \oplus \mathfrak{sp}(1)$	$\bigwedge^3 \mathbb{C}^6 \otimes \mathbb{C}^2$
EIII	$\sigma_2 = \exp(\pi i (H_1' + H_6'))$	$\mathfrak{so}(10) \oplus i\mathbb{R}$	$(M_+ \otimes 1) \oplus (M_- \otimes \overline{1})$
EIV	$\sigma_3 = \tau$	$\mathfrak{f}_4$	V_{ω_4}
EV	$\sigma_3 = \exp(\pi i (H_1' + H_0'))$	$\mathfrak{su}(8)$	$\bigwedge^4 \mathbb{C}^8$
EVI	$\sigma_1 = \exp(\pi i H_2')$	$\mathfrak{so}(12) \oplus \mathfrak{sp}(1)$	$M_+ \otimes \mathbb{C}^2$
EVII	$\sigma_2 = \exp(\pi i H_0')$	$\mathfrak{e}_6 \oplus i\mathbb{R}$	$(V_{\omega_1} \otimes 1) \oplus (V_{\omega_6} \otimes \overline{1})$
EVIII	$\sigma_2 = \exp(\pi i (H_1' + H_2'))$	$\mathfrak{so}(16)$	M_+
EIX	$\sigma_1 = \exp(\pi i H_1')$	$\mathfrak{e}_7 \oplus \mathfrak{sp}(1)$	$V_{\omega_7} \otimes \mathbb{C}^2$
FI	$\sigma_1 = \exp(\pi i H_1')$	$\mathfrak{sp}(3) \oplus \mathfrak{sp}(1)$	$V_{\omega_3} \otimes \mathbb{C}^2$
FII	$\sigma_2 = \exp(\pi i H_4')$	$\mathfrak{so}(9)$	M
G	$\sigma = \exp(\pi i H_1')$	$\mathfrak{sp}(1) \oplus \mathfrak{sp}(1)$	$\mathrm{Sym}^3 \mathbb{C}^2 \otimes \mathbb{C}^2$

Table 1. Symmetric pairs and isotropic modules (exceptional Lie algebras case).

compact Lie group with Lie $H_s = [\mathfrak{k}_0, \mathfrak{k}_0]$ (then Lie $H = \mathfrak{k}_0 = \mathfrak{u}_0^\theta$). Then we have a surjective homomorphism

$$\pi : H \to \mathrm{Aut}(\mathfrak{u}_0)$$

determined by $\mathfrak{g}$ as a $\mathfrak{k}_0$-module. With this construction, it is clear that $\mathrm{Im}(\pi) = \mathrm{Aut}(\mathfrak{u}_0)_0^\theta$ and $\ker \pi$ is determined by $\mathfrak{k}_0$ and its module $\mathfrak{p}$ (as described in Table 1). By Proposition 4.1 and Corollary 4.4, we can also determine the number of connected components of $\mathrm{Aut}(\mathfrak{u}_0)^\theta$. Then we could find elements outside $\mathrm{Aut}(\mathfrak{u}_0)_0^\theta$ to generate $\mathrm{Aut}(\mathfrak{u}_0)^\theta$ together with $\mathrm{Aut}(\mathfrak{u}_0)_0^\theta$. We show the detailed argument in most cases below. The results about the symmetric subgroups $\mathrm{Aut}(\mathfrak{u}_0)^\theta$ are given in the last column of Table 2. The information about the first three columns of Table 2 is contained in [Knapp 2002, pp. 408–426]. The fourth column is from Section 3.

5A. ***Type* $\mathbf{E_6}$.** Now $\mathfrak{u}_0 = \mathfrak{e}_6$. Consider an outer automorphism $\theta = \sigma_3$ or σ_4. By Corollary 4.4, any element in $\mathrm{Int}(\mathfrak{u}_0)^\theta - \mathrm{Aut}(\mathfrak{u}_0)_0^\theta$ acts on $\mathfrak{u}_0^\theta$ as an outer automorphism. Note that $\mathfrak{u}_0^\theta \cong \mathfrak{sp}(4)$ or $\mathfrak{f}_4$, so it has no outer automorphisms. By Corollary 4.4, it follows that $\mathrm{Int}(\mathfrak{u}_0)^\theta = \mathrm{Aut}(\mathfrak{u}_0)_0^\theta$ and $\mathrm{Aut}(\mathfrak{u}_0)^\theta = \mathrm{Aut}(\mathfrak{u}_0)_0^\theta \times \langle\theta\rangle$. Moreover, $\mathrm{Aut}(\mathfrak{u}_0)_0^\theta$ is of adjoint type by Corollary 4.4.

Consider an inner automorphism $\theta = \sigma_1$ or σ_2. Let $\theta' \in \mathrm{E}_6$ be an involution which maps to θ under the covering $\pi : \mathrm{E}_6 \to \mathrm{Int}(\mathfrak{e}_6)$. We have

$$\mathrm{Int}(\mathfrak{e}_6)^\theta = \{g \in \mathrm{E}_6 \mid \theta' g \theta'^{-1} g^{-1} \in Z(\mathrm{E}_6)\}/Z(\mathrm{E}_6),$$

$$\mathrm{Int}(\mathfrak{e}_6)_0^\theta = \{g \in \mathrm{E}_6 \mid \theta' g \theta'^{-1} g^{-1} = 1\}/Z(\mathrm{E}_6),$$

Type	$(\mathfrak{u}_0, \mathfrak{k}_0)$	rank	θ	symmetric subgroup $\mathrm{Aut}(\mathfrak{u}_0)^\theta$
AI	$(\mathfrak{su}(n), \mathfrak{so}(n))$	$n-1$	$\overline{X}$	$(O(n)/\langle -I\rangle)\times\langle\theta\rangle$
AII	$(\mathfrak{su}(2n), \mathfrak{sp}(n))$	$n-1$	$J_n\overline{X}J_n^{-1}$	$(\mathrm{Sp}(n)/\langle -I\rangle)\times\langle\theta\rangle$
AIII $p<q$	$(\mathfrak{su}(p+q), \mathfrak{s}(\mathfrak{u}(p)+\mathfrak{u}(q)))$	p	$I_{p,q}XI_{p,q}$	$(S(U(p)\times U(q))/Z_{p+q})\rtimes\langle\tau\rangle$ $\mathrm{Ad}(\tau)=$ complex conjugation
AIII $p=q$	$(\mathfrak{su}(2p), \mathfrak{s}(\mathfrak{u}(p)+\mathfrak{u}(p)))$	p	$I_{p,p}XI_{p,p}$	$(S(U(p)\times U(p))/Z_{2p})\rtimes\langle\tau, J_p\rangle$ $\mathrm{Ad}(J_p)(X,Y)=(Y,X)$
BDI $p<q$	$(\mathfrak{so}(p+q), \mathfrak{so}(p)+\mathfrak{so}(q))$	p	$I_{p,q}XI_{p,q}$	$(O(p)\times O(q))/\langle(-I_p,-I_q)\rangle$
DI $p>4$	$(\mathfrak{so}(2p), \mathfrak{so}(p)+\mathfrak{so}(p))$	p	$I_{p,p}XI_{p,p}$	$((O(p)\times O(p))/\langle(-I_p,-I_p)\rangle)\rtimes\langle J_p\rangle$ $\mathrm{Ad}(J_p)(X,Y)=(Y,X)$
DI $p=4$	$(\mathfrak{so}(8), \mathfrak{so}(4)+\mathfrak{so}(4))$	4	$I_{4,4}XI_{4,4}$	$((\mathrm{Sp}(1)^4)/Z')\rtimes S_4$ S_4 acts by permutations
DIII	$(\mathfrak{so}(2n), \mathfrak{u}(n))$	n	$J_nXJ_n^{-1}$	$(U(n)/\{\pm I\})\rtimes\langle I_{n,n}\rangle$ $\mathrm{Ad}(I_{n,n})=$ complex conjugation
CI	$(\mathfrak{sp}(n), \mathfrak{u}(n))$	n	$(\mathbf{i}I)X(\mathbf{i}I)^{-1}$	$(U(n)/\{\pm I\})\rtimes\langle\mathbf{j}I\rangle$ $\mathrm{Ad}(\mathbf{j}I)=$ complex conjugation
CII $p<q$	$(\mathfrak{sp}(p+q), \mathfrak{sp}(p)+\mathfrak{sp}(q))$	p	$I_{p,q}XI_{p,q}$	$(\mathrm{Sp}(p)\times\mathrm{Sp}(q))/\langle(-I_p,-I_q)\rangle$
CII $p=q$	$(\mathfrak{sp}(2p), \mathfrak{sp}(p)+\mathfrak{sp}(p))$	p	$I_{p,p}XI_{p,p}$	$((\mathrm{Sp}(p)\times\mathrm{Sp}(p)/\langle(-I_p,-I_p)\rangle)\rtimes\langle J_p\rangle$ $\mathrm{Ad}(J_p)(X,Y)=(Y,X)$
EI	$(\mathfrak{e}_6, \mathfrak{sp}(4))$	6	σ_4	$(\mathrm{Sp}(4)/\langle -1\rangle)\times\langle\theta\rangle$
EII	$(\mathfrak{e}_6, \mathfrak{su}(6)+\mathfrak{sp}(1))$	4	σ_1	$(SU(6)\times\mathrm{Sp}(1)/\langle(e^{\frac{2\pi i}{3}}I,1),(-I,-1)\rangle)\rtimes\langle\tau\rangle$ $\mathfrak{k}_0^\tau=\mathfrak{sp}(3)\oplus\mathfrak{sp}(1)$
EIII	$(\mathfrak{e}_6, \mathfrak{so}(10)+i\mathbb{R})$	2	σ_2	$(\mathrm{Spin}(10)\times U(1)/\langle(c,i)\rangle)\rtimes\langle\tau\rangle$ $\mathfrak{k}_0^\tau=\mathfrak{so}(9)$
EIV	$(\mathfrak{e}_6, \mathfrak{f}_4)$	2	σ_3	$F_4\times\langle\theta\rangle$
EV	$(\mathfrak{e}_7, \mathfrak{su}(8))$	7	σ_3	$(SU(8)/\langle iI\rangle)\rtimes\langle\omega\rangle$ $\mathfrak{k}_0^\omega=\mathfrak{sp}(4)$
EVI	$(\mathfrak{e}_7, \mathfrak{so}(12)+\mathfrak{sp}(1))$	4	σ_1	$(\mathrm{Spin}(12)\times\mathrm{Sp}(1))/\langle(c,1),(-1,-1)\rangle$
EVII	$(\mathfrak{e}_7, \mathfrak{e}_6+i\mathbb{R})$	3	σ_2	$((E_6\times U(1))/\langle(c,e^{\frac{2\pi i}{3}})\rangle)\rtimes\langle\omega\rangle$ $\mathfrak{k}_0^\omega=\mathfrak{f}_4$
EVIII	$(\mathfrak{e}_8, \mathfrak{so}(16))$	8	σ_2	$\mathrm{Spin}(16)/\langle c\rangle$
EIX	$(\mathfrak{e}_8, \mathfrak{e}_7+\mathfrak{sp}(1))$	4	σ_1	$E_7\times\mathrm{Sp}(1)/\langle(c,-1)\rangle$
FI	$(\mathfrak{f}_4, \mathfrak{sp}(3)+\mathfrak{sp}(1))$	4	σ_1	$(\mathrm{Sp}(3)\times\mathrm{Sp}(1))/\langle(-I,-1)\rangle$
FII	$(\mathfrak{f}_4, \mathfrak{so}(9))$	1	σ_2	$\mathrm{Spin}(9)$
G	$(\mathfrak{g}_2, \mathfrak{sp}(1)+\mathfrak{sp}(1))$	2	σ	$(\mathrm{Sp}(1)\times\mathrm{Sp}(1))/\langle(-1,-1)\rangle$

Table 2. Symmetric pairs and symmetric subgroups. (When $n=4$, DIII is identical to BDI when $p=2$ and $q=6$.)

(use Proposition 4.1 here). If $\{g \in \mathrm{E}_6 \mid \theta' g \theta'^{-1} g^{-1} \in Z(\mathrm{E}_6)\} \neq \mathrm{E}_6^{\theta}$, then there exists $g \in \mathrm{E}_6$ such that $\theta' g \theta'^{-1} g^{-1} = c \in Z(E_6)$. Then $g\theta' g^{-1} = \theta' c^{-1}$. But $o(\theta') = 2 \neq 6 = o(\theta' c^{-1})$. So $g\theta' g^{-1} \neq \theta' c^{-1}$. Then $\{g \in \mathrm{E}_6 \mid \theta(g) g^{-1} \in Z(\mathrm{E}_6)\} = \mathrm{E}_6^{\theta}$ and so $\mathrm{Int}(\mathfrak{e}_6)^{\theta} = \mathrm{Int}(\mathfrak{e}_6)_0^{\theta}$. Since σ_1, σ_2 commutes with τ,

$$\mathrm{Aut}(\mathfrak{e}_6)^{\theta} = \mathrm{Int}(\mathfrak{e}_6)_0^{\theta} \rtimes \langle \tau \rangle.$$

The conjugation action of τ on $\mathrm{Int}(\mathfrak{e}_6)_0^{\theta}$ is determined by its action on $\mathfrak{k}_0 = \mathfrak{u}_0^{\theta}$, and

$$(\mathfrak{e}_6^{\sigma_1})^{\tau} = \mathfrak{sp}(3) \oplus \mathfrak{sp}(1), \quad (\mathfrak{e}_6^{\sigma_2})^{\tau} = \mathfrak{so}(9).$$

5B. *Type* E₇. Now $\mathfrak{u}_0 = \mathfrak{e}_7$ and $\mathrm{Aut}(\mathfrak{e}_7) = \mathrm{Int}(\mathfrak{e}_7)$ is connected. Let $\pi : \mathrm{E}_7 \to \mathrm{Aut}(\mathfrak{e}_7)$ be the adjoint homomorphism, which is a 2-fold covering. Let

$$\begin{aligned} \sigma_1' &= \exp(\pi i H_2') \in \mathrm{E}_7, \\ \sigma_2' &= \exp\left(\pi i \frac{H_2' + H_5' + H_7'}{2}\right) \in \mathrm{E}_7, \\ \sigma_3' &= \exp\left(\pi i \frac{2H_1' + H_2' + H_5' + H_7'}{2}\right) \in \mathrm{E}_7 . \end{aligned}$$

Then $\pi(\sigma_i') = \sigma_i$, $o(\sigma_1') = 2$, $o(\sigma_2') = 4$ and $o(\sigma_3') = 4$. One has

$$\begin{aligned} \mathrm{Aut}(\mathfrak{e}_7)^{\sigma_i} &\cong \{g \in \mathrm{E}_7 \mid g\sigma_i' g^{-1} \sigma_i'^{-1} \in Z(\mathrm{E}_7)\}/Z(\mathrm{E}_7), \\ \mathrm{Aut}(\mathfrak{e}_7)_0^{\sigma_i} &\cong \{g \in \mathrm{E}_7 \mid g\sigma_i' g^{-1} \sigma_i'^{-1} = 1\}/Z(\mathrm{E}_7) \end{aligned}$$

(use Proposition 4.1 here), where $Z(\mathrm{E}_7) = \langle \exp(\pi i (H_2' + H_5' + H_7')) \rangle \cong \mathbb{Z}/2\mathbb{Z}$ is the center of E_7.

For $\theta = \sigma_1$, suppose that there exists $g \in \mathrm{E}_7$ such that

$$g\sigma_1' g^{-1} (\sigma_1')^{-1} = \exp(\pi i (H_2' + H_5' + H_7')).$$

Then $g \exp(\pi i H_2') g^{-1} = \exp(\pi i (H_5' + H_7'))$. Then there exists $w \in W$ such that $w(\exp(\pi i H_2')) = \exp(\pi i (H_5' + H_7'))$. Since $w(\exp(\pi i H_{\alpha_2}')) = \exp(\pi i H_{w(\alpha_2)}')$, we get $\exp(\pi i H_{w(\alpha_2)}') = \exp(\pi i (H_5' + H_7'))$. Then

$$w(\alpha_2) \in (\alpha_5 + \alpha_7) + 2\,\mathrm{span}_{\mathbb{Z}}\{\alpha_1, \alpha_2, \alpha_3, \alpha_4, \alpha_5, \alpha_6, \alpha_7\}.$$

There are no roots in $(\alpha_5 + \alpha_7) + 2\,\mathrm{span}_{\mathbb{Z}}\{\alpha_1, \alpha_2, \alpha_3, \alpha_4, \alpha_5, \alpha_6, \alpha_7\}$, so there are no $g \in \mathrm{E}_7$ such that $(g\sigma_1' g^{-1})\sigma_1'^{-1} = \exp(\pi i (H_2' + H_5' + H_7'))$. Then

$$\{g \in \mathrm{E}_7 \mid (g\sigma_1' g^{-1})\sigma_1'^{-1} \in Z(\mathrm{E}_7)\} = \mathrm{E}_7^{\sigma_1'} .$$

So $\mathrm{Aut}(\mathfrak{e}_7)^{\sigma_1} = \mathrm{Aut}(\mathfrak{e}_7)_0^{\sigma_1}$.

For $\theta = \sigma_2$ or σ_3, let

$$\omega = \exp\left(\frac{\pi (X_{\alpha_2} - X_{-\alpha_2})}{2}\right) \exp\left(\frac{\pi (X_{\alpha_5} - X_{-\alpha_5})}{2}\right) \exp\left(\frac{\pi (X_{\alpha_7} - X_{-\alpha_7})}{2}\right).$$

Then

$$\omega\sigma_2'\omega^{-1} = \sigma_2'^{-1} = \sigma_2' \exp(\pi i (H_2' + H_5' + H_7')),$$
$$\omega\sigma_3'\omega^{-1} = \sigma_3'^{-1} = \sigma_3' \exp(\pi i (H_2' + H_5' + H_7')),$$

and $\omega^2 = 1$. Then $\mathrm{Aut}(\mathfrak{e}_7)^\theta = \mathrm{Aut}(\mathfrak{e}_7)_0^\theta \rtimes \langle\omega\rangle$. The conjugation action of ω on $\mathrm{Aut}(\mathfrak{e}_7)_0^\theta$ is determined by its action on $\mathfrak{k}_0 = \mathfrak{u}_0^\theta$, and we have

$$(\mathfrak{e}_7^{\sigma_2})^\omega = \mathfrak{f}_4, \qquad (\mathfrak{e}_7^{\sigma_3})^\omega = \mathfrak{sp}(4).$$

Further, ω acts on $\mathfrak{h}$ as $s_{\alpha_2} s_{\alpha_5} s_{\alpha_7}$, where s_α in the Weyl group is the reflection corresponding to the root α.

5C. ***Types* E₈, F₄, G₂.** If $\mathfrak{u}_0 = \mathfrak{e}_8, \mathfrak{f}_4, \mathfrak{g}_2$, then $\mathrm{Aut}(\mathfrak{u}_0)$ is connected and simply connected. By Proposition 4.1, $\mathrm{Aut}(\mathfrak{u}_0)^\theta$ is connected. Then they are determined by $\mathfrak{u}_0^\theta$ and $\mathfrak{p} = \mathfrak{g}^{-\theta}$.

6. Klein four-subgroups of $\mathrm{Aut}(\mathfrak{u}_0)$

In this section, we classify Klein four-subgroups Γ (called simply Klein subgroups) in $\mathrm{Aut}(\mathfrak{u}_0)$ up to conjugation. We also determine the fixed-point subgroups $\mathrm{Aut}(\mathfrak{u}_0)^\Gamma$. Note that such a Γ is equal to $\{1, \theta, \sigma, \theta\sigma\}$ for two commuting involutions $\theta \neq \sigma$. Fix an involution θ; the conjugacy class of Γ is determined by the conjugacy classes of the involution $\sigma(\neq \theta)$ in $\mathrm{Aut}(\mathfrak{u}_0)^\theta$.

6A. ***Ordered commuting pairs of involutions and semisimple symmetric pairs.*** For a compact simple Lie algebra $\mathfrak{u}_0$ and its complexification $\mathfrak{g}$, the isomorphism classes of semisimple symmetric pairs $(\mathfrak{g}_0, \mathfrak{h}_0)$ with $\mathfrak{g}_0$ a real form of $\mathfrak{g}$ and $\mathfrak{h}_0(\neq \mathfrak{g}_0)$ noncompact are in one-to-one correspondence with the conjugacy classes of ordered commuting pairs of involutions (θ, σ) in $\mathrm{Aut}(\mathfrak{u}_0)$ with $\theta \neq \sigma$. One direction of this correspondence is as follows: let $\mathfrak{u}_{i,j}$ $(i, j = 0 \text{ or } 1)$ be the joint eigenspace of θ and σ where θ acts on it as $(-1)^i$ and σ acts on it as $(-1)^j$. Then we have a decomposition

$$\mathfrak{u}_0 = \mathfrak{u}_{0,0} \oplus \mathfrak{u}_{0,1} \oplus \mathfrak{u}_{1,0} \oplus \mathfrak{u}_{1,1}.$$

Then $\mathfrak{k}_0 = \mathfrak{u}_0^\theta = \mathfrak{u}_{0,0} \oplus \mathfrak{u}_{0,1}$ and $i\mathfrak{p}_0 = \mathfrak{u}_0^{-\theta} = \mathfrak{u}_{1,0} \oplus \mathfrak{u}_{1,1}$. Extend θ, σ to holomorphic automorphisms of $\mathfrak{g}$ and let

$$\mathfrak{g}_0 = \mathfrak{k}_0 + \mathfrak{p}_0 = \mathfrak{u}_{0,0} + \mathfrak{u}_{0,1} + i(\mathfrak{u}_{1,0} + \mathfrak{u}_{1,1}) \quad \text{and} \quad \mathfrak{h}_0 = \mathfrak{g}_0^\sigma = \mathfrak{u}_{0,0} + i\mathfrak{u}_{1,0}.$$

Then $\mathfrak{g}_0$ is a real form of $\mathfrak{g}$ and $(\mathfrak{g}_0, \mathfrak{h}_0)$ is a semisimple symmetric pair with $\mathfrak{h}_0 \neq \mathfrak{g}_0$ and noncompact. The other direction of this correspondence needs a more sophisticated argument.

When θ is fixed, the conjugacy classes of the pairs (θ, σ) in $\mathrm{Aut}(\mathfrak{u}_0)$ are in one-to-one correspondence with the $\mathrm{Aut}(\mathfrak{u}_0)^\theta$-conjugacy classes of involutions in $\mathrm{Aut}(\mathfrak{u}_0)^\theta - \{\theta\}$.

$\mathfrak{u}_0$	Γ_i	$\mathfrak{l}_0=\mathfrak{u}_0^{\Gamma_i}$	Type
$\mathfrak{su}(p+q)$	$\Gamma_{p,q}=\langle\tau,I_{p,q}\rangle$	$\mathfrak{so}(p)+\mathfrak{so}(q)$	**AI-AI-AIII**, S
$\mathfrak{su}(2p)$	$\Gamma_p=\langle\tau,J_p\rangle$	$\mathfrak{u}(p)$	**AI-AII-AIII**, N
$\mathfrak{su}(2p+2q)$	$\Gamma'_{p,q}=\langle\tau J_{p+q},I'_{p,q}\rangle$	$\mathfrak{sp}(p)+\mathfrak{sp}(q)$	**AII-AII-AIII**, S
$\mathfrak{su}(p+q+r+s)$	$\Gamma_{p,q,r,s}$	$\mathfrak{s}(\mathfrak{u}(p)+\mathfrak{u}(q)+\mathfrak{u}(r)+\mathfrak{u}(s))$	**AIII-AIII-AIII**, NSV
$\mathfrak{su}(2p)$	$\Gamma_p=\langle I_{p,p},J_p\rangle$	$\mathfrak{su}(p)$	**AIII-AIII-AIII**, V
$\mathfrak{so}(p+q+r+s)$	$\Gamma_{p,q,r,s}$	$\mathfrak{so}(p)+\mathfrak{so}(q)+\mathfrak{so}(r)+\mathfrak{so}(s))$	**BDI-BDI-BDI**, NSV
$\mathfrak{so}(2p)$	$\Gamma_p=\langle J_p,I_{p,p}\rangle$	$\mathfrak{so}(p)$	**DI-DI-DIII**, S
$\mathfrak{so}(2p+2q)$	$\Gamma_{p,q}=\langle J_{p+q},I'_{p,q}\rangle$	$\mathfrak{u}(p)+\mathfrak{u}(q)$	**DI-DIII-DIII**, S
$\mathfrak{so}(4p)$	$\Gamma'_p=\langle J_{2p},K_p\rangle$	$\mathfrak{sp}(p)$	**DIII-DIII-DIII**, V
$\mathfrak{sp}(p)$	$\Gamma_p=\langle\mathbf{i}I,\mathbf{j}I\rangle$	$\mathfrak{so}(p)$	**CI-CI-CI**, V
$\mathfrak{sp}(p+q)$	$\Gamma_{p,q}=\langle\mathbf{i}I,I_{p,q}\rangle$	$\mathfrak{u}(p)+\mathfrak{u}(q)$	**CI-CI-CII**, S
$\mathfrak{sp}(2p)$	$\Gamma'_p=\langle\mathbf{i}I,\mathbf{j}J_p\rangle$	$\mathfrak{sp}(p)$	**CI-CII-CII**, S
$\mathfrak{sp}(p+q+r+s)$	$\Gamma_{p,q,r,s}$	$\mathfrak{sp}(p)+\mathfrak{sp}(q)+\mathfrak{sp}(r)+\mathfrak{sp}(s)$	**CII-CII-CII**, NSV

Table 3. Klein subgroups in $\mathrm{Aut}(\mathfrak{u}_0)$ for the classical cases. (When $p=1$, $q=3$, $\Gamma_{1,3}$ is very special since $\mathrm{Ad}(I_{2,6})\sim\mathrm{Ad}(J_4)$.)

For an exceptional compact simple Lie algebra $\mathfrak{u}_0$ and any representative θ of involution classes in Section 3, we give the representatives of classes of involutions in $\mathrm{Aut}(\mathfrak{u}_0)^\theta-\{\theta\}$ and identify their classes in $\mathrm{Aut}(\mathfrak{u}_0)$. For any classical compact simple Lie algebra $\mathfrak{u}_0$ and a representative θ of an involution class, we have a similar classification of involutions in $\mathrm{Aut}(\mathfrak{u}_0)^\theta-\{\theta\}$; we omit it here but remark that the representatives can be constructed from Table 3. This gives a new proof to Berger's classification of semisimple symmetric pairs.

In most cases the symmetric subgroup $\mathrm{Aut}(\mathfrak{u}_0)^\theta$ is a product of classical groups with some twisting, for which we can classify their involution classes by matrix calculations. In the remaining cases, $\mathfrak{u}_0^\theta=\mathfrak{s}_0\oplus\mathfrak{z}$ for an exceptional simple Lie algebra $\mathfrak{s}_0$ and an algebra $\mathfrak{z}=0$, $i\mathbb{R}$ or $\mathfrak{sp}(1)$. We have a homomorphism

$$p:\mathrm{Aut}(\mathfrak{u}_0)^\theta\to\mathrm{Aut}(\mathfrak{s}_0).$$

Then what we need to do is to classify involutions in $p^{-1}(\sigma)$ for $\sigma\in\mathrm{Aut}(\mathfrak{s}_0)$ an involution or the identity element, which is not hard in general.

For an exceptional compact simple Lie algebra $\mathfrak{u}_0$, the conjugacy class of an involution $\sigma\in\mathrm{Aut}(\mathfrak{u}_0)$ is determined by $\dim\mathfrak{g}^\sigma$. (This is an accidental phenomenon observed by Helgason [2001, pp. 517–518].) For any involution $\sigma\in\mathrm{Aut}(\mathfrak{u}_0)^\theta-\{\theta\}$, the class of σ in $\mathrm{Aut}(\mathfrak{u}_0)$ is determined by $\dim\mathfrak{g}^\sigma=\dim\mathfrak{k}^\sigma+\dim\mathfrak{p}^\sigma$ and the dimensions $\dim\mathfrak{k}^\sigma$, $\dim\mathfrak{p}^\sigma$ can be calculated from the class of σ in $\mathrm{Aut}(\mathfrak{u}_0)^\theta$. The coroots H'_i are defined in (2) and (5) and the involutions σ_i, σ, τ are defined in Section 3.

Type $\mathbf{E_6}$. Now $\mathfrak{u}_0 = \mathfrak{e}_6$. For $\theta = \sigma_1 = \exp(\pi i H_2')$, one has

$$\mathrm{Aut}(\mathfrak{u}_0)^{\sigma_1} = (\mathrm{SU}(6) \times \mathrm{Sp}(1)/\langle (e^{2\pi i/3} I, 1), (-I, -1)\rangle) \rtimes \langle \tau \rangle,$$

$\sigma_1 = (I, -1) = (-I, 1)$, where $\mathrm{Ad}(\tau)(X, Y) = (J_3 \overline{X} J_3^{-1}, Y)$. Then, in $\mathrm{Aut}(\mathfrak{u}_0)$,

$$\left(\begin{pmatrix} -I_4 & 0 \\ 0 & I_2 \end{pmatrix}, 1\right) \sim \sigma_2, \quad \left(\begin{pmatrix} -I_2 & 0 \\ 0 & I_4 \end{pmatrix}, 1\right) \sim \sigma_1,$$

$$\left(\begin{pmatrix} iI_5 & 0 \\ 0 & -iI_1 \end{pmatrix}, \mathbf{i}\right) \sim \sigma_2, \quad \left(\begin{pmatrix} iI_3 & 0 \\ 0 & -iI_3 \end{pmatrix}, \mathbf{i}\right) \sim \sigma_1,$$

$$\tau \sim \sigma_3, \qquad \tau\sigma_1 \sim \sigma_4, \qquad \tau(J_3, \mathbf{i}) \sim \sigma_4.$$

These elements represent all the conjugacy classes of involutions in $\mathrm{Aut}(\mathfrak{u}_0)^\theta - \{\theta\}$.

For $\theta = \sigma_2 = \exp(\pi i (H_1' + H_6'))$, one has

$$\mathrm{Aut}(\mathfrak{u}_0)^{\sigma_2} = \big((\mathrm{Spin}(10) \times \mathrm{U}(1))/\langle (c, i)\rangle\big) \rtimes \langle \tau \rangle, \quad \sigma_2 = (-1, 1) = (1, -1),$$

where $c = e_1 e_2 \cdots e_{10}$ and $\mathrm{Ad}(\tau)(x, z) = ((e_1 e_2 \cdots e_9) x (e_1 e_2 \cdots e_9)^{-1}, z^{-1})$. Then, in $\mathrm{Aut}(\mathfrak{u}_0)$,

$$(e_1e_2e_3e_4, 1) \sim \sigma_1, \quad (e_1 e_2 \cdots e_8, 1) \sim \sigma_2,$$

$$\left(\delta, \frac{1+i}{\sqrt{2}}\right) \sim \sigma_2, \quad \left(-\delta, \frac{1+i}{\sqrt{2}}\right) \sim \sigma_1,$$

$$\tau \sim \sigma_3, \quad \tau(e_1e_2e_3e_4, 1) \sim \sigma_4,$$

where

$$\delta = \frac{1+e_1e_2}{\sqrt{2}} \frac{1+e_3e_4}{\sqrt{2}} \cdots \frac{1+e_9e_{10}}{\sqrt{2}}.$$

These elements represent all the conjugacy classes of involutions in $\mathrm{Aut}(\mathfrak{u}_0)^\theta - \{\theta\}$.

For $\theta = \sigma_3 = \tau$, one has $\mathrm{Aut}(\mathfrak{u}_0)^{\sigma_3} = \mathrm{F}_4 \times \langle \tau \rangle$. Let τ_1, τ_2 be involutions in F_4 with

$$\mathfrak{f}_4^{\tau_1} \cong \mathfrak{sp}(3) \oplus \mathfrak{sp}(1), \quad \mathfrak{f}_4^{\tau_2} \cong \mathfrak{so}(9).$$

Then, in $\mathrm{Aut}(\mathfrak{u}_0)$,

$$\tau_1 \sim \sigma_1, \quad \tau_2 \sim \sigma_2,$$

$$\sigma_3\tau_1 \sim \sigma_4, \quad \sigma_3\tau_2 \sim \sigma_3,$$

these elements represent all the conjugacy classes of involutions in $\mathrm{Aut}(\mathfrak{u}_0)^\theta - \{\theta\}$.

For $\theta = \sigma_4 = \tau \exp(\pi i H_2')$, one has $\mathrm{Aut}(\mathfrak{u}_0)^{\sigma_4} = (\mathrm{Sp}(4)/\langle -I\rangle) \times \langle \sigma_4 \rangle$. Let

$$\tau_1 = \mathbf{i} I, \quad \tau_2 = \begin{pmatrix} -I_2 & 0 \\ 0 & I_2 \end{pmatrix}, \quad \tau_3 = \begin{pmatrix} -1 & 0 \\ 0 & I_3 \end{pmatrix}.$$

Then, in $\mathrm{Aut}(\mathfrak{u}_0)$,

$$\tau_1 \sim \sigma_1, \qquad \tau_2 \sim \sigma_2, \qquad \tau_3 \sim \sigma_1,$$
$$\sigma_4\tau_1 \sim \sigma_4, \quad \sigma_4\tau_2 \sim \sigma_4, \quad \sigma_4\tau_3 \sim \sigma_3.$$

These elements represent all the conjugacy classes of involutions in $\mathrm{Aut}(\mathfrak{u}_0)^\theta - \{\theta\}$.

Type $\mathbf{E_7}$. Now $\mathfrak{u}_0 = \mathfrak{e}_7$. For $\theta = \sigma_1 = \exp(\pi i H_2')$, one has

$$\mathrm{Aut}(\mathfrak{u}_0)^{\sigma_1} = (\mathrm{Spin}(12) \times \mathrm{Sp}(1))/\langle (c, 1), (-1, -1)\rangle,$$

where $\sigma_1 = (-1, 1) = (1, -1)$, $c = e_1e_2 \cdots e_{12}$. Let

$$\delta = \frac{1+e_1e_2}{\sqrt{2}}\,\frac{1+e_3e_4}{\sqrt{2}}\cdots\frac{1+e_{11}e_{12}}{\sqrt{2}}.$$

Then, in $\mathrm{Aut}(\mathfrak{u}_0)$,

$$(e_1e_2e_3e_4, 1) \sim \sigma_1, \quad (e_1e_2, \mathbf{i}) \sim \sigma_2, \quad (e_1e_2\cdots e_6, \mathbf{i}) \sim \sigma_3,$$
$$(\delta, 1) \sim \sigma_2, \quad (-\delta, 1) \sim \sigma_3, \qquad (e_1\delta e_1, \mathbf{i}) \sim \sigma_1.$$

These elements represent all conjugacy classes of involutions in $\mathrm{Aut}(\mathfrak{u}_0)^\theta - \{\theta\}$. Moreover,

$$\langle \sigma_1, (e_1e_2e_3e_4, 1)\rangle \sim F_2, \quad \langle \sigma_1, (e_1\delta e_1, \mathbf{i})\rangle \sim F_1.$$

For $\theta = \sigma_2 = \tau = \exp\left(\pi i \frac{H_2'+H_5'+H_7'}{2}\right)$, one has

$$\mathrm{Aut}(\mathfrak{u}_0)_0^{\sigma_2} = ((\mathrm{E}_6 \times \mathrm{U}(1))/\langle (c, e^{\frac{2\pi i}{3}})\rangle) \rtimes \langle \omega\rangle,$$

where c is a nontrivial central element of E_6 with $o(c) = 3$, $\sigma_2 = (1, -1)$ and $(\mathfrak{e}_6 \oplus i\mathbb{R})^\omega = \mathfrak{f}_4 \oplus 0$. Let τ_1, τ_2 be involutions in E_6 with

$$\mathfrak{e}_6^{\tau_1} \cong \mathfrak{su}(6) \oplus \mathfrak{sp}(1), \quad \mathfrak{e}_6^{\tau_2} \cong \mathfrak{so}(10) \oplus i\mathbb{R}.$$

Then, in $\mathrm{Aut}(\mathfrak{u}_0)$,

$$\tau_1 \sim \sigma_1, \qquad \tau_2 \sim \sigma_1,$$
$$\tau_1\sigma_2 \sim \sigma_3, \quad \tau_2\sigma_2 \sim \sigma_2,$$
$$\omega \sim \sigma_2, \qquad \omega\eta \sim \sigma_3,$$

where $\eta \in \mathrm{F}_4 = \mathrm{E}_6^\omega$ is an involution with $(\mathfrak{f}_4)^\eta \cong \mathfrak{sp}(3) \oplus \mathfrak{sp}(1)$. These elements represent all the conjugacy classes of involutions in $\mathrm{Aut}(\mathfrak{u}_0)^\theta - \{\theta\}$.

For

$$\theta = \sigma_3 = \exp\left(\pi i \frac{H_2'+H_5'+H_7'+2H_1'}{2}\right),$$

one has

$$\mathrm{Aut}(\mathfrak{u}_0)_0^{\sigma_3} = (\mathrm{SU}(8)/\langle iI\rangle) \rtimes \langle \omega\rangle, \quad \sigma_3 = \frac{1+i}{\sqrt{2}}I,$$

where $\mathrm{Ad}(\omega)X = J_4 \overline{X} J_4^{-1}$. Let $\tau_1 = \begin{pmatrix} -I_2 & \\ & I_6 \end{pmatrix}$, $\tau_2 = \begin{pmatrix} -I_4 & \\ & I_4 \end{pmatrix}$. Then, in $\mathrm{Aut}(\mathfrak{u}_0)$,

$$\tau_1 \sim \sigma_1, \quad \tau_2 \sim \sigma_1, \quad \tau_1\sigma_3 \sim \sigma_2, \quad \tau_2\sigma_3 \sim \sigma_3,$$
$$\omega \sim \sigma_2, \quad \omega\sigma_3 \sim \sigma_3, \quad \omega J_4 \sim \sigma_3.$$

These elements represent all conjugacy classes of involutions in $\mathrm{Aut}(\mathfrak{u}_0)^\theta - \{\theta\}$.

Type $\mathbf{E_8}$. Now $\mathfrak{u}_0 = \mathfrak{e}_8$. For $\theta = \sigma_1 = \exp(\pi i H_2')$, one has

$$\mathrm{Aut}(\mathfrak{u}_0)^{\sigma_1} \cong (\mathrm{E}_7 \times \mathrm{Sp}(1))/\langle (c, -1)\rangle,$$

where $\sigma_1 = (1, -1) = (c, 1)$. Let τ_1, τ_2 denote the elements in E_7 with $\tau_1^2 = \tau_2^2 = c$ and $\mathfrak{e}_7^{\tau_1} \cong \mathfrak{e}_6 \oplus i\mathbb{R}$, $\mathfrak{e}_7^{\tau_2} \cong \mathfrak{su}(8)$. Let τ_3, τ_4 be involutions in E_7 such that there exist Klein subgroups $\Gamma, \Gamma' \subset E_7$ with three nonidentity elements in Γ all conjugate to τ_3, three nonidentity elements in Γ' all conjugate to τ_4, and $\mathfrak{e}_7^\Gamma \cong \mathfrak{su}(6) \oplus (i\mathbb{R})^2$, $\mathfrak{e}_7^{\Gamma'} \cong \mathfrak{so}(8) \oplus (\mathfrak{sp}(1))^3$. Then, in $\mathrm{Aut}(\mathfrak{u}_0)$,

$$(\tau_1, \mathbf{i}) \sim \sigma_1, \quad (\tau_2, \mathbf{i}) \sim \sigma_2, \quad (\tau_3, 1) \sim \sigma_1, \quad (\tau_4, 1) \sim \sigma_2.$$

These elements represent all conjugacy classes of involutions in $\mathrm{Aut}(\mathfrak{u}_0)^\theta - \{\theta\}$.

For $\theta = \sigma_2 = \exp(\pi i (H_2' + H_1'))$, one has $\mathrm{Aut}(\mathfrak{u}_0)^{\sigma_2} \cong \mathrm{Spin}(16)/\langle c\rangle$, where $\sigma_2 = -1$, $c = e_1 e_2 \cdots e_{16}$. Let

$$\delta = \frac{1+e_1e_2}{\sqrt{2}} \frac{1+e_3e_4}{\sqrt{2}} \cdots \frac{1+e_{15}e_{16}}{\sqrt{2}},$$
$$\tau_1 = e_1e_2e_3e_4, \quad \tau_2 = e_1e_2e_3\cdots e_8, \quad \tau_3 = \delta, \quad \tau_4 = -\delta.$$

Then, in $\mathrm{Aut}(\mathfrak{u}_0)$,

$$\tau_1 \sim \sigma_1, \quad \tau_2 \sim \sigma_2, \quad \tau_3 \sim \sigma_1, \quad \tau_4 \sim \sigma_2.$$

These elements represent all the conjugacy classes of involutions in $\mathrm{Aut}(\mathfrak{u}_0)^\theta - \{\theta\}$.

Type $\mathbf{F_4}$. When $\mathfrak{u}_0 = \mathfrak{f}_4$, for $\theta = \sigma_1 = \exp(\pi i H_1')$,

$$\mathrm{Aut}(\mathfrak{u}_0)^{\sigma_1} \cong \mathrm{Sp}(3) \times \mathrm{Sp}(1)/\langle(-I, -1)\rangle,$$

where $\sigma_1 = (-I, 1) = (I, -1)$. Let

$$\tau_1 = \left(\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, 1 \right), \quad \tau_2 = \left(\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, 1 \right), \quad \tau_3 = (\mathbf{i}I, \mathbf{i}).$$

Then, in $\mathrm{Aut}(\mathfrak{u}_0)$,

$$\tau_1 \sim \sigma_1, \quad \tau_2 \sim \sigma_2, \quad \tau_3 \sim \sigma_1.$$

These elements represent all conjugacy classes of involutions in $\mathrm{Aut}(\mathfrak{u}_0)^\theta - \{\theta\}$.

For $\theta = \sigma_2 = \exp(\pi i H_4')$, one has $\mathrm{Aut}(\mathfrak{u}_0)^{\sigma_2} \cong \mathrm{Spin}(9)$, $\sigma_2 = -1$. Let $\tau_1 = e_1e_2e_3e_4$, $\tau_2 = e_1e_2e_3\cdots e_8$. Then, in $\mathrm{Aut}(\mathfrak{u}_0)$, we have $\tau_1 \sim \sigma_1$ and $\tau_2 \sim \sigma_2$. These elements represent all conjugacy classes of involutions in $\mathrm{Aut}(\mathfrak{u}_0)^{\theta} - \{\theta\}$.

Type $\mathbf{G_2}$. When $\mathfrak{u}_0 = \mathfrak{g}_2$ and $\theta = \sigma = \exp(\pi i H_1')$, one has

$$\mathrm{Aut}(\mathfrak{u}_0)^{\sigma_1} \cong \mathrm{Sp}(1) \times \mathrm{Sp}(1)/\langle(-1, -1)\rangle,$$

where $\sigma_1 = (-1, 1) = (1, -1)$. Denote $\tau = (\mathbf{i}, \mathbf{i})$. Then, in $\mathrm{Aut}(\mathfrak{u}_0)$, we have $\tau \sim \sigma$, and τ represents the unique conjugacy class of involutions in $\mathrm{Aut}(\mathfrak{u}_0)^{\theta} - \{\theta\}$.

By the above, we have reproved Berger's classification of semisimple symmetric pairs. The next proposition is an immediate consequence of this classification.

Proposition 6.1. *There are* 23, 19, 8, 5, *and* 1 *isomorphism classes of nontrivial* (*that is*, $\mathfrak{h}_0 \neq \mathfrak{g}_0$) *semisimple symmetric pairs* $(\mathfrak{g}_0, \mathfrak{h}_0)$ *with* $\mathfrak{g}_0$ *noncompact and* $\mathfrak{g} = \mathfrak{g}_0 \otimes_{\mathbb{R}} \mathbb{C}$ *a complex simple Lie algebra of types* $\mathbf{E_6}$, $\mathbf{E_7}$, $\mathbf{E_8}$, $\mathbf{F_4}$, *and* $\mathbf{G_2}$, *respectively.*

6B. ***Klein subgroups, speciality, regularity and centralizers.*** For a Klein group $\Gamma \subset \mathrm{Aut}(\mathfrak{u}_0)$, we call the conjugacy classes of the involutions in Γ the *involution type* of Γ, and the classes of Riemannian symmetric pairs corresponding to the involutions in Γ the *symmetric space type* of Γ. Since there is a one-to-one correspondence between these two types, we simply say *type* of Γ for either involution type or symmetric space type.

For a compact simple Lie algebra $\mathfrak{u}_0$, a Klein subgroup Γ of $\mathrm{Aut}(\mathfrak{u}_0)$ is called *regular* if any two distinct conjugate (in $\mathrm{Aut}(\mathfrak{u}_0)$) elements $\sigma, \theta \in \Gamma$ are conjugate by an element $g \in \mathrm{Aut}(\mathfrak{u}_0)$ commuting with $\theta\sigma$ (that is, $g \in \mathrm{Aut}(\mathfrak{u}_0)^{\theta\sigma}$).

A Klein subgroup $\Gamma \subset \mathrm{Aut}(\mathfrak{u}_0)$ is called *special* if there are two (distinct) elements of Γ which are conjugate in $\mathrm{Aut}(\mathfrak{u}_0)$. It is called *very special* if three involutions of Γ are pairwise conjugate in $\mathrm{Aut}(\mathfrak{u}_0)$. Otherwise it is called nonspecial. The definition of special is due to [Ōshima and Sekiguchi 1984].

In Tables 3 and 4, we list some Klein subgroups $\Gamma_i \subset \mathrm{Aut}(\mathfrak{u}_0)$ for each compact simple Lie algebra $\mathfrak{u}_0$ together with their symmetric space types (when $\mathfrak{u}_0$ is classical) or involution types (when $\mathfrak{u}_0$ is exceptional). These subgroups are not conjugate to each other since their fixed point subalgebras $\mathfrak{u}_0^{\Gamma_i}$ are nonisomorphic. In the last column we also indicate whether they are special or not. For brevity, we write N to mean nonspecial, S to mean special but not very special, V to mean very special. The speciality of the subgroups $\Gamma_{p,q,r,s}$ depends on the parameters. In general they can be nonspecial, special or very special; in this case we use NSV to denote their speciality. The reader can determine for which parameters they are nonspecial, special or very special. The notation $I_{p,q}$, J_p, etc. is defined in Section 2C.

Theorem 6.2. *For a compact simple Lie algebra* $\mathfrak{u}_0$, *any Klein subgroup* $\Gamma \subset \mathrm{Aut}(\mathfrak{u}_0)$ *is conjugate to one in Table 3 or Table 4 and they are all regular.*

$\mathfrak{u}_0$	Γ_i	$\mathfrak{l}_0=\mathfrak{u}_0^{\Gamma_i}$	Type
$\mathfrak{e}_6$	$\Gamma_1=\langle\exp(\pi i H_2'),\exp(\pi i H_4')\rangle$	$(\mathfrak{su}(3))^2\oplus(i\mathbb{R})^2$	$(\sigma_1,\sigma_1,\sigma_1)$, V
$\mathfrak{e}_6$	$\Gamma_2=\langle\exp(\pi i H_4'),\exp(\pi i(H_3'+H_4'+H_5'))\rangle$	$\mathfrak{su}(4)\oplus(\mathfrak{sp}(1))^2\oplus i\mathbb{R}$	$(\sigma_1,\sigma_1,\sigma_2)$, S
$\mathfrak{e}_6$	$\Gamma_3=\langle\exp(\pi i(H_2'+H_1')),\exp(\pi i(H_4'+H_1'))\rangle$	$\mathfrak{su}(5)\oplus(i\mathbb{R})^2$	$(\sigma_1,\sigma_2,\sigma_2)$, S
$\mathfrak{e}_6$	$\Gamma_4=\langle\exp(\pi i(H_1'+H_6')),\exp(\pi i(H_3'+H_5'))\rangle$	$\mathfrak{so}(8)\oplus(i\mathbb{R})^2$	$(\sigma_2,\sigma_2,\sigma_2)$, V
$\mathfrak{e}_6$	$\Gamma_5=\langle\exp(\pi i H_2'),\tau\rangle$	$\mathfrak{sp}(3)\oplus\mathfrak{sp}(1)$	$(\sigma_1,\sigma_3,\sigma_4)$, N
$\mathfrak{e}_6$	$\Gamma_6=\langle\exp(\pi i H_2'),\tau\exp(\pi i H_4')\rangle$	$\mathfrak{so}(6)\oplus i\mathbb{R}$	$(\sigma_1,\sigma_4,\sigma_4)$, S
$\mathfrak{e}_6$	$\Gamma_7=\langle\exp(\pi i(H_1'+H_6')),\tau\rangle$	$\mathfrak{so}(9)$	$(\sigma_2,\sigma_3,\sigma_3)$, S
$\mathfrak{e}_6$	$\Gamma_8=\langle\exp(\pi i(H_1'+H_6')),\tau\exp(\pi i H_2')\rangle$	$\mathfrak{so}(5)\oplus\mathfrak{so}(5)$	$(\sigma_2,\sigma_4,\sigma_4)$, S
$\mathfrak{e}_7$	$\Gamma_1=\langle\exp(\pi i H_2'),\exp(\pi i H_4')\rangle$	$\mathfrak{su}(6)\oplus(i\mathbb{R})^2$	$(\sigma_1,\sigma_1,\sigma_1)$, V
$\mathfrak{e}_7$	$\Gamma_2=\langle\exp(\pi i H_2'),\exp(\pi i H_3')\rangle$	$\mathfrak{so}(8)\oplus(\mathfrak{sp}(1))^3$	$(\sigma_1,\sigma_1,\sigma_1)$, V
$\mathfrak{e}_7$	$\Gamma_3=\langle\exp(\pi i H_2'),\tau\rangle$	$\mathfrak{so}(10)\oplus(i\mathbb{R})^2$	$(\sigma_1,\sigma_2,\sigma_2)$, S
$\mathfrak{e}_7$	$\Gamma_4=\langle\exp(\pi i H_1'),\tau\rangle$	$\mathfrak{su}(6)\oplus\mathfrak{sp}(1)\oplus i\mathbb{R}$	$(\sigma_1,\sigma_2,\sigma_3)$, N
$\mathfrak{e}_7$	$\Gamma_5=\langle\exp(\pi i H_2'),\tau\exp(\pi i H_1')\rangle$	$\mathfrak{su}(4)\oplus\mathfrak{su}(4)\oplus i\mathbb{R}$	$(\sigma_1,\sigma_3,\sigma_3)$, S
$\mathfrak{e}_7$	$\Gamma_6=\langle\tau,\omega\rangle$	$\mathfrak{f}_4$	$(\sigma_2,\sigma_2,\sigma_2)$, V
$\mathfrak{e}_7$	$\Gamma_7=\langle\tau,\omega\exp(\pi i H_1')\rangle$	$\mathfrak{sp}(4)$	$(\sigma_2,\sigma_3,\sigma_3)$, S
$\mathfrak{e}_7$	$\Gamma_8=\langle\tau\exp(\pi i H_1'),\omega\exp(\pi i H_3')\rangle$	$\mathfrak{so}(8)$	$(\sigma_3,\sigma_3,\sigma_3)$, V
$\mathfrak{e}_8$	$\Gamma_1=\langle\exp(\pi i H_2'),\exp(\pi i H_4')\rangle$	$\mathfrak{e}_6\oplus(i\mathbb{R})^2$	$(\sigma_1,\sigma_1,\sigma_1)$, V
$\mathfrak{e}_8$	$\Gamma_2=\langle\exp(\pi i H_2'),\exp(\pi i H_1')\rangle$	$\mathfrak{so}(12)\oplus(\mathfrak{sp}(1))^2$	$(\sigma_1,\sigma_1,\sigma_2)$, S
$\mathfrak{e}_8$	$\Gamma_3=\langle\exp(\pi i H_2'),\exp(\pi i(H_1'+H_4'))\rangle$	$\mathfrak{su}(8)\oplus i\mathbb{R}$	$(\sigma_1,\sigma_2,\sigma_2)$, S
$\mathfrak{e}_8$	$\Gamma_4=\langle\exp(\pi i(H_2'+H_1')),\exp(\pi i(H_5'+H_1'))\rangle$	$\mathfrak{so}(8)\oplus\mathfrak{so}(8)$	$(\sigma_2,\sigma_2,\sigma_2)$, V
$\mathfrak{f}_4$	$\Gamma_1=\langle\exp(\pi i H_2'),\exp(\pi i H_1')\rangle$	$\mathfrak{su}(3)\oplus(i\mathbb{R})^2$	$(\sigma_1,\sigma_1,\sigma_1)$, V
$\mathfrak{f}_4$	$\Gamma_2=\langle\exp(\pi i H_3'),\exp(\pi i H_2')\rangle$	$\mathfrak{so}(5)\oplus(\mathfrak{sp}(1))^2$	$(\sigma_1,\sigma_1,\sigma_2)$, S
$\mathfrak{f}_4$	$\Gamma_3=\langle\exp(\pi i H_4'),\exp(\pi i H_3')\rangle$	$\mathfrak{so}(8)$	$(\sigma_2,\sigma_2,\sigma_2)$, V
$\mathfrak{g}_2$	$\Gamma=\langle\exp(\pi i H_1'),\exp(\pi i H_2')\rangle$	$(i\mathbb{R})^2$	(σ,σ,σ), V

Table 4. Klein four-subgroups in $\mathrm{Aut}(\mathfrak{u}_0)$ for the exceptional cases.

Proof. When $\mathfrak{u}_0$ is a classical compact simple Lie algebra, we can do matrix calculation to show Table 3 is complete and any Klein subgroup is regular. When $\mathfrak{u}_0$ is an exceptional compact simple Lie algebra, from Klein subgroups we get nonconjugate commuting pairs of involutions (θ_1,θ_2) distinguished by the isomorphism type of $\mathfrak{u}_0^{\langle\theta_1,\theta_2\rangle}$ or the distribution of the classes of the (ordered) tuples $(\theta_1,\theta_2,\theta_3)$. When $\mathfrak{u}_0$ is of type $\mathbf{E_6}$, $\mathbf{E_7}$, $\mathbf{E_8}$, $\mathbf{F_4}$, or $\mathbf{G_2}$, we get (at least) 23, 19, 8, 5, or 1 nonconjugate commuting pairs, respectively. By Proposition 6.1, they represent all conjugacy classes of commuting pairs of involutions. So Table 4 is complete.

For an exceptional simple Lie algebra $\mathfrak{u}_0$, suppose that some Klein subgroup fails to be regular. Then we can construct nonconjugate commuting pairs (θ_1,θ_2) and (θ_1',θ_2') $(=(\theta_2,\theta_1))$ with $\langle\theta_1,\theta_2\rangle=\langle\theta_1',\theta_2'\rangle$, $\theta_1\sim\theta_1'$, $\theta_2\sim\theta_2'$, $\theta_1\theta_2\sim\theta_1'\theta_2'$. Then there should exist more isomorphism classes of semisimple symmetric pairs. But it is not the case, and it follows that any Klein subgroup is regular. □

Another way of proving all Klein subgroups of $\mathrm{Aut}(\mathfrak{u}_0)$ are regular is as follows. First we just need to check for any commuting pair of involutions $\theta_1, \theta_2 \in \mathrm{Aut}(\mathfrak{u}_0)$ with $\theta_1 \sim \theta_2$ (in $\mathrm{Aut}(\mathfrak{u}_0)$), θ_1, θ_2 are conjugate in $\mathrm{Aut}(\mathfrak{u}_0)^{\theta}$, where $\theta = \theta_1\theta_2$. Fix θ as a representative in Section 3, when $\mathfrak{u}_0$ is an exceptional simple Lie algebra. This was already checked in the last subsection; when $\mathfrak{u}_0$ is a classical simple Lie algebra, we can check this from the data in Table 3 (list of Klein groups with symmetric space type) and Table 2 (symmetric subgroups).

A statement equivalent to the regularity of all Klein subgroups (Theorem 6.2) is that two commuting pairs of involutions (θ, σ) and (θ', σ') are conjugate in $\mathrm{Aut}(\mathfrak{u}_0)$ if and only if

$$\theta \sim \theta', \quad \sigma \sim \sigma', \quad \theta\sigma \sim \theta'\sigma'$$

and the Klein subgroups $\langle\theta, \sigma\rangle$, $\langle\theta', \sigma'\rangle$ are conjugate. This statement clearly implies the second statement in Theorem 6.2. To derive this statement from Theorem 6.2, give two pairs (θ, σ) and (θ', σ') with $\theta \sim \theta'$, $\sigma \sim \sigma'$, $\theta\sigma \sim \theta'\sigma'$ and $\langle\theta, \sigma\rangle \sim \langle\theta', \sigma'\rangle$. After replacing (θ', σ') by a pair conjugate to it, we may assume $\langle\theta, \sigma\rangle = \langle\theta', \sigma'\rangle$, that is, (θ, σ) and (θ', σ') generate the same Klein subgroup. By Theorem 6.2, $\langle\theta, \sigma\rangle$ is regular, so (θ, σ) and (θ', σ') are conjugate. Since any Klein subgroup of $\mathrm{Aut}(\mathfrak{u}_0)$ is regular, a conjugacy class of Klein subgroups gives 6, 3, or 1 isomorphism types of semisimple symmetric pairs when it is nonspecial, special but not very special, or very special, respectively.

The fact that all Klein subgroups in $\mathrm{Aut}(\mathfrak{u}_0)$ are regular is an interesting phenomenon. The property of regularity can be generalized to closed subgroups of any Lie group; a vast array of examples of nonregular subgroups is given in [Larsen 1994].

From Tables 1 and 4, we can abstract the following facts.

Proposition 6.3. *When* $\mathfrak{u}_0$ *is an exceptional compact simple Lie algebra, any two classes of involutions have commuting representatives*; *for any Klein group* $\Gamma \subset \mathrm{Aut}(\mathfrak{u}_0)$ *the centralizer* $\mathrm{Aut}(\mathfrak{u}_0)^{\Gamma}$ *intersects of* $\mathrm{Aut}(\mathfrak{u}_0)$.

For classical compact simple Lie algebras, both statements of the above proposition fail in general. For example, in $\mathrm{Aut}(\mathfrak{su}(2n))$ and for an odd p with $1 \leq p \leq n-1$, $\tau \circ \mathrm{Ad}(I_{n,n})$ ($\tau =$ complex conjugation) doesn't commute with any involution conjugate to $\mathrm{Ad}(I_{p,2n-p})$; in $\mathrm{Aut}(\mathfrak{so}(4n))$, $\mathrm{Aut}(\mathfrak{so}(4n))^{\Gamma_n} \subset \mathrm{Int}(\mathfrak{so}(4n))$ (see Table 3 for the definition of Γ_n).

For each Klein subgroup Γ listed in Table 3 or 4 with two generators $\theta, \sigma \in \mathrm{Aut}(\mathfrak{u}_0)$, we get the centralizer $\mathrm{Aut}(\mathfrak{u}_0)^{\Gamma}$ by calculating $(\mathrm{Aut}(\mathfrak{u}_0)^{\theta})^{\sigma}$. The results about $\mathrm{Aut}(\mathfrak{u}_0)^{\Gamma}$ are listed in Table 5 for classical compact simple Lie algebras and in Table 6 for exceptional compact simple Lie algebras.

$\mathfrak{u}_0$	Γ_i	$L=\mathrm{Aut}(\mathfrak{u}_0)^{\Gamma_i}$
$\mathfrak{su}(p+q), p\neq q$	$\Gamma_{p,q}$	$((O(p)\times O(q))/\langle(-I_p,-I_q)\rangle)\times\langle\tau\rangle$
$\mathfrak{su}(2p)$	$\Gamma_{p,p}$	$((O(p)\times O(p))/\langle(-I_p,-I_p)\rangle)\rtimes\langle\tau,J_p\rangle$, $\mathrm{Ad}(J_p)(X,Y)=(Y,X)$, $\mathrm{Ad}(\tau)=1$
$\mathfrak{su}(2p)$	Γ'_p	$(U(p)/\langle -I_p\rangle)\rtimes\langle\tau,z\rangle$, $\mathrm{Ad}(z)=1$
$\mathfrak{su}(2p+2q), p\neq q$	$\Gamma'_{p,q}$	$((\mathrm{Sp}(p)\times\mathrm{Sp}(q))/\langle(-I_p,-I_q)\rangle)\times\langle\tau J_{p+q}\rangle$
$\mathfrak{su}(4p)$	$\Gamma'_{p,p}$	$((\mathrm{Sp}(p)\times\mathrm{Sp}(p))/\langle(-I_p,-I_p)\rangle)\rtimes\langle\tau J_{2p},J_p\rangle$, $\mathrm{Ad}(J_p)(X,Y)=(Y,X)$, $\mathrm{Ad}(\tau J_{2p})=1$
$\mathfrak{su}(p+q+r+s)$	$\Gamma_{p,q,r,s}$	$((S(U(p)\times U(q)\times U_r\times U_s)/\langle Z_{p+q+r+s}\rangle)\rtimes\langle\tau\rangle$ $\mathrm{Ad}(\tau)=$ complex conjugation
$\mathfrak{su}(2p+2r), p\neq r$	$\Gamma_{p,p,r,r}$	$((S(U(p)\times U(p)\times U_r\times U_r)/\langle Z_{2p+2r}\rangle)\rtimes\langle\tau,J_{p,r}\rangle$ $\mathrm{Ad}(J_{p,r})(X_1,X_2,X_3,X_4)=(X_2,X_1,X_4,X_3)$
$\mathfrak{su}(4p)$	$\Gamma_{p,p,p,p}$	$((S(U(p)\times U(p)\times U(p)\times U(p))/\langle Z_{4p}\rangle)\rtimes\langle\tau,J_{2p},J_{p,p}\rangle$ $\mathrm{Ad}(J_{2p})(X_1,X_2,X_3,X_4)=(X_3,X_4,X_1,X_2)$
$\mathfrak{su}(2p)$	Γ_p	$PSU(p)\rtimes\langle F_p,\tau\rangle$ $\mathrm{Ad}(\tau)=$ complex conjugation, $\mathrm{Ad}(F_p)=1$
$\mathfrak{so}(p+q+r+s)$	$\Gamma_{p,q,r,s}$	$(O(p)\times O(q)\times O(r)\times O(s))/\langle -I_{p+q+r+s}\rangle$
$\mathfrak{so}(2p+2r), p\neq r$	$\Gamma_{p,p,r,r}$	$((O(p)\times O(p)\times O(r)\times O(r))/\langle -I_{2p+2r}\rangle))\rtimes\langle J_{p,r}\rangle$ $\mathrm{Ad}(J_{p,r})(X_1,X_2,X_3,X_4)=(X_2,X_1,X_4,X_3)$
$\mathfrak{so}(4p)$, $p\neq 2$	$\Gamma_{p,p,p,p}$	$((O(p))^4/\langle -I_{4p}\rangle)\rtimes\langle J_{2p},J_{p,p}\rangle$ $\mathrm{Ad}(J_{2p})(X_1,X_2,X_3,X_4)=(X_3,X_4,X_1,X_2)$
$\mathfrak{so}(8)$	$\Gamma_{2,2,2,2}$	$(U(1)^4/Z')\rtimes\langle\epsilon_{1,2},\epsilon_{1,3},\epsilon_{1,4},S_4\rangle$ $\mathrm{Ad}(\epsilon_{1,2})(X_1,X_2,X_3,X_4)=(-X_1,-X_2,X_3,X_4)$,etc S_4 acts by permutations
$\mathfrak{so}(2p)$	Γ_p	$(O(p)/\langle -I_p\rangle)\times F_p$
$\mathfrak{so}(2p+2q), p\neq q$	$\Gamma_{p,q}$	$((U(p)\times U(q))/\langle(-I_p,-I_q)\rangle)\rtimes\langle\tau\rangle$ $\mathrm{Ad}(\tau)=$ complex conjugation
$\mathfrak{so}(4p)$	$\Gamma_{p,p}$	$((U(p)\times U(p))/\langle(-I_p,-I_p)\rangle)\rtimes\langle\tau,J_p\rangle$, $\mathrm{Ad}(J_p)(X,Y)=(Y,X)$
$\mathfrak{so}(4p)$	Γ'_p	$(\mathrm{Sp}(p)/\langle -I_p\rangle)\times F'_p$
$\mathfrak{sp}(n)$	Γ_p	$(O(n)/\langle -I_n\rangle)\times F_p$
$\mathfrak{sp}(p+q), p\neq q$	$\Gamma_{p,q}$	$((U(p)\times U(q))/\langle(-I_p,-I_q)\rangle)\times\langle\tau\rangle$
$\mathfrak{sp}(2p)$	$\Gamma_{p,p}$	$((U(p)\times U(p))/\langle(-I_p,-I_p)\rangle)\rtimes\langle\tau,J_p\rangle$, $\mathrm{Ad}(\tau)=$ complex conjugation, $\mathrm{Ad}(J_p)(X,Y)=(Y,X)$
$\mathfrak{sp}(2p)$	Γ'_p	$(\mathrm{Sp}(p)/\langle -I_p\rangle)\times F'_p$
$\mathfrak{sp}(p+q+r+s)$	$\Gamma_{p,q,r,s}$	$(\mathrm{Sp}(p)\times\mathrm{Sp}(q)\times\mathrm{Sp}(r)\times\mathrm{Sp}(s))/\langle -I_{p+q+r+s}\rangle$
$\mathfrak{sp}(2p+2r), p\neq r$	$\Gamma_{p,p,r,r}$	$((\mathrm{Sp}(p)\times\mathrm{Sp}(p)\times\mathrm{Sp}(r)\times\mathrm{Sp}(r))/\langle -I_{2p+2r}\rangle)\rtimes\langle J_{p,r}\rangle$ $\mathrm{Ad}(J_{p,r})(X_1,X_2,X_3,X_4)=(X_2,X_1,X_4,X_3)$
$\mathfrak{sp}(4p)$	$\Gamma_{p,p,p,p}$	$((\mathrm{Sp}(p))^4/\langle -I_{4p}\rangle)\rtimes\langle J_{2p},J_{p,p}\rangle$ $\mathrm{Ad}(J_{2p})(X_1,X_2,X_3,X_4)=(X_3,X_4,X_1,X_2)$

Table 5. Fixed point subgroups of Klein four-subgroups: classical cases.

$\mathfrak{u}_0$	Γ_i	$L=\mathrm{Aut}(\mathfrak{u}_0)^{\Gamma_i}$
$\mathfrak{e}_6$	Γ_1	$((SU(3)\times SU(3)\times U(1)\times U(1))/\langle(e^{\frac{2\pi i}{3}}I,I,e^{\frac{2\pi i}{3}},1),(I,e^{\frac{2\pi i}{3}}I,e^{\frac{-2\pi i}{3}},1)\rangle)\rtimes\langle z,\tau\rangle$, $\mathrm{Ad}(\tau)(X,Y,\lambda,\mu)=(\overline{Y},\overline{X},\lambda,\mu)$, $\mathrm{Ad}(z)(X,Y,\lambda,\mu)=(Y,X,\lambda^{-1},\mu^{-1})$
$\mathfrak{e}_6$	Γ_2	$(SU(4)\times\mathrm{Sp}(1)\times\mathrm{Sp}(1)\times U(1))/\langle(iI,-1,1,i),(I,-1,-1,-1)\rangle)\rtimes\langle\tau\rangle$, $\mathrm{Ad}(\tau)(X,y,z,\lambda)=(J_2\overline{X}(J_2)^{-1},y,z,\lambda^{-1})$
$\mathfrak{e}_6$	Γ_3	$(SU(5)\times U(1)\times U(1))\rtimes\langle\tau'\rangle$, $\mathrm{Ad}(\tau')(X,\lambda,\mu)=(\overline{X},\lambda^{-1},\mu^{-1})$
$\mathfrak{e}_6$	Γ_4	$((\mathrm{Spin}(8)\times U(1)\times U(1))/\langle(-1,-1,1),(c,1,-1)\rangle)\rtimes\langle\tau\rangle$, $\mathrm{Ad}(\tau)(x,\lambda,\mu)=(x,\lambda^{-1},\mu^{-1})$
$\mathfrak{e}_6$	Γ_5	$((\mathrm{Sp}(3)\times\mathrm{Sp}(1))/\langle(-I,-1)\rangle)\times\langle\tau\rangle$
$\mathfrak{e}_6$	Γ_6	$((SO(6)\times U(1))/\langle(-I,-1)\rangle)\rtimes\langle\tau',z\rangle$, $\mathrm{Ad}(z)(X,\lambda)=(I_{3,3}XI_{3,3},\lambda^{-1})$, $\mathrm{Ad}(\tau')=1$
$\mathfrak{e}_6$	Γ_7	$\mathrm{Spin}(9)\times\langle\tau\rangle$
$\mathfrak{e}_6$	Γ_8	$((\mathrm{Spin}(5)\times\mathrm{Spin}(5))/\langle(-1,-1)\rangle)\rtimes\langle\tau',z\rangle$, $\mathrm{Ad}(z)(x,y)=(y,x)$
$\mathfrak{e}_7$	Γ_1	$((SU(6)\times U(1)\times U(1))/\langle(e^{\frac{2\pi i}{3}}I,e^{\frac{-2\pi i}{3}},1),(-I,1,1)\rangle)\rtimes\langle z\rangle$, $\mathrm{Ad}(z)(X,\lambda,\mu)=(J_3\overline{X}J_3^{-1},\lambda^{-1},\mu^{-1})$
$\mathfrak{e}_7$	Γ_2	$(\mathrm{Spin}(8)\times\mathrm{Sp}(1)^3)/\langle(c,-1,1,1),(1,-1,-1,-1),(-1,-1,-1,1)\rangle$
$\mathfrak{e}_7$	Γ_3	$((\mathrm{Spin}(10)\times U(1)\times U(1))/\langle(c,i,1)\rangle)\rtimes\langle z\rangle$, $\mathrm{Ad}(z)(x,\lambda,\mu)=(e_1xe_1^{-1},\lambda^{-1},\mu^{-1})$
$\mathfrak{e}_7$	Γ_4	$((SU(6)\times\mathrm{Sp}(1)\times U(1))/\langle(e^{\frac{2\pi i}{3}}I,1,e^{\frac{-2\pi i}{3}}),(-I,-1,1)\rangle)\rtimes\langle z\rangle$, $\mathrm{Ad}(z)(X,y,\lambda)=(J_3\overline{X}J_3^{-1},y,\lambda^{-1})$
$\mathfrak{e}_7$	Γ_5	$((\mathrm{Spin}(6)\times\mathrm{Spin}(6)\times U(1))/\langle(c,c',1),(1,-1,-1)\rangle)\rtimes\langle z_1,z_2\rangle$, $\mathrm{Ad}(z_1)(x,y,\lambda)=(y,x,\lambda^{-1})$, $\mathrm{Ad}(z_2)(x,y,\lambda)=(e_1xe_1^{-1},e_1ye_1^{-1},\lambda^{-1})$
$\mathfrak{e}_7$	Γ_6	$F_4\times\langle\tau,\omega\rangle$
$\mathfrak{e}_7$	Γ_7	$(\mathrm{Sp}(4)/\langle -I\rangle)\times\langle\tau,\omega'\rangle$
$\mathfrak{e}_7$	Γ_8	$(SO(8)/\langle -I\rangle)\times\langle\tau',\omega'\rangle$
$\mathfrak{e}_8$	Γ_1	$((E_6\times U(1)\times U(1))/\langle(c,e^{\frac{2\pi i}{3}},1)\rangle)\rtimes\langle z\rangle$, $\mathfrak{l}_0^z=\mathfrak{f}_4\oplus 0\oplus 0$
$\mathfrak{e}_8$	Γ_2	$(\mathrm{Spin}(12)\times\mathrm{Sp}(1)\times\mathrm{Sp}(1))/\langle(c,-1,1),(-1,-1,-1)\rangle$
$\mathfrak{e}_8$	Γ_3	$((SU(8)\times U(1))/\langle(-I,1),(iI,-1)\rangle)\rtimes\langle z\rangle$, $\mathfrak{l}_0^z=\mathfrak{sp}(4)\oplus 0$
$\mathfrak{e}_8$	Γ_4	$((\mathrm{Spin}(8)\times\mathrm{Spin}(8))/\langle(-1,-1),(c,c)\rangle)\rtimes\langle z\rangle$, $\mathrm{Ad}(z)(x,y)=(y,x)$
$\mathfrak{f}_4$	Γ_1	$((SU(3)\times U(1)\times U(1))/\langle(e^{\frac{2\pi i}{3}}I,e^{\frac{-2\pi i}{3}},1)\rangle)\rtimes\langle z\rangle$, $\mathfrak{l}_0^z=\mathfrak{so}(3)\oplus 0\oplus 0$
$\mathfrak{f}_4$	Γ_2	$((\mathrm{Sp}(2)\times\mathrm{Sp}(1)\times\mathrm{Sp}(1))/\langle(-I,-1,-1)\rangle$
$\mathfrak{f}_4$	Γ_3	$\mathrm{Spin}(8)$
$\mathfrak{g}_2$	Γ	$(U(1)\times U(1))\rtimes\langle z\rangle$, $\mathrm{Ad}(z)(\lambda,\mu)=(\lambda^{-1},\mu^{-1})$

Table 6. Fixed point subgroups of Klein four-subgroups: exceptional cases.

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FRACTAL ENTROPY OF NONAUTONOMOUS SYSTEMS

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We define formulas of entropy dimension for a nonautonomous dynamical system consisting of a sequence of continuous self-maps of a compact metric space. This study reveals analogues of basic propositions for entropy dimension, such as the power rule, product rule and commutativity, etc. These properties allow us to convert to an equality an inequality found by de Carvalho (1997) concerning the product rule for the autonomous dynamical system. We also prove a subadditivity rule of entropy dimension for one-dimensional dynamics based on our previous work.

1. Introduction

Entropies are important factors in the study of autonomous (i.e., deterministic) dynamical systems that are induced by iterations of a single transformation. The concept of topological entropy was originally introduced by Adler, Konheim and McAndrew [Adler et al. 1965] as an invariant of topological conjugacy and a numerical measure for the complexity of a dynamical system. Later on, Bowen [1971] and Dinaburg [1971] gave an equivalent definition when the space is metrizable. Other studies [Brucks and Bruin 2004; Katok and Hasselblatt 1995; Pollicott and Yuri 1998; Walters 1982] and the references therein discuss related definitions and properties. In the 1990s, various authors introduced several refinements of the notion of entropy, leading to significant findings in many different directions.

The commutativity formula for topological entropy (and measure theoretic entropy) was proved first in [Dana and Montrucchio 1986]. With the development of the study of nonautonomous dynamical systems, Kolyada and Snoha [1996] introduced and studied the notion of topological entropy for a sequence of continuous

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self-maps of a compact metric space. Many properties for such dynamical systems were studied in [Cánovas 2011; Huang et al. 2008; Kolyada et al. 1999; 2004; Mouron 2007] and elsewhere. Particularly, the commutativity of the topological entropy was proved and announced in [Kolyada and Snoha 1996]. This kind of problem for nonautonomous dynamical systems has been studied for many years by several authors. A good discussion of these properties and applications appears in [Balibrea et al. 1999; Cánovas and Linero 2002; 2005; Hric 1999; 2000; Kolyada and Snoha 1996; Zhu et al. 2006].

Although systems with positive entropy are much more complicated than those with zero entropy, zero entropy systems have various complexities; see [de Carvalho 1997; Dou et al. 2011; Ferenczi and Park 2007; Huang et al. 2007; Misiurewicz 1981; Misiurewicz and Smítal 1988; Misiurewicz and Szlenk 1980]. These studies give some methods of classifying zero entropy dynamical systems. De Carvalho [1997] introduced a notion of entropy dimension to distinguish zero topological entropy systems and obtained some basic properties of entropy dimension. Cheng and Li [2010] presented some examples to show that every number in (0, 1) can be attained by the entropy dimensions of the dynamical systems and a dynamical system whose entropy dimension is one and topological entropy is zero. These findings answered the question asked in [de Carvalho 1997].

This paper analyzes a nonautonomous discrete dynamical system $(X, T_{1,\infty})$ given by a compact metric space X and a sequence $T_{1,\infty} = \{T_i\}_{i=1}^{\infty}$ of continuous self-maps of X. The trajectory of a fixed point x is defined as the sequence $x, T_1(x), T_2(T_1(x)), \ldots$. Our goal is to study the properties of fractal entropy of nonautonomous dynamical systems. The paper is organized as follows. Section 2 defines and studies the entropy dimension $D(T_{1,\infty})$ of a nonautonomous dynamical system given by a sequence $T_{1,\infty} = \{T_i\}_{i=1}^{\infty}$ of continuous maps of a compact metric space X into itself. Section 3 investigates some formulas of entropy dimension for nonautonomous dynamical systems. These include the power rule, product rule and topological equisemiconjugacy. Applying these results shows that the commutativity of entropy dimension is also true for nonautonomous dynamical systems and the product rule holds for the autonomous dynamics, which was given just as an inequality in [de Carvalho 1997]. Section 4 focuses on continuous maps on the unit interval [0, 1]. To show the subadditivity of entropy dimension, this paper uses the main result in [Cheng and Li 2010] to consider two continuous commuting interval maps. Finally, we discuss the notion of the asymptotical entropy dimension.

2. Equivalent definitions

Topological entropy is one of the most fundamental dynamical invariants associated to a continuous map. It roughly measures the orbit structure complexity of the map.

For nonautonomous dynamical systems, a sequence of continuous maps $\{T_i\}_{i=1}^{\infty}$ is considered. The s-topological entropy dimension of a nonautonomous dynamical system is introduced in this section. After that, we give different types of equivalent definitions.

Let (X, d) be a compact metric space and $\{T_i\}_{i=1}^{\infty}$ be a sequence of continuous maps from X to itself. Denote by $T_{1,\infty}$ the sequence $\{T_i\}_{i=1}^{\infty}$ and by $(X, T_{1,\infty})$ the induced nonautonomous dynamical system.

For any $i \in \mathbb{N}$, let $T_i^0 = \mathrm{Id}$, where Id is the identity map on X. Set

$$T_i^n = T_{i+(n-1)} \circ \cdots \circ T_{i+1} \circ T_i \quad \text{and} \quad T_i^{-n} = T_i^{-1} \circ T_{i+1}^{-1} \circ \cdots \circ T_{i+(n-1)}^{-1}.$$

For any open cover $\mathscr{A}$ of X, define

$$T_i^{-n}(\mathscr{A}) = \{T_i^{-n}(A) : A \in \mathscr{A}\}$$

and

$$\begin{aligned}\mathscr{A}_i^n(T_{1,\infty}) &= \textstyle\bigvee_{j=0}^{n-1} T_i^{-j}(\mathscr{A}) \\ &= \left\{A_{i_0} \cap T_i^{-1}(A_{i_1}) \cap \cdots \cap T_i^{-(n-1)}(A_{i_{n-1}}) : A_{i_j} \in \mathscr{A}, 1 \le j \le n-1\right\}.\end{aligned}$$

We write $\mathscr{A}_1^n$ for simplicity instead of $\mathscr{A}_i^n(T_{1,\infty})$ if there is no confusion. Let $\mathcal{N}(\mathscr{A})$ be the minimal possible cardinality of a subcover chosen from $\mathscr{A}$.

Definition 2.1. Let $T_i : X \to X$, $i = 1, 2, 3, \ldots$, be a sequence of continuous maps and $s \ge 0$ be a real number. The s-topological entropy of $T_{1,\infty}$ is defined as

$$D(s, T_{1,\infty}) = \sup_{\mathscr{A}} D(s, T_{1,\infty}, \mathscr{A}),$$

where $\mathscr{A}$ ranges over all open covers of X and

$$D(s, T_{1,\infty}, \mathscr{A}) = \limsup_{n\to\infty} \frac{1}{n^s} \log \mathcal{N}(\mathscr{A}_1^n).$$

When $T_i = T$ for all $i \in \mathbb{N}$, $D(s, T_{1,\infty})$ is just the s-topological entropy of T defined in [Cheng and Li 2010] (denoted by $D(s, T)$). Furthermore, if $s = 1$ and $T_i = T$ for all $i \in \mathbb{N}$, it is trivial that $D(s, T_{i,\infty})$ is just the topological entropy of T (usually denoted by $h(T)$).

From Definition 2.1 it follows that the s-topological entropy $D(s, T_{1,\infty})$ enjoys the following properties.

Proposition 2.2. (i) *The map $s > 0 \mapsto D(s, T_{1,\infty})$ is nonnegative and decreasing with s.*

(ii) *There exists $s_0 \in [0, +\infty]$ such that*

$$D(s, T_{1,\infty}) = \begin{cases} +\infty & \text{if } 0 < s < s_0, \\ 0 & \text{if } s > s_0. \end{cases}$$

Proposition 2.2(ii) indicates that the value of $D(s, T_{1,\infty})$ jumps from infinity to 0 at both sides of some point s_0, which is similar to a fractal measure. Analogously to the fractal dimension, define the entropy dimension of $T_{1,\infty}$ as follows.

Definition 2.3. Let $(X, T_{1,\infty})$ be a nonautonomous dynamical system. Define the entropy dimension of $T_{1,\infty}$ to be

$$D(T_{1,\infty}) = \sup\{s > 0 : D(s, T_{1,\infty}) = \infty\} = \inf\{s > 0 : D(s, T_{1,\infty}) = 0\}.$$

When $T_i = T$ for all $i \in \mathbb{N}$, then $D(T_{1,\infty}) = D(T)$, where $D(T)$ is the entropy dimension of T defined in [Cheng and Li 2010; Dou et al. 2011].

We now turn to definitions motivated by analogues of the topological entropy. Let $n \in \mathbb{N}$ and define a new (Bowen) metric d_n on X by

$$d_n(x, y) = \max_{0 \le i < n} d(T_1^i(x), T_1^i(y)),$$

where $x, y \in X$.

Definition 2.4. A set $F \subset X$ is called an (n, ε)-spanning set of X for $T_{1,\infty}$ if, for any $x \in X$, there exists $y \in F$ with $d_n(x, y) \le \varepsilon$. A dual definition is as follows. A set $E \subset X$ is called an (n, ε)-separated set of X for $T_{1,\infty}$ if $d_n(x, y) > \varepsilon$ for every pair of distinct point $x, y \in E$, $x \neq y$.

Define

$$r(T_{1,\infty}, n, \varepsilon) = \min\{\#F : F \subset X \text{ is an } (n, \varepsilon)\text{-spanning set for } T_{1,\infty}\},$$
$$s(T_{1,\infty}, n, \varepsilon) = \max\{\#E : E \subset X \text{ is an } (n, \varepsilon)\text{-separated set for } T_{1,\infty}\},$$

where $\#E$ is the number of elements in E. The following lemma describes the relationship among these two quantities and the number of covering sets.

Lemma 2.5. *Let $T_i : X \to X$ be a sequence of continuous maps of a compact metric space (X, d).*

(i) *For any open cover $\mathcal{A}$ of X with Lebesgue number δ,*

$$\mathcal{N}(\mathcal{A}_1^n) \le r(T_{1,\infty}, n, \delta/2) \le s(T_{1,\infty}, n, \delta/2). \tag{2-1}$$

(ii) *For any $\varepsilon > 0$ and open cover $\mathcal{A}$ with* $\operatorname{diam}(\mathcal{A}) := \max\{\operatorname{diam}(A) : A \in \mathcal{A}\} \le \varepsilon$,

$$r(T_{1,\infty}, n, \varepsilon) \le s(T_{1,\infty}, n, \varepsilon) \le \mathcal{N}(\mathcal{A}_1^n). \tag{2-2}$$

Proof. (i) Since any maximal (n, ε)-separated set of X for $T_{1,\infty}$ is (n, ε)-spanning, the second inequality of (2-1) holds. Thus, it suffices to prove the first inequality. Let F be a $(n, \delta/2)$-spanning set for X of cardinality $r(T_{1,\infty}, n, \delta/2)$. Then

$$X = \bigcup_{x \in F} \bigcap_{i=0}^{n-1} T_1^{-i} B(T_1^i x, \delta/2).$$

Note that $B(T^i x, \delta/2)$ is a subset of a member of $\mathscr{A}$ for any $0 \le i \le n-1$ and $x \in F$; thus,

$$\mathcal{N}(\mathscr{A}_1^n) \le r(T_{1,\infty}, n, \varepsilon).$$

(ii) The first inequality of (2-2) holds, as in (i). It suffices to prove the second inequality of (2-2). Let E be an (n, ε)-separated set of cardinality $s(T_{1,\infty}, n, \varepsilon)$. Then no member of the cover $\mathscr{A}_1^n$ can contain two elements of E since $\operatorname{diam}(\mathscr{A}) \le \varepsilon$. This implies

$$s(T_{1,\infty}, n, \varepsilon) \le \mathcal{N}(\mathscr{A}_1^n). \qquad \square$$

Lemma 2.5 immediately implies the following property, which indicates that the s-topological entropy for $T_{1,\infty}$ can be equivalently defined by the spanning and separated sets.

Proposition 2.6. *Let $T_i : X \to X$, $i = 1, 2, 3, \ldots$, be a sequence of continuous maps and $s \ge 0$ a real number. Then*

$$D(s, T_{1,\infty}) = \lim_{\varepsilon\to 0} \limsup_{n\to\infty} \frac{1}{n^s} \log r(T_{1,\infty}, n, \varepsilon) = \lim_{\varepsilon\to 0} \limsup_{n\to\infty} \frac{1}{n^s} \log s(T_{1,\infty}, n, \varepsilon).$$

3. Dynamical propositions

The entropy dimension we defined for a nonautonomous dynamical system is a topological equiconjugacy invariant. Thus, we can consider those two entropy zero dynamical systems as being not the same or being not equivalent by different entropy dimension. The main idea of this section is quite similar to that of Kolyada and Snoha's approximations. The basic proposition of entropy dimension is the power rule. The inequality of the power rule can be shown as follows.

Lemma 3.1 [Kolyada and Snoha 1996]. *Let $\mathscr{A}$, $\mathscr{B}$ be any two open covers of X. Then*

(i) $\mathcal{N}(\mathscr{A} \vee \mathscr{B}) \le \mathcal{N}(\mathscr{A})\mathcal{N}(\mathscr{B})$;

(ii) $\mathcal{N}(T_i^{-n}\mathscr{A}) \le \mathcal{N}(\mathscr{A})$;

(iii) $T^{-1}(\mathscr{A} \vee \mathscr{B}) = T^{-1}(\mathscr{A}) \vee T^{-1}(\mathscr{B})$;

(iv) $\mathcal{N}(\mathscr{A}) \ge \mathcal{N}(\mathscr{B})$ *when $\mathscr{A}$ is finer than $\mathscr{B}$ (denoted by $\mathscr{A} \succ \mathscr{B}$).*

Proposition 3.2. *Let X be a compact topological space and $T_{1,\infty}$ a sequence of continuous maps from X to itself. Then*

$$D(s, T_{1,\infty}^m) \le m^s D(s, T_{1,\infty}) \tag{3-1}$$

for any $s > 0$ and $m \in \mathbb{N}$, where $T_{1,\infty}^m = \{T_{im+1}^{(i+1)m}\}_{i=0}^{\infty}$. As a consequence,

$$D(T_{1,\infty}^m) \le D(T_{1,\infty}).$$

Proof. Let $\mathscr{A}$ be any open cover of X. For any $n \in \mathbb{N}$,

$$\mathscr{A} \vee T_1^{-1}(\mathscr{A}) \vee T_1^{-2}(\mathscr{A}) \vee \cdots \vee T_1^{-(nm-1)}(\mathscr{A}) \succ \mathscr{A} \vee T_1^{-m}(\mathscr{A}) \vee T_1^{-2m}(\mathscr{A}) \vee \cdots \vee T_1^{-(n-1)m}(\mathscr{A}),$$

so by Lemma 3.1(iv),

$$\mathcal{N}\big(\mathscr{A} \vee T_1^{-1}(\mathscr{A}) \vee \cdots \vee T_1^{-(nm-1)}(\mathscr{A})\big) \geq \mathcal{N}\big(\mathscr{A} \vee T_1^{-m}(\mathscr{A}) \vee \cdots \vee T_1^{-(n-1)m}(\mathscr{A})\big).$$

Note that

$$\begin{aligned}\mathscr{A} \vee T_1^{-m}(\mathscr{A}) \vee T_1^{-2m}(\mathscr{A}) \vee \cdots \vee T_1^{-(n-1)m}(\mathscr{A}) &= \mathscr{A} \vee (T_1^m)^{-1}(\mathscr{A}) \vee (T_1^m)^{-1} \circ (T_{m+1}^m)^{-1}(\mathscr{A}) \vee \cdots \\ &\quad \vee (T_1^m)^{-1} \circ (T_{m+1}^m)^{-1} \circ \cdots \circ (T_{(n-2)m+1}^m)^{-1}(\mathscr{A}),\end{aligned}$$

and thus

$$\limsup_{n\to\infty} \frac{1}{(mn)^s} \log \mathcal{N}\big(\mathscr{A} \vee T_1^{-1}(\mathscr{A}) \vee T_1^{-2}(\mathscr{A}) \vee \cdots \vee T_1^{-(nm-1)}(\mathscr{A})\big) \geq \frac{1}{m^s} D(s, T_{1,\infty}^m, \mathscr{A}).$$

Therefore,

$$\begin{aligned}D(s, T_{1,\infty}, \mathscr{A}) &= \limsup_{k\to\infty} \frac{1}{k^s} \log \mathcal{N}(\mathscr{A}_1^k) \geq \limsup_{n\to\infty} \frac{1}{(nm)^s} \log \mathcal{N}(\mathscr{A}_1^{nm}) \\ &= \limsup_{n\to\infty} \frac{1}{(nm)^s} \log \mathcal{N}\big(\mathscr{A} \vee T_1^{-1}(\mathscr{A}) \vee T_1^{-2}(\mathscr{A}) \vee \cdots \vee T_1^{-(nm-1)}(\mathscr{A})\big) \\ &\geq \frac{1}{m^s} D(s, T_{1,\infty}^m, \mathscr{A}).\end{aligned}$$

Thus, $D(s, T_{1,\infty}^m) \leq m^s D(s, T_{1,\infty})$.

For the entropy dimension, assume $t > D(T_{1,\infty})$ is any real number. Then $D(t, T_{1,\infty}) = 0$, which, combined with (3-1), implies $D(t, T_{1,\infty}^m) = 0$, so $t \geq D(T_{1,\infty}^m)$. Therefore, $D(T_{1,\infty}^m) \leq D(T_{1,\infty})$ by the arbitrariness of t. □

[Kolyada and Snoha 1996] gives an example showing that the inequality in (3-1) can be sharp when $s = 1$. The following two propositions indicate that the inequality in (3-1) can be an equality under some conditions.

Proposition 3.3 (power rule). *Let X be a compact topological space and $T_{1,\infty}$ be a sequence of continuous maps from X to itself. If $T_{1,\infty}$ is periodic with period $m \in \mathbb{N}$, that is, $T_{im+j} = T_j$ for any $1 \leq j \leq m$ and $i \geq 0$, then*

$$D(s, T_{1,\infty}^m) = m^s D(s, T_{1,\infty})$$

for any $s > 0$. As a consequence, $D(T_{1,\infty}^m) = D(T_{1,\infty})$.

Proof. Assume $m \geq 2$ since the case $m = 1$ is trivial. From Proposition 3.2, it is only necessary to prove $D(s, T_{1,\infty}^m) \geq m^s D(s, T_{1,\infty})$.

Let $\mathscr{A}$ be any open cover of X and $k = nm + r$, where $n \geq 1$ and $1 \leq r \leq m$. Combining $T_{1,\infty} = \{T_1, T_2, \ldots, T_m, T_1, T_2, \ldots, T_m, \ldots\}$ and $T_{1,\infty}^m = \{T_1^m, T_1^m, \ldots\}$ with Lemma 3.1(iii),

$$\begin{aligned}
&T_1^{-im}(\mathscr{A}) \vee T_1^{-(im+1)}(\mathscr{A}) \vee \cdots \vee T_1^{-((i+1)m-1)}(\mathscr{A}) \\
&\qquad = T_1^{-im}\big(\mathscr{A} \vee T_{im+1}^{-1}(\mathscr{A}) \vee \cdots \vee T_{im+1}^{-(m-1)}(\mathscr{A})\big) \\
&\qquad = T_1^{-im}\big(\mathscr{A} \vee T_1^{-1}(\mathscr{A}) \vee \cdots \vee T_1^{-(m-1)}(\mathscr{A})\big) \\
&\qquad = (T_1^{im})^{-1}\big(\mathscr{A} \vee T_1^{-1}(\mathscr{A}) \vee \cdots \vee T_1^{-(m-1)}(\mathscr{A})\big)
\end{aligned}$$

for $i = 0, 1, 2, \ldots$. Therefore, $\mathscr{A}_1^k(T_{1,\infty})$ can be written as

$$\begin{aligned}
&\big(\mathscr{A} \vee T_1^{-1}(\mathscr{A}) \vee \cdots \vee T_1^{-(m-1)}(\mathscr{A})\big) \vee \big(T_1^{-m}(\mathscr{A}) \vee T_1^{-(m+1)}(\mathscr{A}) \vee \cdots \vee T_1^{-(2m-1)}(\mathscr{A})\big) \\
&\qquad \vee \cdots \vee \big(T_1^{-(n-1)m}\mathscr{A} \vee T_1^{-((n-1)m+1)}(\mathscr{A}) \vee \cdots \vee T_1^{-(nm-1)}(\mathscr{A})\big) \\
&\qquad \vee \big(T_1^{-nm}\mathscr{A} \vee T_1^{-(nm+1)}(\mathscr{A}) \vee \cdots \vee T_1^{-(nm+r-1)}(\mathscr{A})\big) \\
&= \big(\mathscr{A} \vee T_1^{-1}(\mathscr{A}) \vee \cdots \vee T_1^{-(m-1)}(\mathscr{A})\big) \vee (T_1^m)^{-1}\big(\mathscr{A} \vee T_1^{-1}(\mathscr{A}) \vee \cdots \vee T_1^{-(m-1)}(\mathscr{A})\big) \\
&\qquad \vee \cdots \vee (T_1^{(n-1)m})^{-1}\big(\mathscr{A} \vee T_1^{-1}(\mathscr{A}) \vee \cdots \vee T_1^{-(m-1)}(\mathscr{A})\big) \\
&\qquad \vee (T_1^{nm})^{-1}\big(\mathscr{A} \vee T_1^{-1}(\mathscr{A}) \vee \cdots \vee T_1^{-(r-1)}(\mathscr{A})\big) \\
&= \mathscr{A}_1^m \vee (T_1^m)^{-1}(\mathscr{A}_1^m) \vee \cdots \vee (T_1^{(n-1)m})^{-1}(\mathscr{A}_1^m) \vee (T_1^{nm})^{-1}(\mathscr{A}_1^r) \\
&= (\mathscr{A}_1^m(T_{1,\infty}))_1^n(T_{1,\infty}^m) \vee (T_1^{nm})^{-1}(\mathscr{A}_1^r(T_{1,\infty})).
\end{aligned}$$

Combining parts (i) and (iii) of Lemma 3.1, we obtain

$$\begin{aligned}
\mathcal{N}(\mathscr{A}_1^{nm+r}(T_{1,\infty})) &= \mathcal{N}\big((\mathscr{A}_1^m(T_{1,\infty}))_1^n(T_{1,\infty}^m) \vee (T_1^{nm})^{-1}(\mathscr{A}_1^r(T_{1,\infty}))\big) \\
&\leq \mathcal{N}\big((\mathscr{A}_1^m(T_{1,\infty}))_1^n(T_{1,\infty}^m)\big)\mathcal{N}(\mathscr{A}_1^r(T_{1,\infty})).
\end{aligned}$$

Thus,

$$\begin{aligned}
D\big(s, T_{1,\infty}^m, \mathscr{A}_1^m(T_{1,\infty})\big) &= \limsup_{n\to\infty} n^{-s} \log \mathcal{N}\big((\mathscr{A}_1^m(T_{1,\infty}))_1^n(T_{1,\infty}^m)\big) \\
&\geq \limsup_{n\to\infty} n^{-s}\big(\log \mathcal{N}(\mathscr{A}_1^{nm+r}(T_{1,\infty})) - \log \mathcal{N}(\mathscr{A}_1^r(T_{1,\infty}))\big) \\
&= \limsup_{n\to\infty} n^{-s} \log \mathcal{N}(\mathscr{A}_1^{nm+r}(T_{1,\infty})) \\
&= m^s \limsup_{n\to\infty} (nm+r)^{-s} \log \mathcal{N}(\mathscr{A}_1^{nm+r}(T_{1,\infty})) \\
&= m^s \limsup_{k\to\infty} k^{-s} \log \mathcal{N}(\mathscr{A}_1^k(T_{1,\infty})) = m^s D(s, T_{1,\infty}, \mathscr{A}),
\end{aligned}$$

which implies that $D(s, T_{1,\infty}^m) \geq m^s D(s, T_{1,\infty})$ by the arbitrariness of $\mathscr{A}$. □

Applying Proposition 3.3 to the case of one map as a sequence leads to the following, which solves a problem in [de Carvalho 1997], where the author gave an inequality.

Corollary 3.4. *Let (X, T) be a topological dynamical system. Then*

$$D(s, T^m) = m^s D(s, T)$$

for any $s > 0$ and $m \in \mathbb{N}$. In particular, $D(T^m) = D(T)$.

Now let us consider the sequence of equicontinuous maps from X to itself; that is, $T_{1,\infty} = \{T_i\}_{i=1}^{\infty}$ is equicontinuous on X. More precisely, for any $x \in X$ and $\varepsilon > 0$, there exists $\delta > 0$ such that $d(T_i x, T_i y) < \varepsilon$ for all $i = 1, 2, \ldots$ whenever $d(x, y) < \delta$. We know that δ can be independent of the choice of x when X is compact.

Proposition 3.5 (power rule). *Let (X, d) be a compact metric space and $T_{1,\infty}$ be a sequence of equicontinuous maps from X to itself. Then*

$$D(s, T_{1,\infty}^m) = m^s D(s, T_{1,\infty})$$

for any $s > 0$.

Proof. By Proposition 3.2, it suffices to prove $D(s, T_{1,\infty}^m) \geq m^s D(s, T_{1,\infty})$ for $m \geq 2$. For any $\varepsilon > 0$, let

$$\delta(\varepsilon) = \varepsilon + \sup_{i \geq 1} \max_{k=1,\ldots,m-1} \sup_{x,y \in X} \left\{ d(T_i^k(x), T_i^k(y)) : d(x, y) \leq \varepsilon \right\}.$$

Since X is compact and $T_{1,\infty}$ is equicontinuous, we have:

(i) if $\varepsilon \to 0$, then $\delta(\varepsilon) \to 0$;

(ii) if $d(x, y) \leq \varepsilon$, then $d(T_i^k(x), T_i^k(y)) \leq \delta(\varepsilon)$ for any $i \geq 1$ and $k = 1, 2, \ldots, m-1$.

Let E be any $(nm, \delta(\varepsilon))$-separated set for $T_{1,\infty}$. Then, E is an (n, ε)-separated set for $T_{1,\infty}^m$ and $s_{nm}(T_{1,\infty}, \delta(\varepsilon)) \leq s_n(T_{1,\infty}^m, \varepsilon)$.

Therefore, writing $k = nm + r$ with $1 \leq r \leq m$, we have the following calculation:

$$\begin{aligned}
D(s, T_{1,\infty}^m) &= \lim_{\varepsilon \to 0} \limsup_{n \to \infty} \frac{1}{n^s} \log s_n(T_{1,\infty}^m, \varepsilon) \\
&\geq \lim_{\varepsilon \to 0} \limsup_{n \to \infty} \frac{1}{n^s} \log s_{(n-1)m+r}(T_{1,\infty}, \delta(\varepsilon)) \\
&= m^s \lim_{\varepsilon \to 0} \limsup_{n \to \infty} \frac{1}{((n-1)m+r)^s} \log s_{(n-1)m+r}(T_{1,\infty}, \delta(\varepsilon)) \\
&\geq m^s \lim_{\delta(\varepsilon) \to 0} \limsup_{k \to \infty} \frac{1}{k^s} \log s_k(T_{1,\infty}, \delta(\varepsilon)) \\
&= m^s D(s, T_{1,\infty}).
\end{aligned}$$

□

Proposition 3.6 (monotonicity). *Let X be a compact topological space and $T_{1,\infty}$ a sequence of continuous maps from X to itself. Then*

$$D(s, T_{i,\infty}) \le D(s, T_{j,\infty}) \tag{3-2}$$

for any $s > 0$ and $1 \le i \le j \le +\infty$.

Proof. Let $\mathscr{A}$ be any open cover of X. Lemma 3.1(i) implies

$$\mathcal{N}(\mathscr{A}_i^n) = \mathcal{N}\left(\bigvee_{j=0}^{n-1} T_i^{-j}(\mathscr{A})\right) = \mathcal{N}\left(\mathscr{A} \vee \bigvee_{j=1}^{n-1} T_i^{-j}(\mathscr{A})\right) \le \mathcal{N}(\mathscr{A})\, \mathcal{N}\left(\bigvee_{j=1}^{n-1} T_i^{-j}(\mathscr{A})\right). \tag{3-3}$$

Lemma 3.1(ii) shows that

$$\mathcal{N}\left(\bigvee_{j=1}^{n-1} T_i^{-j}(\mathscr{A})\right) = \mathcal{N}\left(T_i^{-1}\left(\bigvee_{j=0}^{n-2} T_{i+1}^{-j}(\mathscr{A})\right)\right) \le \mathcal{N}\left(\bigvee_{j=0}^{n-2} T_{i+1}^{-j}(\mathscr{A})\right) = \mathcal{N}(\mathscr{A}_{i+1}^{n-2}). \tag{3-4}$$

Combining (3-3) and (3-4) leads to

$$\mathcal{N}(\mathscr{A}_i^n) \le \mathcal{N}(\mathscr{A})\mathcal{N}(\mathscr{A}_{i+1}^{n-2}).$$

Therefore,

$$D(s, T_{i,\infty}, \mathscr{A}) = \limsup_{n\to\infty} \frac{1}{n^s} \log \mathcal{N}(\mathscr{A}_i^n) \le \limsup_{n\to\infty} \frac{1}{n^s} \log\bigl(\mathcal{N}(\mathscr{A})\mathcal{N}(\mathscr{A}_{i+1}^{n-2})\bigr).$$

Thus,

$$D(s, T_{i,\infty}, \mathscr{A}) \le \limsup_{n\to\infty} \frac{1}{(n-2)^s} \log \mathcal{N}(\mathscr{A}_{i+1}^{n-2}) = D(s, T_{i+1,\infty}, \mathscr{A}),$$

and $D(s, T_{i,\infty}) \le D(s, T_{i+1,\infty})$ by the arbitrariness of $\mathscr{A}$. Hence, (3-2) holds. □

Applying the monotonicity shows that the s-topological entropy for the composition of two maps does not depend on the order, as the following theorem indicates.

Theorem 3.7 (commutativity). *Let X be a compact topological space and let T, S be two continuous maps from X to itself. Then*

$$D(s, T \circ S) = D(s, S \circ T)$$

for any $s > 0$.

Proof. From Proposition 3.6, we obtain

$$D(s, \{S, T, S, T, \dots\}) \le D(s, \{T, S, T, S, \dots\}) \le D(s, \{S, T, S, T \dots\}),$$

which implies

$$D(s, \{S, T, S, T, \dots\}) = D(s, \{T, S, T, S, \dots\}).$$

By Proposition 3.3,

$$\begin{aligned} D(s, T\circ S) &= D(s, \{T\circ S, T\circ S, \dots\}) = 2^s D(s, \{S, T, S, T, \dots\}) \\ &= 2^s D(s, \{T, S, T, S, \dots\}) = D(s, \{S\circ T, S\circ T, \dots\}) = D(s, S\circ T). \quad \square \end{aligned}$$

Corollary 3.8. *Let X be a compact topological space and T_i $(i = 1, 2, \dots, n)$ be the continuous self-maps on X. Then, for any $1 < i \le n$ and $s > 0$,*

$$D(s, T_n \circ \cdots \circ T_2 \circ T_1) = D(s, T_{i-1} \circ \cdots \circ T_2 \circ T_1 \circ T_n \circ \cdots \circ T_i).$$

Proof. By Theorem 3.7,

$$\begin{aligned} D(s, T_n\circ\cdots\circ T_i\circ T_{i-1}\circ\cdots\circ T_2\circ T_1) &= D(s, (T_n\circ\cdots\circ T_i)\circ(T_{i-1}\circ\cdots\circ T_2\circ T_1)) \\ &= D(s, (T_{i-1}\circ\cdots\circ T_2\circ T_1)\circ(T_n\circ\cdots\circ T_i)) \\ &= D(s, T_{i-1}\circ\cdots\circ T_2\circ T_1\circ T_n\circ\cdots\circ T_i). \quad \square \end{aligned}$$

The following corollary was given in [Cheng and Li 2010]; however, this paper provides a quick proof from the commutativity (Theorem 3.7).

Corollary 3.9. *Let X be a compact topological spaces and T_1, T_2 be two continuous maps on X. If (X, T_1) is conjugate to (Y, T_2), then $D(s, T_1) = D(s, T_2)$ for any $s > 0$.*

Proof. Let ϕ be a conjugacy between T_1 and T_2. Since $T_2 = \phi\circ T_1\circ\phi^{-1}$, Theorem 3.7 shows that

$$D(s, T_2) = D(s, (\phi \circ T_1) \circ \phi^{-1}) = D(s, T_1). \quad \square$$

As Corollary 3.9 shows, the s-topological entropy $D(s, T)$ for an autonomous dynamical system is a conjugate invariant quantity. For the nonautonomous case, the definition of conjugacy must be adapted to the following.

Definition 3.10. Let $(X, \{T_i\}_{i=1}^{\infty})$ and $(Y, \{S_i\}_{i=1}^{\infty})$ be two nonautonomous dynamical systems. Denote by $\pi_{1,\infty} = \{\pi_i\}_{i=1}^{\infty}$ a sequence of equicontinuous surjective maps from X to Y. If

$$\pi_{i+1} \circ T_i = S_i \circ \pi_i$$

for every $i \ge 1$, we say that $\pi_{1,\infty}$ is a topological equisemiconjugacy between $T_{1,\infty}$ and $S_{1,\infty}$, and the dynamical system $(X, T_{1,\infty})$ is topologically equisemiconjugate with $(Y, S_{1,\infty})$. Furthermore, if $\pi_{1,\infty}$ is an equicontinuous sequence of homeomorphisms such that the sequence $\pi_{1,\infty}^{-1} = \{\pi_i^{-1}\}_{i=1}^{\infty}$ of inverse homeomorphisms is also equicontinuous, we say that $\pi_{1,\infty}$ is a topological equiconjugacy between $T_{1,\infty}$ and $S_{1,\infty}$, and the dynamical system $(X, T_{1,\infty})$ is topologically equiconjugate with $(Y, S_{1,\infty})$.

Theorem 3.11. *Let (X, d) and (Y, ρ) be compact metric spaces and $T_{1,\infty}$ and $S_{1,\infty}$ be the sequences of continuous maps from X and Y into themselves, respectively. If the system $(X, T_{1,\infty})$ is equisemiconjugate with $(Y, S_{1,\infty})$, then*

$$D(s, S_{1,\infty}) \le D(s, T_{1,\infty}) \tag{3-5}$$

for any $s > 0$.

Proof. Let $\pi_{1,\infty}$ be the equisemiconjugacy between X and Y. For any given $\varepsilon > 0$, noting that $\pi_{1,\infty}$ is a sequence of equicontinuous maps from X onto Y and X is compact, there exists $\delta(\varepsilon) > 0$ such that if $\rho(\pi_i(x), \pi_i(y)) > \varepsilon$ for some $i \ge 1$, then $d(x, y) > \delta(\varepsilon)$. Let $E \subset Y$ be an (n, ε)-separated set for $S_{1,\infty}$ with maximal cardinality $s(S_{1,\infty}, n, \varepsilon)$. Choose one point from each fiber $\pi_1^{-1}(y)$, $y \in E$ and denote by E_X the set of such points. Then $E_X \subset X$ is an $(n, \delta(\varepsilon))$-separated set for $T_{1,\infty}$. Therefore, $s(T_{1,\infty}, n, \delta(\varepsilon)) \ge s(S_{1,\infty}, n, \varepsilon)$, which implies (3-5). □

Apply Theorem 3.11, the following statement holds.

Corollary 3.12. *Let (X, d) and (Y, ρ) be compact metric spaces and $T_{1,\infty}$ and $S_{1,\infty}$ be the sequences of continuous maps from X and Y into themselves, respectively. If the system $(X, T_{1,\infty})$ is equiconjugate with $(Y, S_{1,\infty})$, then*

$$D(s, S_{1,\infty}) = D(s, T_{1,\infty})$$

for any $s > 0$. As a result, $D(S_{1,\infty}) = D(T_{1,\infty})$.

Theorem 3.13 (product rule). *Let (X, d) and (Y, ρ) be compact metric spaces. Let $\{T_i\}_{i=1}^{\infty}$ and $\{S_i\}_{i=1}^{\infty}$ be two sequences of continuous maps on X and Y, respectively. Define a metric d^* on $X \times Y$ by $d^*((x_1, y_1), (x_2, y_2)) = \max\{d(x_1, x_2), \rho(y_1, y_2)\}$ and a sequence of transformations on $X \times Y$ by $(T_i \times S_i)(x, y) = (T_i x, S_i y)$. Then*

$$D(s, T_{1,\infty} \times S_{1,\infty}) \le D(s, T_{1,\infty}) + D(s, S_{1,\infty})$$

for any $s > 0$, where $T_{1,\infty} \times S_{1,\infty} = \{T_i \times S_i\}_{i=1}^{\infty}$.

Proof. We know that balls in the n-Bowen metric d_n^* are products of balls on X and Y since balls in the product metric d^* are products of balls on X and Y. Therefore,

$$r(T_{1,\infty} \times S_{1,\infty}, n, \varepsilon) \le r(T_{1,\infty}, n, \varepsilon) r(S_{1,\infty}, n, \varepsilon).$$

Thus $D(s, T_{1,\infty} \times S_{1,\infty}) \le D(s, T_{1,\infty}) + D(s, S_{1,\infty})$. □

4. Subadditivity

For S, T two continuous functions from the compact metric space X to itself, some additional conditions are necessary to obtain some interesting results. It is natural to assume that S and T commute, that is, $S \circ T = T \circ S$. For instance, in [Hu 1993], the subadditivity of topological entropy $h(S \circ T) \le h(S) + h(T)$ was proved for diffeomorphisms on C^∞ compact Riemannian manifolds. This section also investigates the subadditivity for entropy dimension in one-dimensional dynamics. For convenience, the following two definitions use the same concept and notation adopted in [Cheng and Li 2010].

Definition 4.1. An interval map $T:[0,1]\to[0,1]$ is called piecewise monotone continuous if there exist points $0=a_0<a_1<\cdots<a_N=1$ such that $T|_{(a_{i-1},a_i)}$ is continuous and monotone.

Definition 4.2. Let T be a piecewise monotone continuous map. If J is a maximal interval on which $T|_J$ is continuous and monotone, then $T:J\to T(J)$ is called a branch or lap of T. The number of laps of T is denoted by $l(T)$.

Rothschild [1971] and Misiurewicz and Szlenk [1980] independently obtained the topological entropy formula for a piecewise monotone map (see [Brucks and Bruin 2004; Pollicott and Yuri 1998]). The following theorem gives a generalized s-topological entropy formula.

Theorem 4.3 [Cheng and Li 2010]. *Let $T:[0,1]\to[0,1]$ be a piecewise monotone continuous map and $s>0$ a real number. Then*

$$D(s,T)=\limsup_{n\to\infty}\frac{\log l(T^n)}{n^s}. \tag{4-1}$$

Theorem 4.4 (subadditivity). *Let T, S be piecewise monotone continuous maps such that $T\circ S=S\circ T$ and let $s>0$ be a real number. Then*

$$D(s,S\circ T)\le D(s,S)+D(s,T).$$

Hence, we have the inequality

$$D(S\circ T)\le\max\{D(S),D(T)\}. \tag{4-2}$$

Proof. Since $S\circ T=T\circ S$, it is trivial that $S^p\circ T^q=T^q\circ S^p$ for all $p,q\in\mathbb{N}$.

The number of intervals of monotonicity of $S^n\circ T^n$ is smaller than or equal to $l(T^n)l(S^n)$. Thus, we obtain that $l((S\circ T)^n)\le l(S^n)l(T^n)$. The previous theorem gives that

$$\begin{aligned}D(s,S\circ T)&=\limsup_{n\to\infty}\frac{\log l((S\circ T)^n)}{n^s}\le\limsup_{n\to\infty}\frac{\log l(S^n)l(T^n)}{n^s}\\&\le\limsup_{n\to\infty}\frac{\log l(S^n)}{n^s}+\limsup_{n\to\infty}\frac{\log l(T^n)}{n^s}=D(s,S)+D(s,T).\end{aligned}$$

For any $t>\max\{D(S),D(T)\}$, it is clear that $D(t,S)=D(t,T)=0$ by the definition of entropy dimension. Thus, $D(t,S\circ T)=0$, which implies $D(S\circ T)\le t$. It follows that $D(S\circ T)\le\max\{D(S),D(T)\}$ by the arbitrariness of t. ☐

Corollary 4.5. *Let T, S be piecewise monotone continuous maps such that $T \circ S = S \circ T$. If $D(S) = D(T) = 0$, then $D(S \circ T) = 0$.*

Note that in general from $D(S) > 0$ or $D(T) > 0$, it may not possible to deduce that $D(S \circ T) > 0$. To find a result in this setting, calculate the left shift S and right shift T on the symbolic space $\{1, 2\}^{\mathbb{Z}}$. Then $S \circ T$ is the identity map. It is trivial that $D(S) = 1$ and $D(T) = 1$. However, $D(S \circ T) = 0$. This example also indicates that the inequality in (4-2) can be sharp. On the other hand, it is easy to see that the inequality can be an equality. For example, if S is the identity map, then $D(S) = 0$, and $D(S \circ T) = D(T) = \max\{D(S), D(T)\}$. Some related properties of topological entropy of composition, $S \circ T$, can be found in [Goodwyn 1972; Raith 2004].

Consider a sequence $T_{1,\infty} = \{T_i\}_{i=1}^{\infty}$ of continuous functions from a compact metric space X to itself. Proposition 3.6 shows a kind of monotonicity of $\{D(s, T_{i,\infty})\}$ on $i \in \mathbb{N}$. Here, we can introduce the notion of the asymptotical entropy dimension of the considered system as the limit of entropy dimension in

$$D^*(T_\infty) = \lim_{i\to\infty} D(T_{i,\infty}),$$

where $T_{i,\infty}$ is the tail $T_i, T_{i+1}, \ldots$ of the sequence $T_{1,\infty}$.

Theorem 4.6. *Let $T_{1,\infty} = \{T_i\}_{i=1}^{\infty}$ be a sequence of monotone continuous functions from X to itself, where X is the unit interval $[0, 1]$ or unit circle S^1. Then the entropy dimension is $D(T_{1,\infty}) = 0$. Consequently, $D^*(T_\infty) = 0$.*

Proof. Consider the unit interval case first. Assume that $E = \{x_1, x_2, \ldots, x_k\}$ is a subset of $[0, 1]$ with $x_1 \le x_2 \le \cdots \le x_k$. Since the functions $T_1, T_2, T_3, \ldots$ are monotone, for every $j = 0, 1, 2, 3, \ldots$, we obtain either

$$T_1^j(x_1) \le T_1^j(x_2) \le T_1^j(x_3) \le \cdots \le T_1^j(x_k)$$

or

$$T_1^j(x_1) \ge T_1^j(x_2) \ge T_1^j(x_3) \ge \cdots \ge T_1^j(x_k).$$

This implies that the set E is an (n, ϵ)-separated set if and only if for every $i = 1, 2, \ldots, k-1$, the set $\{x_i, x_{i+1}\}$ is (n, ϵ)-separated. Denote the integer part of a number z by $[z]$. Since the length of the unit interval $[0, 1]$ is 1, at most $[\frac{1}{\epsilon}]$ of the distances $|T_1^j(x_1) - T_1^j(x_2)|, |T_1^j(x_2) - T_1^j(x_3)|, \ldots, |T_1^j(x_{k-1}) - T_1^j(x_k)|$ are longer than ϵ. Therefore, at most $n[\frac{1}{\epsilon}]$ sets of the form $\{x_i, x_{i+1}\}$, $i = 1, 2, \ldots, k-1$ are (n, ϵ)-separated. Thus, if E is (n, ϵ)-separated, then $k-1 \le n[\frac{1}{\epsilon}]$. By definition, $D(s, T_{1,\infty}) = 0$ for any $s > 0$, which implies $D(T_{1,\infty}) = 0$. Similarly, $D(T_{j,\infty}) = 0$ for any $j > 1$. Thus, $D^*(T_\infty) = 0$

Next, consider the case $X = S^1$. The proof is similar to that of the unit interval case when the order of the points on S^1 is the angle of points on S^1. Therefore, $D^*(T_\infty) = 0$ is also obtained in this case. □

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A GJMS CONSTRUCTION FOR 2-TENSORS AND THE SECOND VARIATION OF THE TOTAL Q-CURVATURE

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We construct a series of conformally invariant differential operators acting on weighted trace-free symmetric 2-tensors by a method similar to that of Graham, Jenne, Mason, and Sparling. For compact conformal manifolds of dimension even and greater than or equal to four with vanishing ambient obstruction tensor, one of these operators is used to describe the second variation of the total Q-curvature. An explicit formula for conformally Einstein manifolds is given in terms of the Lichnerowicz Laplacian of an Einstein representative metric.

Introduction

Let $(M, [g])$ be a conformal manifold of dimension $n \geq 3$. The k-th GJMS operator [Graham et al. 1992] is a conformally invariant differential operator acting on densities $\mathscr{E}(-n/2+k) \to \mathscr{E}(-n/2-k)$, which is defined for all $k \in \mathbb{Z}_+$ if n is odd and for integers within the range $1 \leq k \leq n/2$ if n is even. This operator has a universal expression in terms of any representative metric $g \in [g]$ with leading term the k-th power of the Laplacian. The idea for the construction is realizing densities as functions on the metric cone $\mathscr{G}$ and computing the obstruction of its formal harmonic extension to the ambient space $(\tilde{\mathscr{G}}, \tilde{g})$, where $\tilde{g}$ is an ambient metric of Fefferman and Graham [1985; 2012]. After the appearance of [Graham et al. 1992], other GJMS-like conformally invariant differential operators have been constructed in, e.g., [Branson and Gover 2005; Gover and Peterson 2006].

In this article, we establish another variant of the GJMS construction. Our operators P_k act on weighted trace-free symmetric (covariant) 2-tensors:

$$P_k : \mathscr{S}_0\left(-\frac{n}{2}+2+k\right) \to \mathscr{S}_0\left(-\frac{n}{2}+2-k\right).$$

Here, the values that k takes are the same as in the density case, $\mathscr{S}_0$ is the space of trace-free symmetric 2-tensors on M, and $\mathscr{S}_0(w) = \mathscr{S}_0 \otimes \mathscr{E}(w)$. The main tool of

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our construction is the Lichnerowicz Laplacian of the ambient metric $\tilde{g}$, which is defined by

$$\tilde{\Delta}_{\mathrm{L}} := \tilde{\Delta} + 2\widetilde{\mathrm{Ric}}^{\circ} - 2\mathring{\tilde{R}},$$

where $\tilde{\Delta} = \tilde{\nabla}^{*}\tilde{\nabla}$ is the connection Laplacian and $\widetilde{\mathrm{Ric}}^{\circ}$, $\mathring{\tilde{R}}$ are the following tensorial actions of the Ricci and Riemann curvature tensors of $\tilde{g}$:

$$\begin{aligned}\big(\widetilde{\mathrm{Ric}}^{\circ}\tilde{\sigma}\big)(X,Y) &:= \tfrac{1}{2}\big(\langle\widetilde{\mathrm{Ric}}(X,\cdot\,),\tilde{\sigma}(Y,\cdot\,)\rangle_{\tilde{g}} + \langle\widetilde{\mathrm{Ric}}(Y,\cdot\,),\tilde{\sigma}(X,\cdot\,)\rangle_{\tilde{g}}\big),\\ \big(\mathring{\tilde{R}}\tilde{\sigma}\big)(X,Y) &:= \langle\tilde{R}(X,\cdot\,,Y,\cdot\,),\tilde{\sigma}\rangle_{\tilde{g}}.\end{aligned}$$

Our intention to study the GJMS construction for 2-tensors is because of its relation to the second variation of the total Q-curvature, i.e., the integral of Branson's Q-curvature [1995]. Recall that, for a 4-dimensional compact conformal manifold $(M,[g])$ of positive definite signature, the Chern–Gauss–Bonnet formula for the total Q-curvature $\overline{Q}$ is

$$\overline{Q} = 8\pi^2\chi(M) - \frac{1}{4}\int_M |W|_g^2\, dV_g,$$

where $\chi(M)$ is the Euler characteristic, W is the Weyl tensor, and $g \in [g]$ is any representative. One can deduce from this that $\overline{Q} \le 8\pi^2\chi(M)$ and the equality holds if and only if $(M,[g])$ is conformally flat. It turns out that there is a partial generalization of this fact to the higher dimensions. Recall that a conformal metric $[g]$ is identified with a weighted 2-tensor $\boldsymbol{g} \in \mathscr{S}(2)$. Let $\mathscr{K}_{[g]}$ be the conformal Killing operator. Then we have the following theorem, which is due to Møller and Ørsted [2009].

Theorem 0.1. *Let S^n be the sphere of even dimension $n \ge 4$. Then, for any smooth 1-parameter family $\boldsymbol{g}_t$ of conformal metrics on S^n such that $\boldsymbol{g}_0 = \boldsymbol{g}_{\mathrm{std}}$ and $\dot{\boldsymbol{g}}_t|_{t=0} \notin \operatorname{image}\mathscr{K}_{[g_{\mathrm{std}}]}$, the total Q-curvature $\overline{Q}_t$ attains a local maximum at $t = 0$.*

Our main theorem contains Theorem 0.1 as a special case. Consider the following decomposition of $\mathscr{S}_0(2)$, which is valid for any compact positive definite conformal manifold $(M,[g])$ and a representative $g \in [g]$ (see [Besse 1987, Section 12.21]):

$$\mathscr{S}_0(2) = \operatorname{image}\mathscr{K}_{[g]} \oplus \mathscr{S}^{g}_{\mathrm{TT}}(2). \tag{0-1}$$

Here $\mathscr{S}^{g}_{\mathrm{TT}}(w)$ is the space of TT-tensors (trace-free and divergence-free tensors) with respect to g. This is an orthogonal decomposition with respect to the L^2-inner product, and if g is Einstein, the Lichnerowicz Laplacian Δ_{L} of g respects this decomposition.

Theorem 0.2. *Let $(M,[g])$ be a compact conformally Einstein manifold of positive definite signature with even dimension $n \ge 4$, and g an Einstein representative with Schouten tensor $P_{ij} = \lambda g_{ij}$. Then, for any smooth 1-parameter family $\boldsymbol{g}_t$ of* *conformal metrics such that* $\boldsymbol{g}_0 = \boldsymbol{g}$, *the second derivative of the total* Q-*curvature at* $t = 0$ *is*

$$\text{(0-2)}\quad \frac{d^2}{dt^2}\overline{Q}_t = -\frac{1}{4}\int_M \left\langle \prod_{m=0}^{n/2-1} (\Delta_{\mathrm{L}} - 4(n-1)\lambda + 4m(n-2m-1)\lambda)\varphi^g_{\mathrm{TT}}, \varphi^g_{\mathrm{TT}} \right\rangle_g ,$$

where φ^g_{TT} *is the* $\mathscr{S}^g_{\mathrm{TT}}(2)$-*component of* $\varphi = \dot{\boldsymbol{g}}_t|_{t=0}$ *with respect to* (0-1). *In particular, suppose there is an Einstein representative* g *with* $\lambda \geq 0$ *such that the smallest eigenvalue* α *of* $\Delta_{\mathrm{L}}|_{\mathscr{S}^g_{\mathrm{TT}}(2)}$ *satisfies*

$$\text{(0-3)}\qquad \alpha > 4(n-1)\lambda.$$

Then, for any $\boldsymbol{g}_t$ *for which* $\varphi \notin \operatorname{image}\mathscr{K}_{[g]}$, *the total* Q-*curvature attains a local maximum at* $t = 0$.

For (S^n, g_{std}), $\lambda = 1/2$ and $\Delta_{\mathrm{L}} = \Delta + 2n$. Therefore the assumption for the latter half of Theorem 0.2 is satisfied, and hence Theorem 0.1 follows.

Some ideas for the proof of Theorem 0.2 are in order. Let $(M, [g])$ be a compact conformal manifold of even dimension $n \geq 4$ (here we may allow arbitrary signature). If we are given a smooth family $\boldsymbol{g}_t$ of conformal metrics on M such that $\boldsymbol{g}_0 = \boldsymbol{g}$, then the derivative $\varphi_t = \dot{\boldsymbol{g}}_t \in \mathscr{S}(2)$ is trace-free with respect to $\boldsymbol{g}_t$. As shown in [Graham and Hirachi 2005], the derivative of $\overline{Q}_t$ is given by

$$\frac{d}{dt}\overline{Q}_t = (-1)^{n/2}\frac{n-2}{2}\int_M \langle \mathcal{O}_t, \varphi_t\rangle_{\boldsymbol{g}_t},$$

where $\mathcal{O}_t$ is the Fefferman–Graham ambient obstruction tensor of $\boldsymbol{g}_t$ [Fefferman and Graham 1985; 2012]. In particular, if $(M, [g])$ has vanishing obstruction tensor, which is the case if $(M, [g])$ is conformally Einstein for instance, then $\overline{Q}_t$ stabilizes at $t = 0$. In this case the second derivative of $\overline{Q}_t$ at $t = 0$ is of interest. It is given by

$$\text{(0-4)}\qquad \left.\frac{d^2}{dt^2}\overline{Q}_t\right|_{t=0} = (-1)^{n/2}\frac{n-2}{2}\int_M \langle \mathcal{O}'_{\boldsymbol{g}}\varphi, \varphi\rangle_{\boldsymbol{g}},$$

where $\mathcal{O}'_{\boldsymbol{g}} : \mathscr{S}_0(2) \to \mathscr{S}_0(2-n)$ is the linearization at $\boldsymbol{g}$ of the obstruction tensor operator ($\mathcal{O}'_{\boldsymbol{g}}\varphi$ is trace-free because $\boldsymbol{g}$ is obstruction-flat). This shows that it suffices to compute $\mathcal{O}'_{\boldsymbol{g}}$ to derive the second variational formula of the total Q-curvature. The construction of our operators P_k leads to the fact that $P = P_{n/2}$ is equal to $\mathcal{O}'_{\boldsymbol{g}}$ up to a constant factor for obstruction-flat manifolds. (For $n = 4$ and 6, since an explicit formula of the obstruction tensor is known, one can directly compute its linearization. In higher dimensions our result is really new, because there is no such concrete formula for $\mathcal{O}$.) Thus our GJMS construction adds new knowledge of $\mathcal{O}'_{\boldsymbol{g}}$, which was previously studied in [Branson 2005; Branson and Gover 2007; 2008].

If we specialize to the case of conformally Einstein manifolds, explicit computation is possible thanks to a well-known associated ambient metric. We will derive a formula of P_k restricted to $\mathcal{S}^g_{\mathrm{TT}}(-n/2+2+k)$ with respect to an Einstein representative g with Schouten tensor $P_{ij} = \lambda g_{ij}$:

$$\text{(0-5)}\quad P_k|_{\mathcal{S}^g_{\mathrm{TT}}(-n/2+2+k)} = \prod_{m=0}^{k-1}\Bigl(\Delta_{\mathrm{L}} - 4(n-1)\lambda - 2\Bigl(-\frac{n}{2}+k-2m\Bigr)\Bigl(\frac{n}{2}+k-2m-1\Bigr)\lambda\Bigr).$$

Then Theorem 0.2 is an immediate consequence.

This article is organized as follows. Preliminaries about ambient metrics and some preparatory lemmas are included in Section 1. In Section 2, our operators P_k are constructed. One of the characterizations of P_k is that it gives the obstruction to dilation-annihilating TT-harmonic extension of $\varphi \in \mathcal{S}_0(-n/2+2+k)$ with respect to the ambient Lichnerowicz Laplacian $\tilde{\Delta}_{\mathrm{L}}$. In Section 3, we first show that the variation of the normal-form ambient metric modified by adding a certain tensor in the image of the Killing operator of $\tilde{g}$ is a best possible approximate solution to the harmonic extension problem mentioned above. Using this fact, we prove that the trace-free part of $\mathcal{O}'_g$ equals P in general. In Section 4, we work on conformally Einstein manifolds and prove Theorem 0.2.

In this article, "conformal manifolds" are of arbitrary signature unless otherwise stated. Index notation is used throughout. On ambient spaces we use $I, J, K, \dots$ as indices, while on the original manifolds $i, j, k, \dots$ are used.

1. Preliminaries

Let $(M, [g])$ be a conformal manifold of dimension n of signature (p, q) with metric cone $\mathcal{G}$. With a fixed representative metric $g \in [g]$, $\mathcal{G}$ is trivialized as

$$\mathcal{G} \cong \mathbb{R}_+ \times M, \quad t^2 g_x \mapsto (t, x).$$

Let $\tilde{\mathcal{G}}$ be the associated ambient space:

$$\tilde{\mathcal{G}} := \mathcal{G} \times \mathbb{R} \cong \mathbb{R}_+ \times M \times \mathbb{R} = \{(t, x, \rho)\}.$$

In our index notation, if $\tilde{\mathcal{G}}$ is trivialized as above, we use the indices 0 and ∞ for the t- and ρ-components, respectively.

The space $\mathcal{G}$ carries a natural $\mathbb{R}_+$-bundle structure. The dilation δ_s, $s \in \mathbb{R}^\times$, is by definition the action of $s^2 \in \mathbb{R}_+$, and the infinitesimal dilation field is denoted by T. The spaces of the densities, weighted 1-forms, and weighted covariant symmetric 2-tensors (all of weight w) are denoted by $\mathcal{E}(w)$, $\mathcal{T}(w)$, and $\mathcal{S}(w)$. By the metric cone $\mathcal{G}$, these spaces are realized as follows:

$$\begin{aligned} \mathcal{E}(w) &= \{ f \in C^\infty(\mathcal{G}, \mathbb{R}) \mid Tf = wf \}, \\ \mathcal{T}(w) &= \{ \tau \in C^\infty(\mathcal{G}, T^*\mathcal{G}) \mid T \lrcorner \tau = 0, \quad \mathcal{L}_T \tau = w\tau \}, \\ \mathcal{S}(w) &= \{ \sigma \in C^\infty(\mathcal{G}, \operatorname{Sym}^2 T^*\mathcal{G}) \mid T \lrcorner \sigma = 0, \quad \mathcal{L}_T \sigma = w\sigma \}. \end{aligned} \tag{1-1}$$

The $\mathbb{R}_+$-action extends to $\tilde{\mathcal{G}} = \mathcal{G} \times \mathbb{R}$ and so does T. In terms of the extended T, we define

$$\begin{aligned} \tilde{\mathcal{E}}(w) &:= \{ \tilde{f} \in C^\infty(\tilde{\mathcal{G}}, \mathbb{R}) \mid T\tilde{f} = w\tilde{f} \}, \\ \tilde{\mathcal{T}}(w) &:= \{ \tilde{\tau} \in C^\infty(\tilde{\mathcal{G}}, T^*\tilde{\mathcal{G}}) \mid \mathcal{L}_T \tilde{\tau} = w\tilde{\tau} \}, \\ \tilde{\mathcal{S}}(w) &:= \{ \tilde{\sigma} \in C^\infty(\tilde{\mathcal{G}}, \operatorname{Sym}^2 T^*\tilde{\mathcal{G}}) \mid \mathcal{L}_T \tilde{\sigma} = w\tilde{\sigma} \}. \end{aligned}$$

When $\tilde{\sigma} \in \tilde{\mathcal{S}}(w)$ satisfies $(T \lrcorner \tilde{\sigma})|_{T\mathcal{G}} = 0$, then $\tilde{\sigma}|_{T\mathcal{G}}$ makes sense as a section in $\mathcal{S}(w)$ via the identification (1-1). We use the notation $\tilde{\sigma}|_{TM}$ to express this weighted tensor.

Let $\tilde{g}$ be a preambient metric. This means that $\tilde{g} \in \tilde{\mathcal{S}}(2)$ is a homogeneous pseudo-Riemannian metric of signature $(p+1, q+1)$ defined on a dilation-invariant open neighborhood of $\mathcal{G}$ in $\tilde{\mathcal{G}}$ such that its pullback to $\mathcal{G}$ is equal to $\boldsymbol{g} \in \mathcal{S}(2)$. In the sequel we only work asymptotically near $\mathcal{G}$, so we may assume that all preambient metrics are defined on the whole $\tilde{\mathcal{G}}$. We next introduce the *straightness* condition:

$$\tilde{\nabla} T = \mathrm{id}. \tag{1-2}$$

If this is true, the differential of the canonical defining function $r = |T|^2_{\tilde{g}}$ of $\mathcal{G}$ is

$$dr = 2T \lrcorner \tilde{g}. \tag{1-3}$$

Recall that it follows immediately from (1-2) that

$$T^I \tilde{R}_{IJKL} = 0, \quad \text{and hence} \quad T^I \widetilde{\mathrm{Ric}}_{IJ} = 0. \tag{1-4}$$

The Fefferman–Graham theorem states that there is a straight preambient metric $\tilde{g}$ with

$$\widetilde{\mathrm{Ric}} = \begin{cases} O(r^\infty) & \text{if } n \text{ is odd}, \\ O(r^{n/2-1}) & \text{if } n \text{ is even}. \end{cases}$$

In this article, such a metric $\tilde{g}$ is called an *ambient metric*. When n is odd, ambient metrics are unique modulo $O(r^\infty)$ and the action of dilation-invariant diffeomorphisms on $\tilde{\mathcal{G}}$ leaving points on $\mathcal{G}$ fixed (such diffeomorphisms are called *ambient-equivalence maps* in the sequel). If n is even, the situation is subtle. For a 1-form $\tilde{\tau} \in \tilde{\mathcal{T}}(w)$, we define

$$\begin{aligned} \tilde{\tau} = O^-(r^m) &\iff \tilde{\tau} = O(r^{m-1}) \quad \text{and} \quad (r^{1-m}\tilde{\tau})|_{T\mathcal{G}} \text{ vanishes} \\ &\iff \tilde{\tau} = O(r^m) \quad \operatorname{mod} r^{m-1} T \lrcorner \tilde{g}. \end{aligned}$$

We say that $\tilde{\sigma} \in \tilde{\mathcal{S}}(w)$ is $O^+(r^m)$ if

(i) $\tilde{\sigma} = O(r^m)$;

(ii) $T \lrcorner \tilde{\sigma} = O^-(r^{m+1})$ and hence $(r^{-m}\tilde{\sigma})|_{TM}$ makes sense; and

(iii) $(r^{-m}\tilde{\sigma})|_{TM} \in \mathcal{S}(w-2m)$ is trace-free with respect to $\boldsymbol{g}$.

Then, ambient metrics are unique modulo $O^+(r^{n/2})$ and the action of ambient-equivalence maps. By [Fefferman and Graham 2012, Equation (3.13)], the condition $\widetilde{\mathrm{Ric}} = O(r^{n/2-1})$ for ambient metrics actually forces

$$\widetilde{\mathrm{Ric}} = O^+(r^{n/2-1}).$$

Let $g \in [g]$ and consider the induced trivialization $\tilde{\mathcal{G}} \cong \mathbb{R}_+ \times M \times \mathbb{R}$. If a straight preambient metric $\tilde{g}$ is near $\mathcal{G}$ of the form

$$\tilde{g} = 2\rho\, dt^2 + 2\rho\, dt\, d\rho + t^2 g_\rho, \tag{1-5}$$

where g_ρ is a 1-parameter family of metrics on M with $g_0 = g$, then $\tilde{g}$ is said to be in *normal form relative to* g. For any straight preambient metric $\tilde{g}$ and a choice of $g \in [g]$, it is known [ibid., Proposition 2.8] that there exists an ambient-equivalence map Φ such that $\Phi^* \tilde{g}$ is in normal form relative to g.

Lemma 1.1. *Let $\tilde{g}$ be a straight preambient metric. For $\tilde{\tau} \in \tilde{\mathcal{T}}(w)$ and $\tilde{\sigma} \in \tilde{\mathcal{S}}(w)$,*

$$\tilde{\nabla}_T \tilde{\tau} = (w-1)\tilde{\tau}, \quad \tilde{\nabla}_T \tilde{\sigma} = (w-2)\tilde{\sigma}.$$

Proof. Let $\tilde{\xi} \in \mathfrak{X}(\tilde{\mathcal{G}})$. Then, since the Levi-Civita connection is torsion-free,

$$\begin{aligned}(\tilde{\nabla}_T \tilde{\tau})(\tilde{\xi}) &= T(\tilde{\tau}(\tilde{\xi})) - \tilde{\tau}(\tilde{\nabla}_T \tilde{\xi}) = T(\tilde{\tau}(\tilde{\xi})) - \tilde{\tau}([T, \tilde{\xi}] + \tilde{\nabla}_{\tilde{\xi}} T) \\ &= T(\tilde{\tau}(\tilde{\xi})) - \tilde{\tau}(\mathcal{L}_T \tilde{\xi}) - \tilde{\tau}(\tilde{\nabla}_{\tilde{\xi}} T) = (\mathcal{L}_T \tilde{\tau})(\tilde{\xi}) - \tilde{\tau}(\tilde{\xi}) = (w-1)\tilde{\tau}(\tilde{\xi}).\end{aligned}$$

The second equality is proved similarly. □

Now let $\tilde{g}$ be a fixed ambient metric. Let $\tilde{\mathcal{S}}_0(w)$ be the subspace of formally trace-free tensors of $\tilde{\mathcal{S}}(w)$, and $\tilde{\mathcal{S}}_{\mathrm{TT}}(w)$ the subspace of formally TT-tensors. Moreover, we define

$$\tilde{\mathcal{S}}^X(w) := \{\tilde{\sigma} \in \tilde{\mathcal{S}}(w) \mid T \lrcorner \tilde{\sigma} = O(r^\infty)\},$$
$$\tilde{\mathcal{S}}^X_0(w) := \tilde{\mathcal{S}}_0(w) \cap \tilde{\mathcal{S}}^X(w), \quad \tilde{\mathcal{S}}^X_{\mathrm{TT}}(w) := \tilde{\mathcal{S}}_{\mathrm{TT}}(w) \cap \tilde{\mathcal{S}}^X(w).$$

If n is odd, these spaces are invariant under $O(r^\infty)$-modifications of $\tilde{g}$. If n is even, we need some technically defined tensor spaces. For $2-n \le w \le 2$, we set

$$\tilde{\mathcal{S}}_{\mathrm{aTT}}(w) := \{\tilde{\sigma} \in \tilde{\mathcal{S}}(w) \mid \mathrm{tr}_{\tilde{g}}\, \tilde{\sigma} = O(r^{\lceil (n-2+w)/2 \rceil}), \quad \delta_{\tilde{g}} \tilde{\sigma} = O^-(r^{\lceil (n-2+w)/2 \rceil})\}$$

("aTT" is for "approximately TT") and

$$\tilde{\mathcal{S}}^X_{\mathrm{aTT}}(w) := \{\tilde{\sigma} \in \tilde{\mathcal{S}}_{\mathrm{aTT}}(w) \mid T \lrcorner \tilde{\sigma} = O^-(r^{\lceil (n-2+w)/2 \rceil + 1})\},$$

where $\delta_{\tilde{g}}$ is the divergence operator $(\delta_{\tilde{g}}\tilde{\sigma})_I = -\tilde{\nabla}^J \tilde{\sigma}_{IJ}$, and $\lceil x \rceil$ is the smallest integer not less than x. Then $\tilde{\mathcal{S}}^X_{\mathrm{aTT}}(w)$ does not depend on the $O^+(r^{n/2})$-ambiguity of $\tilde{g}$. To check this, let $\tilde{g}' = \tilde{g} + A$ be another ambient metric with $A = O^+(r^{n/2})$. Then $T \lrcorner A = O^-(r^{n/2+1})$. Since $\operatorname{tr}_{\tilde{g}'} \tilde{\sigma} = \operatorname{tr}_{\tilde{g}} \tilde{\sigma} + O(r^{n/2})$ for any $\tilde{\sigma}$, the trace condition is not affected. The Christoffel symbol of $\tilde{g}'$ is given by

$$(\tilde{\Gamma}')^K{}_{IJ} = \tilde{\Gamma}^K{}_{IJ} - \tfrac{1}{2}(\tilde{g}'^{-1})^{KL}(DA)_{LIJ} = \tilde{\Gamma}^K{}_{IJ} - \tfrac{1}{2}(DA)^K{}_{IJ} + O(r^{n/2}),$$

where

$$(DA)_{KIJ} = \tilde{\nabla}_K A_{IJ} - \tilde{\nabla}_I A_{KJ} - \tilde{\nabla}_J A_{KI}.$$

Hence

$$(\delta_{\tilde{g}'}\tilde{\sigma})_I = (\delta_{\tilde{g}}\tilde{\sigma})_I + \tfrac{1}{2}(DA)^{JK}{}_I \tilde{\sigma}_{JK} + \tfrac{1}{2}(DA)^{JK}{}_K \tilde{\sigma}_{IJ} + O(r^{n/2}).$$

Let $A = r^{n/2}\overline{A}$. Then

$$(DA)_{KIJ} = nr^{n/2-1}\big(T_K \overline{A}_{IJ} - T_I \overline{A}_{KJ} - T_J \overline{A}_{KI}\big) + O(r^{n/2})$$

and, because $T \lrcorner \overline{A} = O^-(r)$,

$$(DA)_{KI}{}^I = nr^{n/2-1} T_K \overline{A}_I{}^I + O^-(r^{n/2}).$$

Therefore, if $\tilde{\sigma} \in \tilde{\mathcal{S}}^X_{\mathrm{aTT}}(w)$, $\delta_{\tilde{g}'}\tilde{\sigma} = \delta_{\tilde{g}}\tilde{\sigma} + O^-(r^{n/2}) = O^-(r^{\lceil (n-2+w)/2 \rceil})$.

Lemma 1.2. *Let $\tilde{g}$ be an ambient metric and $\varphi \in \mathcal{S}_0(-n/2+2+k)$, where $k \in \mathbb{Z}_+$. If n is odd, then there exists $\tilde{\sigma} \in \tilde{\mathcal{S}}^X_{\mathrm{TT}}(-n/2+2+k)$ such that $\tilde{\sigma}|_{TM} = \varphi$. If n is even, there exists $\tilde{\sigma} \in \tilde{\mathcal{S}}^X_{\mathrm{aTT}}(-n/2+2+k)$ such that $\tilde{\sigma}|_{TM} = \varphi$ as long as $k \le n/2$. In both cases, the restriction $\tilde{\varphi} = \tilde{\sigma}|_{\mathcal{G}}$ is uniquely determined.*

Proof. To prove the existence part, take any $\tilde{\sigma}_{(0)} \in \tilde{\mathcal{S}}^X_0(-n/2+2+k)$ for which $\tilde{\sigma}_{(0)}|_{TM} = \varphi$. We shall inductively construct $\tilde{\sigma}_{(m)} \in \tilde{\mathcal{S}}^X_0(-n/2+2+k)$ for nonnegative integers m such that

$$\tilde{\sigma}_{(m)} = \tilde{\sigma}_{(m-1)} + O(r^{m-1}), \quad \delta_{\tilde{g}}\tilde{\sigma}_{(m)} = O(r^m).$$

Suppose we have $\tilde{\sigma}_{(m-1)} \in \tilde{\mathcal{S}}^X_0(-n/2+2+k)$ with $\delta_{\tilde{g}}\tilde{\sigma}_{(m-1)} = O(r^{m-1})$. If $\tilde{\sigma}_{(m)} \in \tilde{\mathcal{S}}^X_0(-n/2+2+k)$, then $T \lrcorner \delta_{\tilde{g}}\tilde{\sigma}_{(m)} = 0$ is automatically guaranteed:

$$T^I \tilde{\nabla}^J (\tilde{\sigma}_{(m-1)})_{IJ} = \tilde{\nabla}^J\big(T^I (\tilde{\sigma}_{(m-1)})_{IJ}\big) - \big(\tilde{\nabla}^J T^I\big)(\tilde{\sigma}_{(m-1)})_{IJ} = 0 + \tilde{g}^{IJ}(\tilde{\sigma}_{(m-1)})_{IJ} = 0.$$

We seek for $\tilde{\sigma}_{(m)}$ assuming that it is of the form

$$(\tilde{\sigma}_{(m)})_{IJ} = (\tilde{\sigma}_{(m-1)})_{IJ} + 2r^{m-1} T_{(I} V_{J)} + r^{m-1} \tilde{f} T_I T_J - r^m W_{IJ}, \tag{1-6}$$

where $V \in \tilde{\mathcal{T}}(-n/2+2+k-2m)$ satisfies $T^I V_I = 0$, $\tilde{f} \in \tilde{\mathcal{E}}(-n/2+k-2m)$, and $W \in \tilde{\mathcal{S}}^X(-n/2+2+k-2m)$ is such that the whole expression (1-6) is trace-free and vanishes if contracted with T (hence $\operatorname{tr}_{\tilde g} W = \tilde f$, $T^J W_{IJ} = V_I + \tilde f T_I$). Minus of the divergences of the additional three terms on the right-hand side of (1-6) are

$$\begin{aligned}\tilde\nabla^J\bigl(2r^{m-1}T_{(I}V_{J)}\bigr) &= r^{m-1}\cdot\bigl((n/2+2+k)V_I + T_I\tilde\nabla^J V_J\bigr) + O(r^m),\\ \tilde\nabla^J\bigl(r^{m-1}\tilde f T_I T_J\bigr) &= r^{m-1}\cdot(n/2+1+k)\tilde f T_I + O(r^m),\\ \tilde\nabla^J(-r^m W_{IJ}) &= r^{m-1}\cdot(-2m)\bigl(V_I+\tilde f T_I\bigr) + O(r^m).\end{aligned}$$

Therefore, we first put $V = (n/2+2+k-2m)^{-1}r^{-m+1}\delta_{\tilde g}\tilde\sigma_{(m-1)}$, and set $\tilde f = -(n/2+1+k-2m)^{-1}\tilde\nabla^J V_J$ so that the $O(r^{m-1})$-term of the divergence of (1-6) vanishes. This is possible for all m if n is odd, and until $m = \lfloor n/2+k\rfloor$ if n is even. Applying Borel's lemma, the proof of the existence for n odd is complete. When n is even, we get $\tilde\sigma = \tilde\sigma_{(\lfloor(n/2+k)/2\rfloor)}$. Furthermore, if $n/2+1+k$ is an even number, then $\delta_{\tilde g}\tilde\sigma$ can be made $O^-(r^{(n/2+1+k)/2})$. Anyway, $\delta_{\tilde g}\tilde\sigma$ finally becomes $O^-(r^{\lceil(n/2+k)/2\rceil})$, and the existence for n even is proved.

Let us once again take $\tilde\sigma_{(0)}$ as we did in the beginning of this proof. If $\tilde\sigma$ is as in the statement, then since $(T\lrcorner\tilde\sigma)|_{\mathcal G} = 0$ and $\tilde\sigma|_{TM} = \varphi$, $\tilde\sigma$ must be written as

$$\tilde\sigma = \tilde\sigma_{(0)} + 2T_{(I}V_{J)} - rW_{IJ},$$

where $T^I V_I = O(r)$. Moreover, in order for $T\lrcorner\tilde\sigma = O(r^2)$ to be satisfied, $T^J W_{IJ}$ should be $V_I + r^{-1}T_I T^J V_J + O(r)$. Then

$$\tilde\nabla^J\bigl(2T_{(I}V_{J)} - rW_{IJ}\bigr) = \Bigl(\frac{n}{2}+k\Bigr)V_I + T_I\bigl(\tilde\nabla^J V_J - 2r^{-1}T^J V_J\bigr) + O(r).$$

Therefore, $V_I \bmod O^-(r)$ is determined by the condition $\delta_{\tilde g}\tilde\sigma = O^-(r)$. If we put $\tilde f T_I$ into V_I, then the right-hand side will be $(n+2k-2)\tilde f T_I$. Thus V_I is uniquely determined in order to satisfy $\delta_{\tilde g}\tilde\sigma = O(r)$. □

We call $\tilde\varphi$ in Lemma 1.2 the *ambient lift* of $\varphi \in \mathcal S(-n/2+2+k)$.

2. A GJMS construction for trace-free symmetric 2-tensors

Let $(M,[g])$ be a conformal manifold of dimension $n \ge 3$ and $\tilde g$ an ambient metric. We shall play with the following three operators:

$$\begin{aligned} &x : \tilde{\mathcal S}(w) \to \tilde{\mathcal S}(w+2), && \tilde\sigma \mapsto \tfrac14 r\tilde\sigma,\\ &y : \tilde{\mathcal S}(w) \to \tilde{\mathcal S}(w-2), && \tilde\sigma \mapsto \tilde\Delta_{\mathrm L}\tilde\sigma,\\ &h : \tilde{\mathcal S}(w) \to \tilde{\mathcal S}(w), && \tilde\sigma \mapsto \Bigl(\tilde\nabla_T + \frac{n+2}{2}\Bigr)\tilde\sigma = \Bigl(w + \frac{n}{2} - 1\Bigr)\tilde\sigma.\end{aligned}$$

Just as in the case of the classical GJMS construction, one can verify the following.

Proposition 2.1. *The operators x, y, h enjoy the $\mathfrak{sl}(2)$ commutation relations*:

$$[h,x] = 2x,\quad [h,y] = -2y,\quad [x,y] = h.$$

The proof is left to the reader. Consequently we have the following identities:

$$[y^m, x] = -my^{m-1}(h - m + 1), \tag{2-1}$$

$$[x^m, y] = mx^{m-1}(h + m - 1), \tag{2-2}$$

$$y^{m-1}x^{m-1} = (-1)^{m-1}(m-1)!\, h(h+1)\cdots(h+m-2) + xZ_m, \tag{2-3}$$

where Z_m is some polynomial in x, y, h.

We are going to verify that x, y, and h preserve the subspaces $\tilde{\mathcal{S}}^X_{\mathrm{TT}}(w)$ when n is odd and $\tilde{\mathcal{S}}^X_{\mathrm{aTT}}(w)$ when n is even. For this we need two lemmas.

Lemma 2.2. *For $\tilde{f} \in \tilde{\mathcal{E}}(w)$, $\tilde{\tau} \in \tilde{\mathcal{T}}(w)$,*

$$\tilde{f} = O(r^m) \Longrightarrow \tilde{\Delta}\tilde{f} = O(r^{m-1}), \tag{2-4}$$

$$\tilde{\tau} = O^-(r^m) \Longrightarrow \tilde{\Delta}\tilde{\tau} = O^-(r^{m-1}). \tag{2-5}$$

In (2-5), *we may also replace $\tilde{\Delta}$ with the Hodge Laplacian $\tilde{\Delta}_{\mathrm{H}}$.*

Proof. First we compute $\tilde{\Delta}(r^m)$:

$$\tilde{\Delta}(r^m) = -\tilde{\nabla}^I\tilde{\nabla}_I(r^m) = -\tilde{\nabla}^I(2mr^{m-1}T_I) = -2m(2m+n)r^{m-1}.$$

Hence it is clear that $\tilde{f} = O(r^m)$ implies $\tilde{\Delta}\tilde{f} = O(r^{m-1})$ and that $\tilde{\tau} = O(r^m)$ implies $\tilde{\Delta}\tilde{\tau} = O(r^{m-1})$. So, to prove (2-5), it remains to show that $\tilde{\Delta}(r^{m-1}\tilde{f}T_I)$ is $O^-(r^{m-1})$. This is checked directly:

$$\tilde{\nabla}_J\bigl(r^{m-1}\tilde{f}T_I\bigr) = 2(m-1)r^{m-2}\tilde{f}T_I\,T_J + r^{m-1}\tilde{f}\tilde{g}_{IJ} + r^{m-1}T_I\,\tilde{\nabla}_J\tilde{f}$$

and therefore

$$\tilde{\Delta}\bigl(r^{m-1}\tilde{f}T_I\bigr) = -2(m-1)(2m+n+2w)r^{m-2}\tilde{f}T_I + O(r^{m-1}).$$

By Bochner's formula $\tilde{\Delta}_{\mathrm{H}}\tilde{\tau}_I = \tilde{\Delta}\tilde{\tau}_I + \widetilde{\mathrm{Ric}}_I{}^J\tilde{\tau}_J$, $\tilde{\Delta}_{\mathrm{H}}\tilde{\tau} = O^-(r^{m-1})$ is clear. □

Let $\bigl(D\widetilde{\mathrm{Ric}}\bigr)^\circ : \tilde{\mathcal{S}}(w) \to \tilde{\mathcal{T}}(w-4)$ be defined by

$$\bigl(\bigl(D\widetilde{\mathrm{Ric}}\bigr)^\circ\tilde{\sigma}\bigr)_I = \bigl(\tilde{\nabla}_I\widetilde{\mathrm{Ric}}_{JK} - \tilde{\nabla}_J\widetilde{\mathrm{Ric}}_{IK} - \tilde{\nabla}_K\widetilde{\mathrm{Ric}}_{IJ}\bigr)\tilde{\sigma}^{JK}.$$

Then it is known that, on any symmetric 2-tensor,

$$\delta_{\tilde{g}} \circ \tilde{\Delta}_{\mathrm{L}} = \tilde{\Delta}_{\mathrm{H}} \circ \delta_{\tilde{g}} + \bigl(D\widetilde{\mathrm{Ric}}\bigr)^\circ. \tag{2-6}$$

Lemma 2.3. *When n is even and $2 - n \le w \le 2$,*

$$\tilde{\sigma} \in \tilde{\mathcal{S}}^X_{\mathrm{aTT}}(w) \Longrightarrow \bigl(D\widetilde{\mathrm{Ric}}\bigr)^\circ\tilde{\sigma} = O^-(r^{n/2-1}).$$

Proof. Let $\widetilde{\mathrm{Ric}} = r^{n/2-1}\tilde{S}$. Then

$$\tilde{\nabla}_I \widetilde{\mathrm{Ric}}_{JK} = (n-2)r^{n/2-2}T_I\,\tilde{S}_{JK} + O(r^{n/2-1}). \tag{2-7}$$

Therefore

$$\big(\tilde{\nabla}_I \widetilde{\mathrm{Ric}}_{JK}\big)\tilde{\sigma}^{JK} = (n-2)r^{n/2-2}\langle \tilde{S}, \tilde{\sigma}\rangle_{\tilde{g}} T_I + O(r^{n/2-1}).$$

On the other hand, since $T \lrcorner \tilde{\sigma}$ is at least $O^-(r)$, we can write $T^I\tilde{\sigma}_{IJ} = \tilde{f}T_J + O(r)$. Hence, by (2-7) and (1-4),

$$\big(\tilde{\nabla}_J \widetilde{\mathrm{Ric}}_{IK}\big)\tilde{\sigma}^{JK} = (n-2)r^{n/2-2}\tilde{f}T^K\tilde{S}_{IK} + O(r^{n/2-1}) = O(r^{n/2-1}).$$

Consequently, $\big(D\widetilde{\mathrm{Ric}}\big)^\circ\tilde{\sigma} = O^-(r^{n/2-1})$. □

Proposition 2.4. *If n is odd, then, for any w,*

$$x\big(\tilde{\mathscr{S}}^X_{\mathrm{TT}}(w)\big) \subset \tilde{\mathscr{S}}^X_{\mathrm{TT}}(w+2), \quad y\big(\tilde{\mathscr{S}}^X_{\mathrm{TT}}(w)\big) \subset \tilde{\mathscr{S}}^X_{\mathrm{TT}}(w-2), \quad h\big(\tilde{\mathscr{S}}^X_{\mathrm{TT}}(w)\big) \subset \tilde{\mathscr{S}}^X_{\mathrm{TT}}(w).$$

If n is even,

$$\begin{aligned} &x\big(\tilde{\mathscr{S}}^X_{\mathrm{aTT}}(w)\big) \subset \tilde{\mathscr{S}}^X_{\mathrm{aTT}}(w+2), && 2-n \le w \le 0,\\ &y\big(\tilde{\mathscr{S}}^X_{\mathrm{aTT}}(w)\big) \subset \tilde{\mathscr{S}}^X_{\mathrm{aTT}}(w-2), && -n \le w \le 2,\\ &h\big(\tilde{\mathscr{S}}^X_{\mathrm{aTT}}(w)\big) \subset \tilde{\mathscr{S}}^X_{\mathrm{aTT}}(w), && 2-n \le w \le 2. \end{aligned}$$

Proof. Since the case n odd is easier to prove, we discuss the case n even. It is clear that $h(\tilde{\mathscr{S}}^X_{\mathrm{aTT}}(w)) \subset \tilde{\mathscr{S}}^X_{\mathrm{aTT}}(w)$. For $\tilde{\sigma} \in \tilde{\mathscr{S}}^X_{\mathrm{aTT}}(w)$, we have $T \lrcorner (r\tilde{\sigma}) = rT \lrcorner \tilde{\sigma} = O^-(r^{\lceil (n-2+w)/2\rceil+2})$, $\mathrm{tr}_{\tilde{g}}(r\tilde{\sigma}) = r\,\mathrm{tr}_{\tilde{g}}\,\tilde{\sigma} = O(r^{\lceil (n-2+w)/2\rceil+1})$, and

$$\delta_{\tilde{g}}(r\tilde{\sigma}) = -2T \lrcorner \tilde{\sigma} + r\delta_{\tilde{g}}\tilde{\sigma} = O^-\big(r^{\lceil (n-2+w)/2\rceil+1}\big).$$

Hence $x\tilde{\sigma} \in \tilde{\mathscr{S}}^X_{\mathrm{aTT}}(w+2)$. It remains to show that $y\tilde{\sigma} \in \tilde{\mathscr{S}}^X_{\mathrm{aTT}}(w-2)$. The trace of $\tilde{\Delta}_{\mathrm{L}}\tilde{\sigma}$ is $\mathrm{tr}_{\tilde{g}}\,\tilde{\Delta}_{\mathrm{L}}\tilde{\sigma} = \tilde{\Delta}(\mathrm{tr}_{\tilde{g}}\,\tilde{\sigma}) = O(r^{\lceil (n-2+w)/2\rceil-1})$ by (2-4). Furthermore,

$$\tilde{\nabla}_K\big(T^J\tilde{\sigma}_{IJ}\big) = \delta_K{}^J\tilde{\sigma}_{IJ} + T^J\tilde{\nabla}_K\tilde{\sigma}_{IJ} = \tilde{\sigma}_{IK} + T^J\tilde{\nabla}_K\tilde{\sigma}_{IJ}$$

and hence

$$\begin{aligned} \tilde{\Delta}(T^J\tilde{\sigma}_{IJ}) &= -\tilde{\nabla}^K\tilde{\sigma}_{IK} - \tilde{\nabla}^K\big(T^J\tilde{\nabla}_K\tilde{\sigma}_{IJ}\big)\\ &= -2\tilde{\nabla}^K\tilde{\sigma}_{IK} - T^J\tilde{\nabla}^K\tilde{\nabla}_K\tilde{\sigma}_{IJ} = -2\tilde{\nabla}^K\tilde{\sigma}_{IK} + T^J\tilde{\Delta}_{\mathrm{L}}\tilde{\sigma}_{IJ}; \end{aligned}$$

the last equality is because of (1-4). This implies $T \lrcorner \tilde{\Delta}_{\mathrm{L}}\tilde{\sigma} = O^-(r^{\lceil (n-2+w)/2\rceil})$. Finally, (2-6) and Lemma 2.3 show $\delta_{\tilde{g}}\tilde{\Delta}_{\mathrm{L}}\tilde{\sigma} = O^-(r^{\lceil (n-2+w)/2\rceil-1})$. □

Theorem 2.5. *Let $k \in \mathbb{Z}_+$ if n is odd, and $k \in \{1, 2, \ldots, n/2\}$ if n is even. For any $\varphi \in \mathscr{S}_0(-n/2+2+k)$, let $\tilde{\sigma} \in \tilde{\mathscr{S}}(-n/2+2+k)$ be any extension of the ambient lift $\tilde{\varphi}$. Then $\tilde{\Delta}^k_{\mathrm{L}}\tilde{\sigma}|_{\mathscr{G}}$ depends only on φ and not on the extension. Furthermore, $\tilde{\Delta}^k_{\mathrm{L}}\tilde{\sigma}|_{TM}$ makes sense as a section in $\mathscr{S}(-n/2+2-k)$.*

Proof. We work on the case n even only. Any two extensions of $\tilde{\varphi}$ differ by a tensor of the form $r\tilde{\tau}$, where $\tilde{\tau} \in \tilde{\mathcal{S}}_0(-n/2+k)$. Equation (2-1) shows that the commutator $[\tilde{\Delta}_{\mathrm{L}}^k, r]$ vanishes on $\tilde{\mathcal{S}}_0(-n/2+k)$ and hence $\tilde{\Delta}_{\mathrm{L}}^k(r\tilde{\tau})|_{\mathcal{G}} = 0$. In particular, using Lemma 1.2 one can take $\tilde{\sigma} \in \tilde{\mathcal{S}}^X_{\mathrm{aTT}}(-n/2+2+k)$ as an extension of $\tilde{\varphi}$. Then by Proposition 2.4, $\tilde{\Delta}_{\mathrm{L}}^k\tilde{\sigma} \in \tilde{\mathcal{S}}^X_{\mathrm{aTT}}(-n/2+2-k)$ and $\tilde{\Delta}_{\mathrm{L}}^k\tilde{\sigma}|_{TM}$ is defined. □

Theorem 2.6. *Let $k \in \mathbb{Z}_+$ if n is odd, and $k \in \{1, 2, \dots, n/2\}$ if n is even. Let $\varphi \in \mathcal{S}_0(-n/2+2+k)$ and let $\tilde{\varphi}$ be its ambient lift. Then there exists a solution $\tilde{\sigma} \in \tilde{\mathcal{S}}^X_{\mathrm{TT}}(-n/2+2+k)$ if n is odd, and $\tilde{\sigma} \in \tilde{\mathcal{S}}^X_{\mathrm{aTT}}(-n/2+2+k)$ if n is even, to the problem*

$$\tilde{\Delta}_{\mathrm{L}}\tilde{\sigma} = O(r^{k-1}), \quad \tilde{\sigma}|_{\mathcal{G}} = \tilde{\varphi}, \tag{2-8}$$

which is unique modulo $O(r^k)$. For any such $\tilde{\sigma}$, $(r^{1-k}\tilde{\Delta}_{\mathrm{L}}\tilde{\sigma})|_{\mathcal{G}}$ is independent of the ambiguity that lives in $\tilde{\sigma}$, and agrees with $\tilde{\Delta}_{\mathrm{L}}^k\tilde{\sigma}|_{\mathcal{G}}$ up to a constant factor:

$$\big(r^{1-k}\tilde{\Delta}_{\mathrm{L}}\tilde{\sigma}\big)\big|_{\mathcal{G}} = \frac{1}{4^{k-1}(k-1)!^2}\tilde{\Delta}_{\mathrm{L}}^k\tilde{\sigma}|_{\mathcal{G}}. \tag{2-9}$$

Proof. We work on the case n even only. Let us begin with an arbitrary extension $\tilde{\sigma}_{(0)} \in \tilde{\mathcal{S}}^X_{\mathrm{aTT}}(-n/2+2+k)$ of $\tilde{\varphi}$. If an extension $\tilde{\sigma}_{(m-1)}$ satisfies $\tilde{\Delta}_{\mathrm{L}}\tilde{\sigma}_{(m-1)} = O(r^{m-1})$, then it has a modification $\tilde{\sigma}_{(m)} = \tilde{\sigma}_{(m-1)} + r^m\tilde{\sigma}_1$, $\tilde{\sigma}_1 \in \tilde{\mathcal{S}}^X_{\mathrm{aTT}}(-n/2+2+k-2m)$, which is unique modulo $O(r^{m+1})$, satisfying $\tilde{\Delta}_{\mathrm{L}}\tilde{\sigma}_{(m)} = O(r^m)$. In fact, by (2-2), we have

$$\tilde{\Delta}_{\mathrm{L}}(r^m\tilde{\sigma}_1) = 4mr^{m-1}(m-k)\tilde{\sigma}_1 + r^m\tilde{\Delta}_{\mathrm{L}}\tilde{\sigma}_1. \tag{2-10}$$

Thus $\tilde{\sigma}_1$ can be taken so that $\tilde{\Delta}_{\mathrm{L}}\tilde{\sigma}_{(m)} = O(r^m)$ unless $m = k$. Hence there is a $\tilde{\sigma}$ with the property stated in the theorem. Let $\tilde{\Delta}_{\mathrm{L}}\tilde{\sigma} = r^{k-1}\tilde{F}$, with $\tilde{F} \in \tilde{\mathcal{S}}^X_{\mathrm{aTT}}(-n/2+2-k)$. Then, by (2-3), $\tilde{\Delta}_{\mathrm{L}}^k\tilde{\sigma} = 4^{k-1}y^{k-1}x^{k-1}\tilde{F} = 4^{k-1}(k-1)!^2\tilde{F} + O(r)$. Hence (2-9). □

Except in the case where n is even and $k = n/2$, $(\tilde{\Delta}_{\mathrm{L}}^k\tilde{\sigma})|_{TM}$ is trace-free since $\mathrm{tr}_{\tilde{g}}\,\tilde{\Delta}_{\mathrm{L}}^k\tilde{\sigma}$ and $T \lrcorner \tilde{\Delta}_{\mathrm{L}}^k\tilde{\sigma}$ are both $O(r)$.

Definition 2.7. Let $(M, [g])$ be a conformal manifold of dimension $n \geq 3$ and $\tilde{g}$ an ambient metric. We call

$$P_k : \mathcal{S}_0(-n/2+2+k) \to \mathcal{S}_0(-n/2+2-k), \quad P_k\varphi = \mathrm{tf}_{\boldsymbol{g}}\big(\tilde{\Delta}_{\mathrm{L}}^k\tilde{\sigma}|_{TM}\big)$$

the *GJMS operator on trace-free symmetric 2-tensors*, where $\tilde{\sigma} \in \tilde{\mathcal{S}}(-n/2+2+k)$ is any extension of the ambient lift of φ. (One can remove $\mathrm{tf}_{\boldsymbol{g}}$ unless n is even and $k = n/2$.) In particular, when $n = \dim M \geq 4$ is even,

$$P = P_{n/2} : \mathcal{S}_0(2) \to \mathcal{S}_0(2-n)$$

is called the *critical GJMS operator on trace-free symmetric 2-tensors*.

Theorem 2.8. *The GJMS operators on trace-free symmetric* 2*-tensors do not depend on the choice of* $\tilde{g}$, *and hence are conformally invariant differential operators.*

For the case where n is even and $k = n/2$, the direct verification of the conformal invariance is not easy. We will see in Theorem 3.4 that, up to a constant factor, $P\varphi$ is equal to $\operatorname{tf}_{\boldsymbol{g}} \mathcal{O}'_{\boldsymbol{g}}\varphi$, which is clearly conformally invariant. Here, we prove the theorem in the case n odd and the case n even, $k \le n/2 - 1$.

Proof of Theorem 2.8 except the case where $(n, k) = (\mathit{even}, n/2)$. By Theorem 2.6, we may work with $r^{1-k}\tilde{\Delta}_{\mathrm{L}}\tilde{\sigma}$ instead of $\tilde{\Delta}_{\mathrm{L}}^k\tilde{\sigma}$. Let $\tilde{g}$ be an ambient metric, $\varphi \in \mathcal{S}_0(-n/2 + 2 + k)$ and, let $\tilde{\sigma}$ be a solution to the problem stated in Theorem 2.6. Then, if Φ is an ambient-equivalence map, $\Phi^*\tilde{\sigma}$ solves the same problem with respect to $\Phi^*\tilde{g}$. Since $(\Phi^* r)^{1-k}\tilde{\Delta}_{\mathrm{L},\Phi^*\tilde{g}}(\Phi^*\tilde{\sigma}) = \Phi^*(r^{1-k}\tilde{\Delta}_{\mathrm{L}}\sigma)$, the restrictions of $(\Phi^* r)^{1-k}\tilde{\Delta}_{\mathrm{L},\Phi^*\tilde{g}}(\Phi^*\tilde{\sigma})$ and $r^{1-k}\tilde{\Delta}_{\mathrm{L}}\sigma$ to TM coincide. Therefore we may assume that $\tilde{g}$ is in normal form.

When n is odd, the assertion is now clear because $\tilde{g}$ is formally unique if it is in normal form. So we assume that n is even in what follows. It suffices to show that, if $\tilde{g}$, $\hat{\tilde{g}}$ are ambient metrics in normal form and $\tilde{\sigma} \in \tilde{\mathcal{S}}^X_{\mathrm{aTT}}(-n/2 + 2 + k)$,

$$\hat{\tilde{\Delta}}_{\mathrm{L}}\tilde{\sigma} - \tilde{\Delta}_{\mathrm{L}}\tilde{\sigma} = O(\rho^{n/2-2}) \quad \text{and} \quad \hat{\tilde{\Delta}}_{\mathrm{L}}\tilde{\sigma}_{ij} - \tilde{\Delta}_{\mathrm{L}}\tilde{\sigma}_{ij} = O(\rho^{n/2-1}).$$

Let $D^K{}_{IJ} = \hat{\tilde{\Gamma}}^K{}_{IJ} - \tilde{\Gamma}^K{}_{IJ}$. From [Fefferman and Graham 2012, Equation (3.16)], one concludes that $D^K{}_{IJ} = O(\rho^{n/2-1})$ and $\tilde{\nabla}^I D^K{}_{IJ} = O(\rho^{n/2-1})$. Therefore

$$\hat{\tilde{\Delta}}\tilde{\sigma}_{IJ} - \tilde{\Delta}\tilde{\sigma}_{IJ} = \tilde{\nabla}^K\big(2D^L{}_{K(I}\tilde{\sigma}_{J)L}\big) + O(\rho^{n/2-1}) = O(\rho^{n/2-1}).$$

In addition, $\widehat{\widetilde{\mathrm{Ric}}} = \widetilde{\mathrm{Ric}} + O(\rho^{n/2-1})$ and $\hat{\tilde{R}} = \tilde{R} + O(\rho^{n/2-2})$ by [ibid., Equation (6.1)]. Hence $\hat{\tilde{\Delta}}_{\mathrm{L}}\tilde{\sigma} - \tilde{\Delta}_{\mathrm{L}}\tilde{\sigma} = O(\rho^{n/2-2})$. Moreover, if $\tilde{S}_{IJKL} = \hat{\tilde{R}}_{IJKL} - \tilde{R}_{IJKL}$, then

$$\begin{aligned}
&\hat{\tilde{\Delta}}_{\mathrm{L}}\tilde{\sigma}_{ij} - \tilde{\Delta}_{\mathrm{L}}\tilde{\sigma}_{ij} \\
&= -2t^{-4}(g_\rho^{-1})^{km}(g_\rho^{-1})^{ln}\tilde{S}_{ikjl}\tilde{\sigma}_{mn} - 4t^{-3}(g_\rho^{-1})^{km}\tilde{S}_{ikj\infty}\tilde{\sigma}_{m0} + 4t^{-4}\rho(g_\rho^{-1})^{km}\tilde{S}_{ikj\infty}\tilde{\sigma}_{m\infty} \\
&\quad -2t^{-2}\tilde{S}_{i\infty j\infty}\tilde{\sigma}_{00} + 4t^{-3}\rho\tilde{S}_{i\infty j\infty}\tilde{\sigma}_{0\infty} - 8t^{-4}\rho^2\tilde{S}_{i\infty j\infty}\tilde{\sigma}_{\infty\infty} + O(\rho^{n/2-1}).
\end{aligned}$$

Again by [ibid., Equation (6.1)], we have $\tilde{S}_{ijkl} = O(\rho^{n/2-1})$, $\tilde{S}_{ijk\infty} = O(\rho^{n/2-1})$, $\tilde{S}_{i\infty k\infty} = O(\rho^{n/2-2})$ and hence $\hat{\tilde{\Delta}}_{\mathrm{L}}\tilde{\sigma}_{ij} - \tilde{\Delta}_{\mathrm{L}}\tilde{\sigma}_{ij} = O(\rho^{n/2-1})$. □

We close this section with a lemma that is proved just like the construction of $\tilde{\sigma}$ in Theorem 2.6.

Lemma 2.9. *Let* $k \in \mathbb{Z}_+$. *For any* $\tilde{f}_1 \in \tilde{\mathcal{E}}(-n/2-2+k)$, *there exists* $\tilde{f} \in \tilde{\mathcal{E}}(-n/2+k)$ *such that*

$$\tilde{\Delta}\tilde{f} = \tilde{f}_1 + O(r^{k-1}).$$

Likewise, for any $\tilde{\tau}_1 \in \tilde{\mathcal{T}}(-n/2-1+k)$, *there exists* $\tilde{\tau} \in \tilde{\mathcal{T}}(-n/2+1+k)$ *such that*

$$\tilde{\Delta}\tilde{\tau} = \tilde{\tau}_1 + O(r^{k-1}).$$

In both problems, we may arbitrarily prescribe the values along $\mathscr{G}$; *if we prescribe* $\tilde{f}|_{\mathscr{G}}$, $\tilde{\tau}|_{\mathscr{G}}$, *then* $\tilde{f}$, $\tilde{\tau}$ *are unique modulo* $O(r^k)$.

3. The variations of obstruction tensor and Q-curvature

Let $\tilde{g}$ be an ambient metric for a conformal manifold $(M, [g])$ of dimension $n \geq 3$. Recall that, from general calculations on (pseudo-)Riemannian curvature tensors, the differential of the Ricci tensor operator (which we write as Ric here) is

$$\mathrm{Ric}'_{\tilde{g}}\,\tilde{\sigma} = \tfrac{1}{2}\tilde{\Delta}_{\mathrm{L}}\tilde{\sigma} - \delta^*_{\tilde{g}}\mathscr{B}_{\tilde{g}}\tilde{\sigma}, \tag{3-1}$$

where $\delta^*_{\tilde{g}}$ is the dual of the divergence $(\delta^*_{\tilde{g}}\tilde{\tau})_{IJ} = \tilde{\nabla}_{(I}\tilde{\tau}_{J)}$ and $\mathscr{B}_{\tilde{g}}$ is defined by $\mathscr{B}_{\tilde{g}}\tilde{\sigma} = \delta_{\tilde{g}}\tilde{\sigma} + \frac{1}{2}d(\mathrm{tr}_{\tilde{g}}\,\tilde{\sigma})$. Therefore, for n even, a solution $\tilde{\sigma} \in \tilde{\mathscr{S}}^X_{\mathrm{aTT}}(2)$ to the problem in Theorem 2.6 approximately solves $\mathrm{Ric}'_{\tilde{g}}\,\tilde{\sigma} = 0$, and hence it is expected that we can read off $\mathcal{O}'_{\boldsymbol{g}}\varphi$ from the asymptotics of $\tilde{\sigma}$. This will finally turn out to be true, but since the definition of $\mathcal{O}$ depends on the existence theorem of normal-form ambient metrics, in order to capture $\mathcal{O}'_{\boldsymbol{g}}\varphi$ our starting point has to be infinitesimal modifications of ambient metrics in normal form. The differential equation that they (approximately) satisfy is different from $\tilde{\Delta}_{\mathrm{L}}\tilde{\sigma} = 0$. So we shall establish a method for translating solutions of the two equations.

Let $(M, [g])$ be an n-dimensional conformal manifold with $n \geq 4$ even and $\varphi \in \mathscr{S}_0(2)$. Suppose that $\boldsymbol{g}_s$ is a family of conformal metrics (here we use s for the parameter, because t will denote a coordinate on $\tilde{\mathscr{G}}$) with $\boldsymbol{g}_0 = \boldsymbol{g}$ such that $\dot{\boldsymbol{g}}_s|_{s=0} = \varphi$. Let $g \in [g]$ be any representative metric, and g_s the corresponding representatives of $\boldsymbol{g}_s$. By the method of [Fefferman and Graham 2012], we can construct a family of ambient metrics

$$\tilde{g}_s = 2\rho\, dt^2 + 2t\, dt\, d\rho + t^2 g^s_\rho$$

such that $g^s_0 = g_s$ and g^s_ρ smoothly depends on the two variables ρ, s. All these metrics satisfy $\widetilde{\mathrm{Ric}}_s = O(r^{n/2-1})$ and $T \lrcorner \widetilde{\mathrm{Ric}}_s = O^-(r^{n/2})$. Differentiating these equations, we conclude that $\tilde{\sigma} = \tilde{\sigma}_{\mathrm{norm}} = (d/ds)\tilde{g}_s|_{s=0}$ solves

$$\mathrm{Ric}'_{\tilde{g}}\,\tilde{\sigma} = O(r^{n/2-1}), \quad T \lrcorner \mathrm{Ric}'_{\tilde{g}}\,\tilde{\sigma} = O^-(r^{n/2}).$$

Note that it satisfies $T \lrcorner \tilde{\sigma}_{\mathrm{norm}} = 0$, $\mathrm{tr}_{\tilde{g}}\,\tilde{\sigma}_{\mathrm{norm}} = O(r)$, and hence

$$T^I\tilde{\nabla}^J(\tilde{\sigma}_{\mathrm{norm}})_{IJ} = \tilde{\nabla}^J\big(T^I(\tilde{\sigma}_{\mathrm{norm}})_{IJ}\big) - \tilde{g}^{IJ}(\tilde{\sigma}_{\mathrm{norm}})_{IJ} = O(r);$$

therefore it holds that

$$T \lrcorner \mathcal{B}_{\tilde{g}} \tilde{\sigma}_{\mathrm{norm}} = T \lrcorner \delta_{\tilde{g}} \tilde{\sigma}_{\mathrm{norm}} + \tfrac{1}{2} T (\operatorname{tr}_{\tilde{g}} \tilde{\sigma}_{\mathrm{norm}}) = O(r). \tag{3-2}$$

Since the obstruction tensor $\mathcal{O} = \mathcal{O}_s$ is defined by

$$\mathcal{O}_s = c_n \big(r^{1-n/2} \widetilde{\mathrm{Ric}}_s \big)|_{TM}, \quad c_n = (-1)^{n/2-1} \frac{2^{n-2}(n/2-1)!^2}{n-2},$$

we have

$$\mathcal{O}'_{g} \varphi = c_n \big(r^{1-n/2} \widetilde{\mathrm{Ric}}'_{\tilde{g}} \tilde{\sigma}_{\mathrm{norm}} \big)|_{TM}.$$

Lemma 3.1. *Let $\tilde{\sigma}_{\mathrm{norm}}$ be as above. Then, there exists a dilation-invariant vector field $\tilde{\xi}$ on $\tilde{\mathcal{G}}$ such that $\tilde{\xi}|_{\mathcal{G}} = 0$ and*

$$\mathcal{B}_{\tilde{g}} \big(\tilde{\sigma}_{\mathrm{norm}} + \mathcal{K}_{\tilde{g}} \tilde{\xi} \big) = O(r^{n/2}),$$

where $\mathcal{K}_{\tilde{g}}$ is the Killing operator: $(\mathcal{K}_{\tilde{g}} \tilde{\xi})_{IJ} = 2 \tilde{\nabla}_{(I} \tilde{\xi}_{J)}$. Such a $\tilde{\xi}$ is unique modulo $O(r^{n/2+1})$ and satisfies $\tilde{g}(T, \tilde{\xi}) = O(r^2)$, $\operatorname{tr}_{\tilde{g}} \mathcal{K}_{\tilde{g}} \tilde{\xi} = O(r)$.

Proof. The equation to be solved is $\mathcal{B}_{\tilde{g}} \mathcal{K}_{\tilde{g}} \tilde{\xi} = -\mathcal{B}_{\tilde{g}} \tilde{\sigma}_{\mathrm{norm}} + O(r^{n/2})$. By a straightforward calculation,

$$\big(\mathcal{B}_{\tilde{g}} \mathcal{K}_{\tilde{g}} \tilde{\xi} \big)_I = \tilde{\Delta} \tilde{\xi}_I - \widetilde{\mathrm{Ric}}_{IJ} \tilde{\xi}^J.$$

Since $\widetilde{\mathrm{Ric}}_{IJ} \tilde{\xi}^J = O(r^{n/2})$ for any $\tilde{\xi}$ satisfying $\tilde{\xi}|_{\mathcal{G}} = 0$, the equation simplifies to $\tilde{\Delta} \tilde{\xi} = -\mathcal{B}_{\tilde{g}} \tilde{\sigma}_{\mathrm{norm}} + O(r^{n/2})$. By Lemma 2.9, $\tilde{\xi}$ is uniquely determined up to an $O(r^{n/2+1})$ ambiguity.

If we write $\tilde{\xi} = rV$, then $\tilde{\Delta} \tilde{\xi} = -2nV + O(r)$. On the other hand, $T \lrcorner \tilde{\Delta} \tilde{\xi} = -2T \lrcorner \mathcal{B}_{\tilde{g}} \tilde{\sigma}_{\mathrm{norm}} + O(r^{n/2})$ should be $O(r)$ by (3-2). Consequently $T \lrcorner V = O(r)$, i.e., $T \lrcorner \tilde{\xi} = O(r^2)$. Moreover, $\operatorname{tr}_{\tilde{g}} \mathcal{K}_{\tilde{g}} \tilde{\xi} = 2 \tilde{\nabla}^I \tilde{\xi}_I = 4 T^I V_I + O(r) = O(r)$. □

Let $\tilde{\sigma} = \tilde{\sigma}_{\mathrm{norm}} + \mathcal{K}_{\tilde{g}} \tilde{\xi} \in \tilde{\mathcal{S}}(2)$. It is a consequence of the fact that the Ricci operator commutes with diffeomorphisms that $\mathrm{Ric}'_{\tilde{g}} \mathcal{K}_{\tilde{g}} \tilde{\xi} = \mathrm{Ric}'_{\tilde{g}} \mathcal{L}_{\tilde{\xi}} \tilde{g} = \mathcal{L}_{\tilde{\xi}} \widetilde{\mathrm{Ric}}$. Since $\tilde{\xi}|_{\mathcal{G}} = 0$, $\widetilde{\mathrm{Ric}} = O(r^{n/2-1})$, and $T \lrcorner \widetilde{\mathrm{Ric}} = O^-(r^{n/2})$, $\mathcal{L}_{\tilde{\xi}} \widetilde{\mathrm{Ric}}$ itself is $O(r^{n/2-1})$ and $T \lrcorner \mathcal{L}_{\tilde{\xi}} \widetilde{\mathrm{Ric}} = O^-(r^{n/2})$. Therefore $\mathrm{Ric}'_{\tilde{g}} \tilde{\sigma} = O(r^{n/2-1})$, $T \lrcorner \mathrm{Ric}'_{\tilde{g}} \tilde{\sigma} = O^-(r^{n/2})$. Moreover, $\mathcal{B}_{\tilde{g}} \tilde{\sigma} = O(r^{n/2})$ and hence $\delta^*_{\tilde{g}} \mathcal{B}_{\tilde{g}} \tilde{\sigma} = O(r^{n/2-1})$, $T \lrcorner \delta^*_{\tilde{g}} \mathcal{B}_{\tilde{g}} \tilde{\sigma} = O^-(r^{n/2})$. Thus we conclude

$$\tilde{\Delta}_{\mathrm{L}} \tilde{\sigma} = O(r^{n/2-1}), \quad T \lrcorner \tilde{\Delta}_{\mathrm{L}} \tilde{\sigma} = O^-(r^{n/2}). \tag{3-3}$$

Lemma 3.2. *Let $\tilde{\sigma}_{\mathrm{norm}}$ and $\tilde{\xi}$ be as in Lemma 3.1. Then $\tilde{\sigma} = \tilde{\sigma}_{\mathrm{norm}} + \mathcal{K}_{\tilde{g}} \tilde{\xi} \in \tilde{\mathcal{S}}^X_{\mathrm{aTT}}(2)$ and it is a solution to* (3-3).

Proof. It remains to show that $\tilde{\sigma} \in \tilde{\mathcal{S}}^X_{\mathrm{aTT}}(2)$. By taking the trace of (3-3), we obtain $\tilde{\Delta}(\operatorname{tr}_{\tilde{g}} \tilde{\sigma}) = O(r^{n/2-1})$. In addition, since $\operatorname{tr}_{\tilde{g}} \mathcal{K}_{\tilde{g}} \tilde{\xi} = O(r)$, we have $(\operatorname{tr}_{\tilde{g}} \tilde{\sigma})|_{\mathcal{G}} = 0$.

Hence, by Lemma 2.9, $\operatorname{tr}_{\tilde g}\tilde\sigma = O(r^{n/2})$. Then $\mathcal{B}_{\tilde g}\tilde\sigma = O(r^{n/2})$ implies $\delta_{\tilde g}\tilde\sigma = O^-(r^{n/2})$. Furthermore,

$$\tilde\Delta(T^J\tilde\sigma_{IJ}) = T^J\tilde\Delta\tilde\sigma_{IJ} - 2\tilde\nabla^J\tilde\sigma_{IJ} = T^J\tilde\Delta_{\mathrm{L}}\tilde\sigma_{IJ} - 2\tilde\nabla^J\tilde\sigma_{IJ} = O^-(r^{n/2})$$

and

$$T^J\tilde\sigma_{IJ} = T^J(\mathcal{K}_{\tilde g}\tilde\xi)_{IJ} = T^J\tilde\nabla_I\tilde\xi_J + T^J\tilde\nabla_J\tilde\xi_I = \tilde\nabla_I(T^J\tilde\xi_J) = O(r).$$

Since $\tilde\Delta(r^{n/2}\tilde f T_I) = -2nr^{n/2-1}\tilde f T_I + O(r^{n/2})$ for $\tilde f\in\tilde{\mathcal{E}}(-n)$, one can determine $\tilde f$ so that $\tilde\Delta(T^J\tilde\sigma_{IJ} + r^{n/2}\tilde f T_I) = O(r^{n/2})$. Then $T^J\tilde\sigma_{IJ} + r^{n/2}\tilde f T_I$ is still $O(r)$, and hence $T\lrcorner\tilde\sigma = O^-(r^{n/2+1})$ by Lemma 2.9. □

Lemma 3.3. *Let $\tilde\sigma_{\mathrm{norm}}$ and $\tilde\xi$ be as in Lemma 3.1 and set $\tilde\sigma = \tilde\sigma_{\mathrm{norm}} + \mathcal{K}_{\tilde g}\tilde\xi$. Then $\tilde\Delta_{\mathrm{L}}\tilde\sigma - 2\,\mathrm{Ric}'_{\tilde g}\,\tilde\sigma_{\mathrm{norm}} = O(r^{n/2-1})$, and $(r^{1-n/2}(\tilde\Delta_{\mathrm{L}}\tilde\sigma - 2\,\mathrm{Ric}'_{\tilde g}\,\tilde\sigma_{\mathrm{norm}}))|_{T\mathcal{G}}$ vanishes.*

Proof. Recall that

$$\tfrac12\tilde\Delta_{\mathrm{L}}\tilde\sigma - \mathrm{Ric}'_{\tilde g}\,\tilde\sigma_{\mathrm{norm}} = \mathrm{Ric}'_{\tilde g}\,\mathcal{K}_{\tilde g}\tilde\xi - \delta^*_{\tilde g}\mathcal{B}_{\tilde g}\tilde\sigma = \mathcal{L}_{\tilde\xi}\widetilde{\mathrm{Ric}} - \delta^*_{\tilde g}\mathcal{B}_{\tilde g}\tilde\sigma.$$

Let $\widetilde{\mathrm{Ric}} = r^{n/2-1}S$ and $\tilde\xi = rV$. We proved in Lemma 3.1 that $T^IV_I = O(r)$. As in the proof of Lemma 1.1, we compute

$$\big(\mathcal{L}_{\tilde\xi}\widetilde{\mathrm{Ric}}\big)_{IJ} = \tilde\xi^K\tilde\nabla_K\widetilde{\mathrm{Ric}}_{IJ} + 2\widetilde{\mathrm{Ric}}_{K(I}\tilde\nabla_{J)}\tilde\xi^K = 4r^{n/2-1}S_{K(I}T_{J)}\,V^K + O(r^{n/2}).$$

Thus $(r^{1-n/2}\mathcal{L}_{\tilde\xi}\widetilde{\mathrm{Ric}})|_{T\mathcal{G}}$ vanishes. On the other hand, if we write $\mathcal{B}_{\tilde g}\tilde\sigma = r^{n/2}\tilde\tau$, then

$$(\delta^*_{\tilde g}\mathcal{B}_{\tilde g}\tilde\sigma)_I = \tilde\nabla_{(I}(r^{n/2}\tilde\tau)_{J)} = nr^{n/2-1}T_{(I}\,\tilde\tau_{J)} + O(r^{n/2}),$$

and hence $(r^{1-n/2}\delta^*_{\tilde g}\mathcal{B}_{\tilde g}\tilde\sigma)|_{T\mathcal{G}} = 0$. This completes the proof. □

Theorem 3.4. *Let $(M,[g])$ be a conformal manifold of even dimension n. Then the differential of the obstruction tensor $\mathcal{O}'_{\boldsymbol g}$ is given by*

$$\mathcal{O}'_{\boldsymbol g}\varphi = \frac{(-1)^{n/2-1}}{2(n-2)}P\varphi + \frac{1}{n+2}\langle\mathcal{O},\varphi\rangle_{\boldsymbol g}\,\boldsymbol g. \tag{3-4}$$

Proof. Let $\tilde\sigma_{\mathrm{norm}}$, $\tilde\xi$ as in Lemma 3.1 and $\tilde\sigma = \tilde\sigma_{\mathrm{norm}} + \mathcal{K}_{\tilde g}\tilde\xi$. By Lemma 3.2, $P\varphi$ is equal to the trace-free part of $2^{n-2}(n/2-1)!^2(r^{1-n/2}\tilde\Delta_{\mathrm{L}}\tilde\sigma)|_{TM}$. By the previous lemma, $(r^{1-n/2}\tilde\Delta_{\mathrm{L}}\tilde\sigma)|_{TM} = (2r^{1-n/2}\,\mathrm{Ric}'_{\tilde g}\,\tilde\sigma_{\mathrm{norm}})|_{TM} = c_n^{-1}\mathcal{O}'_{\boldsymbol g}\varphi$. Therefore,

$$\mathrm{tf}_{\boldsymbol g}\,\mathcal{O}'_{\boldsymbol g}\varphi = \frac{(-1)^{n/2-1}}{2(n-2)}P\varphi.$$

On the other hand, $\operatorname{tr}_{\boldsymbol g}\mathcal{O}'_{\boldsymbol g}\varphi = \langle\mathcal{O},\varphi\rangle_{\boldsymbol g}$, for $\operatorname{tr}_{\boldsymbol g}\mathcal{O} = 0$ for any $\boldsymbol g$. Hence (3-4). □

Combining the theorem above and (0-4), we obtain the following.

Corollary 3.5. *Let $(M, [g])$ be a compact conformal manifold of even dimension $n \geq 4$ with vanishing obstruction tensor. Let $\boldsymbol{g}_t$ be a family of conformal structures such that $\boldsymbol{g}_0 = \boldsymbol{g}$. Then the second derivative of the total Q-curvature at $t = 0$ is*

$$\frac{d^2}{dt^2}\bar{Q}_t\bigg|_{t=0} = -\frac{1}{4}\int_M \langle P\varphi, \varphi\rangle_{\boldsymbol{g}},$$

where $\varphi = \dot{\boldsymbol{g}}_t|_{t=0}$ and $P : \mathcal{S}_0(2) \to \mathcal{S}_0(2-n)$ is the critical GJMS operator on trace-free symmetric 2-tensors.

4. Explicit calculations for conformally Einstein manifolds

Recall that, for $g \in [g]$ Einstein with $\mathrm{Ric}_{ij} = 2\lambda(n-1)g_{ij}$ so that $P_{ij} = \lambda g_{ij}$, the following formula gives an ambient metric that is genuinely Ricci-flat:

$$\tilde{g} = 2\rho\, dt^2 + 2t\, dt\, d\rho + t^2(1+\lambda\rho)^2 g. \tag{4-1}$$

The inverse of $\tilde{g}$ is

$$(\tilde{g}^{-1})^{IJ} = \begin{pmatrix} 0 & 0 & t^{-1} \\ 0 & t^{-2}(1+\lambda\rho)^{-2}g^{ij} & 0 \\ t^{-1} & 0 & -2t^{-2}\rho \end{pmatrix}$$

and the Christoffel symbol of $\tilde{g}$ is given by

$$\tilde{\Gamma}^0{}_{IJ} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & -\lambda t(1+\lambda\rho)g_{ij} & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \tilde{\Gamma}^k{}_{IJ} = \begin{pmatrix} 0 & t^{-1}\delta_j{}^k & 0 \\ t^{-1}\delta_i{}^k & \Gamma^k{}_{ij} & \lambda(1+\lambda\rho)^{-1}\delta_i{}^k \\ 0 & \lambda(1+\lambda\rho)^{-1}\delta_j{}^k & 0 \end{pmatrix},$$

$$\tilde{\Gamma}^\infty{}_{IJ} = \begin{pmatrix} 0 & 0 & t^{-1} \\ 0 & -(1+\lambda\rho)(1-\lambda\rho)g_{ij} & 0 \\ t^{-1} & 0 & 0 \end{pmatrix}.$$

A direct computation shows that $\tilde{W}_{ijkl} = t^2 W_{ijkl}$, where $\tilde{W}$ and W are the Weyl tensors of $\tilde{g}$ and g, respectively (the latter is extended to $\tilde{\mathcal{G}} = \mathbb{R}_+ \times M \times \mathbb{R}$ in the trivial way). The other components of $\tilde{W}$ are zero.

Lemma 4.1. *Let $\tilde{g}$ be as above, and suppose that $\tilde{\sigma} \in \tilde{\mathcal{S}}(w)$ is of the form*

$$\tilde{\sigma}_{ij} = t^w(1+\lambda\rho)^w\sigma_{ij},$$

where σ_{ij} is a symmetric 2-tensor on (M, g). Then

$$\tilde{\Delta}_{\mathrm{L}}\tilde{\sigma} = t^{w-2}(1+\lambda\rho)^{w-2}\big(\Delta_{\mathrm{L}} - 4(n-1)\lambda - 2(w-2)(n+w-3)\lambda\big)\sigma, \tag{4-2}$$

where $\Delta_{\mathrm{L}} = \Delta + 4n\lambda - 2\mathring{W}$ is the Lichnerowicz Laplacian of g.

Proof. The first covariant derivative of $\tilde{\sigma}$ is as follows:

$$\begin{aligned}
\tilde{\nabla}_\infty \tilde{\sigma}_{ij} &= \partial_\rho \tilde{\sigma}_{ij} - 2\tilde{\Gamma}^k{}_{\infty(i}\tilde{\sigma}_{j)k} = t^w(1+\lambda\rho)^{w-1}(w-2)\lambda\sigma_{ij}\,,\\
\tilde{\nabla}_0 \tilde{\sigma}_{ij} &= \partial_t \tilde{\sigma}_{ij} - 2\tilde{\Gamma}^k{}_{0(i}\tilde{\sigma}_{j)k} = t^{w-1}(1+\lambda\rho)^{w}(w-2)\sigma_{ij}\,,\\
\tilde{\nabla}_k \tilde{\sigma}_{ij} &= \partial_{x^k} \tilde{\sigma}_{ij} - 2\tilde{\Gamma}^l{}_{k(i}\tilde{\sigma}_{j)l} = t^w(1+\lambda\rho)^{w}\nabla_k\sigma_{ij}\,,\\
\tilde{\nabla}_k \tilde{\sigma}_{i\infty} &= -\tilde{\Gamma}^l{}_{k\infty}\tilde{\sigma}_{il} = -t^w(1+\lambda\rho)^{w-1}\lambda\sigma_{ik}\,,\\
\tilde{\nabla}_k \tilde{\sigma}_{i0} &= -\tilde{\Gamma}^l{}_{k0}\tilde{\sigma}_{il} = -t^{w-1}(1+\lambda\rho)^{w}\sigma_{ik}\,.
\end{aligned}$$

Therefore,

$$\begin{aligned}
\tilde{\nabla}_0\tilde{\nabla}_\infty \tilde{\sigma}_{ij} &= \partial_t \tilde{\nabla}_\infty \tilde{\sigma}_{ij} - \tilde{\Gamma}^\infty{}_{0\infty}\tilde{\nabla}_\infty\tilde{\sigma}_{ij} - 2\tilde{\Gamma}^k{}_{0(i|}\tilde{\nabla}_\infty\tilde{\sigma}_{|j)k}\\
&= t^{w-1}(1+\lambda\rho)^{w-1}(w-2)(w-3)\lambda\sigma_{ij}\,,\\
\tilde{\nabla}_\infty\tilde{\nabla}_0 \tilde{\sigma}_{ij} &= \tilde{\nabla}_0\tilde{\nabla}_\infty \tilde{\sigma}_{ij} - 2\tilde{R}_{\infty 0}{}^k{}_{(i}\tilde{\sigma}_{j)k} = \tilde{\nabla}_0\tilde{\nabla}_\infty \tilde{\sigma}_{ij}\,,\\
\tilde{\nabla}_\infty\tilde{\nabla}_\infty \tilde{\sigma}_{ij} &= \partial_\rho \tilde{\nabla}_\infty \tilde{\sigma}_{ij} - 2\tilde{\Gamma}^k{}_{\infty(i|}\tilde{\nabla}_\infty\tilde{\sigma}_{|j)k} = t^w(1+\lambda\rho)^{w-2}(w-2)(w-3)\lambda^2\sigma_{ij}\,,\\
g^{kl}\tilde{\nabla}_k\tilde{\nabla}_l \tilde{\sigma}_{ij} &= \partial_{x^k}\tilde{\nabla}_l\tilde{\sigma}_{ij} - \tilde{\Gamma}^m{}_{kl}\tilde{\nabla}_m\tilde{\sigma}_{ij} - 2\tilde{\Gamma}^m{}_{k(i|}\tilde{\nabla}_l\tilde{\sigma}_{|j)m}\\
&\qquad - \tilde{\Gamma}^\infty{}_{kl}\tilde{\nabla}_\infty\tilde{\sigma}_{ij} - 2\tilde{\Gamma}^\infty{}_{k(i|}\tilde{\nabla}_l\tilde{\sigma}_{|j)\infty} - \tilde{\Gamma}^0{}_{kl}\tilde{\nabla}_0\tilde{\sigma}_{ij} - 2\tilde{\Gamma}^0{}_{k(i|}\tilde{\nabla}_l\tilde{\sigma}_{|j)0}\\
&= -t^w(1+\lambda\rho)^w\big(\Delta\sigma_{ij} - 2(n(w-2)-2)\lambda\sigma_{ij}\big)
\end{aligned}$$

and hence

$$\begin{aligned}
\tilde{\Delta}\tilde{\sigma}_{ij} &= -2t^{-1}\tilde{\nabla}_0\tilde{\nabla}_\infty\tilde{\sigma}_{ij} + 2t^{-2}\rho\tilde{\nabla}_\infty\tilde{\nabla}_\infty\tilde{\sigma}_{ij} - t^{-2}(1+\lambda\rho)^{-2}g^{kl}\tilde{\nabla}_k\tilde{\nabla}_l\tilde{\sigma}_{ij}\\
&= t^{w-2}(1+\lambda\rho)^{w-2}\big(\Delta + 4\lambda - 2(w-2)(n+w-3)\lambda\big)\sigma_{ij}\,.
\end{aligned}$$

Consequently, $\tilde{\Delta}_{\mathrm{L}}\tilde{\sigma} = (\tilde{\Delta} - 2\mathring{\tilde{W}})\tilde{\sigma}$ is given by (4-2). □

Theorem 4.2. *Let $(M, [g])$ be a conformally Einstein manifold with* $\dim M = n \geq 3$, *and $g \in [g]$ an Einstein representative with Schouten tensor $P_{ij} = \lambda g_{ij}$. Then, the action of P_k restricted to $\mathcal{S}^g_{\mathrm{TT}}(-n/2+2+k)$ is given by* (0-5).

Proof. Let $\varphi = t^{-n/2+2+k}\overline{\varphi} \in \mathcal{S}^g_{\mathrm{TT}}(-n/2+2+k)$ and $\tilde{\sigma} = (1+\lambda\rho)^{-n/2+2+k}\varphi$. Then

$$\tilde{\nabla}_k\tilde{\sigma}_{ij} = t^{-n/2+2+k}(1+\lambda\rho)^{-n/2+2+k}\nabla_k\overline{\varphi}_{ij}\,,\quad \tilde{\nabla}_\infty\tilde{\sigma}_{0i} = \tilde{\nabla}_0\tilde{\sigma}_{\infty i} = \tilde{\nabla}_\infty\tilde{\sigma}_{\infty i} = 0.$$

Since $\overline{\varphi}$ is a TT-tensor on (M, g), $\tilde{\sigma}$ itself is a TT-tensor with respect to $\tilde{g}$, and hence is an extension of the ambient lift of φ. We may compute $\tilde{\Delta}^k_{\mathrm{L}}\tilde{\sigma}$ by Lemma 4.1. By taking the value along $\mathcal{G}$ and trivializing with respect to g, we obtain (0-5). □

Now we prove our main theorem.

Proof of Theorem 0.2. Let $\varphi = \mathcal{K}_{[g]}\xi + \varphi^g_{\mathrm{TT}}$ be the decomposition of $\varphi = \dot{\boldsymbol{g}}_t|_{t=0}$ with respect to (0-1) and Ξ_t the flow generated by ξ. Then $\boldsymbol{g}'_t = \Xi^*_{-t}\boldsymbol{g}_t$ satisfies

$\dot{\boldsymbol{g}}_t'|_{t=0} = \varphi_{\mathrm{TT}}^g$ and the total Q-curvature of $\boldsymbol{g}_t'$ is equal to $\overline{Q}_t$. Therefore

$$\frac{d^2}{dt^2}\overline{Q}_t\bigg|_{t=0} = \frac{d^2}{dt^2}\overline{Q}_t'\bigg|_{t=0} = -\frac{1}{4}\int_M \langle P\varphi_{\mathrm{TT}}^g, \varphi_{\mathrm{TT}}^g\rangle,$$

and thus (0-2) follows from Theorem 4.2. Under the assumption of the latter half of the theorem, any eigenvalue of $\Delta_{\mathrm{L}}|_{\mathcal{S}^g_{\mathrm{TT}(2)}} - 4(n-1)\lambda + 4m(n-2m-1)\lambda$ is strictly positive for $0 \le m \le n/2-1$. Therefore, if $\varphi_{\mathrm{TT}}^g \ne 0$, the second derivative of $\overline{Q}_t$ at $t=0$ is negative. □

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DROPLET CONDENSATION AND ISOPERIMETRIC TOWERS

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We consider a variational problem in a planar convex domain, motivated by the statistical mechanics of crystal growth in a saturated solution. The minimizers are constructed explicitly and are completely characterized.

1. Introduction

In understanding the physical phenomenon of droplet condensation or crystal growth, the central issue is to explain how a particular macroscopic shape of the growing droplet or crystal is determined by microscopic interactions of its constituent particles.

According to Gibbs' formulation of statistical mechanics, the probability of a microscopic configuration σ is proportional to $\exp(-\beta H(\sigma))$, where $\beta > 0$ is the inverse temperature and $H(\cdot)$ is the Hamiltonian defining the energy of the system. Therefore the most probable configurations are the ones with minimal energy. In the "thermodynamical" limit of a large number of particles, this minimum becomes very sharp: the overall configuration of the system settles, up to minute fluctuations, to a well-defined deterministic structure.

It turns out that the microscopic laws of atomic interactions give rise to a certain macroscopic quantity, the surface tension, which determines the droplet shape via minimization of the surface energy. Phenomenology of surface tension was proposed by Gibbs in the late 1870s. In an important contribution, G. Wulff suggested in 1900 that for a growing crystal, its equilibrium shape is that of a ball in a metric generated by the surface tension (the *Wulff shape*).

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It has been furthermore observed experimentally that flat facets of a growing crystal may carry macroscopic but monomolecular "islands", whose shape is also determined by the surface tension. A mathematical approach to explaining this phenomenon has been developed by S. Shlosman and collaborators in a series of works [Schonmann and Shlosman 1996a; Ioffe and Shlosman 2008; 2010], building upon his earlier work with R. L. Dobrushin and R. Kotecky [Dobrushin et al. 1992].

A typical setting in this approach is represented by the following discrete model of crystal growth, which is a variant of the Ising model: fix an open domain $\Omega \subset \mathbb{R}^2$ of unit area and consider the three-dimensional lattice obtained by intersecting the cylinder $\Omega \times [-1, 1] \subset \mathbb{R}^3$ with $(1/N)\big(\mathbb{Z}^3 + \big(0, 0, \frac{1}{2}\big)\big)$, where N is a large integer parameter. At each node t of this lattice there is a variable σ_t (the *spin*) taking values $+1$ (interpreted as "t belongs to the free phase") and -1 (interpreted as "t belongs to the condensed phase"). The collection $\sigma = (\sigma_t)$ is called the microscopic configuration of the system.

Fix now the Ising Hamiltonian $H(\sigma) = -\sum_{s,t:|s-t|=1} \sigma_s \sigma_t$, which describes a "ferromagnetic" interaction between nearest neighbors (equal values have smaller energy than opposite ones), and consider the canonical probability distribution $p(\sigma) = \exp(-\beta H(\sigma))/Z$. Here the normalization coefficient $Z = \sum_\sigma \exp(-\beta H(\sigma))$ is defined by summation over all configurations that satisfy the so-called *Dobrushin boundary condition*: spins at outermost nodes (x, y, z) of the lattice have values $+1$ if $z > 0$ and -1 if $z < 0$.

It turns out that in the limit of large N the main contribution to probability comes from configurations where the lower and upper halves of the lattice are filled, respectively, with -1's and $+1$'s. In this equilibrium state, the numbers of $+1$'s and -1's are asymptotically equal, so that $S_N = \sum_t \sigma_t \sim 0$, and fluctuations of the flat surface dividing the two phases are logarithmic in N.

A more interesting situation occurs when, in addition to the Dobrushin boundary values, the system is conditioned to have macroscopically more -1's than $+1$'s:

$$S_N = \sum_t \sigma_t = -mN^2$$

with $m > 0$. In this case, depending on the value of m, the most probable state of the system may feature one or more monomolecular layers on top of the surface $z = 0$ in the box $\Omega \times [-1, 1]$. A detailed account of the observed equilibrium states as m changes can be found in [Ioffe and Shlosman 2010].

As proved in [Schonmann and Shlosman 1996a], the behavior of this model in the continuous limit $N \to \infty$ is closely related to the following variational problem: given an open set $\Omega \subset \mathbb{R}^n$ and a value $m \in [0, +\infty)$, find

$$\min\left\{ \int_\Omega \varphi^*(Du) : u \in BV(\mathbb{R}^n),\, u = 0 \text{ on } \mathbb{R}^n \setminus \Omega,\, u(\,\cdot\,) \in \mathbb{N},\, \int_\Omega u\, dx = m \right\}, \tag{1-1}$$

where φ^* is some given general norm on $\mathbb{R}^n$. Of course, in the application to the Ising model we are discussing here one has $n = 2$, the two-dimensional case; however the case of generic dimension n of the ambient space $\mathbb{R}^n$ also makes sense from the mathematical point of view. The growth of a droplet and formation of new layers of the solid is described by the growth of profile u as m increases.

The norm $\varphi^*(\,\cdot\,)$ here is related to the surface tension as follows. The surface tension $\gamma^{3D}(\,\cdot\,)$ is a function defined over $\mathbb{S}^2$, the two-dimensional unit sphere in $\mathbb{R}^3$, and satisfying $\gamma^{3D}(\nu) \geq 0$ and $\gamma^{3D}(-\nu) = \gamma^{3D}(\nu)$ for all $\nu \in \mathbb{S}^2$. The surface energy of a closed surface $M^2 \subset \mathbb{R}^3$ is defined to be

$$H(M^2) = \int_{M^2} \gamma^{3D}(\nu_s)\, ds,$$

where ν_s is the unit normal to M^2 at $s \in M^2$. While γ^{3D} defines the $3D$ shape of a crystal growing in space, the shape of monolayers growing on facets is given by the restricted $2D$ surface tension defined for $n \in \mathbb{S}^1$ by

$$\gamma^{2D}(\nu) = \frac{\partial}{\partial \nu}\, \gamma^{3D}\Big|_{\nu_s=(0,0,1)},$$

where the derivatives are taken at the "north pole" $\nu_s = (0, 0, 1) \in \mathbb{S}^2$ along all tangents $\nu \in \mathbb{S}^1$ to $\mathbb{S}^2$ [Ioffe and Shlosman 2010]. The function γ^{2D} can then be extended to all of $\mathbb{R}^2$ by homogeneity of degree one, and $\varphi^*(\,\cdot\,)$ is defined as the convex hull of the thus defined $\gamma^{2D}(\,\cdot\,)$. However in the sequel φ^* will be fixed, without any assumptions of smoothness or strict convexity: indeed one of the examples in Section 5 corresponds to a crystalline norm.

It is easy to see that the functional minimized in (1-1) is the one-dimensional surface energy for the restricted surface tension. It turns out that minimization of this surface energy alone is sufficient to reconstruct most of the physics of monomolecular layer growth described in [Ioffe and Shlosman 2010]. In particular, if $\varphi^*(\,\cdot\,)$ is the Euclidean norm and Ω a unit square, then as m grows, the first four monomolecular layers start as Wulff circles and then develop into "Wulff plaquettes" while from the fifth layer on all new layers appear as Wulff plaquettes identical to underlying layers (Section 5).

In contrast, this simple variational model does not capture the thermodynamic fluctuations, which render Wulff circles below a certain size unstable and prevent their formation for small m. Neither does it capture the microscopic (that is, "finite-N") structure of the Wulff plaquettes, whose boundaries are in fact separated with gaps that vanish in the continuous limit. A first-principle approach that takes proper account of these phenomena is due to R. Dobrushin, S. Shlosman and their coauthors and is presented in [Dobrushin et al. 1992; Schonmann and Shlosman 1996a; 1996b; Ioffe and Shlosman 2008; 2010].

It is worth observing that a similar problem with the additional restriction that u be a characteristic function of some set (that is, that the droplet has exactly one layer) in the two-dimensional situation (that is when $n = 2$), the set Ω is convex, and the norm φ^* is Euclidean, has been studied in [Stredulinsky and Ziemer 1997], and for more general anisotropic norms (but for a somewhat different functional, namely, with penalization on the volume instead of the volume constraint), in [Novaga and Paolini 2005]. The latter problem will play an important role also in the present paper. Eventually, one has to mention that it is also very similar to the well-known Cheeger problem, the solutions of the latter being so-called Cheeger sets; see for instance [Buttazzo et al. 2007; Kawohl and Novaga 2008; Kawohl and Lachand-Robert 2006; Caselles et al. 2010].

Our aim in this paper is to study the variational problem (1-1) in the two-dimensional case (that is, when $n = 2$). This geometric optimization problem is considered without resort to the underlying lattice model or its continuous limit, allowing us to treat an arbitrary open domain Ω and an arbitrary norm φ^* that is not necessarily strictly convex. In this setting we completely characterize the minimizers and the possible levels of u when the domain Ω is convex. In particular it turns out that except some degenerate situation, which can however happen only when Ω is not strictly convex, the number of nonzero levels of u is at most two.

The basic tool we use is the auxiliary problem when u is a priori required to have a single nonzero level (that is, is requested to be a characteristic function); namely, we show that in the two-dimensional case ($n = 2$) when Ω is convex, the nonzero levels of solutions to the latter problem corresponding to different values of m as m grows can be arranged as a family of sets ordered by inclusion. Thus, solutions to problem (1-1) can be seen as "towers" with levels solving the auxiliary problem. The assumption of convexity of Ω is essential, as shown by a counterexample at the end of Section 4A. The main result of the paper is formulated as Theorem 4.10. We conclude with an explicit example of solutions to (1-1) for the case of a square $\Omega = [0, 1]^2$ with a strictly convex (Euclidean) norm and a crystalline norm.

This work was inspired by some seminar talks of Senya Shlosman. After it was completed, we learned that a full description of the solutions to the variational problem (1-1) when Ω is a square and φ^* is generated by a physical Hamiltonian (in particular, when it is the Euclidean norm) has been independently obtained by him and Ioffe by a rigorous continuous limit of a suitable lattice model (S. Shlosman, private communication, 2012). Their proof, together with an analysis of the microscopic structure of the solution and its behavior under thermal perturbations, has not yet been published.

2. Notation and preliminary results

For a set $E \subset \mathbb{R}^n$ we denote by $|E|$ its Lebesgue measure, by $\mathbf{1}_E$ its characteristic function, by $\bar{E}$ its closure, by ∂E its topological boundary, and by E^c its complement.

In the following φ will denote the given (not necessarily Euclidean) norm over $\mathbb{R}^n$. Given $E \subset \mathbb{R}^n$ and $x \in \mathbb{R}^n$, we set

$$\mathrm{dist}_\varphi(x, E) := \inf_{y \in E} \varphi(x - y), \quad d_\varphi^E(x) := \mathrm{dist}_\varphi(x, E) - \mathrm{dist}_\varphi(x, E^c).$$

The value $d_\varphi^E(x)$ is the signed distance from x to ∂E and is positive outside E. Notice that at each point where d_φ^E is differentiable one has (see [Bellettini et al. 2001])

$$\varphi^*(\nabla d_\varphi^E) = 1, \qquad \nu \cdot \nabla d_\varphi^E = 1 \quad \text{for all } \nu \in \partial\varphi^*(\nabla d_\varphi^E), \tag{2-1}$$

where φ^* denotes the dual norm of φ defined as

$$\varphi^*(\xi) := \max_{\eta:\, \varphi(\eta) \le 1} \xi \cdot \eta$$

and $\partial\varphi^*$ denotes the subdifferential of φ^* in the sense of convex analysis. In particular

$$\nabla d_\varphi^E = \frac{\nu^E}{\varphi^*(\nu^E)}$$

where ν^E is the exterior Euclidean unit normal to ∂E.

We define the anisotropic perimeter of a set $E \subseteq \mathbb{R}^n$ as

$$P_\varphi(E) := \sup\left\{ \int_E \mathrm{div}\, \eta \, dx : \eta \in C_0^1(\mathbb{R}^n), \varphi(\eta) \le 1 \right\} = \int_{\partial^* E} \varphi^*(\nu^E) d\mathcal{H}^{n-1}, \tag{2-2}$$

where $\partial^* E$ is the reduced boundary of E according to De Giorgi. We will usually identify a set E of finite perimeter with the set of its density points (that is, points of density 1).

Given an open set $\Omega \subset \mathbb{R}^n$ we define the BV-seminorm of $v \in BV(\Omega)$ as

$$\int_\Omega \varphi^*(Dv) := \sup\left\{ \int_\Omega v \, \mathrm{div}\, \eta \, dx : \ \eta \in C_0^1(\mathbb{R}^n), \varphi(\eta) \le 1 \right\},$$

where $C_0^1(\mathbb{R}^n)$ stands for the set of continuously differentiable functions with compact support is $\mathbb{R}^n$.

We let $W_\varphi := \{x \mid \varphi(x) < 1\}$, usually called the *Wulff shape*, be the unit ball of φ. Observe that $P_\varphi(W_\varphi) = n|W_\varphi|$.

In the sequel, given $x \in \mathbb{R}^n$ and $r > 0$, we set $W_r(x) := x + rW_\varphi$ (a *Wulff ball* of radius r with center x). In this notation the reference to a norm φ is not retained for the sake of brevity, but always silently assumed. When φ is the Euclidean norm, we will use a more common notation $B_r(x)$ instead of $W_r(x)$ and P instead of P_φ.

Definition 2.1. Given an $r > 0$, we say that E satisfies the rW_φ-condition, if for every $x \in \partial E$ there exists an $y \in \mathbb{R}^n$ such that $W_r(y) \subset E$ and $x \in \partial W_r(y)$.

Observe that, if E is convex, then E^c satisfies the rW_φ-condition for all $r > 0$.

We conclude the section by recalling the following isoperimetric inequality [Taylor 1975].

Proposition 2.2. *For all $E \subset \mathbb{R}^n$ such that $|E| < +\infty$ there holds*

$$P_\varphi(E) \geq \frac{|E|^{\frac{n-1}{n}}}{|W_\varphi|^{\frac{n-1}{n}}} P_\varphi(W_\varphi). \tag{2-3}$$

3. Existence of minimizers

Notice that, since the total variation is lower semicontinuous and the constraints are closed under weak BV convergence, by direct method one immediately gets existence of minimizers of (1-1).

Proposition 3.1. *For any $m \geq 0$ there exists a* (*possibly nonunique*) *minimizer of* (1-1).

For every $u \in L^1(\mathbb{R}^n)$ and $j \in \mathbb{N}$ we set

$$E_j := \{u \geq j\}. \tag{3-1}$$

It is worth observing that whenever $u(\,\cdot\,)$ takes values in $\mathbb{N}$,

$$u = \sum_{i=1}^{\infty} \mathbf{1}_{E_i} \tag{3-2}$$

and

$$\int_{\mathbb{R}^n} \varphi^*(Du) = \sum_{i=1}^{\infty} P_\varphi(E_i). \tag{3-3}$$

Remark 3.2. If we let u_m be a minimizer of (1-1) for a given $m > 0$, then the normalized functions $v_m := u_m/m$ converge, as $m \to \infty$, up to a subsequence, to a minimizer of the problem

$$\min\left\{\int_\Omega \varphi^*(Dv) : v \in BV(\mathbb{R}^n),\, v = 0 \text{ on } \Omega^c,\, \int_\Omega v\,dx = 1\right\},$$

which is closely related to the *Cheeger problem* in Ω [Kawohl and Novaga 2008].

Proposition 3.3. *If u is a minimizer of* (1-1), *then $u \in L^\infty(\mathbb{R}^n)$.*

Proof. Assume by contradiction that $|E_j| > 0$ for all $j \in \mathbb{N}$. Notice that

$$\lim_{j\to\infty} |E_j| = 0$$

(since otherwise u would not be integrable). Given $x_0 \in \Omega$ we let

$$u_j := \min(u, j) + \mathbf{1}_{W_{R_j}(x_0)}$$

where the radius R_j is such that

$$\int_\Omega u_j = \int_\Omega u = m,$$

that is (keeping in mind (3-2)),

$$|W_\varphi| R_j^n = \sum_{i>j} |E_i|,$$

and choose $j \in \mathbb{N}$ big enough so that $W_{R_j}(x_0) \subset \Omega$.

Letting

$$f(t) := n|W_\varphi|^{\frac{1}{n}}\, t^{\frac{n-1}{n}} \quad \text{so that } P_\varphi(W_{R_j}(x_0)) = f(|W_\varphi| R_j^n),$$

we have

$$\begin{aligned}
\int_\Omega \varphi^*(Du_j) &\le \int_\Omega \varphi^*(D\min(u, j)) + P_\varphi(W_{R_j}(x_0)) \\
&= \int_\Omega \varphi^*(D\min(u, j)) + f(|W_\varphi| R_j^n) \\
&\le \int_\Omega \varphi^*(D\min(u, j)) + \sum_{i>j} f(|E_i|) \qquad \text{by the concavity of } f \\
&\le \int_\Omega \varphi^*(D\min(u, j)) + \sum_{i>j} P_\varphi(E_i) \qquad \text{by (2-3)} \\
&= \int_\Omega \varphi^*(Du) \qquad \text{by (3-3)},
\end{aligned}$$

the second inequality being strict unless $|E_i| = |E_k|$ for all $i > j$, $k > j$, thus leading to a contradiction. □

Proposition 3.4. *Let $\Omega \subset \mathbb{R}^n$ be star-shaped. Then the problem* (1-1) *is equivalent to the following relaxed problem*:

$$\min\left\{ \int_\Omega \varphi^*(Du) : u \in BV(\mathbb{R}^n),\ u = 0 \text{ on } \Omega^c,\ u(\cdot) \in \mathbb{N},\ \int_\Omega u\, dx \ge m \right\}. \tag{3-4}$$

Namely, the minimum values and the minimizers are the same for both problems.

Proof. It is enough to show that any minimizer u of (3-4) satisfies

$$\int_\Omega u\,dx = m. \tag{3-5}$$

To this aim let Ω be star-shaped with respect to x_0 and assume by contradiction that (3-5) is violated. Let $u_\lambda(x) := u(x_0+\lambda(x-x_0))$ for any $\lambda > 0$, so that $u_\lambda \in BV(\mathbb{R}^n)$, $u_\lambda(\cdot) \in \mathbb{N}$, while, by star-shapedness of Ω, one has $u_\lambda = 0$ outside of Ω for every $\lambda \geq 1$. Then there exists a $\lambda > 1$ such that (3-5) holds with u replaced by u_λ. However,

$$\int_\Omega \varphi^*(Du_\lambda) = \lambda^{1-n} \int_{x_0+\lambda(\Omega-x_0)} \varphi^*(Du) = \lambda^{1-n} \int_\Omega \varphi^*(Du) < \int_\Omega \varphi^*(Du)$$

(the second equality is due to the fact that $\Omega \subset x_0 + \lambda(\Omega - x_0)$ for $\lambda > 1$, while $u = 0$ outside of Ω), contradicting the minimality of u. □

4. The convex two-dimensional case

In this section we shall assume that $n = 2$ and $\Omega \subset \mathbb{R}^2$ is a convex open set.

Given $E \subset \mathbb{R}^2$ and an $r > 0$ we define the set $E^r \subset E$ by the formula

$$E^r := \begin{cases} \bigcup\{W_r(x) : W_r(x) \subset E\} & \text{if } r > 0, \\ E & \text{if } r = 0. \end{cases} \tag{4-1}$$

Notice that, if E is a convex set, then E^r is convex and satisfies the rW_φ-condition. The set E^r is called the *Wulff plaquette* of radius r relative to E.

The following assertion holds:

Lemma 4.1. *Let $E \subset \mathbb{R}^2$ be a convex open set satisfying the rW_φ-condition for some $r > 0$. Then $E = E^r$.*

Proof. One has $E^r \subset E$. On the other hand, $\partial E \subset \partial E^r$ because E satisfies the rW_φ-condition. Minding that E, and hence E^r, is convex, we get $E = E^r$. □

The convexity of set E is essential in Lemma 4.1. In fact, if A, B and C are the vertices of an equilateral triangle $\triangle ABC$ with side length 1, then letting

$$E := B_{1/2}(A) \cup B_{1/2}(B) \cup B_{1/2}(C) \cup \triangle ABC$$

we have that E satisfies the $\frac{1}{2}W_\varphi$-condition with respect to the Euclidean norm, but

$$E^{1/2} = B_{1/2}(A) \cup B_{1/2}(B) \cup B_{1/2}(C) \neq E.$$

4A. ***Isoperimetric sets.*** We consider the constrained isoperimetric problem

$$\min\{P_\varphi(E) : E \subset \Omega,\ |E| = m \in [0, |\Omega|]\}, \tag{4-2}$$

which corresponds to the problem (1-1) under the additional constraint that u is a characteristic function. Clearly, the minimizers of this problem exist and the assertion of Proposition 3.4 remains valid for this problem.

Let $R_\Omega > 0$ be the maximal radius R such that $W_R(x) \subseteq \Omega$ for some $x \in \Omega$, and let $r_\Omega \in [0, R_\Omega]$ be the maximal radius r such that Ω satisfies the rW_φ-condition (we set for convenience $r_\Omega = 0$ if Ω does not satisfy any rW_φ-condition). Observe that in the Euclidean case one has

$$r_\Omega = \frac{1}{\|\kappa\|_{L^\infty(\partial\Omega)}}$$

where κ stands for the curvature of $\partial\Omega$.

Lemma 4.2. *Let $m \in (0, |\Omega|)$, and let E be a minimizer of* (4-2). *Then E is convex and there exists an $r > 0$ (depending on m) such that E satisfies the rW_φ-condition and each connected component of $\partial E \cap \Omega$ is contained in $\partial W_r(x)$, for some Wulff ball $W_r(x) \subset \Omega$ (with x depending on the connected component of $\partial E \cap \Omega$).*

Remark 4.3. Recall that here and in the sequel when speaking of the properties of a set E of finite perimeter we actually refer to the respective properties of the set of its density points. In particular, a minimizer E of (4-2) is not necessarily convex, but the set of its density points is (and hence, in particular, the closure $\bar{E}$ is convex).

Proof. STEP 1. We first show the convexity of E. As in [Ambrosio et al. 2001, Theorem 2] we can uniquely decompose E as a union of (measure theoretic) connected components $\{E_i\}_{i\in I}$, where I is finite or countable, such that

$$|E| = \sum_{i\in I} |E_i| \quad \text{and} \quad P_\varphi(E) = \sum_{i\in I} P_\varphi(E_i).$$

As in [Ambrosio et al. 2002, Proposition 6.12], one shows by the isoperimetric inequality and the minimality of E that the number of connected components is finite and the boundary of each connected component E_i is parametrized by a finite number of pairwise disjoint Jordan curves. In particular, the boundaries of two different connected components do not intersect. Further, using Lemma 6.9 from [Ambrosio et al. 2002], one has that the perimeter $P_\varphi(E_i)$ of a measure theoretic connected component E_i that has its boundary parametrized by Jordan curves $\{\theta_i^j\}_{j=1}^{N_i}$ (all parametrized, say, over [0, 1]) is given by

$$P_\varphi(E_i) = \sum_{j=1}^{N_i} \int_0^1 \psi(\dot{\theta}_i^j(t))\,dt,$$

where $\psi : \mathbb{R}^2 \to \mathbb{R}$ is some convex and 1-homogeneous function (in fact, $\psi := \varphi^* \circ R$, R being the clockwise rotation of $\mathbb{R}^2$ by $\pi/2$; see Corollary 6.10 from [Ambrosio et al. 2002]). Hence, using Jensen inequality one shows that the convex envelope of E_i has lower (anisotropic) perimeter than E_i itself, and minding that is also has greater volume (as well as the fact that the assertion of Proposition 3.4 is valid for the problem (4-2)), one has that each E_i is convex.

Finally, if E is not connected, recalling that Ω is convex we can translate a connected component inside Ω in such a way that its boundary touches the boundary of another connected component (this changes neither the perimeter nor the volume), and taking the convex envelope of the resulting set we obtain again a set with greater volume and strictly lower anisotropic perimeter, hence a contradiction which shows that E is convex.

STEP 2. Reasoning as in [Novaga and Paolini 2005, Theorem 4.5], where the related problem

$$\min\left\{P_\varphi(E) - \lambda|E| : E \subset \Omega, \lambda \geq 0\right\}$$

was considered instead of (4-2), one gets that each connected component of $\partial E \cap \Omega$ is contained in $\partial W_r(x)$, for some $x \in \mathbb{R}^2$ and $r > 0$.

Moreover, as in [Ambrosio et al. 2002, Theorem 6.19] one can show the existence of a (possibly nonunique) Lipschitz continuous vector field $n : \partial E \to \mathbb{R}^2$ such that $n(x) \in \partial\varphi^*(\nu(x))$ for $\mathcal{H}^1$-a.e. $x \in \partial E$. In particular $\mathrm{div}_\tau n \in L^\infty(\partial E)$, where $\mathrm{div}_\tau n := \partial_\tau(n \cdot \tau)$ denotes the tangential divergence of n and corresponds to the anisotropic curvature of ∂E; see [Taylor 1975; Bellettini et al. 2001]. (Here and below τ and ν denote respectively the Euclidean unit tangent and exterior normal vectors to ∂E.)

Without loss of generality we may assume that $\mathrm{div}_\tau n$ is constant along every maximal segment contained in ∂E (if not, we can substitute n over the segment by a convex combination of its values on the endpoints of the segment; one would then still have $n \in \partial\varphi^*(\nu)$ along the segment because ν is constant there and $\partial\varphi^*(\,\cdot\,)$ is convex). In particular, if a connected component Σ of $\partial E \cap \Omega$ is contained in $\partial W_r(x)$, then $n(y) = (y-x)/(r\varphi(y-x))$ for $\mathcal{H}^1$-a.e. $y \in \Sigma$.

STEP 3. We now prove that E satisfies the rW_φ-condition for some $r > 0$. Since E is convex, it is enough to show that

$$\mathrm{div}_\tau n \leq \frac{1}{r} \quad \mathcal{H}^1\text{-a.e. on } \partial E. \tag{4-3}$$

This follows by a local variation argument as in the proof of Lemma 4.9 below. Let us fix $x_1 \in \Sigma$, where Σ is a connected component of $\partial E \cap \Omega$, and $x_2 \in \partial E \setminus \bar{\Sigma}$. We know from the previous step that Σ is contained in $\partial W_r(x)$ for some $x \in \mathbb{R}^2$ and $r > 0$. We distinguish four cases.

Case 1. There are two disjoint open sets U_i, $i = 1, 2$, such that $x_i \in U_i$ and $U_i \cap \partial E$ do not contain segments. Let ψ_1, ψ_2 be two nonnegative smooth functions, with support on U_1, U_2 respectively, such that

$$\int_{U_1\cap\partial E} \psi_1(z)\varphi^*(\nu(z))\, d\mathcal{H}^1(z) = \int_{U_2\cap\partial E} \psi_2(z)\varphi^*(\nu(z))\, d\mathcal{H}^1(z). \tag{4-4}$$

We consider a family of diffeomorphisms such that

$$\Psi(\varepsilon, x) := x + \varepsilon\psi_1(x)n(x) - \varepsilon\psi_2(x)n(x) + o(\varepsilon)$$

for $\varepsilon > 0$ small enough. By (4-4), the term $o(\varepsilon)$ can be chosen in such a way that

$$|E^\varepsilon| = |E| \quad \text{for all } \varepsilon > 0 \text{ small enough,} \tag{4-5}$$

with $E^\varepsilon := \Psi(\varepsilon, E) \subset \Omega$. We then have

$$P_\varphi(E^\varepsilon) = P_\varphi(E) + \frac{\varepsilon}{r}\int_{U_1\cap\partial E} \psi_1(z)\varphi^*(\nu(z))\, d\mathcal{H}^1(z) \\ -\varepsilon\int_{U_2\cap\partial E} \psi_2(z)\mathrm{div}_\tau n(z)\varphi^*(\nu(z))\, d\mathcal{H}^1(z) + o(\varepsilon),$$

where ν stands for the exterior Euclidean unit normal to ∂E. As $\varepsilon \to 0^+$, by minimality of E, we get

$$\frac{1}{r}\int_{U_1\cap\partial E} \psi_1(z)\varphi^*(\nu(z))\, d\mathcal{H}^1(z) \geq \int_{U_2\cap\partial E} \psi_2(z)\mathrm{div}_\tau n(z)\varphi^*(\nu(z))\, d\mathcal{H}^1(z),$$

which in view of (4-4) gives (4-3).

Case 2. We can find two maximal segments $\ell_1, \ell_2 \subset \partial E$ such that $x_i \in \ell_i$, and we define E^ε by shifting ℓ_1 by $c_1\varepsilon$ parallel to itself outside E, and by shifting ℓ_2 by $c_2\varepsilon$ inside of E, with c_1, c_2 so that (4-5) holds, that is

$$c_1|\ell_1| = c_2|\ell_2|. \tag{4-6}$$

By [Novaga and Paolini 2005, Lemma 4.4] we have

$$P_\varphi(E^\varepsilon) = P_\varphi(E) + c_1\alpha_1\varepsilon - c_2\alpha_2\varepsilon + o(\varepsilon),$$

where α_1, α_2 are respectively the (Euclidean) length of the face of W_φ parallel to ℓ_1, ℓ_2. By minimality of E, letting $\varepsilon \to 0^+$ we obtain $c_1\alpha_1 \geq c_2\alpha_2$. Recalling (4-6), we finally get

$$\frac{1}{r} = \frac{\alpha_1}{|\ell_1|} \geq \frac{\alpha_2}{|\ell_2|} = \mathrm{div}_\tau n(z) \quad \text{for } z \in \ell_2.$$

Case 3. There is a maximal segment $\ell_1 \subset \partial E$ and an open set U_2 such that $x_1 \in \ell_1$, $x_2 \in U_2$ and $U_2 \cap \partial E$ does not contain segments. We proceed by combining the previous strategies and we define the set E^ε by shifting ℓ_1 by ε parallel to itself outside E, and then taking the image of the resulting set through the diffeomorphism

$$\Psi(\varepsilon, x) := x - \varepsilon \psi_2(x) n(x) + o(\varepsilon),$$

where ψ_2 is a nonnegative smooth function supported on U_2 satisfying

$$\int_{U_2 \cap \partial E} \psi_2(z) \varphi^*(\nu(z))\, d\mathcal{H}^1(z) = |\ell_1|. \tag{4-7}$$

This condition guarantees that the volume change after these two operations is of order $o(\varepsilon)$, so that the extra term $o(\varepsilon)$ in the definition of Ψ is chosen in such a way that (4-5) holds. Reasoning as above, we get

$$P_\varphi(E^\varepsilon) = P_\varphi(E) + \alpha_1 \varepsilon - \varepsilon \int_{U_2 \cap \partial E} \psi_2(z) \operatorname{div}_\tau n(z) \varphi^*(\nu(z))\, d\mathcal{H}^1(z) + o(\varepsilon),$$

which gives, by minimality of E,

$$\alpha_1 = \frac{|\ell_1|}{r} \geq \int_{U_2 \cap \partial E} \psi_2(z) \operatorname{div}_\tau n(z) \varphi^*(\nu(z))\, d\mathcal{H}^1(z),$$

which gives (4-3), recalling (4-7).

Case 4. There is a maximal segment $\ell_2 \subset \partial E$ and an open set U_1 such that $x_1 \in U_1$, $x_2 \in \ell_2$ and $U_1 \cap \partial E$ does not contain segments. This case can be dealt with reasoning as in the previous case, by shifting ℓ_2 by ε inside E and defining

$$\Psi(\varepsilon, x) := x + \varepsilon \psi_1(x) n_2(x) + o(\varepsilon).$$

STEP 4. From (4-3) it follows that the radius r in Step 3 does not depend on the connected component Σ. In particular, every connected component of $\partial E \cap \Omega$ is contained in $\partial W_r(x)$, for a fixed $r > 0$ (while x depends in general on the connected component). □

Consider now the function $v(r) := |\Omega^r|$. It is clearly constantly equal to $|\Omega|$ for $r \leq r_\Omega$ and to zero for $r > R_\Omega$, while over $[r_\Omega, R_\Omega]$ it is continuous and monotone decreasing. In particular, for all $m \in [|\Omega^{R_\Omega}|, |\Omega|]$ there exists a unique value $r_m \in [r_\Omega, R_\Omega]$ such that $v(r_m) = m$.

From the isoperimetric inequality (2-3) and Lemma 4.2, we get the following statement.

Proposition 4.4. *Let $\Omega \subset \mathbb{R}^2$ be convex, and let E be a minimizer of* (4-2) *with $m \in [0, |\Omega|]$. Then either*

(a) $\bar{E} = \bar{\Omega}^{r_m}$, *if $m > |\Omega^{R_\Omega}|$, or*

(b) *$\bar{E}$ is the closure of some convex union of Wulff balls of radius R_Ω, if $m \in [R_\Omega^2|W_\varphi|, |\Omega^{R_\Omega}|]$, or*

(c) *$\bar{E} = \bar{W}_{\sqrt{m/|W_\varphi|}}(x)$ for some $x \in \Omega$, if $m \le R_\Omega^2|W_\varphi|$.*

Proof. We can assume $m \in (0, |\Omega|)$. By Lemma 4.2, there exists an $r > 0$ (depending on m) such that $\bar{E}$ is the closure of a union of Wulff balls of radius r, hence $\bar{E} \subset \bar{\Omega}^r$ and $r \le R_\Omega$.

If $m > |\Omega^{R_\Omega}|$, then necessarily $r < R_\Omega$ and $\bar{E} = \bar{\Omega}^r$, since otherwise we could find a connected component of $\partial E \cap \Omega$ that is not contained in the boundary of a Wulff ball, contradicting Lemma 4.2. In particular, we have $r = r_m$.

If $m \in [R_\Omega^2|W_\varphi|, |\Omega^{R_\Omega}|]$ then $r = R_\Omega$, since otherwise $\bar{E}$ would coincide with the set $\bar{\Omega}^r$ (with $r < R_\Omega$), which has volume strictly greater than $|\Omega^{R_\Omega}|$.

If $m \le R_\Omega^2|W_\varphi|$ the result follows by the isoperimetric inequality (2-3). □

Remark 4.5. It is worth noticing that, if Ω is strictly convex, then there exists a *unique* ball $W_{R_\Omega}(x) \subset \Omega$, and thus $\Omega^{R_\Omega} = W_{R_\Omega}(x)$. In other words, the case (b) of the above Proposition 4.4 reduces to case (c). Therefore, either $\bar{E} = \bar{\Omega}^{r_m}$, if $m \ge |\Omega^{R_\Omega}|$, or $\bar{E} = \bar{W}_{\sqrt{m/|W_\varphi|}}(x)$ for some $x \in \Omega$, if $m \le |\Omega^{R_\Omega}|$.

We now state an easy consequence of Proposition 4.4 showing that solutions to the problem (4-2) with decreasing volumes may be arranged as a decreasing sequence of sets.

Corollary 4.6. *Let Ω be convex and let m_j be a decreasing sequence such that $m_j \in (0, |\Omega|)$, for all j. There exists a sequence of sets E_j such that $E_{j+1} \subset E_j \subset \Omega$, $|E_j| = m_j$ and each E_j is a minimizer of* (4-2) *with $m := m_j$.*

Note that the convexity assumption on the set Ω is essential in the above result. In fact, reasoning as in [Kawohl and Lachand-Robert 2006, Section 6] with the example of Ω a couple of circles connected by a thin tube (like a barbell considered in [Kawohl and Lachand-Robert 2006, Section 6]), one provides a family of minimizers of (4-2) with decreasing volumes which cannot be arranged as a decreasing sequence of sets (see Figure 1).

4B. ***Isoperimetric towers.*** We return now to the original problem (1-1). Here and below we let $u \in L^1(\mathbb{R}^2)$ be an arbitrary minimizer of this problem and E_j be its level set corresponding to a $j \in \mathbb{N}$, as defined by (3-1). The following result follows directly from Corollary 4.6.

Proposition 4.7. *If Ω is convex, then for all $j \in \mathbb{N}$ the set E_j is a minimizer of the problem* (4-2) *with $m := |E_j|$ (in particular E_j is convex).*

Proof. If the assertion is not true, then considering a sequence of sets E'_j of minimizers of (4-2) (with $m := |E_j|$) such that $E'_{j+1} \subset E'_j \subset \Omega$, $|E'_j| := |E_j|$ (the

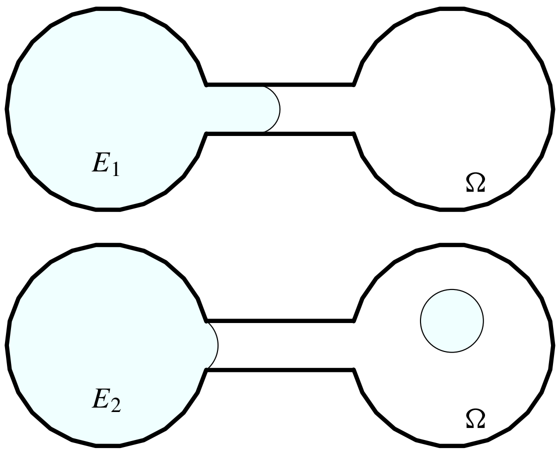

Figure 1. Example of $\Omega \subset \mathbb{R}^2$ nonconvex: two circles connected with a thin tube. E_1 and E_2 (which has two connected components) are two minimizers of (4-2) that are not included into one another.

existence of such a sequence is guaranteed by Corollary 4.6), and setting

$$u' := \sum_j \mathbf{1}_{E'_j},$$

we get

$$\int_{\mathbb{R}^2} \varphi^*(Du') = \sum_j P_\varphi(E'_j) < \sum_j P_\varphi(E_j) = \int_{\mathbb{R}^2} \varphi^*(Du),$$

the strict inequality being due to the fact that one of E_j is not a minimizer of (4-2) (with $m := |E_j|$) by assumption. On the other hand,

$$\int_\Omega u'\,dx = \int_\Omega u\,dx = m,$$

since the level sets of u' and u have the same volume by construction. This would mean that u is not a solution to the problem (1-1). □

Remark 4.8. By Proposition 4.7 and Lemma 4.2, each set E_i is convex and each connected component of $\partial E_i \cap \Omega$ is contained in $\partial W_{r_i}(x_i)$ for some Wulff ball $W_{r_i}(x_i) \subset \Omega$.

Lemma 4.9. *Let S_i, S_j be connected components of $\partial E_i \cap \Omega$ and $\partial E_j \cap \Omega$, respectively, with $j > i$, such that*

$$S_i \subset \partial W_{r_i}(x_i) \subset \bar{\Omega}, \quad S_j \subset \partial W_{r_j}(x_j) \subset \bar{\Omega}, \quad \frac{1}{r_i}(S_i - x_i) \subset \frac{1}{r_j}(S_j - x_j), \tag{4-8}$$

for some $x_i, x_j \in \mathbb{R}^2$, $r_i, r_j > 0$. Then $r_i \geq r_j$.

Proof. It is enough to consider the case $j = i + 1$. We can also assume $S_i \neq S_{i+1}$, otherwise there is nothing to prove. As in Figure 2, there are two cases to consider.

Case 1. There are two points $y_i \in S_i$, $y_{i+1} \in S_{i+1}$ and two disjoint open sets $U_i \subset \Omega$ and $U_{i+1} \subset \Omega$ such that $y_i \in U_i$, $y_{i+1} \in U_{i+1}$, and that $U_i \cap S_i$ and $U_{i+1} \cap S_{i+1}$ do not contain segments. Consider a smooth function ψ_i with support on U_i. It generates a one-parameter family of diffeomorphisms of E_i defined by

$$\Psi_i(\varepsilon, x) := x - \varepsilon\psi_i(x)n_i(x)$$

for all sufficiently small $\varepsilon > 0$, where

$$n_i(x) := \frac{x - x_i}{r_i\varphi(x - x_i)}\,.$$

Consider now a one-parameter family $\{\Psi_{i+1}(\varepsilon, \cdot\,)\}$ of diffeomorphisms of E_{i+1} such that $\Psi_{i+1}(0, x) = x$ for all $x \in E_{i+1}$, $\Psi_{i+1}(\varepsilon, \cdot\,) - \mathrm{Id}$ is supported in U_{i+1} for all $\varepsilon > 0$, while

$$\Psi_{i+1}(\varepsilon, x) := x + \varepsilon\psi_{i+1}(x)n_{i+1}(x) + o(\varepsilon)$$

as $\varepsilon \to 0^+$, where ψ_{i+1} is some smooth function (with support in U_{i+1}), and

$$n_{i+1}(x) := \frac{x - x_{i+1}}{r_{i+1}\,\varphi(x - x_{i+1})}\,.$$

We choose Ψ_{i+1} so that the sets $E_i^\varepsilon := \Psi_i(\varepsilon, E_i)$ and $E_{i+1}^\varepsilon := \Psi_{i+1}(\varepsilon, E_{i+1})$ satisfy

$$|E_i^\varepsilon| + |E_{i+1}^\varepsilon| = |E_i| + |E_{i+1}|$$

for all sufficiently small $\varepsilon > 0$. Denote by ν_j the exterior Euclidean unit normal to ∂E_j. Since

$$|E_i^\varepsilon| = |E_i| - \varepsilon \int_{\partial E_i \cap U_i} \psi_i(z)\varphi^*(\nu_i(z))\, d\mathcal{H}^1(z) + o(\varepsilon),$$
$$|E_{i+1}^\varepsilon| = |E_{i+1}| + \varepsilon \int_{\partial E_{i+1} \cap U_{i+1}} \psi_{i+1}(z)\varphi^*(\nu_{i+1}(z))\, d\mathcal{H}^1(z) + o(\varepsilon),$$

as $\varepsilon \to 0^+$, we have

$$\int_{\partial E_i \cap U_i} \psi_i(z)\varphi^*(\nu_i(z))\, d\mathcal{H}^1(z) = \int_{\partial E_{i+1} \cap U_{i+1}} \psi_{i+1}(z)\varphi^*(\nu_{i+1}(z))\, d\mathcal{H}^1(z). \tag{4-9}$$

Letting now

$$u_\varepsilon := u - \mathbf{1}_{E_i} - \mathbf{1}_{E_{i+1}} + \mathbf{1}_{E_i^\varepsilon} + \mathbf{1}_{E_{i+1}^\varepsilon} = \sum_{\substack{k \neq i \\ k \neq i+1}} \mathbf{1}_{E_k} + \mathbf{1}_{E_i^\varepsilon} + \mathbf{1}_{E_{i+1}^\varepsilon},$$

we have $\int_\Omega u_\varepsilon\,dx = \int_\Omega u\,dx$ for all sufficiently small $\varepsilon > 0$. Recall that

$$\int_\Omega \varphi^*(Du_\varepsilon) = \int_\Omega \varphi^*(Du) - \varepsilon \int_{\partial E_i \cap U_i} \frac{1}{r_i}\psi_i(z)\varphi^*(\nu_i(z))\,d\mathcal{H}^1(z) \\ +\varepsilon \int_{\partial E_{i+1}\cap U_{i+1}} \frac{1}{r_{i+1}}\psi_{i+1}(z)\varphi^*(\nu_{i+1}(z))\,d\mathcal{H}^1(z) + o(\varepsilon).$$

As $\varepsilon \to 0^+$, by minimality of u, we get

$$-\frac{1}{r_i}\int_{\partial E_i\cap U_i} \psi_i(z)\varphi^*(\nu_i(z))\,d\mathcal{H}^1(z) + \frac{1}{r_{i+1}}\int_{\partial E_{i+1}\cap U_{i+1}} \psi_{i+1}(z)\varphi^*(\nu_{i+1}(z))\,d\mathcal{H}^1(z) \\ \geq 0,$$

which together with (4-9) implies the thesis.

Case 2. We can find two maximal line segments $\ell_i \subset S_i$ and $\ell_{i+1} \subset S_{i+1}$. We define then E_i^ε by shifting the segment ℓ_i by $c_i\varepsilon$ parallel to itself inside E_i and E_{i+1}^ε by shifting the segment ℓ_{i+1} parallel to itself outside of E_{i+1} by $c_{i+1}\varepsilon$ with c_i and c_{i+1} so as to satisfy

$$|E_i^\varepsilon| + |E_{i+1}^\varepsilon| = |E_i| + |E_{i+1}|$$

for all $\varepsilon > 0$ sufficiently small. Since

$$|E_i^\varepsilon| = |E_i| - c_i|\ell_i|\varepsilon + o(\varepsilon),$$
$$|E_{i+1}^\varepsilon| = |E_{i+1}| + c_{i+1}|\ell_{i+1}|\varepsilon + o(\varepsilon),$$

as $\varepsilon \to 0^+$, we have

$$c_i|\ell_i| = c_{i+1}|\ell_{i+1}|. \tag{4-10}$$

Letting again, as in Case 1,

$$u_\varepsilon := u - \mathbf{1}_{E_i} - \mathbf{1}_{E_{i+1}} + \mathbf{1}_{E_i^\varepsilon} + \mathbf{1}_{E_{i+1}^\varepsilon} = \sum_{\substack{k\neq i\\ k\neq i+1}} \mathbf{1}_{E_k} + \mathbf{1}_{E_i^\varepsilon} + \mathbf{1}_{E_{i+1}^\varepsilon},$$

we have $\int_\Omega u_\varepsilon\,dx = \int_\Omega u\,dx$ for all sufficiently small $\varepsilon > 0$. On the other hand, by [Novaga and Paolini 2005, Lemma 4.4],

$$\int_\Omega \varphi^*(Du_\varepsilon) = \int_\Omega \varphi^*(Du) - c_i\alpha_i\varepsilon + c_{i+1}\alpha_{i+1}\varepsilon + o(\varepsilon),$$

where α_i, α_{i+1} are the (Euclidean) lengths of the face of W_φ parallel to ℓ_i, ℓ_{i+1}, respectively. By minimality of u, letting $\varepsilon \to 0^+$ we obtain $c_i\alpha_i \leq c_{i+1}\alpha_{i+1}$. Recalling (4-10), we get $r_i = |\ell_i|/\alpha_i \geq |\ell_{i+1}|/\alpha_{i+1} = r_{i+1}$.

Notice that in this proof we do not have to deal with the situation depicted in Cases 3 and 4 of the proof of Lemma 4.2 due to condition (4-8). In fact, the latter implies that if S_i contains a line segment ℓ_i, then the line segment $\ell_j :=$

$x_j + (l_i - x_i)r_j/r_i$ is contained in S_j. Otherwise, if there is a neighborhood U_i of a point of S_i such that $S_i \cap U_i$ does not contain any line segment, then $U_j := x_j + (U_i - x_i)r_j/r_i$ is a neighborhood of a point in S_j such that $S_j \cap U_j$ does not contain any line segment. ☐

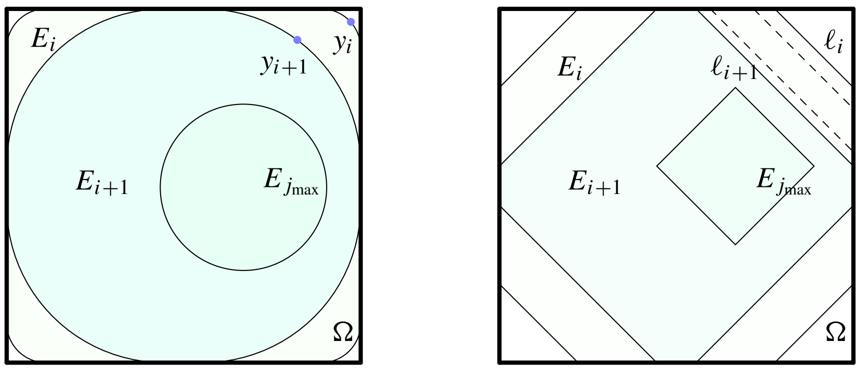

Figure 2. The two possible cases in the proof of Lemma 4.9.

We are now able to prove the following result giving the complete characterization of solutions to the problem (1-1).

Theorem 4.10. *Let $\Omega \subset \mathbb{R}^2$ be convex and set $j_{\max} := \|u\|_\infty$. Then one of the following cases holds.*

(a) *There exists an $\bar{r} \in [r_\Omega, R_\Omega)$ such that $\bar{E}_j = \bar{\Omega}^{\bar{r}}$ for all $j \le j_{\max}$. In this case*

$$u = j_{\max} \mathbf{1}_{\Omega^{\bar{r}}}$$

(*in particular, if $\bar{r} = r_\Omega$, then $u = j_{\max} \mathbf{1}_\Omega$*).

(b) *There exists an $\bar{r} \in (r_\Omega, R_\Omega)$ such that $\bar{E}_{j_{\max}} = \bar{W}_{\bar{r}}(x)$ for some $x \in \Omega$ such that $W_{\bar{r}}(x) \subset \Omega^{\bar{r}}$, and $\bar{E}_j = \bar{\Omega}^{\bar{r}}$ for all $j < j_{\max}$. In this case*

$$u = \mathbf{1}_{W_{\bar{r}}(x)} + (j_{\max} - 1)\mathbf{1}_{\Omega^{\bar{r}}}.$$

(c) *There exists an $\bar{r} \in (0, r_\Omega]$ such that $\bar{E}_{j_{\max}} = \bar{W}_{\bar{r}}(x)$ for some $x \in \Omega$ such that $W_{\bar{r}}(x) \subset \Omega$, and $\bar{E}_j = \bar{\Omega}$ for all $j < j_{\max}$. In this case*

$$u = \mathbf{1}_{W_{\bar{r}}(x)} + (j_{\max} - 1)\mathbf{1}_\Omega$$

(*note that this condition may hold only when $r_\Omega > 0$*).

(d) *Every $\bar{E}_j$ is the closure of a convex union of Wulff balls of radius R_Ω for all $j \le j_{\max}$. In this case*

$$u = \sum_{j=1}^{j_{\max}} \mathbf{1}_{E_j}.$$

Remark 4.11. Observe that Case (d) of Theorem 4.10 is the only case where the number of nonzero level sets of the minimizer may be bigger than two.

Proof. We may assume $j_{\max} > 1$, since otherwise the result follows directly from Proposition 4.4.

By Remark 4.8, for all $i \le j_{\max}$ the set E_i is convex and each connected component of $\partial E_i \cap \Omega$ is contained, up to a translation, in $\partial W_{r_i}(x_i)$ for some $r_i > 0$, $x_i \in \mathbb{R}^2$. Moreover, if $\partial E_i \cap \Omega$ and $\partial E_{i+1} \cap \Omega$ are nonempty, from the inclusion $E_{i+1} \subset E_i$ it follows that we can always find two connected components $S_i \subset \partial E_i \cap \Omega$ and $S_{i+1} \subset \partial E_{i+1} \cap \Omega$ satisfying the assumptions of Lemma 4.9. By Lemma 4.9 we then get $r_i \ge r_{i+1}$ for all $i < j_{\max}$.

Recalling Propositions 4.7 and 4.4, this leaves only the following possibilities:

(i) $\bar{E}_i = \bar{\Omega}^{r_i}$, $\bar{E}_{i+1} = \bar{\Omega}^{r_{i+1}}$ with $r_i \ge r_{i+1}$. If $r_i > r_\Omega$ (hence $\Omega^{r_i} \ne \Omega$), then minding $\bar{E}_{i+1} \subset \bar{E}_i$ we have in this case $r_i = r_{i+1}$ hence $\bar{E}_i = \bar{E}_{i+1} = \bar{\Omega}^{r_i}$, while if $r_{i+1} \le r_i \le r_\Omega$ we have $\bar{E}_i = \bar{E}_{i+1} = \bar{\Omega}$, and we may just set $r_i = r_{i+1} := r_\Omega$ so that still $\bar{E}_i = \bar{E}_{i+1} = \bar{\Omega}^{r_i}$ (because $\Omega^{r_\Omega} = \Omega$).

(ii) $\bar{E}_i = \bar{\Omega}^{r_i}$, $\bar{E}_{i+1} = \bar{W}_{r_{i+1}}(x_{i+1})$ with $r_i \ge r_{i+1}$.

(iii) $\bar{E}_i = \bar{W}_{r_i}(x_i)$, $\bar{E}_{i+1} = \bar{W}_{r_{i+1}}(x_{i+1})$ with $r_i \ge r_{i+1}$.

(iv) $\bar{E}_i$ is a closure of some convex union of Wulff balls of radius R_Ω and $E_{i+1} = \bar{W}_{r_{i+1}}(x_{i+1})$ with $R_\Omega > r_{i+1}$.

(v) Both $\bar{E}_i$ and $\bar{E}_{i+1}$ are closures of some convex unions of Wulff balls of radius R_Ω.

(Note that the case when $\bar{E}_{i+1}$ is a closure of a convex union of Wulff balls of radius R_Ω and $\bar{E}_i = \bar{W}_{r_i}(x_i)$ with $R_\Omega < r_i$ is impossible.) Thus there is a $\bar{j} \in \{0, \dots, j_{\max}\}$ and an $r_1 \in [r_\Omega, R_\Omega)$ such that either

(A) for every $i \le \bar{j}$ one has $\bar{E}_i = \bar{\Omega}^{r_1}$ or

(B) for every $i \le \bar{j}$ each $\bar{E}_i$ is a closure of a convex union of Wulff balls of radius R_Ω (in particular, just a single closed Wulff ball),

while $\bar{E}_i = \bar{W}_{r_i}(x_i)$, $r_i < R_\Omega$ for all $i > \bar{j}$, with $\{r_i\}$ decreasing.

Consider now an arbitrary $i > \bar{j}$ such that $E_i \ne \varnothing$. Note that either $r_i \le r_1 < R_\Omega$ (Case A) or $r_i < R_\Omega$ (Case B).

It remains to show that $E_j = \varnothing$ for all $j > i$. Suppose the contrary, namely, that $E_{i+1} \ne \varnothing$. We may assume without loss of generality all level sets are open convex by Proposition 4.7, and, further, $\bar{E}_{l+1} \subset E_l$ for all $l \in \{\bar{j}, \dots, j_{\max}\}$) (if not, from what has been already proven it follows that we may just shift appropriately all the respective level sets, which would maintain both $\int_\Omega \varphi^*(Du)$ and $\int_\Omega u$). Choose now $\varepsilon > 0$ and $\varepsilon' > 0$ sufficiently small so that for $r'_{i+1} := r_{i+1} - \varepsilon'$ and $r_i := r_i + \varepsilon$ one would have

$$r_i'^2 + r_{i+1}'^2 = r_i^2 + r_{i+1}^2 \tag{4-11}$$

and $\bar{W}_{r'_i}(x_i) \subset E_{i-1}$, $\bar{E}_{i+2} \subset W_{r'_{i+1}}(x_{i+1})$. From (4-11) one gets $\varepsilon' = (r_i/r_{i+1})\varepsilon + o(\varepsilon)$, and hence

$$\frac{P_\varphi(W_{r'_{i+1}}(x_{i+1})) + P_\varphi(W_{r'_i}(x_i))}{P_\varphi(W_{r_{i+1}}(x_{i+1})) + P_\varphi(W_{r_i}(x_i))} = \frac{r'_{i+1} + r'_i}{r_{i+1} + r_i} = 1 - \varepsilon \frac{r_{i+1} - r_i}{r_{i+1}(r_{i+1} + r_i)} + o(\varepsilon),$$

where the error term $o(\varepsilon)$ is negative when $r_i = r_{i+1}$. Therefore, representing u as $u = \tilde{u} + \mathbf{1}_{E_{i+1}} + \mathbf{1}_{E_i}$, and letting

$$u'_\varepsilon := \tilde{u} + \mathbf{1}_{W_{r'_{i+1}}(x_{i+1})} + \mathbf{1}_{W_{r'_i}(x_i)},$$

we get $\int_\Omega \varphi^*(Du'_\varepsilon) < \int_\Omega \varphi^*(Du)$ for sufficiently small $\varepsilon > 0$; but $\int_{\mathbb{R}^2} u\,dx = \int_{\mathbb{R}^2} u'_\varepsilon\,dx$, contrary to the optimality of u, which proves the claim.

One has therefore either $\bar{j} = j_{\max} - 1$ or $\bar{j} = j_{\max}$, which concludes the proof. □

5. An explicit example

5A. ***A square with Euclidean norm.*** Let now $\Omega := [0, 1]^2$ and let φ be the Euclidean norm on $\mathbb{R}^2$. From Theorem 4.10 we obtain the following characterization for the minimizers of (1-1).

Proposition 5.1. *Let $\Omega = [0, 1]^2$.*

(1) *If $m \in (n-1, n\pi/4)$, with $1 \le n \le 4$, we have $j_{\max} = n$, $\bar{E}_{j_{\max}} = \bar{B}_r(x_0) \subset \bar{\Omega}$ and $\bar{E}_j = \bar{\Omega}^r$ for $j < j_{\max}$, with*

$$r = \sqrt{\frac{n-m-1}{4(n-1) - n\pi}}.$$

(2) *If $m \in [n\pi/4, n]$, with $1 \le n \le 4$, we have $j_{\max} = n$ and $\bar{E}_j = \bar{\Omega}^r$ for $j \le j_{\max}$, with $r = \sqrt{(1 - m/n)/(4-\pi)}$.*

(3) *If $m > 4$ we have*

$$j_{\max} \in \left\{ \left\lfloor \frac{2+\sqrt{\pi}}{2\sqrt{\pi}} m \right\rfloor, \left\lfloor \frac{2+\sqrt{\pi}}{2\sqrt{\pi}} m \right\rfloor + 1 \right\} \tag{5-1}$$

and $\bar{E}_j = \bar{\Omega}^r$ for $j \le j_{\max}$, with $r = \sqrt{(1 - m/j_{\max})/(4-\pi)}$.

Proof. By Theorem 4.10 for all $m > 0$ we have one of the following two possibilities.

Case A. $\bar{E}_j = \bar{\Omega}^r$ for all $j \le j_{\max}$ with

$$m = j_{\max}|\Omega^r| = j_{\max}\big(1-(4-\pi)r^2\big) \quad r \in \big[0, \tfrac{1}{2}\big].$$

It then follows that

$$r = r_A(j_{\max}) := \sqrt{\frac{j_{\max}-m}{(4-\pi)\,j_{\max}}}$$

and $\sum_{j=1}^{j_{\max}} P(E_j) = F_A(j_{\max})$, where

$$F_A(x) := x\,P(\Omega^{r_A(x)}) = 4x - 2\sqrt{4-\pi}\,\sqrt{x(x-m)}\,.$$

Notice that

$$F_A'(x) = 4 - \sqrt{4-\pi}\,\frac{2x-m}{\sqrt{x(x-m)}}\,,$$

which implies that $F_A(x)$ is increasing for $x > ((2+\sqrt{\pi})/2\sqrt{\pi})m$, while it is decreasing for $m \le x < ((2+\sqrt{\pi})/2\sqrt{\pi})m$. As a consequence we have

$$j_{\max} \in \{j^A, j^A{+}1\}, \quad \text{where } j^A := \left\lfloor \frac{2+\sqrt{\pi}}{2\sqrt{\pi}} m \right\rfloor. \tag{5-2}$$

Case B. $\bar{E}_{j_{\max}} = \bar{B}_r(x_0) \subset \bar{\Omega}$ and $\bar{E}_j = \bar{\Omega}^r$ for all $j < j_{\max}$ with

$$\begin{aligned} m &= \pi r^2 + (j_{\max}-1)|\Omega^r| \\ &= (j_{\max}-1)\left(1-\left(4-\frac{j_{\max}}{j_{\max}-1}\pi\right)r^2\right) \quad r \in \big(0, \tfrac{1}{2}\big). \end{aligned}$$

It follows

$$r_B(j_{\max}) := \sqrt{\frac{j_{\max}-1-m}{(4-\pi)(j_{\max}-1)-\pi}} > r_A(j_{\max}-1)$$

and $\sum_{j=1}^{j_{\max}} P(E_j) = F_B(j_{\max})$, where

$$\begin{aligned} F_B(x) &:= (x-1)P(\Omega^{r_B(x)}) + 2\pi r_B(x) \\ &= 4(x-1) - 2\sqrt{4-\pi}\,\sqrt{\Big(x-1-\frac{\pi}{4-\pi}\Big)(x-1-m)}. \end{aligned}$$

Notice that the derivative

$$F_B'(x) = 4 - \sqrt{4-\pi}\,\frac{2(x-1)-m-\dfrac{\pi}{4-\pi}}{\sqrt{\Big(x-1-\dfrac{\pi}{4-\pi}\Big)(x-1-m)}}\,.$$

Assuming $x > 4/(4-\pi)$, we then have that F_B is increasing for

$$x-1 > \frac{2+\sqrt{\pi}}{2\sqrt{\pi}}m - \frac{\sqrt{\pi}}{2(2+\sqrt{\pi})}$$

and decreasing otherwise, so that

$$j_{\max} \in \{j^B, j^B+1\}, \quad \text{where } j^B := \left\lfloor \frac{2+\sqrt{\pi}}{2\sqrt{\pi}}m + \frac{4+\sqrt{\pi}}{2(2+\sqrt{\pi})} \right\rfloor \tag{5-3}$$

as soon as $j_{\max} \geq 5$.

Observe that, if $m < 5\pi/4$, we have $j_{\max} \leq 4$ and there is only one choice for the minimizers E_j. In particular, we are in Case A or Case B depending on the value of m. On the other hand, when $m > 5\pi/4$, we have to determine which one between Cases A and B is energetically more convenient. However, since $\min\{F_B(j^B), F_B(j^B+1)\} > \min\{F_A(j^A), F_A(j^A+1)\}$ for all $m > 5\pi/4$, it follows that Case B can never occur as a minimizer, thus implying the thesis. □

It is worth remarking that $2\pi/(2+\pi)$ is the volume of the (unique) Cheeger set C_Ω of Ω, so that Proposition 5.1 implies that the functions $u_m/j_{\max}$ converge to the characteristic function of C_Ω, according to the Remark 3.2.

5B. *A square with a crystalline norm.* Now we set $\Omega = [0, 1]^2$ as above and $\varphi(\nu) = \max\{|\nu_1|, |\nu_2|\}$. Notice that φ is a crystalline norm with Wulff shape

$$W_\varphi = \{(x, y) \in \mathbb{R}^2 : |x| + |y| \leq 1\}.$$

As before, we are able to characterize completely the minimizers of (1-1).

Proposition 5.2. *Let Ω and φ be as above.*

(i) *If $m \in \left(0, \frac{1}{2}\right]$, we have $j_{\max} = 1$ and $\bar{E}_1 = \bar{W}_r(x_0) \subset \bar{\Omega}$, with $r = \sqrt{m/2}$.*

(ii) *If $m \in \left[\frac{1}{2}, 1\right)$, we have $j_{\max} = 1$ and $\bar{E}_1 = \bar{\Omega}^r$, with $r = \sqrt{(1-m)/2}$.*

(iii) *If $m = 1$, then either $j_{\max} = 1$ and $\bar{E}_1 = \Omega$, or $j_{\max} = 2$, $\bar{E}_1 = \bar{\Omega}^r$ and $\bar{E}_2 = \bar{W}_r(x_0) \subset \Omega$, with $r \in \left(0, \frac{1}{2}\right]$.*

(iv) *If $m > 1$, we have*

$$j_{\max} \in \left\{ \left\lfloor \frac{1+\sqrt{2}}{2}m \right\rfloor, \left\lfloor \frac{1+\sqrt{2}}{2}m \right\rfloor + 1 \right\} \tag{5-4}$$

and $\bar{E}_j = \bar{\Omega}^r$ for $j \leq j_{\max}$, with $r = \sqrt{(1-m/j_{\max})/2}$.

Proof. The proof is similar to that of Proposition 5.1.

If $m \leq \frac{1}{2}$, then $j_{\max} = 1$ and $\bar{E}_1 = \bar{W}_r(x_0) \subset \Omega$, since the (rescaled) Wulff shape solves the isoperimetric problem. By Theorem 4.10, for all $m \geq \frac{1}{2}$ we have one of the following two possibilities.

Case A. $\bar{E}_j = \bar{\Omega}^r$ for all $j \le j_{\max}$ with

$$m = j_{\max}|\Omega^r| = j_{\max}(1-2r^2), \quad r \in \left[0, \tfrac{1}{2}\right],$$

which gives

$$r = \frac{1}{\sqrt{2}}\sqrt{1-\frac{m}{j_{\max}}},$$

and $\sum_{j=1}^{j_{\max}} P_\varphi(E_j) = F_A(j_{\max})$, where

$$F_A(x) = x(4-4r) = 4x - 4\sqrt{\frac{x^2 - mx}{2}}\,.$$

Since the function F_A is increasing for $x > (1+\sqrt{2})m/2$ and decreasing for $m \le x < (1+\sqrt{2})m/2$, we have

$$j_{\max} \in \{j^A, j^A+1\}, \quad \text{where } j^A := \left\lfloor \frac{1+\sqrt{2}}{2} m \right\rfloor.$$

Case B. $\bar{E}_{j_{\max}} = \bar{W}_r(x_0) \subset \bar{\Omega}$ and $\bar{E}_j = \bar{\Omega}^r$ for all $j < j_{\max}$, with $r \in \left(0, \tfrac{1}{2}\right]$ and

$$m = 2r^2 + (j_{\max}-1)\left(1-2r^2\right),$$

and hence $m \ge 1$ because $j_{\max} \ge 2$ and $r \le \frac{1}{2}$.

If $m = 1$ then $j_{\max} = 2$ and we can take any $r \in \left(0, \tfrac{1}{2}\right]$.

If $m > 1$ then $j_{\max} \ge m+1$ and we get

$$r = \sqrt{\frac{j_{\max} - m - 1}{2(j_{\max}-2)}}$$

and $\sum_{j=1}^{j_{\max}} P_\varphi(E_j) = F_B(j_{\max})$, where

$$F_B(x) = 4(x-1) - 4(x-2)\sqrt{\frac{x-m-1}{2(x-2)}}\,.$$

Since the function F_B is increasing for $x > (1+\sqrt{2})m/2 + (3-\sqrt{2})/2$ and decreasing otherwise, we have

$$j_{\max} \in \{j^B, j^B+1\}, \quad \text{where } j^B := \left\lfloor \frac{1+\sqrt{2}}{2} m + \frac{3-\sqrt{2}}{2} \right\rfloor.$$

As in the proof of Proposition 5.1, when $m > 1$ we have to determine which of Cases A and B is energetically more convenient. Since $\min\{F_B(j^B), F_B(j^B+1)\} > \min\{F_A(j^A), F_A(j^A+1)\}$ (by a calculation as in the example with the Euclidean norm), it follows that Case B can never occur. □

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BRAUER'S HEIGHT ZERO CONJECTURE FOR METACYCLIC DEFECT GROUPS

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We prove that Brauer's height zero conjecture holds for p-blocks of finite groups with metacyclic defect groups. If the defect group is nonabelian and contains a cyclic maximal subgroup, we obtain the distribution into p-conjugate and p-rational irreducible characters. The Alperin–McKay conjecture then follows provided $p = 3$. Along the way we verify a few other conjectures. Finally we consider more closely the extraspecial defect group of order p^3 and exponent p^2 for an odd prime. Here for blocks with inertial index 2 we prove the Galois–Alperin–McKay conjecture by computing $k_0(B)$. Then for $p \le 11$ also Alperin's weight conjecture follows. This improves results of Gao (2012), Holloway, Koshitani, Kunugi (2010) and Hendren (2005).

1. Introduction

An important task in representation theory is the determination of the invariants of a block of a finite group when its defect group is given. For a p-block B of a finite group G we are interested in the number $k(B)$ of irreducible ordinary characters and the number $l(B)$ of irreducible Brauer characters of B. Let D be a defect group of B. Then the irreducible ordinary characters split into $k_i(B)$ characters of height $i \ge 0$. Here the *height* $h(\chi)$ of a character χ in B is defined by $\chi(1)_p = p^{h(\chi)}|G : D|_p$.

If $p = 2$, the block invariants for several defect groups were obtained in the last years. In particular the invariants are known if the defect group is metacyclic; see [Sambale 2012]. However, for odd primes p the situation is more complicated. Here even in the smallest interesting example of an elementary abelian defect group of order 9, the block invariants are not determined completely; see [Kiyota 1984]. Nevertheless Brauer's $k(B)$-conjecture and Olsson's conjecture were proved for all blocks with metacyclic defect groups in [Gao 2011; Yang 2011]. Following these lines, we obtain in this paper that also Brauer's height zero conjecture is fulfilled for these blocks. The proof uses the notion of lower defect groups and inequalities from [Héthelyi et al. 2012]. Moreover, if G is p-solvable, we obtain the algebra

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structure of B with respect to an algebraically closed field of characteristic p. If one restricts to blocks with maximal defect, the precise invariants were determined in [Gao 2012]. We can confirm at least some of these values. For principal blocks there is even a perfect isometry between B and its Brauer correspondent in $\mathrm{N}_G(D)$ by the main theorem of [Horimoto and Watanabe 2012].

In the second part of the paper we consider the (unique) nonabelian p-group with a cyclic subgroup of index p as a special case. Here the difference $k(B)-l(B)$ is known from [Gao and Zeng 2011]. We confirm this result and derive the distribution into p-conjugate and p-rational irreducible characters. We also show that $k_i(B)=0$ for $i\ge 2$. This implies various numerical conjectures. Moreover, it turns out that the Alperin–McKay conjecture holds provided $p=3$. This is established by computing $k_0(B)$. Here in the case $|D|\le 3^4$ we even obtain the other block invariants $k(B)$, $k_i(B)$ and $l(B)$, which leads to a proof of Alperin's weight conjecture in this case. This generalizes some results from [Holloway et al. 2010], where these blocks were considered under additional assumptions on G.

The smallest nonabelian example for a metacyclic defect group for an odd prime is the extraspecial defect group p_-^{1+2} of order p^3 and exponent p^2. For this special case Hendren [2005] obtained some inequalities on the invariants. In [Schulz 1980] one can find results for these blocks under the hypothesis that G is p-solvable. The present paper improves both of these works. In particular if the inertial index $e(B)$ of B is 2, we verify the Galois–Alperin–McKay conjecture (see [Isaacs and Navarro 2002]), a refinement of the Alperin–McKay conjecture. As a consequence, for $p\le 11$ we are able to determine the block invariants $k(B)$, $k_i(B)$ and $l(B)$ completely without any restrictions on G. Then we use the opportunity to prove several conjectures including Alperin's weight conjecture for this special case. As far as I know, these are the first nontrivial examples of Alperin's conjecture for a nonabelian defect group for an odd prime.

2. Brauer's height zero conjecture

Let B be a p-block of a finite group G with metacyclic defect group D. Since for $p=2$ the block invariants are known and most of the conjectures are verified (see [Sambale 2012]), we assume $p>2$ for the rest of the paper. If D is abelian, Brauer's height zero conjecture is true by [Kessar and Malle 2011] (using the classification). Hence, we can also assume that D is nonabelian. Then we have to distinguish whether D splits or not. In the nonsplit case the main theorem of [Gao 2011] says that B is nilpotent. Again, the height zero conjecture holds. Thus, let us assume that D is a nonabelian split metacyclic group. Then D has a presentation of the form

$$D=\langle x,y\mid x^{p^m}=y^{p^n}=1,\ yxy^{-1}=x^{1+p^l}\rangle \tag{2-1}$$

with $0 < l < m$ and $m - l \le n$. Many of the results in this paper will depend on these parameters. Assume that the map $x \to x^{\alpha_1}$ generates an automorphism of $\langle x \rangle$ of order $p - 1$. Then by Theorem 2.5 in [Gao 2011], the map α with $\alpha(x) = x^{\alpha_1}$ and $\alpha(y) = y$ is an automorphism of D of order $p - 1$. By the Schur–Zassenhaus theorem applied to $\mathrm{O}_p(\mathrm{Aut}(D)) \trianglelefteq \mathrm{Aut}(D)$, $\langle \alpha \rangle$ is unique up to conjugation in $\mathrm{Aut}(D)$. In particular the isomorphism type of the semidirect product $D \rtimes \langle \alpha \rangle$ does not depend on the choice of α. We denote the inertial quotient of B by $I(B)$; in particular $e(B) = |I(B)|$. It is known that $I(B)$ is a p'-subgroup of the outer automorphism group $\mathrm{Out}(D)$. Hence, we may assume that $I(B) \le \langle \alpha \rangle$. Sometimes we regard α as an element of $\mathrm{N}_G(D)$ by a slight abuse of notation.

We fix a Brauer correspondent b_D of B in $\mathrm{C}_G(D)$. For an element $u \in D$ we have a B-subsection $(u, b_u) \in (D, b_D)$. Here b_u is a Brauer correspondent of B in $\mathrm{C}_G(u)$. Let $\mathcal{F}$ be the fusion system of B. Then by Proposition 5.4 in [Stancu 2006], $\mathcal{F}$ is controlled. In particular $\mathrm{C}_D(u)$ is a defect group of b_u; see Theorem 2.4(ii) in [Linckelmann 2006]. In case $l(b_u) = 1$ we denote the unique irreducible Brauer character of b_u by φ_u. Then the generalized decomposition numbers d^u_{ij} form a vector $d^u := (d^u_{\chi\varphi_u} : \chi \in \mathrm{Irr}(B))$. More generally we have subpairs $(R, b_R) \le (D, b_D)$ for every subgroup $R \le D$. In particular $I(B) = \mathrm{N}_G(D, b_D)/D\,\mathrm{C}_G(D)$. For $r \in \mathbb{N}$ we set $\zeta_r := e^{2\pi i/r}$.

Proposition 2.1. *Let B be a p-block of a finite group with a nonabelian metacyclic defect group for an odd prime p. Then $l(B) \ge e(B)$.*

Proof. We use the notation above. If D is nonsplit, we have $e(B) = l(B) = 1$. Thus, assume that D is given by (2-1). Let $m(d)$ be the multiplicity of $d \in \mathbb{N}$ as an elementary divisor of the Cartan matrix of B. It is well-known that $m(p^{m+n}) = m(|D|) = 1$. Hence, it suffices to show $m(p^n) \ge e(B) - 1$.

By Corollary V.10.12 in [Feit 1982], we have

$$m(p^n) = \sum_{R \in \mathcal{R}} m_B^{(1)}(R)$$

where $\mathcal{R}$ is a set of representatives for the G-conjugacy classes of subgroups of G of order p^n. After combining this with the formula (2S) of [Broué and Olsson 1986] we get

$$m(p^n) = \sum_{(R, b_R) \in \mathcal{R}'} m_B^{(1)}(R, b_R)$$

where $\mathcal{R}'$ is a set of representatives for the G-conjugacy classes of B-subpairs (R, b_R) such that R has order p^n.

Thus, it suffices to prove $m_B^{(1)}(\langle y \rangle, b_y) \ge e(B) - 1$. By (2Q) [ibid.] we have $m_B^{(1)}(\langle y \rangle, b_y) = m_{B_y}^{(1)}(\langle y \rangle)$ where $B_y := b_y^{\mathrm{N}_G(\langle y \rangle, b_y)}$. It is easy to see that $\mathrm{N}_D(\langle y \rangle) = \mathrm{C}_D(y)$, because $D/\langle x \rangle \cong \langle y \rangle$ is abelian. Since B is controlled and $I(B)$ acts trivially on $\langle y\rangle$, we get $\mathrm{N}_G(\langle y\rangle, b_y) = \mathrm{C}_G(y)$ and $B_y = b_y$. Thus, it remains to prove $m_{b_y}^{(1)}(\langle y\rangle) \geq e(B) - 1$. Let $x^i y^j \in \mathrm{C}_D(y) \setminus \langle y\rangle$. Then $x^i \in \mathrm{Z}(D)$. Hence, by Theorem 2.3(2)(iii) in [Gao 2011] we have $\mathrm{C}_D(y) = \mathrm{Z}(D)\langle y\rangle = \langle x^{p^{m-l}}\rangle \times \langle y\rangle$. By Proposition 2.1(b) in [An 2011], also b_y is a controlled block. Observe that $(\mathrm{C}_D(y), b_{\mathrm{C}_D(y)})$ is a maximal b_y-subpair. Since $\alpha \in \mathrm{N}_{\mathrm{C}_G(y)}(\mathrm{C}_D(y), b_{\mathrm{C}_D(y)})$, we see that $e(b_y) = e(B)$.

As usual, b_y dominates a block of $\mathrm{C}_G(y)/\langle y\rangle$ with cyclic defect group

$$\mathrm{C}_D(y)/\langle y\rangle \cong \langle x^{p^{m-l}}\rangle.$$

Hence, p^n occurs as elementary divisor of the Cartan matrix of b_y with multiplicity $e(b_y) - 1 = e(B) - 1$ (see [Dade 1966; Fujii 1980]). By Corollary 3.7 in [Olsson 1980] every lower defect group of b_y must contain $\langle y\rangle$. This implies $m_{b_y}^{(1)}(\langle y\rangle) = e(B) - 1$. □

Since Alperin's weight conjecture would imply that $l(B) = e(B)$, it is reasonable that $\langle y\rangle$ and D are the only (nontrivial) lower defect groups of D up to conjugation. However, we do not prove this. We remark that Proposition 2.1 would be false for abelian metacyclic defect groups; see [Kiyota 1984].

We introduce a general lemma.

Lemma 2.2. *Let B be a controlled block of a finite group G with Brauer correspondent b_D in $\mathrm{C}_G(D)$. If $(u, b_u) \in (D, b_D)$ is a subsection such that*

$$\mathrm{N}_G(D, b_D) \cap \mathrm{C}_G(u) \subseteq \mathrm{C}_D(u)\,\mathrm{C}_G(\mathrm{C}_D(u)),$$

then $e(b_u) = l(b_u) = 1$.

Proof. By Proposition 2.1 in [An 2011], b_u is a controlled block with Sylow b_u-subpair $(\mathrm{C}_D(u), b_{\mathrm{C}_D(u)})$. Hence,

$$e(b_u) = |\mathrm{N}_{\mathrm{C}_G(u)}(\mathrm{C}_D(u), b_{\mathrm{C}_D(u)})/\,\mathrm{C}_D(u)\,\mathrm{C}_G(\mathrm{C}_D(u))|.$$

Every $\mathcal{F}$-automorphism on $\mathrm{C}_D(u)$ is a restriction from $\mathrm{Aut}_{\mathcal{F}}(D)$. This gives

$$\mathrm{N}_{\mathrm{C}_G(u)}(\mathrm{C}_D(u), b_{\mathrm{C}_D(u)}) \subseteq (\mathrm{N}_G(D, b_D) \cap \mathrm{C}_G(u))\,\mathrm{C}_G(\mathrm{C}_D(u)) \subseteq \mathrm{C}_D(u)\,\mathrm{C}_G(\mathrm{C}_D(u)).$$

Thus, we have $e(b_u) = 1$. Since b_u is controlled, it follows that b_u is nilpotent and $l(b_u) = 1$. □

Theorem 2.3. *Let B be a p-block of a finite group with a nonabelian split metacyclic defect group for an odd prime p. Then*

$$k(B) \geq \left(\frac{p^l + p^{l-1} - p^{2l-m-1} - 1}{e(B)} + e(B)\right)p^n.$$

Proof. If $e(B) = 1$, the block B is nilpotent. Then the claim follows from Theorem 2.3(2)(iii) in [Gao 2011] and Remark 2.4 in [Héthelyi and Külshammer 2011]. So, assume $e(B) > 1$. The idea is to use Brauer's formula [Nagao and Tsushima 1989, Theorem 5.9.4]. Let $u \in D$. Then b_u has metacyclic defect group $\mathrm{C}_D(u)$. Assume first that $u \in \mathrm{C}_D(I(B))$. Since $I(B)$ acts freely on $\langle x\rangle$, we see that $u \in \langle y\rangle$. As in the proof of Proposition 2.1 (for $u = y$), we get $e(b_u) = e(B)$. If $\mathrm{C}_D(u)$ is nonabelian, Proposition 2.1 implies $l(b_u) \geq e(B)$. Now suppose that $\mathrm{C}_D(u)$ is abelian. Since $y \in \mathrm{C}_D(u)$, it follows that $\mathrm{C}_D(u) = \mathrm{C}_D(y) = \langle x^{p^{m-l}}\rangle \times \langle y\rangle$. Thus, by Theorem 1 in [Watanabe 1991] we have $l(b_u) = l(b_y) = e(B)$.

Now assume that u is not $\mathcal{F}$-conjugate to an element of $\mathrm{C}_D(I(B)) = \langle y\rangle$. We are going to show that $e(b_u) = l(b_u) = 1$ by using Lemma 2.2. For this let $\gamma \in (\mathrm{N}_G(D, b_D) \cap \mathrm{C}_G(u)) \setminus \mathrm{C}_D(u)\,\mathrm{C}_G(\mathrm{C}_D(u))$ by way of contradiction. Since $D\,\mathrm{C}_G(D) \cap \mathrm{C}_G(u) = \mathrm{C}_G(D)\,\mathrm{C}_D(u) \subseteq \mathrm{C}_D(u)\,\mathrm{C}_G(\mathrm{C}_D(u))$, γ is not a p-element. Hence, after replacing γ by a suitable power if necessary, we may assume that γ is a nontrivial p'-element modulo $\mathrm{C}_G(D)$. By the Schur–Zassenhaus Theorem (in our special situation one could use more elementary theorems) applied to $D/\mathrm{Z}(D) \trianglelefteq \mathrm{Aut}_{\mathcal{F}}(D)$, γ is D-conjugate to a nontrivial power of α (modulo $\mathrm{C}_G(D)$). But then u is D-conjugate to an element of $\langle y\rangle$. Contradiction. Hence, we have $\mathrm{N}_G(D, b_D) \cap \mathrm{C}_G(u) \subseteq \mathrm{C}_D(u)\,\mathrm{C}_G(\mathrm{C}_D(u))$ and $e(b_u) = l(b_u) = 1$ by Lemma 2.2.

It remains to determine a set $\mathcal{R}$ of representatives for the $\mathcal{F}$-conjugacy classes of D; see Lemma 2.4 in [Sambale 2011a]. Since the powers of y are pairwise nonconjugate in $\mathcal{F}$, we get p^n subsections (u, b_u) such that $l(b_u) \geq e(B)$ (including the trivial subsection).

By Theorem 2.3(2)(iii) in [Gao 2011] we have $|D'| = p^{m-l}$ and $|\mathrm{Z}(D)| = p^{n-m+2l}$. Hence, Remark 2.4 in [Héthelyi and Külshammer 2011] implies that D has precisely $p^{n-m+2l-1}(p^{m-l+1} + p^{m-l} - 1)$ conjugacy classes. Let C be one of these classes that do not intersect $\langle y\rangle$. Assume $\alpha^i(C) = C$ for some $i \in \mathbb{Z}$ such that $\alpha^i \neq 1$. Then there are elements $u \in C$ and $w \in D$ such that $\alpha^i(u) = wuw^{-1}$. Hence $\gamma := w^{-1}\alpha^i \in \mathrm{N}_G(D, b_D) \cap \mathrm{C}_G(u)$. Since γ is not a p-element, we get a contradiction as above. This shows that no nontrivial power of α can fix C as a set. Thus, all these conjugacy classes split in

$$\frac{p^{m-l+1} + p^{m-l} - p^{m-2l+1} - 1}{e(B)}\,p^{n-m+2l-1}$$

orbits of length $e(B)$ under the action of $I(B)$. For every element u in one of these classes we have $l(b_u) = 1$ as above. This gives

$$k(B) = \sum_{u \in \mathcal{R}} l(b_u) \geq e(B)p^n + \frac{p^l + p^{l-1} - p^{2l-m-1} - 1}{e(B)}\,p^n. \qquad \square$$

The results for blocks with maximal defect in [Gao 2012] show that the bound in Theorem 2.3 is sharp (after evaluating the geometric series [ibid., Theorem 1.1]).

Theorem 2.4. *Let B be a p-block of a finite group with a nonabelian split metacyclic defect group D for an odd prime p. Then*

$$k_0(B) \le \left(\frac{p^l-1}{e(B)} + e(B)\right)p^n \le p^{n+l} = |D:D'|,$$

$$\sum_{i=0}^{\infty} p^{2i} k_i(B) \le \left(\frac{p^l-1}{e(B)} + e(B)\right)p^{n+m-l} \le p^{n+m} = |D|,$$

$$k_i(B) = 0 \quad \textit{for } i > \min\left\{2(m-l), \frac{m+n-1}{2}\right\}.$$

In particular $k_0(B) < k(B)$; that is, Brauer's height zero conjecture holds for B.

Proof. We consider the subsection (y, b_y). We have already seen that $l(b_y) = e(B)$ and $C_D(y)/\langle y\rangle$ is cyclic of order p^l. Hence, Proposition 2.5(i) in [Héthelyi et al. 2012] implies the first inequality. For the second we consider $u := x^{p^{m-l}} \in Z(D)$. Since u is not D-conjugate to a power of y, the proof of Theorem 2.3 gives $l(b_u) = 1$. Moreover, $|\mathrm{Aut}_{\mathcal{F}}(\langle u\rangle)| = e(B)$. Thus, Theorem 4.10 in the same reference shows the second claim. Since $k_0(B) > 0$, it follows at once that $k_i(B) = 0$ for $i > (n+m-1)/2$. On the other hand Corollary V.9.10 in [Feit 1982] implies $k_i(B) = 0$ for $i > 2(m-l)$.

Now we discuss the claim $k_0(B) < k(B)$. By Theorem 2.3 it suffices to show

$$\left(\frac{p^l-1}{e(B)} + e(B)\right)p^n < \left(\frac{p^l+p^{l-1}-p^{2l-m-1}-1}{e(B)} + e(B)\right)p^n.$$

This reduces to $l < m$, one of our hypotheses. □

Again for blocks with maximal defect, the bound on $k_0(B)$ in Theorem 2.4 is sharp; see [Gao 2012]. On the other hand the bound on the height of the irreducible characters is probably not sharp in general.

Corollary 2.5. *Let B be a p-block of a finite group with a nonabelian split metacyclic defect group for an odd prime p. Then*

$$k(B) \le \left(\frac{p^l-1}{e(B)} + e(B)\right)(p^{n+m-l-2} + p^n - p^{n-2}).$$

Proof. In view of Theorem 2.4, the number $k(B)$ is maximal if $k_0(B)$ is maximal and $k_1(B) = k(B) - k_0(B)$. Then

$$k_1(B) \le \left(\frac{p^l-1}{e(B)} + e(B)\right)(p^{n+m-l-2} - p^{n-2})$$

and the result follows. □

Apart from a special case covered in [Schulz 1980], it seems that there are no results about B in the literature for p-solvable groups. We take the opportunity to give such a result, which also holds in a more general situation.

Theorem 2.6. *Let B be a controlled block of a p-solvable group over an algebraically closed field F of characteristic p. If $I(B)$ is cyclic, then B is Morita equivalent to the group algebra $F[D \rtimes I(B)]$ where D is the defect group of B. In particular $k(B) = k(D \rtimes I(B))$ and $l(B) = e(B)$.*

Proof. Let $P \trianglelefteq D$, H and $\overline{H}$ as in Theorem A in [Külshammer 1981]. As before let $\mathcal{F}$ be the fusion system of B. Then parts (iii) and (v) of that theorem imply that P is $\mathcal{F}$-radical. Moreover, the Hall–Higman lemma gives

$$\mathrm{C}_D(P)\,\mathrm{O}_{p'}(H)/\,\mathrm{O}_{p'}(H) \subseteq \mathrm{C}_{\overline{H}}(\mathrm{O}_p(\overline{H})) \subseteq \mathrm{O}_p(\overline{H}) = P\,\mathrm{O}_{p'}(H)/\,\mathrm{O}_{p'}(H).$$

Since P is normal in H, we have $\mathrm{C}_D(P) \subseteq P$. In particular P is also $\mathcal{F}$-centric. Now let $g \in \mathrm{N}_G(P, b_P)$. Since B is controlled, there exists a $h \in \mathrm{N}_G(D, b_D)$ such that $h^{-1}g \in \mathrm{C}_G(P)$. Hence, $g \in \mathrm{N}_G(D, b_D)\,\mathrm{C}_G(P)$ and

$$D\,\mathrm{C}_G(P)/P\,\mathrm{C}_G(P) \trianglelefteq \mathrm{N}_G(P, b_P)/P\,\mathrm{C}_G(P).$$

Since P is $\mathcal{F}$-radical, it follows that $P\,\mathrm{C}_G(P) = D\,\mathrm{C}_G(P)$. Now $\mathrm{C}_D(P) = \mathrm{Z}(P)$ implies $P = D$. Hence, $\overline{H} \cong D \rtimes I(B)$. Observe at this point that $I(B)$ can be regarded as a subgroup of $\mathrm{Aut}(D)$ by the Schur–Zassenhaus Theorem. Moreover, this subgroup is unique up to conjugation in $\mathrm{Aut}(D)$. Hence, the isomorphism type of $D \rtimes I(B)$ is uniquely determined. Since $I(B)$ is cyclic, the 2-cocycle γ appearing in [ibid.] is trivial. Thus, the result follows from Theorem A(iv). □

Let us consider the opposite situation where G is quasisimple. Then the main theorem of [An 2011] tells us that B cannot have nonabelian metacyclic defect groups. Thus, in order to settle the general case it would be sufficient to reduce the situation to quasisimple groups.

For the convenience of the reader we collect the results about metacyclic defect groups.

Theorem 2.7. *Let B be a block of a finite group with metacyclic defect group. Then Brauer's $k(B)$-conjecture, Brauer's height zero conjecture and Olsson's conjecture are satisfied for B.*

In the next sections we make restrictions on the parameters p, m, n and l in order to prove stronger results.

3. The group $M_{p^{m+1}}$

Let $n = 1$. Then $m = l + 1$ and D is the unique nonabelian group of order p^{m+1} with exponent p^m. We denote this group by $M_{p^{m+1}}$ (compare with [Holloway et al.

2010]). It follows from Theorem 2.4 that $k_i(B) = 0$ for $i > 2$. We will see that the same holds for $i = 2$.

Theorem 3.1. *Let B be a block of a finite group with defect group $M_{p^{m+1}}$ where p is an odd prime and $m \geq 2$. Then $k_i(B) = 0$ for $i \geq 2$. In particular the following conjectures are satisfied for B:*

- *Eaton's conjecture* [2003],
- *Eaton–Moretó conjecture* [2011],
- *Robinson's conjecture* [1996],
- *Malle–Navarro conjecture* [2006].

Proof. Assume $k_2(B) > 0$. We are going to show that the following inequality from Theorem 2.4 is not satisfied:

$$k_0(B) + p^2 k_1(B) + p^4 k_2(B) \leq \left(\frac{p^{m-1}-1}{e(B)} + e(B)\right) p^2. \tag{3-1}$$

In order to do so, we may assume $k_2(B) = 1$. Moreover, taking Theorem 2.3 into account, we assume

$$k_0(B) = \left(\frac{p^{m-1}-1}{e(B)} + e(B)\right) p, \qquad k_1(B) = \frac{p^{m-1}-p^{m-2}}{e(B)} - 1.$$

Now (3-1) gives the contradiction

$$p^4 \leq (e(B)+1)p^2 - \frac{p^2-p}{e(B)} - e(B)p \leq p^3.$$

Hence, $k_2(B) = 0$. In particular Eaton's conjecture is in fact equivalent to Brauer's $k(B)$-conjecture and Olsson's conjecture. Also the Eaton–Moretó conjecture is trivially satisfied. Robinson's conjecture, stated in the introduction of [Robinson 1996], reads: If D is nonabelian, then $p^{h(\chi)} < |D : \mathrm{Z}(D)|$ for all $\chi \in \mathrm{Irr}(B)$. This is true in our case. It remains to verify the Malle–Navarro conjecture. For this, observe

$$\frac{k(B)}{l(B)} \leq \left(\frac{p^{m-1}-1}{e(B)^2} + 1\right)(p+1-p^{-1}) \leq p^m + p^{m-1} - p^{m-2} = k(D)$$

by Corollary 2.5 and Remark 2.4 in [Héthelyi and Külshammer 2011]. Now we establish a lower bound for $k_0(B)$. From Theorem 2.4 we get

$$k_1(B) \leq \frac{p^{m-1}-1}{e(B)} + e(B) - 1.$$

This gives

$$k_0(B) = k(B) - k_1(B) \geq \frac{p^m - p^{m-2} - p + 1}{e(B)} + e(B)(p-1) + 1. \tag{3-2}$$

The other inequality of the Malle–Navarro conjecture reads

$$k(B) \le k_0(B)k(D') = k_0(B)p.$$

After a calculation using (3-2) and Corollary 2.5, this boils down to

$$p^m + 2p^{m-1} + p^2 \le p^{m+1} + 2p + 1,$$

which is obviously true. □

The argument in the proof of Theorem 3.1 can also be used to improve the general bound for the heights in Theorem 2.4 at least in some cases. However, it does not suffice to prove $k_i(B) = 0$ for $i > m - l$ (which is conjectured). The next theorem also appears in [Gao and Zeng 2011].

Theorem 3.2. *Let B be a block of a finite group with defect group $M_{p^{m+1}}$ where p is an odd prime and $m \ge 2$. Then*

$$k(B) - l(B) = \frac{p^m + p^{m-1} - p^{m-2} - p}{e(B)} + e(B)(p-1).$$

Proof. By the proof of Theorem 2.3, it suffices to show $l(b_u) = e(B)$ for $1 \ne u \in \langle y \rangle$. Since $n = 1$, we have $\mathrm{C}_D(u) = \mathrm{Z}(D)\langle y \rangle = \langle x^p \rangle \times \langle y \rangle$. Thus, by Theorem 1 in [Watanabe 1991] we have $l(b_u) = e(B)$. □

This result leads to the distribution of the irreducible characters into p-conjugate and p-rational characters. We need this later for the study of decomposition numbers. We denote the Galois group of $\mathbb{Q}(\zeta_{|G|})|\mathbb{Q}(\zeta_{|G|_{p'}})$ by $\mathcal{G}$. Then restriction gives an isomorphism $\mathcal{G} \cong \mathrm{Gal}(\mathbb{Q}(\zeta_{|G|_p})|\mathbb{Q})$. In particular since p is odd, $\mathcal{G}$ is cyclic of order $|G|_p(p-1)/p$. We often identify both groups.

Proposition 3.3. *Let B be a block of a finite group with defect group $M_{p^{m+1}}$ where p is an odd prime and $m \ge 2$. Then the ordinary irreducible characters of B split into orbits of p-conjugate characters of the following lengths*:

- *two orbits of length $p^{m-2}(p-1)/e(B)$,*
- *one orbit of length $p^i(p-1)/e(B)$ for every $i = 0, \dots, m-3$,*
- *$(p-1)/e(B) + e(B)$ orbits of length $p-1$,*
- *$(p-1)/e(B)$ orbits of length $p^i(p-1)$ for every $i = 1, \dots, m-2$,*
- *$l(B)$ ($\ge e(B)$) p-rational characters.*

Proof. By Brauer's permutation lemma (Lemma IV.6.10 in [Feit 1982]) it suffices to reveal the orbits of $\mathcal{G}$ on the columns of the generalized decomposition matrix. The ordinary decomposition numbers are all integral, so the action on these columns is trivial. This gives $l(B)$ p-rational characters. Now we consider a set of representatives for the B-subsections as in Theorem 2.3.

There are $(p^{m-1}-1)/e(B)$ nontrivial major subsections (z, b_z). All of them satisfy $l(b_z)=1$ and $\mathrm{Aut}_{\mathcal{F}}(\langle z\rangle)=I(B)$. So these columns form $m-1$ orbits of lengths $p^{m-2}(p-1)/e(B)$, $p^{m-3}(p-1)/e(B), \dots, (p-1)/e(B)$, respectively. Now for $u\in\langle x\rangle\setminus \mathrm{Z}(D)$ we have $l(b_u)=1$ and $\mathrm{Aut}_{\mathcal{F}}(\langle u\rangle)=\langle y\rangle\times I(B)$. This gives another orbit of length $p^{m-2}(p-1)/e(B)$. Next let $1\neq u\in\langle y\rangle$. Then $l(b_u)=e(B)$ and $\mathrm{Aut}_{\mathcal{F}}(\langle u\rangle)=1$. Hence, we get $e(B)$ orbits of length $p-1$ each.

Finally let $u:=x^iy^j\in D\setminus\langle x\rangle$ such that u is not conjugate to an element of $\langle y\rangle$. As in the proof of Theorem 2.3, $p^l\nmid i$ holds. Since $|D'|=p$, we have $(x^iy^j)^p=x^{ip}$ by Hilfssatz III.1.3 in [Huppert 1967]. In particular $D'\subseteq\langle u\rangle$ and $\mathrm{N}_D(\langle u\rangle)=D$. Moreover, $|D:\mathrm{Z}(D)|=p^2$ and $|\mathrm{Aut}_D(\langle u\rangle)|=p$. Since $I(B)$ acts trivially on $D/\langle x\rangle\cong\langle y\rangle$, we see that $|\mathrm{Aut}_{\mathcal{F}}(\langle u\rangle)|=p$. The calculation above shows that u has order $p^{m-\log i}$. We have exactly $p^{m-\log i-1}(p-1)^2$ such elements of order $p^{m-\log i}$. These split in $p^{m-\log i-2}(p-1)^2/e(B)$ conjugacy classes. In particular we get $(p-1)/e(B)$ orbits of length $p^{m-i-2}(p-1)$ each for every $i=0,\dots,l-1=m-2$. □

It should be emphasized that the proof of Proposition 3.3 heavily relies on the fact $\mathrm{Aut}_{\mathcal{F}}(\langle u\rangle)=1$ whenever $l(b_u)>1$. Since otherwise it would be not clear, whether some Brauer characters of b_u are conjugate under $\mathrm{N}_G(\langle u\rangle, b_u)$. In other words, generally the knowledge of $k(B)-l(B)$ does not provide the distribution into p-conjugate and p-rational characters.

For $p=3$ the inequalities Theorem 2.3 and Corollary 2.5 almost coincide. This allows us to prove the Alperin–McKay conjecture.

Theorem 3.4. *Let B be a nonnilpotent block of a finite group with defect group $M_{3^{m+1}}$ where $m\geq 2$. Then*

$$e(B)=2,\qquad k_0(B)=\frac{3^m+9}{2},$$
$$k_1(B)\in\{3^{m-2},3^{m-2}+1\},\qquad k_i(B)=0 \quad \text{for } i\geq 2,$$
$$k(B)\in\left\{\frac{11\cdot 3^{m-2}+9}{2},\frac{11\cdot 3^{m-2}+11}{2}\right\},\qquad l(B)\in\{2,3\}.$$

In particular the Alperin–McKay conjecture holds for B.

Proof. Since B is nonnilpotent, we must have $e(B)=2$. From Theorem 2.3 we get $k(B)\geq(11\cdot 3^{m-2}+9)/2$. On the other hand Corollary 2.5 implies $k(B)\leq(11\cdot 3^{m-2}+11)/2$. Hence, $l(B)\in\{2,3\}$ by Theorem 3.2. Moreover, we have $(3^m+7)/2\leq k_0(B)\leq(3^m+9)/2$ by Theorem 2.4 (otherwise $k_1(B)$ would be too large). Now Corollary 1.6 in [Landrock 1981] shows that $k_0(B)=(3^m+9)/2$. Since we get the same number for the Brauer correspondent of B in $\mathrm{N}_G(D)$, the Alperin–McKay conjecture follows. □

The next aim is to show that even Alperin's weight conjecture holds in the situation of Theorem 3.4 provided $m \le 3$. Moreover, we verify the ordinary weight conjecture [Robinson 2004] in this case using the next proposition.

Proposition 3.5. *Let B be a block of a finite group with defect group $M_{p^{m+1}}$ where p is an odd prime and $m \ge 2$. Then the ordinary weight conjecture for B is equivalent to the equalities*

$$k_0(B) = \left(\frac{p^{m-1}-1}{e(B)} + e(B)\right)p, \qquad k_1(B) = \frac{p-1}{e(B)}p^{m-2}.$$

Proof. We use the version in Conjecture 6.5 in [Kessar 2007]. Let Q be an $\mathcal{F}$-centric and $\mathcal{F}$-radical subgroup of D. Since $|D : \mathrm{Z}(D)| = p^2$ and $\mathrm{C}_D(Q) \le Q$, we have $|D : Q| \le p$. Assume $|D : Q| = p$. Then $D/Q \le \mathrm{Aut}_{\mathcal{F}}(Q)$. Since $\mathcal{F}$ is controlled, all $\mathcal{F}$-automorphisms on Q come from automorphisms on D. In particular $D/Q \trianglelefteq \mathrm{Aut}_{\mathcal{F}}(Q)$. But then Q cannot be $\mathcal{F}$-radical. Hence, we have seen that D is the only $\mathcal{F}$-centric and $\mathcal{F}$-radical subgroup of D. It follows that the set $\mathcal{N}_D$ in [Kessar 2007] only consists of the trivial chain. Since $I(B)$ is cyclic, all 2-cocycles appearing in the same paper are trivial. Hence, we see that

$$\mathbf{w}(D, d) = \sum_{\chi \in \mathrm{Irr}^d(D)/I(B)} |I(B) \cap I(\chi)|$$

where $\mathrm{Irr}^d(D)$ is the set of irreducible characters of D of defect $d \ge 0$ and

$$I(B) \cap I(\chi) := \{\gamma \in I(B) : {}^{\gamma}\chi = \chi\}.$$

Now the ordinary weight conjecture predicts that $k^d(B) = \mathbf{w}(D, d)$ where $k^d(B)$ is the number of irreducible characters of B of defect $d \ge 0$. For $d < m$ both numbers vanish. Now consider $d \in \{m, m+1\}$. Let us look at a part of the character table of D:

D	x	x^p	y
χ_{ij}	$\zeta_{p^{m-1}}^i$	$\zeta_{p^{m-2}}^i$	ζ_p^j
ψ_k	0	$p\zeta_{p^{m-1}}^k$	0

Here $i, k \in \{0, \dots, p^{m-1} - 1\}$, $j \in \{0, \dots, p - 1\}$ and $\gcd(k, p) = 1$. The characters of degree p are induced from $\mathrm{Irr}(\langle x\rangle)$. It can be seen that the linear characters of D split into $(p^m - p)/e(B)$ orbits of length $e(B)$ and p stable characters under the action of $I(B)$. This gives

$$\mathbf{w}(D, m+1) = \left(\frac{p^{m-1}-1}{e(B)} + e(B)\right)p.$$

Similarly, the irreducible characters of D of degree p split into $p^{m-2}(p-1)/e(B)$ orbits of length $e(B)$. Hence,

$$\mathbf{w}(D, m) = \frac{p-1}{e(B)} p^{m-2}.$$

The claim follows. □

We introduce another lemma, which will be needed at several points.

Lemma 3.6. *Let q be the integral quadratic form corresponding to the Dynkin diagram A_r, and let $a \in \mathbb{Z}^r$.*

(i) *If $q(a) = 1$, then $a = \pm(0, \dots, 0, 1, 1, \dots, 1, 0, \dots, 0)$.*

(ii) *If $q(a) = 2$, then one of the following holds*:

- $a = \pm(0, \dots, 0, 1, 1, \dots, 1, 0, 0, \dots, 0, 1, 1, \dots, 1, 0, \dots, 0)$,
- $a = \pm(0, \dots, 0, 1, 1, \dots, 1, 0, 0, \dots, 0, -1, -1, \dots, -1, 0, \dots, 0)$,
- $a = \pm(0, \dots, 0, 1, 1, \dots, 1, 2, 2, \dots, 2, 1, 1, \dots, 1, 0, \dots, 0)$.

Here $s, \dots, s$ includes the possibility of no $s \in \mathbb{Z}$ at all.

Proof. Without loss of generality, $r \geq 2$. Let $a = (a_1, \dots, a_r)$. Then

$$q(a) = \sum_{i=1}^{r} a_i^2 - \sum_{i=1}^{r-1} a_i a_{i+1} = \tfrac{1}{2}\left(a_1^2 + \sum_{i=1}^{r-1} (a_i - a_{i+1})^2 + a_r^2\right). \tag{3-3}$$

Assume first that $q(a) = 1$ and $a_i \neq 0$ for some $i \in \{1, \dots, r\}$. After replacing a with $-a$ if necessary, we have $a_i > 0$. By the equation above we see that the difference between two adjacent entries of a is at most 1. Going from i to the left and to the right, we see that a has the stated form.

Now assume $q(a) = 2$. If one of $\{a_1, a_r\}$ is ± 2, so must be the other, since each two adjacent entries of a must coincide. But this contradicts (3-3). Hence, $a_1, a_r \in \{\pm 1, 0\}$. Now let $|a_i| \geq 3$ for some $i \in \{2, \dots, r-1\}$. Going from i to the left we get at least two nonvanishing summands in (3-3). The same holds for the entries on the right side of i. Thus, we end up with a configuration where $a_1 \neq 0$. This is again a contradiction. It follows that $a_i \in \{\pm 1, \pm 2, 0\}$ for $i = 2, \dots, r-1$. In particular we have only finitely many solutions for a. If no ± 2 is involved in a, it is easy to see that a must be one of the given vectors in the statement of the lemma. Thus, let us consider $a_i = 2$ for some $i \in \{2, \dots, r-1\}$ (after changing signs if necessary). Then $a_{i-1}, a_{i+1} \in \{1, 2\}$, since otherwise $(a_i - a_{i-1})^2 \geq 4$ or $(a_{i+1} - a_i)^2 \geq 4$. Now we can repeat this argument with a_{i-1} and a_{i+1} until we get the desired form for a. □

Theorem 3.7. *Let B be a nonnilpotent block of a finite group with defect group $M_{3^{m+1}}$ where $m \in \{2, 3\}$. Then*

$$k_0(B) = \frac{3^m + 9}{2}, \quad k_1(B) = 3^{m-2}, \quad k(B) = \frac{11 \cdot 3^{m-2} + 9}{2}, \quad l(B) = e(B) = 2.$$

In particular Alperin's weight conjecture and Robinson's ordinary weight conjecture [Robinson 2004] *are satisfied for B.*

Proof. Since B is nonnilpotent, we must have $e(B) = 2$. The case $m = 2$ is very easy and will be handled in the next section together with some more information. Hence, we assume $m = 3$ (that is, $|D| = 81$) for the rest of the proof. By Theorem 3.4 we already know $k_0(B) = 18$. By way of contradiction we assume $k(B) = 22$, $k_1(B) = 4$ and $l(B) = 3$.

We consider the vector d^z for $z := x^3 \in \mathrm{Z}(D)$. As in [Héthelyi et al. 2012] (we will use this paper a lot) we can write $d^z = \sum_{i=0}^{5} a_i \zeta_9^i$ for integral vectors a_i. We will show that $(a_0, a_i) = 0$ for $i \geq 1$. By Lemma 4.7 [ibid.] this holds unless $i = 3$. But in this case we have $(a_3, a_3) = 0$ and $a_3 = 0$ by Proposition 4.4 [ibid.]. If we follow the proof of Theorem 4.10 [ibid.] closely, it turns out that the vectors a_i are spanned by a_0, a_1 and a_4. So we can also write

$$d^z = a_0 + a_1 \tau + a_4 \sigma$$

where τ and σ are certain linear combinations of powers of ζ_9. Of course, one could give more precise information here, but this is not necessary in this proof. By Lemma 4.7 [ibid.] we have $(a_0, a_0) = 27$.

Let q be the quadratic form corresponding to the Dynkin diagram of type A_3. We set $a(\chi) := (a_0(\chi), a_1(\chi), a_4(\chi))$ for $\chi \in \mathrm{Irr}(B)$. Since the subsection (z, b_z) gives equality in Theorem 4.10 [ibid.], we have

$$k_0(B) + 9k_1(B) = \sum_{\chi \in \mathrm{Irr}(B)} q(a(\chi)) = 54.$$

This implies $q(a(\chi)) = 3^{2h(\chi)}$ for $\chi \in \mathrm{Irr}(B)$. Assume that there is a character $\chi \in \mathrm{Irr}(B)$ such that $a_0(\chi)a_i(\chi) > 0$ for some $i \in \{1, 4\}$. Since $(a_0, a_i) = 0$, there must be another character $\chi' \in \mathrm{Irr}(B)$ such that $a_0(\chi')a_i(\chi') < 0$. However, then $q(a(\chi')) > 3^{2h(\chi)}$ by Lemma 3.6. Thus, we have shown that $a_0(\chi)a_i(\chi) = 0$ for all $\chi \in \mathrm{Irr}(B)$ and $i \in \{1, 4\}$. Moreover, if $a_0(\chi) \neq 0$, then $a_0(\chi) = \pm 3^{h(\chi)}$ again by Lemma 3.6.

In the next step we determine the number β of integral numbers $d^z(\chi)$ for characters χ of height 1. Since $(a_0, a_0) = 27$, we have $\beta < 4$. Let $\psi \in \mathrm{Irr}(B)$ of height 1 such that $d^z(\psi) \notin \mathbb{Z}$. Then we can form the orbit of $d^z(\psi)$ under the Galois group $\mathcal{H}$ of $\mathbb{Q}(\zeta_9) | (\mathbb{Q}(\zeta_9) \cap \mathbb{R})$. The length of this orbit must be $|\mathcal{H}| = 3$. In particular $\beta = 1$.

This implies that $d^z(\chi) = a_0(\chi) = \pm 1$ for all 18 characters $\chi \in \mathrm{Irr}(B)$ of height 0. In the following we derive a contradiction using the orthogonality relations of decomposition numbers. In order to do so, we repeat the argument with the subsection (x, b_x). Again we get equality in Theorem 4.10, but this time for $k_0(B)$ instead of $k_0(B) + 9k_1(B)$. Hence, $d^x(\chi) = 0$ for characters $\chi \in \mathrm{Irr}(B)$ of height 1. Again we can write $d^x = \sum_{i=0}^{17} \bar{a}_i \zeta_{27}^i$ where $\bar{a}_i$ are integral vectors. Lemma 4.7 [ibid.] implies $(\bar{a}_0, \bar{a}_0) = 9$. Using Lemma 3.6 we also have $\bar{a}_0(\chi) \in \{0, \pm 1\}$ in this case. This gives the final contradiction $0 = (d^z, d^x) = (a_0, \bar{a}_0) \equiv 1 \pmod 2$.

Hence, we have proved that $k(B) = 21$, $k_1(B) = 3$ and $l(B) = 2$. Since B is controlled, Alperin's weight conjecture asserts that $l(B) = l(b)$ where b is the Brauer correspondent of B in $\mathrm{N}_G(D)$. Since $e(b) = e(B)$, the claim follows at once. the ordinary weight conjecture follows from Proposition 3.5. This completes the proof. □

4. The group p_-^{1+2}

In this section we restrict further to the case $n = 1$ and $m = 2$, that is,

$$D = \langle x, y \mid x^{p^2} = y^p = 1,\, yxy^{-1} = x^{1+p} \rangle$$

is extraspecial of order p^3 and exponent p^2. We denote this group by p_-^{1+2} (compare with [Hendren 2005]). In particular we can use the results from the last section. One advantage of this restriction is that the bounds are slightly sharper than in the general case.

Inequalities. Our first theorem says that the block invariants fall into an interval of length $e(B)$.

Theorem 4.1. *Let B be a block of a finite group with defect group p_-^{1+2} for an odd prime p. Then*

$$\frac{p^2-1}{e(B)} + e(B)p \le k(B) \le \frac{p^2-1}{e(B)} + e(B)p + e(B) - 1,$$

$$\left(\frac{p-1}{e(B)} + e(B)\right)p - e(B) + 1 \le k_0(B) \le \left(\frac{p-1}{e(B)} + e(B)\right)p,$$

$$\frac{p-1}{e(B)} \le k_1(B) \le \frac{p-1}{e(B)} + e(B) - 1,$$

$$k_i(B) = 0 \quad \textit{for } i \ge 2,$$

$$e(B) \le l(B) \le 2e(B) - 1,$$

$$k(B) - l(B) = \frac{p^2-1}{e(B)} + (p-1)e(B).$$

Proof. The formula for $k(B)-l(B)$ comes from Theorem 3.2. The lower bounds for $l(B)$ and $k(B)$ follow from Proposition 2.1 and Theorem 2.3. The upper bound for $k_0(B)$ comes from Theorem 2.4. The same theorem gives also

$$k_1(B) \le \frac{p-1}{e(B)} + e(B) - 1.$$

Adding this to the upper bound for $k_0(B)$ results in the stated upper bound for $k(B)$. Now the upper bound for $l(B)$ follows from $k(B)-l(B)$. A lower bound for $k_0(B)$ is given by

$$\begin{aligned} k_0(B) &= k(B) - k_1(B) \\ &\ge \frac{p^2-1}{e(B)} + e(B)p - \frac{p-1}{e(B)} - e(B) + 1 = \left(\frac{p-1}{e(B)} + e(B)\right)p - e(B) + 1 \end{aligned}$$

Moreover,

$$k_1(B) = k(B) - k_0(B) \ge \frac{p^2-1}{e(B)} + e(B)p - \left(\frac{p-1}{e(B)} + e(B)\right)p = \frac{p-1}{e(B)}. \quad \square$$

Since we already know that the upper bound for $k_0(B)$ and the lower bound for $k(B)$ are sharp (for blocks with maximal defect), it follows at once that the lower bound for $k_1(B)$ in Theorem 4.1 is also sharp (compare with Proposition 3.5).

If $e(B)$ is as large as possible, we can prove slightly more.

Proposition 4.2. *Let B be a block of a finite group with defect group p_-^{1+2} for an odd prime p. If $e(B) = p-1$, then $k(B) \le p^2 + p - 2$, $l(B) \le 2e(B) - 2$ and $k_0(B) \ne p^2 - r$ for $r \in \{1, 2, 4, 5, 7, 10, 13\}$.*

Proof. By way of contradiction, assume $k(B) = p^2 + p - 1$. By Theorem 4.1 we have $k_0(B) = p^2$ and $k_1(B) = p-1$. Set $z := x^p \in \mathrm{Z}(D)$. Then we have $l(b_z) = 1$. Since $I(B)$ acts regularly on $\mathrm{Z}(D) \setminus \{1\}$, the vector d^z is integral. By Lemma 4.1 in [Héthelyi et al. 2012] we have $0 \ne d^z_{\chi\varphi_z} \equiv 0 \pmod p$ for characters χ of height 1. Hence, d^z must consist of p^2 entries ± 1 and $p-1$ entries $\pm p$. Similarly $l(b_x) = 1$. Moreover, all powers x^i for $(i, p) = 1$ are conjugate under $\mathcal{F}$. Hence, also the vector d^x is integral. Thus, the only nonvanishing entries of d^x are ± 1 for the characters of height 0, because $(d^x, d^x) = p^2$ (again using [ibid., Lemma 4.1]). Now the orthogonality relations imply the contradiction $0 = (d^z, d^x) \equiv 1 \pmod 2$, since p is odd. Thus, we must have $k(B) \le p^2 + p - 2$ and $l(B) \le 2e(B) - 2$.

We have seen that every character of height 0 corresponds to a nonvanishing entry in d^x. If we have a nonvanishing entry for a character of height 1 on the other hand, then Theorem V.9.4 in [Feit 1982] shows that this entry is $\pm p$. However, this contradicts the orthogonality relation $(d^z, d^x) = 0$. Hence, the nonvanishing entries of d^x are in one-to-one correspondence to the irreducible characters of height 0.

Thus, we see that p^2 is the sum of $k_0(B)$ nontrivial integral squares. This gives the last claim. □

Since in case $e(B)=2$ the inequalities are very strong, it seems reasonable to obtain more precise information here. In the last section we proved for arbitrary m that the Alperin–McKay conjecture holds provided $p=3$. As a complementary result we now show the same for all p, but with the restrictions $m=2$ and $e(B)=2$. We even obtain a refinement of the Alperin–McKay conjecture, which is called the Galois–Alperin–McKay conjecture; see Conjecture D in [Isaacs and Navarro 2002].

Theorem 4.3. *Let B be a block of a finite group with defect group p_{-}^{1+2} for an odd prime p and $e(B)=2$. Then $k_0(B)=p(p+3)/2$. In particular the Galois–Alperin–McKay conjecture holds for B.*

Proof. By Theorem 3.4 we may assume $p>3$. For some subtle reasons we also have to distinguish between $p=7$ and $p\neq 7$. Let us assume first that $p\neq 7$. By Theorem 4.1 we have $k_0(B)\in\{p(p+3)/2-1,\,p(p+3)/2\}$. We write $d^x=\sum_{i=0}^{p(p-1)-1}\bar{a}_i\zeta_{p^2}^i$ with integral vectors $\bar{a}_i$. As in Proposition 4.9 of [Héthelyi et al. 2012] we see that $\bar{a}_i=0$ if $(i,p)=1$. Moreover, the arguments in the proof of Proposition 4.8 of the same paper tell us that $\bar{a}_p=0$ and $\bar{a}_{ip}=\bar{a}_{(p-i)p}$ for $i=2,\dots,(p-1)/2$. Now let $\tau_i:=\zeta_p^i+\zeta_p^{-i}$ for $i=2,\dots,(p-1)/2$. Then we can write

$$d^x=a_0+\sum_{i=2}^{(p-1)/2}a_i\tau_i$$

for integral vectors a_i. Here observe that d^x is real, since (x,b_x) and $(x^{-1},b_{x^{-1}})$ are conjugate under $I(B)$. By [ibid., Lemma 4.7] we have $(a_0,a_0)=3p$, $(a_i,a_j)=p$ for $i\neq j$ and $(a_i,a_i)=2p$ for $i\geq 2$. Now let $a(\chi)=(a_i(\chi):i=0,2,3,\dots,(p-1)/2)$ for $\chi\in\mathrm{Irr}(B)$. Moreover, let q be the integral quadratic form corresponding to the Dynkin diagram of type $A_{(p-1)/2}$. Then as in [ibid., Proposition 4.2], we get

$$\sum_{\chi\in\mathrm{Irr}(B)}q(a(\chi))=p\left(3+2\,\frac{p-3}{2}-\frac{p-3}{2}\right)=p\,\frac{p+3}{2}.$$

Let $\chi\in\mathrm{Irr}(B)$ be a character of height 1. Suppose that $a(\chi)\neq 0$. Then we have $k_0(B)=p(p+3)/2-1$ and χ is the only character of height 1 such that $a(\chi)\neq 0$. In particular χ is p-rational and $a(\chi)=a_0(\chi)\in\mathbb{Z}$. Now Theorem V.9.4 in [Feit 1982] implies $p\mid a_0(\chi)$. Since $(a_0,a_0)=3p$, this gives $p=3$, which contradicts our hypothesis. Hence, we have shown that $a(\chi)=0$ for all characters $\chi\in\mathrm{Irr}(B)$ of height 1. In particular

$$\sum_{\substack{\chi\in\mathrm{Irr}(B)\\ h(\chi)=0}}q(a(\chi))=p\,\frac{p+3}{2}.$$

By way of contradiction suppose that $k_0(B) = p(p+3)/2 - 1$. Then there is exactly one character $\chi \in \mathrm{Irr}(B)$ such that $q(a(\chi)) = 2$ (this already settles the case $p = 5$). Now the idea is to show that there is a p-conjugate character ψ also satisfying $q(a(\psi)) > 1$. In order to do so, we discuss the different cases in Lemma 3.6. Here we can of course choose the sign of $a(\chi)$.

First assume

$$a(\chi) = (0, \dots, 0, 1, 1, \dots, 1, 0, 0, \dots, 0, -1, -1, \dots, -1, 0, \dots, 0).$$

Choose an index k corresponding to one of the -1 entries in $a(\chi)$. Let $k' \in \{2, \dots, (p-1)/2\}$ such that $kk' \equiv \pm 1 \pmod p$, and let $\gamma_{k'} \in \mathcal{G}$ be the Galois automorphism which sends ζ_p to $\zeta_p^{k'}$. Then

$$\gamma_{k'}(\tau_k) = -1 - \sum_{i=2}^{(p-1)/2} \tau_i.$$

Apart from this, $\gamma_{k'}$ acts as a permutation on the remaining indices

$$\{2, \dots, (p-1)/2\} \setminus \{k\}.$$

This shows that $a(\gamma_{k'}(\chi))$ contains an entry 2. In particular $\gamma_{k'}(\chi) \neq \chi$. Moreover, Lemma 3.6 gives $q(a(\gamma_{k'}(\chi))) > 1$.

Next suppose that

$$a(\chi) = (0, \dots, 0, 1, 1, \dots, 1, 2, 2, \dots, 2, 1, 1, \dots, 1, 0, \dots, 0).$$

Here we choose k corresponding to an entry 2 in $a(\chi)$. Then the same argument as above implies that $a(\gamma_{k'}(\chi))$ has a -2 on position k_1. Contradiction.

Now let $a(\chi) = (0, 0, \dots, 0, 1, 1, \dots, 1, 0, 0, \dots, 0, 1, 1, \dots, 1, 0, \dots, 0)$ (observe the leading 0). We choose the index k corresponding to a 1 in $a(\chi)$. Let $\gamma_{k'}$ be the automorphism as above. Observe that χ is not p-rational. Thus, Proposition 3.3 implies $\gamma_{k'}(\chi) \neq \chi$. In particular $q(a(\gamma_{k'}(\chi))) = 1$. Hence, we must have $a(\gamma_{k'}(\chi)) = (-1, -1, \dots, -1, 0, 0, \dots, 0)$ where the number of -1 entries is uniquely determined by $a(\chi)$. In particular $a(\gamma_{k'}(\chi))$ is independent of the choice of k. Now choose another index k_1 corresponding to an entry 1 in $a(\chi)$ (always exists). Then we see that $a(\chi)$ and thus χ is fixed by $\gamma_{k'}^{-1}\gamma_{k_1'}$. Proposition 3.3 shows that $\gamma_{k'}^{-1}\gamma_{k_1'}$ must be (an extension of) the complex conjugation. This means $k' \equiv -k_1' \pmod p$ and $k \equiv -k_1 \pmod p$. However this contradicts $2 \leq k, k_1 \leq (p-1)/2$.

Finally let $a(\chi) = (1, 1, \dots, 1, 0, 0, \dots, 0, 1, 1, \dots, 1, 0, \dots, 0)$. Here a quite similar argument shows that $a(\chi)$ only contains one entry 0, say on position k. Now we can use the same trick where $k_1 \geq 2$ corresponds to an entry 1. Here $a(\gamma_{k_1'}(\chi)) = (0, 0, \dots, 0, -1, -1, 0, \dots, 0)$. Let $k_2 \in \{2, \dots, (p-1)/2\}$ such that

$k_2 \equiv \pm kk'_1 \pmod p$. Then the -1 entries of $a(\gamma_{k'_1}(\chi))$ lie on positions k'_1 and k_2. Since these entries lie next to each other, we get $k \pm 1 \equiv \pm k_1 \pmod p$ where the signs are independent. However, this shows that k and k_1 are adjacent. Hence, we proved that $a(\chi) = (1, 0, 1)$ and $p = 7$ ($(1, 1, 0, 1)$ is not possible, since 9 is not a prime). However, this case was excluded. Thus, $k_0(B) = p(p+3)/2$.

It remains to deal with the case $p = 7$. It can be seen that there is in fact a permissible configuration for $k_0(B) = 34$:

$$d^x = (\underbrace{1, \dots, 1}_{13\text{ times}}, \underbrace{1+\tau_2+\tau_3, \dots, 1+\tau_2+\tau_3}_{6\text{ times}}, 1+\tau_2, 1+\tau_3, \tau_2+\tau_3, \underbrace{\tau_2, \dots, \tau_2}_{6\text{ times}}, \underbrace{\tau_3, \dots, \tau_3}_{6\text{ times}}, 0, \dots, 0).$$

Hence, we consider d^z for $z := x^7$. Suppose by way of contradiction that $k_0(B) = 34$. Then $k_1(B) = 4$ and $k(B) = 38$. By Proposition 3.3 we have exactly two 7-rational irreducible characters in $\mathrm{Irr}(B)$. Moreover, the orbit lengths of the 7-conjugate characters are all divisible by 3. Hence, we have precisely one 7-rational character of height 1 and one of height 0. In the same way as above we can write $d^z = a_0 + a_2\tau_2 + a_3\tau_3$; see Proposition 4.8 in [Héthelyi et al. 2012]. Then $(a_0, a_0) = 3 \cdot 7^2$, $(a_i, a_j) = 7^2$ for $i \neq j$ and $(a_i, a_i) = 2 \cdot 7^2$ for $i = 2, 3$. For a character $\chi \in \mathrm{Irr}(B)$ of height 1 we have $7 \mid a_i(\chi)$ for $i = 0, 2, 3$ by [ibid., Lemma 4.1]. Since

$$\sum_{\chi \in \mathrm{Irr}(B)} q(a(\chi)) = 5p^2,$$

it follows that $q(a(\chi)) = 7^2$ for every character $\chi \in \mathrm{Irr}(B)$ of height 1. It is easy to see that $a(\chi) \notin \{\pm 7(0, 1, 1), \pm 7(1, 1, 0)\}$. Hence, the four rows $a(\chi)$ for characters χ of height 1 have to following form up to signs and permutations:

$$7\begin{pmatrix} 1 & \cdot & \cdot \\ \cdot & 1 & \cdot \\ \cdot & \cdot & 1 \\ 1 & 1 & 1 \end{pmatrix}.$$

Thus, for a character $\chi_i \in \mathrm{Irr}(B)$ of height 0 ($i = 1, \dots, 34$) we have

$$d^z(\chi_i) = a_0(\chi_i) \neq 0 \quad \text{and} \quad \sum_{i=1}^{34} a_0(\chi_i)^2 = 7^2.$$

Up to signs and permutations we get $(a_0(\chi_i)) = (4, 1, \dots, 1)$ (taking into account that only χ_1 can be 7-rational). So still no contradiction.

Now consider d_{ij}^y. The Cartan matrix of b_y is $7\left(\begin{smallmatrix}4&3\\3&4\end{smallmatrix}\right)$ up to basic sets; see [Dade 1966; Rouquier 1998]. We can write

$$d^y_{\chi\varphi_1}=\sum_{i=0}^{5}\widetilde{a}_i(\chi)\zeta_7^i \quad\text{and}\quad d^y_{\chi\varphi_2}=\sum_{i=0}^{5}\widetilde{b}_i(\chi)\zeta_7^i$$

for $\chi\in\mathrm{Irr}(B)$. It follows that $(\widetilde{a}_0,\widetilde{a}_0)=(\widetilde{b}_0,\widetilde{b}_0)=8$ (this is basically the same calculation as in Proposition 4.8 in [Héthelyi et al. 2012]). By Corollary 1.15 in [Murai 2000] we have $\widetilde{a}_0(\chi_1)\neq 0$ or $\widetilde{b}_0(\chi_1)\neq 0$. Without loss of generality assume $\widetilde{a}_0(\chi_1)\neq 0$. Then $\widetilde{a}_0(\chi_1)=\pm 1$, since $(a_0,\widetilde{a}_0)=(d^z,\widetilde{a}_0)=0$. On the other hand $\widetilde{a}_0(\chi)=0$ for characters $\chi\in\mathrm{Irr}(B)$ of height 1, because we have equality in Theorem 2.4 in [Héthelyi et al. 2012]. However, this gives the following contradiction:

$$0=(a_0,\widetilde{a}_0)=\sum_{i=1}^{34}a_0(\chi_i)\widetilde{a}_0(\chi_i)\equiv\sum_{i=2}^{34}\widetilde{a}_0(\chi_i)\equiv\sum_{i=2}^{34}\widetilde{a}_0(\chi_i)^2\equiv 7 \pmod 2.$$

Altogether we have proved that $k_0(B)=p(p+3)/2$ for all odd primes p. In order to verify the Galois–Alperin–McKay conjecture we have to consider a p-automorphism $\gamma\in\mathcal{G}$. By Lemma IV.6.10 in [Feit 1982] it suffices to compute the orbits of $\langle\gamma\rangle$ on the columns of the generalized decomposition matrix. For an element $u\in D$ of order p, γ acts trivially on $\langle u\rangle$. If u has order p^2, then γ acts as D-conjugation on $\langle u\rangle$. This shows that γ acts in fact trivially on the columns of the generalized decomposition matrix. In particular all characters of height 0 are fixed by γ. Hence, the Galois–Alperin–McKay conjecture holds. □

The case p ≤ 11. We already know $k_0(B)$ if $e(B)=2$. For small primes it is also possible to obtain $k(B)$.

Theorem 4.4. *Let B be a block of a finite group with defect group p_-^{1+2} for $3\le p\le 11$ and $e(B)=2$. Then*

$$k(B)=\frac{p^2+4p-1}{2},\quad k_0(B)=\frac{p+3}{2}p,\quad k_1(B)=\frac{p-1}{2},\quad l(B)=2.$$

The irreducible characters split into two orbits of $(p-1)/2$ p-conjugate characters, $(p+3)/2$ orbits of length $p-1$, and two p-rational characters. For $p\ge 5$ the p-rational characters have height 0. *In particular Alperin's weight conjecture and Robinson's ordinary weight conjecture* [Robinson 2004] *are satisfied for B.*

Proof. We have $k_0(B)=p(p+3)/2$ by Theorem 4.3. For $p=3$ the block invariants and the distribution into 3-conjugate and 3-rational characters follow at once from Theorem 4.1 and Proposition 4.2. So we may assume $p>3$ for the first part of the proof. Suppose $k(B)=(p^2+4p+1)/2$ and $k_1(B)=(p+1)/2$. Then

$\mathrm{Irr}(B)$ contains exactly three p-rational characters. Moreover, the orbit lengths of the p-conjugate characters are all divisible by $(p-1)/2$. Let $z := x^p$. Then we can write

$$d^z = a_0 + \sum_{i=2}^{(p-1)/2} a_i \tau_i$$

as in Theorem 4.3 where $\tau_i := \zeta_p^i + \zeta_p^{-i}$ for $i = 2, \ldots, (p-1)/2$ (see Proposition 4.8 in [Héthelyi et al. 2012]). Then $(a_0, a_0) = 3p^2$, $(a_i, a_j) = p^2$ for $i \neq j$ and $(a_i, a_i) = 2p^2$ for $i \geq 2$. For a character $\chi \in \mathrm{Irr}(B)$ of height 1 we have $p \mid a_i(\chi)$ by [ibid., Lemma 4.1]. Since

$$\sum_{\chi \in \mathrm{Irr}(B)} q(a(\chi)) = \frac{p+3}{2} p^2,$$

we have $q(a(\chi)) = p^2$ for every character $\chi \in \mathrm{Irr}(B)$ of height 1. If all characters of height 1 are p-rational, we have $p = 5$. But then $(a_0, a_2) = 0$. Hence, exactly one character of height 1 is p-rational. Now choose a non-p-rational character $\psi \in \mathrm{Irr}(B)$ of height 1. Assume $a(\psi) = p(0, \ldots, 0, 1, 1, 1, \ldots, 1, 0, \ldots, 0)$ with at least two entries 1 in a row and at least one entry 0 (see Lemma 3.6).

If $a_0(\psi) = 0$, then $a(\gamma(\psi)) = p(-1, -1, \ldots, -1, 0, 0, \ldots, 0) = a(\gamma'(\psi))$ for two different Galois automorphisms $\gamma, \gamma' \in \mathcal{G}$ (see proof of Theorem 4.3). Moreover, $\gamma^{-1}\gamma'$ is not (an extension of) the complex conjugation. In particular $(\gamma^{-1}\gamma')(\psi) \neq \psi$. Since $(a_2, a_2) = 2p^2$, $\gamma^{-1}\gamma'$ (up to complex conjugation) is the only nontrivial automorphism fixing $d^z(\psi)$. So, $(\gamma^{-1}\gamma')^2$ is (an extension of) the complex conjugation. This gives $4 \mid p-1$ and $p = 5$ again. But for 5 the whole constellation is not possible, since $a(\psi)$ is 2-dimensional in this case.

Finally assume $a(\psi) = p(1, 1, 1, \ldots, 1, 0, 0, \ldots, 0)$. Then we can find again a Galois automorphism γ (corresponding to an entry 0 in $a(\psi)$) such that $a(\gamma(\psi)) = a(\psi)$. So we get the same contradiction in this case too.

Hence, we have seen that $a(\psi)$ contains either one or $(p-1)/2$ entries ± 1. Thus, the rows $a(\chi)$ for characters χ of height 1 have to following form up to signs and permutations:

$$p \begin{pmatrix} 1 & \cdot & \cdots & \cdot \\ \cdot & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \cdot \\ \cdot & \cdots & \cdot & 1 \\ 1 & 1 & \cdots & 1 \end{pmatrix}.$$

In particular, for all characters χ_i of height 0,

$$d^z(\chi_i) = a_0(\chi_i) \neq 0 \quad (i = 1, \ldots, p(p+3)/2).$$

Moreover,

$$\sum_{i=1}^{p(p+3)/2} a_0(\chi_i)^2 = p^2.$$

Subtracting $p(p+3)/2$ on both sides gives

$$\sum_{i=2}^{\infty} r_i(i^2-1) = p\frac{p-3}{2} \tag{4-1}$$

for some $r_i \geq 0$. Choose $r_i' \in \{0, 1, \dots, (p-3)/2\}$ such that $r_i \equiv r_i' \pmod{(p-1)/2}$. Since we have only two p-rational characters of height 0, the following inequality is satisfied: $\sum_{i=2}^{\infty} r_i' \leq 2$. Using this, it turns out that (4-1) has no solution unless $p > 11$. Hence, $k(B) = (p^2+4p-1)/2$.

The orbit lengths of p-conjugate characters follow from Proposition 3.3. If there is a p-rational character of height 1, we must have $p = 5$. Then of course both characters ψ_1, ψ_2 of height 1 must be 5-rational. For these characters we have $d^z(\psi_i) = a_0(\psi_i) = \pm 5$ with the notation above. Now our aim is to show that $\psi_1 - \psi_2$ or $\psi_1 + \psi_2$ vanishes on the 5-singular elements of G. This is true for the elements in $\mathrm{Z}(D)$. Now let (u, b_u) be a nonmajor B-subsection. Assume first that $u \in \langle y \rangle$. Since $l(b_u) = 2$, we have equality in Theorem 2.4 in [Héthelyi et al. 2012]. This implies $d^u_{\psi_i,\varphi_j} = 0$ for $i, j \in \{1, 2\}$. Next suppose $u \in \langle x \rangle$. Then $d^u(\psi_i) \in \mathbb{Z}$. Hence, Theorem V.9.4 in [Feit 1982] implies $5 \mid d^u(\psi_i)$. Since the scalar product of the integral part of d^u is 15 (compare with proof of Theorem 4.3), we get $d^u(\psi_i) = 0$ for $i = 1, 2$ again. It remains to handle the case $u \notin \langle x \rangle$ and $l(b_u) = 1$. Here Lemma 4.7 in [Héthelyi et al. 2012] shows that the scalar product of the integral part of d^u is 10. So by the same argument as before $d^u(\psi_i) = 0$ for $i = 1, 2$. Hence, we have shown that $\psi_1 - \psi_2$ or $\psi_1 + \psi_2$ vanishes on the 5-singular elements of G. Now, one can check that under these circumstances the number 2 is representable by the quadratic form of the Cartan matrix C of B. However, by (the proof of) Proposition 2.1, the elementary divisors of C are 5 and 5^3. In particular every entry of C is divisible by 5. So this cannot happen. Hence, we have shown that the two irreducible characters of height 1 are 5-conjugate.

Now let $3 \leq p \leq 11$ be arbitrary. Then the two conjectures follow as usual. □

If we have $p = 13$ in the situation of Theorem 4.4, then (4-1) has the solution $r_2 = 19$, $r_3 = 1$ and $r_i = 0$ for $i \geq 4$. For larger primes we get even more solutions. With the help of Theorem 3.7 and Theorem 4.4 it is possible to obtain $k(B) - l(B)$ in the following situations:

- $p = 3$, D as in (2-1) with $n = l = 2$ (in particular $|D| \leq 3^6$),
- $3 \leq p \leq 11$, D as in (2-1) with $n = 2$ and $l = 1$ (in particular $|D| \leq p^5$), and $e(B) = 2$.

However, there is no need to do so.

In case $p = 3$, Theorem 4.4 applies to all nonnilpotent blocks. Here we can show even more.

Theorem 4.5. *Let B be a nonnilpotent block of a finite group with defect group 3^{1+2}_-. Then $e(B) = l(B) = 2$, $k(B) = 10$, $k_0(B) = 9$ and $k_1(B) = 1$. There are three pairs of 3-conjugate irreducible characters (of height 0) and four 3-rational irreducible characters. The Cartan matrix of B is given by $3\left(\begin{smallmatrix} 2 & 1 \\ 1 & 5 \end{smallmatrix}\right)$ up to basic sets. Moreover, the gluing problem* [Linckelmann 2004] *for B has a unique solution.*

Proof. Since B is nonnilpotent, we get $e(B) = 2$. It remains to show the last two claims.

It is possible to determine the Cartan matrix C of B by enumerating all decomposition numbers with the help of a computer. However, we give a more theoretical argument which does not rely on computer calculations. By (the proof of) Proposition 2.1, C has elementary divisors 3 and 27. Hence, $\widetilde{C} := \frac{1}{3}C = \left(\begin{smallmatrix} a & b \\ b & c \end{smallmatrix}\right)$ is an integral matrix with elementary divisors 1 and 9. By changing the basic set if necessary, we may assume that $\widetilde{C}$ is reduced as a binary quadratic form; see [Buell 1989]. This means $0 \le 2b \le a \le c$. We derive

$$\tfrac{3}{4}a^2 \le ac - b^2 = \det \widetilde{C} = 9$$

and $a \in \{1, 2, 3\}$. This gives only the following two possibilities for $\widetilde{C}$: $\left(\begin{smallmatrix} 2 & 1 \\ 1 & 5 \end{smallmatrix}\right)$, $\left(\begin{smallmatrix} 1 & 0 \\ 0 & 9 \end{smallmatrix}\right)$. It remains to exclude the second matrix. So assume by way of contradiction that this matrix occurs for $\widetilde{C}$. Let d_1 be the column of decomposition numbers corresponding to the first irreducible Brauer character in B. Then d_1 consists of three entries 1 and seven entries 0.

It can be seen easily that $d^x = (1, \dots, 1, 0)^{\mathrm{T}}$ up to permutations and signs. Since $(d_1, d^x) = 0$, we have $d_1(\chi_{10}) = 1$ where χ_{10} is the unique irreducible character of height 1.

Now consider y. The Cartan matrix of b_y is $3\left(\begin{smallmatrix} 2 & 1 \\ 1 & 2 \end{smallmatrix}\right)$; see [Dade 1966; Rouquier 1998]. We denote the two irreducible Brauer characters of b_y by φ_1 and φ_2 and write $d^y_{\chi\varphi_i} = a_i(\chi) + b_i(\chi)\zeta_3$ for $i = 1, 2$. Then we have

$$\begin{aligned}
6 &= (a_i, a_i) + (b_i, b_i) - (a_i, b_i),\\
0 &= (a_i, a_i) + 2(a_i, b_i)\zeta_3 + (b_i, b_i)\bar{\zeta}_3\\
&= (a_i, a_i) - (b_i, b_i) + (2(a_i, b_i) - (b_i, b_i))\zeta_3,\\
3 &= (a_1, a_2) + (b_1, b_2) + (b_1, a_2)\zeta_3 + (a_1, b_2)\bar{\zeta}_3\\
&= (a_1, a_2) + (b_1, b_2) - (a_1, b_2) + ((b_1, a_2) - (a_1, b_2))\zeta_3,\\
0 &= (a_1, a_2) + ((a_1, b_2) + (b_1, a_2))\zeta_3 + (b_1, b_2)\bar{\zeta}_3\\
&= (a_1, a_2) - (b_1, b_2) + ((a_1, b_2) + (b_1, a_2) - (b_1, b_2))\zeta_3.
\end{aligned}$$

Thus, $(a_i, a_i) = (b_i, b_i) = 4$, $(a_i, b_i) = (a_1, a_2) = (b_1, b_2) = 2$ and $(a_1, b_2) = (a_2, b_1) = 1$ for $i = 1, 2$. It follows that the numbers $d^y_{\chi\varphi_i}$ can be given in the following form (up to signs and permutations):

$$\begin{pmatrix} 1 & 1 & 1+\zeta_3 & 1+\zeta_3 & \zeta_3 & \zeta_3 & \cdot & \cdot & \cdot & \cdot \\ 1 & \cdot & 1+\zeta_3 & \cdot & \zeta_3 & \cdot & 1+\zeta_3 & 1 & \zeta_3 & \cdot \end{pmatrix}^{\mathrm{T}}.$$

But now we see that d_1 cannot be orthogonal to both of these columns. This contradiction gives C up to basic sets.

Finally we investigate the gluing problem for B. For this we use the notation of [Park 2010]. Up to conjugation there are four $\mathcal{F}$-centric subgroups $Q_1 := \langle x^3, y\rangle$, $Q_2 := \langle x\rangle$, $Q_3 := \langle xy\rangle$ and D. This gives seven chains of $\mathcal{F}$-centric subgroups. It can be shown that $\mathrm{Aut}_{\mathcal{F}}(Q_1) \cong S_3$, $\mathrm{Aut}_{\mathcal{F}}(Q_2) \cong C_6$, $\mathrm{Aut}_{\mathcal{F}}(Q_3) \cong C_3$ and $\mathrm{Aut}_{\mathcal{F}}(D) \cong C_3 \times S_3$. It follows that $\mathrm{H}^2(\mathrm{Aut}_{\mathcal{F}}(\sigma), k^\times) = 0$ for all chains σ of $\mathcal{F}$-centric subgroups of D. Consequently, $\mathrm{H}^0([S(\mathcal{F}^c)], \mathcal{A}^2_{\mathcal{F}}) = 0$. Hence, by Theorem 1.1 in [Park 2010] the gluing problem has at least one solution. (Obviously, this should hold in a more general context.)

Now we determine $\mathrm{H}^1([S(\mathcal{F}^c)], \mathcal{A}^1_{\mathcal{F}})$. For a finite group A it is known that $\mathrm{H}^1(A, k^\times) = \mathrm{Hom}(A, k^\times) = \mathrm{Hom}(A/A'\mathrm{O}^{p'}(A), k^\times)$. Using this we observe that $\mathrm{H}^1(\mathrm{Aut}_{\mathcal{F}}(\sigma), k^\times) \cong C_2$ for all chains except $\sigma = Q_3$ and $\sigma = (Q_3 < D)$, in which case we have $\mathrm{H}^1(\mathrm{Aut}_{\mathcal{F}}(\sigma), k^\times) = 0$. Since $[S(\mathcal{F}^c)]$ is partially ordered by taking subchains, one can view $[S(\mathcal{F}^c)]$ as a category where the morphisms are given by the pairs of ordered chains. In particular $[S(\mathcal{F}^c)]$ has exactly 13 morphisms. With the notation of [Webb 2007] the functor $\mathcal{A}^1_{\mathcal{F}}$ is a *representation* of $[S(\mathcal{F}^c)]$ over $\mathbb{Z}$. Hence, we can view $\mathcal{A}^1_{\mathcal{F}}$ as a module $\mathcal{M}$ over the incidence algebra of $[S(\mathcal{F}^c)]$. More precisely, we have

$$\mathcal{M} := \bigoplus_{a \in \mathrm{Ob}[S(\mathcal{F}^c)]} \mathcal{A}^1_{\mathcal{F}}(a) \cong C_2^5.$$

At this point we can apply Lemma 6.2(2) in [Webb 2007]. For this let

$$d : \mathrm{Hom}[S(\mathcal{F}^c)] \to \mathcal{M}$$

a derivation. Then by definition we have $d(\beta) = 0$ for

$$\beta \in \{(Q_3, Q_3), (Q_3, Q_3 < D), (D, Q_3 < D), (Q_3 < D, Q_3 < D)\}.$$

For all identity morphisms $\beta \in \mathrm{Hom}([S(\mathcal{F}^c)])$ we have

$$d(\beta) = d(\beta\beta) = \mathcal{A}^1_{\mathcal{F}}(\beta)d(\beta) + d(\beta) = 2d(\beta) = 0.$$

Since $\beta\gamma$ for $\beta, \gamma \in \mathrm{Hom}([S(\mathcal{F}^c)])$ is only defined if β or γ is an identity, we see that there are no further restrictions on d. On the four morphisms $(Q_1, Q_1 < D)$, $(D, Q_1 < D)$, $(Q_2, Q_2 < D)$ and $(D, Q_2 < D)$ the value of d is arbitrary. It remains to show that d is an inner derivation. For this observe that the map $\mathcal{A}^1_{\mathcal{F}}(\beta)$ is bijective if β is one of the four morphisms above. Now we construct a set $u = \{u_a \in \mathcal{A}^1_{\mathcal{F}}(a) : a \in \mathrm{Ob}[S(\mathcal{F}^c)]\}$ such that d is the inner derivation induced by u. Here we can set $u_{Q_1<D} = 0$. Then the equation

$$d((Q_1, Q_1 < D)) = \mathcal{A}^1_{\mathcal{F}}((Q_1, Q_1 < D))(u_{Q_1})$$

determines u_{Q_1}. Similarly $d((D, Q_1 < D)) = \mathcal{A}^1_{\mathcal{F}}(u_D)$ determines u_D. Then $d((D, Q_2 < D)) = \mathcal{A}^1_{\mathcal{F}}(u_D) - u_{Q_2<D}$ gives $u_{Q_2<D}$ and finally

$$d((Q_2, Q_2 < D)) = \mathcal{A}^1_{\mathcal{F}}(u_{Q_2}) - u_{Q_2<D}$$

determines u_{Q_2}. Hence, Lemma 6.2(2) in [Webb 2007] shows $\mathrm{H}^1([S(\mathcal{F}^c)], \mathcal{A}^1_{\mathcal{F}}) = 0$. So the Gluing Problem has only one solution by Theorem 1.1 in [Park 2010]. □

Whenever one knows the Cartan matrix (up to basic sets) for a specific defect group, one can apply Theorem 2.4 in [Héthelyi et al. 2012]. This gives the following corollary.

Corollary 4.6. *Let B be a 3-block of a finite group and (u, b_u) be a subsection for B such that b_u has defect group Q. If $Q/\langle u\rangle \cong 3^{1+2}_{-}$, then $k_0(B) \le |Q|$. If in addition (u, b_u) is major, we have $k(B) \le |Q|$, and Brauer's $k(B)$-conjecture holds for B.*

Using [Usami 1988; Puig and Usami 1993] one can show that Corollary 4.6 remains true if we replace 3^{1+2}_{-} by the similar group $C_9 \times C_3$.

The next interesting case which comes to mind is $p = 5$ and $e(B) = 4$. Here Proposition 4.2 gives $k(B) \in \{26, 27, 28\}$, $k_0(B) \in \{22, 25\}$, $k_1(B) \in \{1, 2, 3, 4\}$ and $l(B) \in \{4, 5, 6\}$. It is reasonable that one can settle this and other small cases as well, but this will not necessarily lead to any new insights.

We remark that also for the extraspecial group of order p^3 and exponent p some results of Hendren [2007] can be improved. In particular in [Héthelyi et al. 2012] we proved Olsson's conjecture for these blocks provided $p \neq 3$. On the other hand for $p = 3$, Brauer's $k(B)$-conjecture was shown in [Sambale 2011b].

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CONTENTS

Volume 262, no. 1 and no. 2

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