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POLARIZATION, SIGN SEQUENCES AND ISOTROPIC VECTOR SYSTEMS

GERGELY AMBRUS AND SLOAN NIETERT

We determine the order of magnitude of the n-th ℓ_p-polarization constant of the unit sphere S^{d-1} for every $n, d \geqslant 1$ and $p > 0$. For $p = 2$, we prove that extremizers are isotropic vector sets, whereas for $p = 1$, we show that the polarization problem is equivalent to that of maximizing the norm of signed vector sums. Finally, for $d = 2$, we discuss the optimality of equally spaced configurations on the unit circle.

1. Introduction

Let $\omega_n = \{u_1, \ldots, u_n\}$ be a multiset of n unit vectors in $\mathbb{R}^d$, and set $p > 0$. The *ℓ_p-potential* of ω_n at the unit vector $v \in S^{d-1}$ is defined as

$$U^p(\omega_n, v) = \sum_{i=1}^{n} |\langle v, u_i \rangle|^p,$$

where $\langle \cdot, \cdot \rangle$ denotes the standard inner product. This is an analogue of the classical Riesz potential for inner products. The *ℓ_p-polarization of ω_n* is given by

$$M^p(\omega_n) = \max_{v \in S^{d-1}} U^p(\omega_n, v).$$

We are interested in finding the minimum ℓ_p-polarization of $\omega_n \subset S^{d-1}$, for fixed d and n, that is,

$$M_n^p(S^{d-1}) = \min_{\omega_n \subset S^{d-1}} M^p(\omega_n) = \min_{u_1, \ldots, u_n \in S^{d-1}} \max_{v \in S^{d-1}} \sum_{i=1}^{n} |\langle v, u_i \rangle|^p.$$

The quantity $M_n^p(S^{d-1})$ is called the *n-th ℓ_p-polarization (or Chebyshev) constant of S^{d-1}*.

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Related questions for $p \leqslant 0$ have been studied extensively; see, e.g., the recent article of Hardin, Petrache and Saff [Hardin et al. 2019] about general polarization problems. In the planar case, $M_n^p(S^1)$ has a direct connection to the classical notions of Riesz potentials and Chebyshev constants. This connection is described in Section 5. Polarization problems have been subject to very active research in the last 15 years, although their study dates back to at least 1967 [Ohtsuka 1967]. The most relevant results to our present problem are discussed in [Ambrus 2009; Nikolov and Rafailov 2011; 2013; Stolarsky 1975a; 1975b].

Determining the exact value of $M_n^p(S^{d-1})$ is hopeless in general, except for certain cases. Therefore, our first result provides asymptotic bounds. For brevity, we introduce the quantity

$$\mu_{d,p} = \frac{\Gamma\left(\frac{d}{2}\right)\Gamma\left(\frac{p+1}{2}\right)}{\sqrt{\pi}\,\Gamma\left(\frac{d+p}{2}\right)}.$$

Clearly, $\mu_{d,p} = \Theta(d^{-p/2})$. Here, and throughout the paper, we are going to use the standard asymptotic notations following Knuth [1997]: given two positive-valued functions $f(n) > 0$ and $g(n) > 0$, $n \in \mathbb{N}$, we write

$$\begin{aligned}
f(n) &= \mathcal{O}(g(n)) \quad \text{if } \limsup_{n\to\infty} f(n)/g(n) < \infty;\\
f(n) &= o(g(n)) \quad \text{if } \lim_{n\to\infty} f(n)/g(n) = 0;\\
f(n) &= \Omega(g(n)) \quad \text{if } \liminf_{n\to\infty} f(n)/g(n) > 0;\\
f(n) &= \omega(g(n)) \quad \text{if } \lim_{n\to\infty} f(n)/g(n) = \infty;\\
f(n) &= \Theta(g(n)) \quad \text{if } f(n) = \mathcal{O}(g(n)) \text{ and } f(n) = \Omega(g(n)).
\end{aligned}$$

Depending on the number of points compared to the dimension, we derive different estimates.

Theorem 1. *For every $p > 0$,*

$$M_n^p(S^{d-1}) = n\mu_{d,p} + o(nd^{-p/2})$$

as $d, n \to \infty$ and $n = \omega(d^{1+p}\log d)$.

Furthermore, for $0 < p \leqslant 2$,

$$M_n^p(S^{d-1}) = \Theta(nd^{-p/2}),$$

while for $p > 2$,

$$M_n^p(S^{d-1}) = \Omega(n\,d^{-p/2}) \quad \text{and} \quad M_n^p(S^{d-1}) = \mathcal{O}(n\,d^{-1})$$

holds, as $d, n \to \infty$ and $n \geqslant d$.

For special values of p and d, stronger results may be proved. In order to discuss the case $p = 2$, we introduce the following notion: $\omega_n = \{u_1, \dots, u_n\} \subset S^{d-1}$ is an *isotropic set of unit vectors* if

$$\sum_{i=1}^{n} u_i \otimes u_i = \frac{n}{d} I_d,$$

where I_d is the identity operator on $\mathbb{R}^d$. Isotropic sets of unit vectors are also called *unit norm tight frames*; see, e.g., [Benedetto and Fickus 2003].

Theorem 2. *For every $d \geqslant 1$ and $n \geqslant d$,*

$$M_n^2(S^{d-1}) = \frac{n}{d},$$

and the extremal ω_n configurations are exactly the isotropic sets of unit vectors.

For $p = 1$, Theorem 1 provides the exact asymptotics: $M_n^1(S^{d-1}) = \Theta(nd^{-1/2})$. By the following fact, this also provides an estimate to a quantity involving sign sequences:

Proposition 3. *For any set of unit vectors $\omega_n = \{u_1, \dots, u_n\} \subset S^{d-1}$,*

$$\max_{\varepsilon \in \{-1,1\}^n} \left| \sum_{i=1}^{n} \varepsilon_i u_i \right| = M^1(\omega_n).$$

As a consequence of Proposition 3 and Theorem 1, we immediately obtain:

Theorem 4. *For every $d \geqslant 1$ and $n \geqslant d$,*

$$\min_{(u_i)_1^n \subset S^{d-1}} \max_{\varepsilon \in \{\pm 1\}^n} \left| \sum_{i=1}^{n} \varepsilon_i u_i \right| = \Theta\left(\frac{n}{\sqrt{d}} \right). \tag{1}$$

Finally, we discuss the ℓ_p-polarization constants of the unit circle.

Proposition 5. *For $d = 2$ and $0 < p \leqslant 1$ as well as for $p = 2, 4, \dots, 2n-2$, $M^p(\omega_n)$ is minimized by vector sets which are equally distributed on the half-circle. For $p = 2, 4, \dots, 2n-2$, the potential function of any extremal configuration is constant on T, whereas for $0 < p \leqslant 1$,*

$$M_n^p(S^1) = \sum_{k=1}^{n} \left| \cos\left(\frac{k\pi}{n} - \frac{\pi}{2n} \right) \right|^p$$

for even values of n, and

$$M_n^p(S^1) = \sum_{k=1}^{n} \left| \cos\left(\frac{k\pi}{n} \right) \right|^p$$

for odd n.

2. General asymptotics

Proof of Theorem 1. We start with the lower bound, which holds for every $p > 0$ and $n \geqslant d$. Let $\omega_n = \{u_1, \ldots, u_n\} \subset S^{d-1}$ be fixed. Note that

$$M^p(\omega_n) = \max_{v \in S^{d-1}} \sum_{i=1}^{n} |\langle v, u_i\rangle|^p \geqslant \mathbb{E}_v\Big[\sum_{i=1}^{n} |\langle v, u_i\rangle|^p\Big]$$
$$= \sum_{i=1}^{n} \mathbb{E}_v |\langle v, u_i\rangle|^p = n\, \mathbb{E}_v |\langle v, u_1\rangle|^p,$$

where the expectation is taken as v being selected uniformly at random from the sphere. By a standard calculation, we obtain that

$$\mathbb{E}_v |\langle v, u_1\rangle|^p = \frac{2}{\mathrm{B}\big(\frac{1}{2}, \frac{d-1}{2}\big)} \int_0^1 t^p (1-t^2)^{(d-3)/2} \mathrm{d}t = \mu_{d,p}$$

and by the previous arguments,

$$M_n^p(S^{d-1}) \geqslant n \mu_{d,p}. \tag{2}$$

Next, we show that this bound is asymptotically correct when n is large, or when $0 < p \leqslant 2$. First, assume that $n = \Omega(d^{1+p} \log d)$, and select an independent, random uniform sample $\omega_n = \{u_1, \ldots, u_n\}$ from S^{d-1}. We will show that with positive probability, $M^p(\omega_n)$ is of order $O(n\, d^{-p/2})$.

For conciseness, let

$$f(v) = \sum_{i=1}^{n} |\langle v, u_i\rangle|^p. \tag{3}$$

Observe that f is np-Lipschitz, since

$$|f(v) - f(w)| = \sum_{i=1}^{n} \big(|\langle v, u_i\rangle|^p - |\langle w, u_i\rangle|^p\big)$$
$$\leqslant \sum_{i=1}^{n} \big||\langle v, u_i\rangle|^p - |\langle w, u_i\rangle|^p\big|$$
$$\leqslant p \sum_{i=1}^{n} \big||\langle v, u_i\rangle| - |\langle w, u_i\rangle|\big| \leqslant p \sum_{i=1}^{n} |\langle v - w, u_i\rangle|$$
$$\leqslant p \sum_{i=1}^{n} |v - w| = np|v - w|.$$

On the other hand, for any fixed $v \in S^{d-1}$,

$$\mathbb{E}\, f(v) = n\mu_{d,p}, \tag{4}$$

where the expectation refers to the choice of the random base system ω_n. Moreover, since $0 \leqslant |\langle v, u_i\rangle|^p \leqslant 1$, Hoeffding's inequality and (4) yields that for any fixed $v \in S^{d-1}$ and $t > 0$,

$$\mathbb{P}\big(|f(v) - n\mu_{d,p}| > t\big) < 2e^{-2t^2/n}. \tag{5}$$

We are going to bound the maximum of $f(v)$ on S^{d-1} by pinning it down at the points of a δ-net and then exploiting the Lipschitz property. It is well known (see, e.g., [Ball 1997]) that there exists a δ-net (with respect to the Euclidean metric) in S^{d-1} with at most $(4/\delta)^d$ points. Let D be such a δ-net. Choose $v^* \in S^{d-1}$ such that

$$f(v^*) = M^p(\omega_n) = \max_{v \in S^{d-1}} f(v).$$

Since v^* must be within δ of some $w \in D$ and f is np-Lipschitz, we have that $|f(w) - M^p(\omega_n)| \leqslant \delta np$. Then, the union bound and (5) gives that for every $\lambda > 0$,

$$\begin{aligned}\mathbb{P}\big(|M^p(\omega_n) - n\mu_{p,d}| > \lambda\big) &\leqslant \sum_{w \in D} \mathbb{P}\big(|f(w) - n\mu_{p,d}| > \lambda - \delta np\big) \\ &\leqslant 2\Big(\frac{4}{\delta}\Big)^d e^{-2(\lambda-\delta np)^2/n}.\end{aligned}$$

Setting $\delta = \lambda/(2np)$, the bound simplifies to

$$\mathbb{P}\big(|M^p(\omega_n) - n\mu_{p,d}| > \lambda\big) \leqslant 2\Big(\frac{8np}{\lambda}\Big)^d e^{-\lambda^2/(2n)}.$$

Take $\lambda = cnd^{-p/2}$ with some constant $c > 0$. Then

$$\mathbb{P}\big(|M^p(\omega_n) - n\mu_{p,d}| > cnd^{-p/2}\big) \leqslant c'^{\,d} d^{dp/2} e^{-(c^2/2)nd^{-p}}$$

with $c' = 10/c$. Taking logarithm shows that the above probability is guaranteed to be less than one if

$$n > \frac{2\log c'}{c^2} d^{1+p} + \frac{p}{c^2} d^{1+p} \log d.$$

Therefore, when $n = \omega(d^{1+p}\log d)$, we obtain that

$$M_n^p(S^{d-1}) = n\mu_{d,p} + o(nd^{-p/2}) = \Theta(nd^{-p/2}).$$

Let us turn to the estimates valid for smaller values of n. The lower bound (2) still holds, so we only have to prove the upper estimates. Without changing the asymptotic bounds, we may assume that $n = kd$. Let ω_n consist of k copies of an orthonormal basis of $\mathbb{R}^d$. Then,

$$\max_{v \in S^{d-1}} U^p(\omega_n, v) = k \max_{|v|=1} \sum_{i=1}^{d} |v_i|^p = \begin{cases} kd^{1-p/2} & \text{for } 0 < p \leqslant 2, \\ k & \text{for } 2 < p, \end{cases}$$

which implies the upper bounds for arbitrary $n \geqslant d$. $\square$

Remark. The following construction gives a slightly stronger estimate for a small number of points, when $0 < p \leqslant 2$. Let $c_{n,d,p}$ be the infimum of all constants $c \in \mathbb{R}$ satisfying

$$M_n^p(S^{d-1}) \leqslant c\, nd^{-p/2}.$$

Let H and $H^\perp$ be two orthogonal, d-dimensional linear subspaces in $\mathbb{R}^{2d}$. Take ω_n and $\omega_n^\perp$ to be n-element vector sets in H and $H^\perp$, respectively, with $M_n^p(S^{d-1}) = M^p(\omega_n) = M^p(\omega_n^\perp)$. Let $\omega_{2n} = \omega_n \cup \omega_n^\perp \subset \mathbb{R}^{2d}$. Then

$$\begin{aligned} M^p(\omega_{2n}) &= \max_{\substack{v \in H,\, v^\perp \in H^\perp \\ |v|^2 + |v^\perp|^2 = 1}} \bigl(U^p(\omega_n, v) + U^p(\omega_n^\perp, v^\perp)\bigr) \\ &\leqslant \max_{|v|^2+|v^\perp|^2=1} \bigl(|v|^p + |v^\perp|^p\bigr) c_{n,d,p}\, nd^{-p/2} \\ &= \frac{2}{2^{p/2}}\, c_{n,d,p}\, nd^{-p/2} = c_{n,d,p}\,(2n)(2d)^{-p/2}. \end{aligned}$$

Thus, $c_{2n,2d,p} \leqslant c_{n,d,p}$. Using the fact that for $d = 0$, $M_n^p(S^0) = n = nd^{-p/2}$, it follows that for $a, b \in \mathbb{N}$, $a \geqslant b$, we have $c_{2^a,2^b,p} \leqslant 1$. Moreover, for $2^a < n < 2^{a+1}$, it is easy to see that $M_n^p(S^{d-1}) \leqslant 2M_{2^a}^p(S^{d-1})$ (by taking the vectors of ω_n once or twice). Likewise, for $2^b < d < 2^{b+1}$, we know that $M_n^p(S^{d-1}) \leqslant 2^{p/2} M_n^p(S^{2^b-1})$ by keeping the optimal vectors from the $d = 2^b$ case. Therefore, $c_{n,d,p} \leqslant 2^{p/2}$ for all $n \geqslant d$.

3. Isotropic vector sets: $p = 2$

Proof of Theorem 2. Let $\omega_n = \{u_1, \dots, u_n\} \subset S^{d-1}$. Introduce the *frame operator*

$$A = \sum_{i=1}^{n} u_i \otimes u_i,$$

where $u \otimes v = uv^\top$ denotes the tensor product of the two vectors. Then for any vector $v \in S^{d-1}$,

$$v^\top A v = \sum_{i=1}^{n} \langle v, u_i \rangle^2.$$

Therefore, $\max_{v \in S^{d-1}} \sum \langle v, u_i \rangle^2$ is attained at the eigenvector of norm 1 of A belonging to the maximal eigenvalue. Since $\operatorname{tr} A = n$, we obtain that

$$M^2(\omega_n) \geqslant \frac{n}{d},$$

and equality holds if and only if $\sum_{i=1}^n u_i \otimes u_i = (n/d) I_d$, that is, if ω_n is an isotropic vector system. □

Isotropic vector sets also arise in different contexts: in frame theory, they are called *unit norm tight frames* or UNTFs, while in the context of John's theorem, their rescaled copies provide a *decomposition of the identity*. A characterization of them was first given by Benedetto and Fickus [2003] (for a simplified proof, see [Ambrus 2014]): they showed that a set of n unit vectors form an isotropic set if and only if they are the minimizer of the *frame potential* among n-element vector sets in S^{d-1}, defined by

$$\mathrm{FP}(\omega_n) = \sum_{i,j} |\langle u_i, u_j \rangle|^2.$$

In particular, it follows that n-element isotropic sets of d-dimensional unit vectors exist for every $n \geqslant d$.

For $d = 2$ and $d = 3$, the characterization may be simplified by utilizing the connection with complex numbers. Goyal et al. [2001] showed that in $\mathbb{R}^2$, isotropic sets of unit vectors correspond to sequences $\{z_i\}_{i=1}^n \subset \mathbb{C}$ satisfying $|z_i| = 1$ and

$$\sum_{i=1}^n z_i^2 = 0,$$

where the unit circle S^1 of $\mathbb{R}^2$ is identified with the complex unit circle T. For $d = 3$, Benedetto and Fickus [2003] provide a correspondence between isotropic vector sets and sequences $\{z_i\}_{i=1}^n \subset \mathbb{C}$ satisfying $|z_i| \leqslant 1$ and

$$\sum_{i=1}^n |z_i|^2 = \tfrac{2}{3} n, \qquad \sum_{i=1}^n z_i^2 = 0, \qquad \sum_{i=1}^n z_i \sqrt{1 - |z_i|^2} = 0.$$

Here, each point in S^2 is identified with its projection onto the unit disc of the complex plane.

4. Sign sequences: $p = 1$

Proof of Proposition 3. First, we show that $\max_{\varepsilon \in \{-1,1\}^n} \left| \sum_{i=1}^n \varepsilon_i u_i \right| \leqslant M^1(\omega_n)$. Indeed, let ε be an arbitrary sign sequence, and define

$$z = \sum_{i=1}^n \varepsilon_i u_i.$$

Then

$$|z|^2 = \Big|\sum \varepsilon_i u_i\Big|^2 = \sum_{i,j} \varepsilon_i \varepsilon_j \langle u_i, u_j\rangle = \sum \varepsilon_i \langle z, u_i\rangle \leqslant \sum^n |\langle z, u_i\rangle|$$

which shows that

$$\Big|\sum \varepsilon_i u_i\Big| \leqslant U^1\Big(\omega_n, \frac{z}{|z|}\Big) \leqslant M^1(\omega_n).$$

For the reverse direction, introduce the function $f(v) = \sum_{i=1}^n |\langle v, u_i\rangle|$ defined on S^{d-1} as in (3). Applying Lagrange multipliers implies that those critical points of f on S^{d-1} where f is differentiable satisfy

$$v = \frac{\sum \varepsilon_i u_i}{\big|\sum \varepsilon_i u_i\big|}$$

with $\varepsilon_i = \operatorname{sgn}\langle v, u_i\rangle$. By taking inner products of both sides with v we obtain that $\big|\sum \varepsilon_i u_i\big| = U^1(\omega_n, v)$.

Therefore, we only have to rule out the existence of maximizers of f at non-differentiable points. Assume on the contrary that $v \in S^{d-1}$ is a maximizer with $\langle v, u_j\rangle = 0$, where $1 \leqslant j \leqslant k$, and $|\langle v, u_j\rangle| > 0$ for $k < j \leqslant n$. Then for $\delta \in \mathbb{R}$ with sufficiently small absolute value,

$$\begin{aligned} f(v + \delta u_1) &= \sum_{i=1}^n |\langle v + \delta u_1, u_i\rangle| = |\delta| \sum_{i=1}^k |\langle u_1, u_k\rangle| + \sum_{i=k+1}^n |\langle v, u_i\rangle + \delta\langle u_1, u_i\rangle| \\ &= f(v) + \delta \sum_{i=k+1}^n \operatorname{sgn}\langle v, u_i\rangle \cdot \langle u_1, u_i\rangle + |\delta| \sum_{i=1}^k |\langle u_1, u_k\rangle|. \end{aligned}$$

Here, $\sum_{i=1}^k |\langle u_1, u_k\rangle| \geqslant 1$, and thus, for sufficiently small but nonzero δ whose sign agrees with that of $\sum_{i=k+1}^n \operatorname{sgn}\langle v, u_i\rangle \cdot \langle u_1, u_i\rangle$, we obtain that

$$f\Big(\frac{v + \delta u_j}{|v + \delta u_j|}\Big) \geqslant \frac{f(v) + |\delta|}{\sqrt{1 + \delta^2}} > f(v),$$

which contradicts the maximality of v. □

Sign sequences arise in several topics, most prominently in the context of discrepancy theory; see, for example, the famous conjecture of Komlós [Spencer 1987]. Note, however, a fundamental difference: in that setting, one would like to *minimize* the norm of $\sum \varepsilon_i u_i$, whereas here, the goal is to find the *maximizers*. The "dual" question of Theorem 4 was asked by Dvoretzky [1963]: Determine

$$\max_{(u_i)_1^n \in S^{d-1}} \; \min_{\varepsilon \in \{\pm 1\}^n} \Big|\sum_{i=1}^n \varepsilon_i u_i\Big|.$$

Various related games were studied by Spencer [1977]. Bárány and Grinberg [1981] proved a stronger result which implies an $O(d)$ upper bound on the above quantity.

More related to the present question is Bang's lemma [1951], which arose in the context of the well-known plank problem. Its simplest form [Ball 2001] states the following: *If $u_1, \dots, u_n$ are unit vectors in $\mathbb{R}^d$, and the signs $\varepsilon_i = \pm 1$ are chosen so as to maximize the norm $|\sum_1^n \varepsilon_i u_i|$, then $|\langle u_k, \sum_1^n \varepsilon_i u_i \rangle| \geqslant 1$ holds for every k.* Note, however, that this only implies

$$\min \max \left| \sum_1^n \varepsilon_i u_i \right| \geqslant \sqrt{n}.$$

The same estimate follows by taking the average of $\left|\sum \varepsilon_i u_i\right|^2$ over all possible sign sequences.

It remains an open question to determine the extremal point configurations of (1). In general, we have very little information about the extremizers, and a complete description of them can only be hoped for in a few special cases. For $n = d$, the above averaging argument yields that the extremum is uniquely achieved by the vectors e_i of an orthonormal basis, which satisfy $\min \max \left|\sum_1^n \varepsilon_i e_i\right| = \sqrt{d}$. For $n = d+1$, natural intuition and numerical experiments suggest that each extremal configuration is, up to sign changes, the union of the vertex set of an even dimensional regular simplex and an orthonormal basis of the orthogonal complement of its subspace. The following conjecture was stated in a slightly incorrect form in [Brugger et al. 2018] and has been corrected by [Polyanskii 2019].

Conjecture 1. *For any $d \geqslant 1$, and for any configuration of $d+1$ unit vectors $u_i, \dots, u_{d+1} \in S^{d-1}$, there exists a sequence of signs $\varepsilon \in \{\pm 1\}^{d+1}$ so that*

$$\left| \sum_{i=1}^{d+1} \varepsilon_i u_i \right| \geqslant \sqrt{d+2}.$$

Moreover, the above estimate is sharp if and only if, up to sign changes, $(u_i)_1^{d+1}$ is the union of the vertex set of a regular simplex centered at the origin in a subspace H, and an orthonormal basis of $H^\perp$, where H is an even dimensional linear subspace of $\mathbb{R}^d$.

5. Planar case: equidistributed sets

In the plane, finding $M^p(\omega_n)$ is equivalent to maximizing the sum of the p-th powers of the Euclidean distances from a variable unit vector to n fixed unit vectors via the following transformation. Identify S^1 with the complex unit circle T, and let $u_i = e^{i\alpha_i}$, $v = e^{i\phi}$. Introduce $\tilde{u}_i = e^{i2\alpha_i} = u_i^2$ and $\tilde{v} = e^{i(2\phi+\pi)} = -e^{i2\phi}$. Then

$$|\tilde{v} - \tilde{u}_i| = 2\left|\sin \frac{2(\phi+\pi/2) - 2\alpha_i}{2}\right| = 2\left|\cos(\alpha_i - \phi)\right| = 2\left|\langle v, u_i \rangle\right|. \tag{6}$$

Therefore, $M^p(\omega_n)$ may be obtained by finding the point $\tilde{v} \in S^1$ for which $\sum |\tilde{u}_i - \tilde{v}|^p$ is maximal.

Accordingly, we introduce the following quantities for an n-point configuration $\omega_n = \{z_1, \dots, z_n\} \subset T$:

$$\widetilde{U}^p(\omega_n, z) = \sum_{i=1}^{n} |z - z_i|^p$$
$$\widetilde{M}^p(\omega_n) = \max_{z \in T} \widetilde{U}^p(\omega_n, z)$$
$$\widetilde{M}_n^p = \min_{\omega_n \in T^n} \widetilde{M}^p(\omega_n).$$

Analogues of the above notions with negative p are called the Riesz potential and polarization quantities, and have been extensively studied before; see, e.g., [Erdélyi and Saff 2013] for general results in that direction.

By (6), $\widetilde{M}_n^p = 2^p M_n^p(S^1)$, and thus Theorem 1 implies the lower bound

$$\widetilde{M}_n^p \geqslant 2^p \cdot n\mu_{2,p} = n \cdot \tilde{\mu}_p, \tag{7}$$

where

$$\tilde{\mu}_p = 2^p \mu_{2,p} = \frac{2^p \Gamma\left(\frac{p+1}{2}\right)}{\sqrt{\pi}\,\Gamma\left(\frac{p}{2}+1\right)} = \frac{\Gamma(p+1)}{\Gamma\left(\frac{p}{2}+1\right)^2} = \binom{p}{p/2},$$

using the Legendre duplication formula and the natural extension of the binomial coefficient to nonintegers.

The above notions have been studied by Stolarsky [1975a; 1975b], who determined $\widetilde{M}^p(\omega_n^*)$ for $0 < p < 2n$, where ω_n^* is an *equidistributed set* on T:

$$\omega_n^* = \{1, \xi, \xi^2, \dots, \xi^{n-1}\},$$

where $\xi = e^{i2\pi/n}$. He also determined $\widetilde{M}_n^p$ for $n = 3$ and $0 < p \leqslant 2$. Nikolov and Rafailov [2011] determined the value $\widetilde{M}_n^p$ for $n = 3$ and arbitrary $p > 0$ and also discussed the critical points of $\widetilde{U}^p(\omega_n^*, z)$ on T. They showed that if p is an even integer with $2 \leqslant p \leqslant 2n-2$, then $\widetilde{U}^p(\omega_n^*, z)$ is constant on T. Moreover, they proved [Nikolov and Rafailov 2013] that this property (holding for all even integer exponents between 2 and $2n$) characterizes equidistributed sets. They conjectured that the condition holding solely for $p = 2n-2$ is already sufficient for characterization. This was verified by Bosuwan and Ruengrot [2017] (for the case $\omega_n \subset T$, which we assumed anyway). The authors also proved that for $p = 2, 4, \dots, 2n-2$, $\widetilde{M}_n^p$ is attained at the configurations ω_n which satisfy

$$\sum_{z \in \omega_n} z^j = 0$$

for every $j = 1, 2, \dots, n-1$.

On the other hand, Hardin, Kendall and Saff [Hardin et al. 2013], proving a conjecture in [Ambrus et al. 2013], proved the polarization optimality of equidistributed sets on the unit circle for convex potentials. Recently, their result has been extended to more general settings [Farkas et al. 2018].

Proof of Proposition 5. By (6), finding the polarization constants is equivalent to maximizing the quantity $\sum|\tilde{u}_i-\tilde{v}|^p$.

First, we assume $0<p\leqslant 1$. Let $g(t)=-|\sin(t/2)|^p+1$. Then g is nonnegative, nonincreasing and strictly convex on $[0,2\pi]$. Moreover,

$$\tfrac{1}{2}\sum|\tilde{v}-\tilde{u}_i|^p=-\sum g(\psi-\beta_i)+n,$$

where $\tilde{v}=e^{i\psi}$ and $\tilde{u}_i=e^{i\beta_i}$. Therefore, $\widetilde{M}^p(\omega_n)$ is attained when $\sum g(\psi-\beta_i)$ is minimized. Theorem 1 of [Hardin et al. 2013] implies that $\widetilde{M}_n^p$ is achieved by equidistributed points sets; moreover, these are the only optimizers. Accordingly, the lines spanned by an optimal configuration for $M_n^p(S^1)$ are evenly spaced. It is easy to check [Stolarsky 1975a] that for such a configuration, the maximum of the potential function $U^p(\omega_n,\cdot)$ is attained at one of the base points for odd n, and at the midpoint between two consecutive base points for even n.

The case $p=2,4,\dots,2n-2$ is discussed in [Bosuwana and Ruengrot 2017, Theorem 2]. We also give a short proof here. It was shown in [Nikolov and Rafailov 2011] that for these values of p, $\widetilde{U}^p(\omega_n^*,z)$ is constant on T. Therefore, for any n-point configuration ω_n on T,

$$\widetilde{M}^p(\omega_n)\geqslant\frac{1}{n}\sum_{z\in\omega_n^*}\widetilde{U}^p(\omega_n,z)=\frac{1}{n}\sum_{v\in\omega_n}\widetilde{U}^p(\omega_n^*,v)=\widetilde{M}^p(\omega_n^*).\qquad\square$$

For equally distributed point sets, it was proven by Stolarsky [1975a] and by Nikolov and Rafailov [2011] that $\widetilde{M}^p(\omega_n^*)=\max_{z\in T}\sum_{k=0}^{n-1}|z-\xi^k|^p$ is (not necessarily uniquely) attained at z which is, depending on p, either one of the base points ξ^k or is the midpoint between two consecutive base points. More precisely, introduce the *positive-exponent Riesz energy* of $\omega_n\subset T$ defined by

$$E^p(\omega_n)=\sum_{j,k=1}^{n}|z_j-z_k|^p$$

(note that in the previous articles related to Riesz energies, the exponent is taken to be $-p$, therefore the above quantity becomes the negative exponent Riesz energy). For brevity, let $E_n^p=E^p(\omega_n^*)$. Theorem 1.2 of [Stolarsky 1975a] states that for $0<p<2n$, taking $m=\lfloor p/2\rfloor$,

$$\widetilde{M}^p(\omega_n^*)=\begin{cases}\dfrac{E_n^p}{n}, & m\text{ odd},\\[2ex] \dfrac{E_{2n}^p}{2n}-\dfrac{E_n^p}{n}, & m\text{ even}.\end{cases}\tag{8}$$

Furthermore, for $p \geqslant 2n$, Theorem 2 of [Nikolov and Rafailov 2011] implies that

$$\widetilde{M}^p(\omega_n^*) = \begin{cases} \dfrac{E_n^p}{n}, & n \text{ even}, \\ \dfrac{E_{2n}^p}{2n} - \dfrac{E_n^p}{n}, & n \text{ odd}. \end{cases} \tag{9}$$

The asymptotic expansion of E_n^p was given by Brauchart, Hardin and Saff [Brauchart et al. 2009]:

$$E_n^p = n^2 \tilde{\mu}_p + \mathcal{O}(n^{1-p}), \quad n \to \infty.$$

This, along with (7)–(9), and the fact $\widetilde{M}_n^p \leqslant \widetilde{M}^p(\omega_n^*)$, implies that $\widetilde{M}_n^p \sim n\tilde{\mu}_p = n\binom{p}{p/2}$ as $n \to \infty$.

Proposition 5 shows that for integer exponents p with $0 < p < 2n$, $\widetilde{M}_n^p = \widetilde{M}^p(\omega_n^*)$. For these exponents, we provide the explicit value of E_n^p (and, by (8) and (9), of $\widetilde{M}^p(\omega_n^*)$) by a combinatorial argument. If $p = 2m$ for some integer $m < n$,

$$\begin{aligned} E_n^p &= \sum_{j=0}^{n-1} \sum_{k=0}^{n-1} |\xi^j - \xi^k|^{2m} = \sum_{j=0}^{n-1} \sum_{k=0}^{n-1} |1 - \xi^{k-j}|^p \\ &= n \sum_{j=0}^{n-1} |1 - \xi^j|^{2m} = n \sum_{j=0}^{n-1} (1 - \xi^j)^m (1 - \xi^{-j})^m. \end{aligned}$$

Using binomial expansion gives

$$\begin{aligned} E_n^p &= n \sum_{j=0}^{n-1} \sum_{r,s=0}^{m} \binom{m}{r}\binom{m}{s} (-1)^{r+s} (\xi^j)^{r-s} \\ &= n \sum_{r,s=0}^{m} \binom{m}{r}\binom{m}{s} (-1)^{r+s} \sum_{j=0}^{n-1} (\xi^{r-s})^j \\ &= n^2 \sum_{r}^{m} \binom{m}{r}^2 = n^2 \binom{2m}{m} = n^2 \tilde{\mu}_p. \end{aligned}$$

On the other hand, assume that p is odd with $0 < p < 2n$. Noting that for $t \in [0, 2\pi)$,

$$|1 - e^{it}| = i e^{-it/2}(1 - e^{it}),$$

it follows that

$$\begin{aligned} E_n^p &= n \sum_{j=0}^{n-1} |1 - \xi^j|^p = n\, i^p \sum_{j=0}^{n-1} \xi^{-pj/2} (1 - \xi^j)^p \\ &= n\, i^p \sum_{j=0}^{n-1} \sum_{s=0}^{p} \binom{p}{s} (-1)^s \xi^{(s-p/2)j} = n\, i^p \sum_{s=0}^{p} \binom{p}{s} (-1)^s \sum_{j=0}^{n-1} \xi^{(s-p/2)j}. \end{aligned}$$

Now, using that p is odd, we have

$$\begin{aligned} E_n^p &= n\, i^p \sum_{s=0}^{p} \binom{p}{s} (-1)^s \frac{\xi^{n(s-p/2)}-1}{\xi^{s-p/2}-1} \\ &= 2n\, i^p \sum_{s=0}^{p} \binom{p}{s} \frac{(-1)^s}{1-\xi^{s-p/2}}, \end{aligned}$$

since $\xi^{ns}=1$ and $\xi^{-np/2}=-1$. Observing the symmetry of this sum about $p/2$, we can compute

$$\begin{aligned} E_n^p &= 4n\, i^{p+1}\, \operatorname{Im}\biggl(\sum_{s=0}^{\lfloor p/2 \rfloor} \binom{p}{s} \frac{(-1)^s}{1-\xi^{s-p/2}} \biggr) \\ &= n\,(-1)^{(p-1)/2} \sum_{s=0}^{p} \binom{p}{s} (-1)^s \cot\Bigl(\Bigl(\frac{p}{2}-s\Bigr)\frac{\pi}{n}\Bigr). \end{aligned}$$

For $p=1$, this gives $E_n^p = 2n\cot\bigl(\frac{\pi}{2n}\bigr) \sim \frac{4n^2}{\pi} = n^2\tilde{\mu}_1$. In general, as $n\to\infty$, the Taylor expansion of the cotangent gives

$$E_n^p = n\left| \sum_{s=0}^{p} \binom{p}{s} (-1)^s \frac{n}{\pi\bigl(\frac{p}{2}-s\bigr)} + \mathcal{O}(1/n) \right| = n^2\tilde{\mu}_p + \mathcal{O}(1),$$

where the second equality follows from a series computation described in Proposition 2.3 of [Garrappa 2007].

We conclude the paper by restating the following natural conjecture of Bosuwan and Ruengrot [2017], which is also supported by our numerical experiments:

Conjecture 2. *For any $n \geqslant 1$, the vector systems achieving $\widetilde{M}_n^p$ are equally distributed on the circle for every $p \in \mathbb{R}^+ \setminus \{2, 4, \dots, 2n-2\}$.*

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L^p-OPERATOR ALGEBRAS WITH APPROXIMATE IDENTITIES, I

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We initiate an investigation into how much the existing theory of (nonselfadjoint) operator algebras on a Hilbert space generalizes to algebras acting on L^p-spaces. In particular we investigate the applicability of the theory of real positivity, which has recently been useful in the study of L^2-operator algebras and Banach algebras, to algebras of bounded operators on L^p-spaces. In the process we answer some open questions on real positivity in Banach algebras from work of Blecher and Ozawa.

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1. Introduction

In a series of recent papers (see, e.g., [Phillips 2012; 2013a; 2013b; 2014a; 2014b]) the second author has pointed out that the study of algebras of bounded operators on L^p-spaces, henceforth, *L^p-operator algebras*, has been somewhat overlooked, and has initiated the study of these objects. Subsequently others have followed him into this inquiry (for example, Gardella, Thiel, Lupini, and Viola; see, e.g., [Gardella and Thiel 2015a; 2015b; 2019; Gardella and Lupini 2017; Phillips and Viola 2017]). However, as he has frequently stated, these investigations have been very largely focused on examples; one still lacks an abstract general theory in this setting.

Here and in a sequel in preparation we initiate an investigation into how much the existing theory of (nonselfadjoint) L^2-operator algebras (see, e.g., [Arveson 1969; Blecher and Le Merdy 2004; Blecher and Read 2011]) generalizes to the L^p case. We restrict ourselves almost exclusively to the "isometric theory"; we may pursue the isomorphic theory elsewhere. In addition to establishing some general facts about L^p-operator algebras, the main goal of the present paper is to investigate to what extent the first author's theory of real positivity (developed with Read, Neal, Ozawa, and others; see, e.g., [Blecher and Read 2011; 2013; 2014; Blecher and Ozawa 2015]), is applicable to L^p-operator algebras, particularly those which are approximately unital, that is, have contractive approximate identities. As an easy motivation, notice that the canonical approximate identity for the compact operators $\mathbb{K}(l^p)$ is real positive, and the real positive elements span $B(L^p([0, 1]))$ (as they do any unital Banach algebra).

The theory of real positivity was developed as a tool for generalizing certain parts of C^*-algebra theory to more general algebras. In [Blecher and Ozawa 2015] this was extended to Banach algebras (see also [Blecher 2016] for a survey and some additional results). All this theory of course therefore applies to L^p-operator algebras. We refer to the first of these papers frequently, although most of our paper may be read without a deep familiarity with that paper.

Some parts of [Blecher and Ozawa 2015] applied only to certain classes of Banach algebras defined there, which were shown to behave in some respects similarly to L^2-operator algebras. For example, a nonunital approximately unital Banach algebra A was defined there to be *scaled* if the set of restrictions to A of states on the multiplier unitization A^1 equals the quasistate space $Q(A)$ of A (that is, the set of $\lambda\varphi$ for $\lambda \in [0, 1]$ and φ a norm 1 functional on A that extends to a state on A^1). All unital Banach algebras are scaled. In [loc. cit.], there are several pretty equivalent conditions for a Banach algebra to be scaled (see the start of our Section 6 for some of these), and this class of Banach algebras was shown to have several nice theoretical features, such as a Kaplansky density type theorem. Thus it is natural to ask the following:

(1) To which of the classes defined in [Blecher and Ozawa 2015] do L^p-operator algebras belong?

(2) For those classes in [loc. cit.] to which they do not belong, to what extent do the theorems for those classes from that paper still hold for L^p-operator algebras?

(3) To what extent do other parts of the theory of L^2-operator algebras hold for L^p-operator algebras?

We focus mostly here on the parts of the theory of Blecher with Read, Neal, and others referred to above, that were not already extended to the general classes considered in [Blecher and Ozawa 2015]. For example, one may ask if the material in Section 4 of that paper, and in particular the theory of hereditary subalgebras, improves (that is, becomes closer to the L^2-operator case) for L^p-operator algebras. Similarly, one may ask about the *noncommutative topology* (in the sense of Akemann, Pedersen, L. G. Brown, and others) of L^p-operator algebras. In papers of Blecher with Read, Neal, and others referred to above, Akemann's noncommutative topology of C^*-algebras was fused with the classical theory of (generalized) peak sets of function algebras to create a *relative* noncommutative topology for closed subalgebras of C^*-algebras that has proved to have many applications. Examples given in [Blecher and Ozawa 2015] show that not much of this will extend to general Banach algebras, and it is natural to ask if L^p-operator algebras are better in this regard. Most of the present paper and the sequel in preparation is devoted to answering these questions. In the process we also answer some open questions from [loc. cit.].

We admit from the outset that for $p \neq 2$, and for some significant part of the theory, the answer to question (2) above is, so far, in the negative. This may change somewhat in the future, for example if we were able to solve some of the open problems listed at the end of this paper. It should also be admitted that for $p \neq 2$, the "projection lattice" of $B(L^p(X, \mu))$ is problematic from our perspective (see Example 3.2 and the sequel paper), in contrast to the projection lattices of von Neumann algebras and L^2-operator algebras.

Concerning question (1), several classes of Banach algebras introduced and considered in [Blecher and Ozawa 2015] coincide for approximately unital L^p-operator algebras. Indeed the classes of *scaled* and *M-approximately unital* Banach algebras defined in that paper coincide for L^p-operator algebras, and these also turn out to be the approximately unital L^p-operator algebras which satisfy the aforementioned Kaplansky density property. (We remark that the usual Kaplansky density theorem variants for C^*-algebras can be shown to follow easily from the weak* density of the subset of interest in A within the matching set in A^{**}. Our Kaplansky density theorems have the latter flavor.) We show that some approximately unital L^p-operator algebras are scaled and others are not. This answers the questions from [loc. cit.] as to whether every approximately unital Banach algebra is scaled, or has a Kaplansky density property. Also, nonscaled approximately unital L^p-operator algebras may contain no real positive elements (whereas it was shown in [loc. cit.]

that if they are scaled then there is an abundance of real positive elements, e.g., every element in A is a difference of two real positive elements).

Concerning question (3) above, indeed, some aspects of the theory improve. For example, Section 4 of [loc. cit.] improves drastically in our setting, and indeed L^p-operator algebras do support a basic theory of noncommutative topology and hereditary subalgebras, unlike general Banach algebras. This is worked out in the sequel paper in preparation, where the reader will find many more positive results than in the present paper. It is worth remarking that the methods used here do not seem to extend far beyond the class of L^p-operator algebras as we will discuss elsewhere. However, most of our results for L^p-operator algebras in Sections 2 and 4 do generalize to the class of SQ_p*-operator algebras*, by which we mean closed algebras of operators on an SQ_p-space, that is, a quotient of a subspace of an L^p-space. (See, e.g., [Le Merdy 1996] and [Junge 1996]. We thank Eusebio Gardella for suggesting SQ_p-spaces after we listed in a talk the properties needed for our results to work.)

On the other hand, except cosmetically, not much to speak of in Section 3 of [Blecher and Ozawa 2015] improves for L^p-operator algebras, in the sense of becoming significantly more like the L^2-operator algebra case. However several of the concepts appearing throughout the latter paper become much simpler in our setting. For example as we said above, three of the main classes of Banach algebras considered there coincide. Also as we shall see the subscript and superscript $\mathfrak{e}$ which appear often in that paper may be erased in our setting, since we are able to show that all L^p-operator algebras are Hahn–Banach smooth. Then of course the Arens regularity of L^p-operator algebras means that many irritating features of the bidual appearing in that paper disappear, such as mixed identities in A^{**}.

We now describe the contents of the present paper.

We will be assuming that $p \in (1, \infty) \setminus \{2\}$ in all results in the paper unless stated to the contrary. As usual $\frac{1}{p} + \frac{1}{q} = 1$. In the remainder of Section 1 we give some notation and basic definitions. In Section 2 we discuss further notation and background. We also collect a large number of useful general facts, many of which are well known. They concern topics such as duals, bidual algebras, the multiplier unitization, states and real positivity, hermitian elements, representations, etc. We just mention one sample result from this section: if A is an approximately unital L^p-operator algebra with $p \in (1, \infty)$, then there exists a measure space (X, μ) and a unital isometric representation $\theta : A^{**} \to B(L^p(X, \mu))$ which is a weak* homeomorphism onto its range, and such that $\theta(A)$ acts nondegenerately on $L^p(X, \mu)$.

In Section 3 we list the main examples of L^p-operator algebras which we use in this paper for counterexamples, as well as some other basic examples not in the literature. Some of these have real positive approximate identities, and others do not. We also expose some of the aforementioned bad properties of the "projection lattice" of $B(L^p(X, \mu))$.

Section 4 contains many miscellaneous results. Here is a sample of these. We show that the quotient of an L^p-operator algebra by an approximately unital closed ideal satisfying a simple extra condition is again (isometrically) an L^p-operator algebra. An example is presented to prove that this can fail if the ideal is only assumed to be closed and approximately unital. We show that an L^p-operator algebra A need not have a unique unitization, unlike in the case $p = 2$ (Meyer's unitization theorem). However there is a unique unitization if we restrict attention to nondegenerately represented approximately unital L^p-operator algebras. The nonuniqueness above is related to the fact that when $p \neq 2$ the Cayley transform can take a real positive element of A to an element of norm greater than 1. We study support idempotents of elements of A and their properties. We also give some important consequences of the strict convexity of L^p-spaces. For example, a state on a unital L^p-operator algebra that takes the value zero at a real positive idempotent e is zero on the left or right ideal generated by e. We also deduce that an L^p-operator algebra is Hahn–Banach smooth in its multiplier unitization. These results have several significant applications in this paper and its sequel. For example they yield in Section 4 several foundational properties of states and state extensions.

In Section 5 and Section 6 we discuss M-ideals and scaled Banach algebras. Our main result here is that in the setting of approximately unital L^p-operator algebras, the classes of scaled algebras and M-approximately unital algebras coincide. These are also the algebras which satisfy the aforementioned Kaplansky density property, as we show in Section 7. We will see for example that the algebra $\mathbb{K}(L^p(X, \mu))$ of compact operators is in this class if and only if μ is purely atomic (Proposition 5.2). The L^p-operator algebras with a hermitian contractive identity are also in this class. We also show for example in these sections that every M-ideal J in an approximately unital L^p-operator algebra A is an approximately unital closed ideal. Moreover, if in addition A is scaled then so is J (this follows from Theorem 5.4 (3)(a)).

At the end of the paper we provide an index listing some of the main definitions in this paper and where they may be found.

In the sequel paper in preparation we show that the theory of one-sided ideals, hereditary subalgebras, open projections, etc. for L^p-operator algebras is quite similar to the (nonselfadjoint) L^2-operator algebra case. This is particularly so for certain large classes of L^p-operator algebras. We feel that this is important, since hereditary subalgebras play a large role in modern C^*-algebra theory, and thus hopefully will be important for L^p-operator algebras too.

We end our introduction with a few definitions and basic lemmas.

We set $\mathbb{R}_+ = [0, \infty)$.

Notation 1.1. Let E be a normed vector space. Then $\mathrm{Ball}(E)$ is the closed unit ball of E, that is,

$$\mathrm{Ball}(E) = \{\xi \in E : \|\xi\| \leq 1\}.$$

Notation 1.2. Let $p \in [1, \infty]$. Let E and F be normed vector spaces. We denote by $E \oplus^p F$ their L^p direct sum, that is, the algebraic direct sum $E \oplus F$ with the norm given for $\xi \in E$ and $\eta \in F$ by $\|(\xi, \eta)\| = (\|\xi\|^p + \|\eta\|^p)^{1/p}$ if $p < \infty$ and $\|(\xi, \eta)\| = \max(\|\xi\|, \|\eta\|)$ if $p = \infty$.

Although many of our Banach algebras have identities of norm greater than 1, the adjectives "unital" or "approximately unital" for a Banach algebra will carry a norm 1 requirement.

Definition 1.3. A *unital* Banach algebra is a Banach algebra with an identity 1 such that $\|1\| = 1$.

Definition 1.4. A *cai* in a Banach algebra is a contractive approximate identity, that is, an approximate identity $(e_t)_{t \in \Lambda}$ such that $\|e_t\| \leq 1$ for all $t \in \Lambda$. An *approximately unital* Banach algebra is a Banach algebra which has a cai.

When we write L^p or $L^p(X)$ we mean the L^p-space of some measure space (X, μ).

Definition 1.5. Recall that a Banach space E is *strictly convex* if whenever $\xi, \eta \in E \setminus \{0\}$ satisfy

$$\|\xi + \eta\| = \|\xi\| + \|\eta\|,$$

then there is $\lambda \in (0, \infty)$ such that $\xi = \lambda\eta$, and *smooth* if for given $\xi \in E$ with $\|\xi\| = 1$, there is a unique $\eta \in \mathrm{Ball}(E^*)$ with $\langle \xi, \eta \rangle = 1$.

If $1 < p < \infty$, then $L^p(X)$ is strictly convex (by the converse to Minkowski's inequality). Moreover, still assuming $1 < p < \infty$, the space $L^p(X)$ is smooth, with η above given by the function

$$\eta(x) = \begin{cases} \overline{\xi(x)}|\xi(x)|^{p-2}, & \xi(x) \neq 0 \\ 0, & \xi(x) = 0 \end{cases}$$

in $L^q(X)$. We will frequently use the fact that $L^p(X)$ is smooth and strictly convex if $1 < p < \infty$.

Definition 1.6. Let $p \in [1, \infty)$. An *L^p-operator algebra* is a Banach algebra which is isometrically isomorphic to a norm closed subalgebra of the algebra of bounded operators on $L^p(X, \mu)$ for some measure space (X, μ). When $p = 2$ we simply refer to an *operator algebra*. (See the beginning of Section 2.1 of [Blecher and Le Merdy 2004], except that we do not consider matrix norms in the present paper.)

Definition 1.7. Let A be an L^p-operator algebra (not necessarily approximately unital). We say that an L^p-operator algebra B is an *L^p-operator unitization of A* if either A is unital and $B = A$, or if A is nonunital, B is unital (in particular, by our convention, $\|1\| = 1$), and A is a codimension one ideal in B.

Definition 1.8 [Blecher and Le Merdy 2004, (A.9) on p. 364]. Let A be a nonunital approximately unital Banach algebra (as in Definition 1.4). We define its *multiplier unitization* A^1 to be the usual unitization $A + \mathbb{C} \cdot 1$ with the norm

$$\|a + \lambda 1\|_{A^1} = \sup(\{\|ac + \lambda c\| : c \in \operatorname{Ball}(A)\})$$

for $a \in A$ and $\lambda \in \mathbb{C}$. If A is already unital then we set $A^1 = A$.

Remark 1.9. We recall the following easy standard facts.

(1) If A is an approximately unital Banach algebra, then the standard inclusion of A in A^1 is isometric.

(2) Let A be a Banach algebra, and let $(e_t)_{t \in \Lambda}$ be any cai in A. Then

$$\|a + \lambda 1\|_{A^1} = \lim_t \|ae_t + \lambda e_t\| = \sup_t \|ae_t + \lambda e_t\|.$$

(3) If A is any nonunital Banach algebra, and B is a unital Banach algebra which contains A as a codimension 1 subalgebra, then the map $\chi_0 : B \to \mathbb{C}$, given by $\chi_0(a + \lambda 1_B) = \lambda$ for $a \in A$ and $\lambda \in \mathbb{C}$, is contractive.

(4) If A is any nonunital Banach algebra with a cai, and B is a unital Banach algebra which contains A as a codimension 1 subalgebra, then the map $\psi : B \to A^1$, given by $\psi(a + \lambda 1_B) = a + \lambda 1_{A^1}$ for $a \in A$ and $\lambda \in \mathbb{C}$, is a contractive homomorphism. Thus A^1 has the smallest norm of any unitization. This follows, e.g., by a small variant of the proof of Lemma 1.10.

Lemma 1.10. *Suppose that A is a closed subalgebra of a nonunital approximately unital Banach algebra B, and suppose that A has a cai but is not unital. Then for all $a \in A$ and $\lambda \in \mathbb{C}$ we have $\|a + \lambda 1\|_{A^1} \le \|a + \lambda 1\|_{B^1}$.*

Proof. Clearly

$$\sup(\{\|ac + \lambda c\| : c \in \operatorname{Ball}(A)\}) \le \sup(\{\|ac + \lambda c\| : c \in \operatorname{Ball}(B)\}),$$

as desired. □

It is easy to find examples showing that the homomorphism above need not be isometric, for example, with notation as in Example 3.2 (or Example 3.5) below, $\mathbb{C}\, e_2 \otimes c_0 \subseteq M_2^p \otimes c_0$. However we have the following result.

Lemma 1.11. *Let A and B be nonunital approximately unital Banach algebras. Let $\varphi : A \to B$ be a contractive (resp. isometric) homomorphism. Suppose that there is a cai $(e_t)_{t \in \Lambda}$ for A such that $(\varphi(e_t))_{t \in \Lambda}$ is a cai for B. Then the obvious unital homomorphism $A^1 \to B^1$ between the multiplier unitizations is contractive (resp. isometric).*

Proof. If $a \in A$ and $\lambda \in \mathbb{C}$ then

$$\|\varphi(a)\varphi(e_t) + \lambda\varphi(e_t)\| \le \|ae_t + \lambda e_t\|.$$

In the isometric case this is an equality. Taking limits over t and using Remark 1.9 (2) gives the result. □

We recall two further standard facts. The first is that the relation $\mathbb{K}(L^2(X))^{**} = B(L^2(X))$ is true with 2 replaced by any $p \in (1, \infty)$.

Definition 1.12. We recall that the bidual A^{**} of a Banach algebra has in general two canonical products, called the left and right Arens products [Palmer 1994, Definition 1.4.1]. We say that A is *Arens regular* if these two products coincide.

Theorem 1.13. *Let $p \in (1, \infty)$ and let (X, μ) be a measure space. Let $q \in (1, \infty)$ satisfy $\frac{1}{p} + \frac{1}{q} = 1$. Then:*

(1) *There is an isometric isomorphism $\mathbb{K}(L^p(X, \mu))^* \to L^q(X, \mu) \widehat{\otimes} L^p(X, \mu)$ (projective tensor product) which for $\rho \in L^p(X, \mu)$ and $\eta \in L^q(X, \mu)$ sends $\eta \otimes \rho$ to the operator $\xi \mapsto \langle \xi, \eta \rangle \rho$.*

(2) *There is an isometric algebra isomorphism from $\mathbb{K}(L^p(X, \mu))^{**}$ (with either Arens product) onto $B(L^p(X, \mu))$ which extends the inclusion $\mathbb{K}(L^p(X, \mu)) \subseteq B(L^p(X, \mu))$.*

Proof. This follows from results of Grothendieck, as described in the theorem on page 828 of [Palmer 1985], the discussion after that, and Theorems 1–3 there. It is stated there that any Banach space X such that X and X^* have the Radon–Nikodym property and the approximation property, satisfies [Palmer 1985, Theorem 1] and the aforementioned theorem of Grothendieck, giving (1), and also the case of (2) for the first Arens product. By [Palmer 1985, Theorem 2], if X is also reflexive then $\mathbb{K}(X)$ is Arens regular, so (2) holds as stated. See also the discussion on page 24, Corollary 4.13, and Theorem 5.33 of [Ryan 2002] (and we thank M. Mazowita for this reference). The explicit formulas there are useful to check directly the Arens product assertion. One needs to know that $L^p(X, \mu)$ has the Radon–Nikodym property and the approximation property, and this follows, e.g., from [Ryan 2002, Example 4.5 and Corollary 5.45]. □

We remark that the last result and proof works with L^p replaced by any reflexive space with the approximation property, since reflexive spaces have the Radon–Nikodym property, and indeed [Ryan 2002, Corollary 4.7] implies that if E is reflexive and has the approximation property, then so does E^*.

By Theorem 1.13, a net $(x_t)_{t \in \Lambda}$ in $B(L^p(X))$ converges weak* to x if and only if, with $\frac{1}{p} + \frac{1}{q} = 1$,

$$\sum_{k=1}^{\infty} \langle x_t \xi_k, \eta_k \rangle \to \sum_{k=1}^{\infty} \langle x \xi_k, \eta_k \rangle$$

for all $\xi_1, \xi_2, \ldots \in L^p(X)$ and $\eta_1, \eta_2, \ldots \in L^q(X)$ with $\sum_{k=1}^{\infty} \|\xi_k\|_p \|\eta_k\|_q < \infty$ (or equivalently, by the usual trick, with $\sum_{k=1}^{\infty} \|\xi_k\|_p^p < \infty$ and $\sum_{k=1}^{\infty} \|\eta_k\|_q^q < \infty$).

If $(x_t)_{t\in\Lambda}$ is bounded then by Banach duality principles this is equivalent to $x_t \to x$ in the weak operator topology, that is, $\langle x_t\xi, \eta\rangle \to \langle x\xi, \eta\rangle$ for all $\xi \in L^p(X)$ and $\eta \in L^q(X)$. We will not use this here but it is well known that essentially the usual L^2-operator proof shows that the weak operator closure of a convex set in $B(L^p([0, 1]))$ equals the strong operator closure. Indeed, for a Banach space E, the strong operator continuous linear functionals on $B(E)$ are the same as those that are weak operator continuous.

The argument for the following well known lemma will be reused several times, once in the form of an approximate identity bounded by M converging weak* to an identity in A^{**} of norm at most M.

Lemma 1.14. *Let A be an approximately unital Arens regular Banach algebra. Then A^{**} has an identity $1_{A^{**}}$ of norm 1, and any cai for A converges weak* to $1_{A^{**}}$.*

Proof. The argument follows the proof of [Blecher and Le Merdy 2004, Proposition 2.5.8]. Since identities are unique if they exist, it suffices to show that every subnet of any cai in A has in turn a subnet which converges to an identity for A^{**}. Using Alaoglu's theorem and since a subnet of a cai is a cai, one sees that it is enough to show that if $e \in A^{**}$ is the weak* limit of a cai, then e is an identity for A^{**}. Multiplication on A^{**} is separately weak* continuous by [Blecher and Le Merdy 2004, 2.5.3], so $ea = ae = a$ for all $a \in A$. A second application of separate weak* continuity of multiplication shows that this is true for all $a \in A^{**}$. $\square$

2. Notation, background, and general facts

2A. *Dual and bidual algebras.*

Lemma 2.1. *Let $p \in (1, \infty)$. Let A be an L^p-operator algebra* (*resp.* SQ_p*-operator algebra*)*. Then*:

(1) *A is Arens regular.*

(2) *Multiplication on A^{**} is separately weak* continuous.*

(3) *A^{**} is an L^p-operator algebra* (*resp.* SQ_p*-operator algebra*)*.*

Proof. We first recall (Theorem 3.3 (ii) of [Heinrich 1980], or [Le Merdy 1996], or the remarks above Theorem 4.1 in [Daws 2010]) that any ultrapower of L^p-spaces (resp. SQ_p-spaces) is again an L^p-space (resp. SQ_p-space). In the SQ_p-space case this uses the well known fact that ultrapowers behave well with respect to subspaces and quotients (this is obvious for subspaces, for quotients see, e.g., the proof of Proposition 6.5 in [Heinrich 1980]). In particular, such an ultrapower is reflexive, so every L^p-space (resp. SQ_p-space) is superreflexive. (See Proposition 1 of [Daws 2004].)

Now let E be an L^p-space (resp. SQ_p-space). Theorem 1 of [Daws 2004] implies that $B(E)$ is Arens regular. The proof of Theorem 1 of [Daws 2004] embeds

$B(E)^{**}$ isometrically as a subalgebra of $B(F)$ for a Banach space F obtained as an ultrapower of $l^r(E)$ for an arbitrarily chosen $r \in (1, \infty)$ (called p in [Daws 2004]). We may choose $r = p$. Then $l^r(E)$ is isometrically isomorphic to an L^p-space (resp. SQ_p-space). Since ultrapowers of L^p-spaces (resp. SQ_p-spaces) are L^p-spaces (resp. SQ_p-spaces) as we said at the start of this proof, we have shown that $B(E)^{**}$ is an L^p- (resp. SQ_p-) operator algebra.

Now suppose that $A \subseteq B(E)$ is a norm closed subalgebra. Since $B(E)$ is Arens regular, A^{**} is a subalgebra of $B(E)^{**}$ and A is Arens regular by [Blecher and Le Merdy 2004, 2.5.2]. It is now immediate that A^{**} is an L^p- (resp. SQ_p-) operator algebra. It also follows from [Blecher and Le Merdy 2004, 2.5.3] that multiplication on A^{**} is separately weak* continuous. $\square$

It follows from [Daws 2004, Proposition 8] that $B(L^1(X, \mu))$ is not Arens regular unless $L^1(X, \mu)$ is finite-dimensional.

Corollary 2.2. *Let $p \in (1, \infty)$ and let (X, μ) be a measure space. Then multiplication on $B(L^p(X, \mu))$ is separately weak* continuous.*

Proof. We have $\mathbb{K}(L^p(X, \mu))^{**} \cong B(L^p(X, \mu))$ by Theorem 1.13 (2). $\square$

Definition 2.3. Let $p \in (1, \infty)$. A *dual L^p-operator algebra* is a Banach algebra A with a predual such that there is a measure space (X, μ) and an isometric and weak* homeomorphic isomorphism from A to a weak* closed subalgebra of $B(L^p(X, \mu))$.

By Corollary 2.2, the multiplication on a dual L^p-operator algebra is separately weak* continuous.

Corollary 2.4. *Let $p \in (1, \infty)$ and let A be an L^p-operator algebra. Then A^{**} is a dual L^p-operator algebra.*

Proof. The embedding of $B(L^p(X, \mu))^{**}$ in Lemma 2.1 coming from the proof from [Daws 2004] is easily checked to be weak* continuous, hence a weak* homeomorphism onto its range by the Krein–Smulian theorem. Hence $B(L^p(X, \mu))^{**}$ is a dual L^p-operator algebra. It easily follows that A^{**} is too. $\square$

Lemma 2.5. *Let $p \in (1, \infty)$ and let A be a dual L^p-operator algebra. Then*:

(1) *The weak* closure of any subalgebra of A is a dual L^p-operator algebra.*

(2) *If A is approximately unital then A is unital.*

Proof. The proofs are essentially the same as in the case $p = 2$, as done in the proof of Proposition 2.7.4 of [Blecher and Le Merdy 2004]. $\square$

2B. ***States, hermitian elements, and real positivity.*** We take states to be as at the beginning of Section 2 of [Blecher and Ozawa 2015].

Definition 2.6. If A is a unital Banach algebra, then a *state* on A is a linear functional $\omega : A \to \mathbb{C}$ such that $\|\omega\| = \omega(1) = 1$. If A is an approximately unital Banach algebra, we define a *state* on A to be a linear functional $\omega : A \to \mathbb{C}$ such that $\|\omega\| = 1$ and ω is the restriction to A of a state on the multiplier unitization A^1 (Definition 1.8).

We denote by $S(A)$ the set of all states on A, and write $Q(A)$ for the quasistate space (that is, the set of $\lambda\varphi$ for $\lambda \in [0, 1]$ and $\varphi \in S(A)$).

If $\mathfrak{e} = (e_t)_{t\in\Lambda}$ is a cai for A, define

$$S_{\mathfrak{e}}(A) = \{\omega \in \mathrm{Ball}(A^*) : \omega(e_t) \to 1\}$$

and define

$$Q_{\mathfrak{e}}(A) = \{\lambda\varphi : \lambda \in [0, 1] \text{ and } \varphi \in S_{\mathfrak{e}}(A)\}.$$

If A is a C^*-algebra (unital or not), this definition gives the usual states and quasistates on A.

The first part of the following definition is Definition 2.6.1 of [Palmer 1994].

Definition 2.7. Let A be a unital Banach algebra, and let $a \in A$. We define the *numerical range* of a to be $\{\varphi(a) : \varphi \in S(A)\}$.

If E is a Banach space and $a \in B(E)$, we define the *spatial numerical range of a* to be

$$\{\langle a\xi, \eta\rangle : \xi \in \mathrm{Ball}(E) \text{ and } \eta \in \mathrm{Ball}(E^*) \text{ with } \langle \xi, \eta\rangle = 1\}.$$

There are other definitions of the numerical range. For our purposes, only the convex hull is important, and by Theorem 14 of [Lumer 1961], the convex hulls of the numerical range and the spatial numerical range of an element in $B(E)$ are always the same.

Definition 2.8 (see Definition 2.6.5 of [Palmer 1994] and the preceding discussion). Let A be a unital Banach algebra, and let $a \in A$. We say that a is *hermitian* if $\|\exp(i\lambda a)\| = 1$ for all $\lambda \in \mathbb{R}$.

If A is approximately unital we define the hermitian elements of A to be the elements in A which are hermitian in the multiplier unitization A^1 (Definition 1.8).

Lemma 2.9 (see [Palmer 1994, Theorem 2.6.7]). *Let A be a unital Banach algebra, and let $a \in A$. Then a is hermitian if and only if $\varphi(a) \in \mathbb{R}$ for all states φ of A.*

Lemma 2.10. *Let A be an approximately unital Banach algebra, and let $B \subseteq A$ be a closed subalgebra which contains a cai for A. Let $a \in B$. Then a is hermitian as an element of B if and only if a is hermitian as an element of A.*

Proof. By definition, we work in the multiplier unitizations. By Lemma 1.11, B^1 is isometrically a unital subalgebra of A^1. The Hahn–Banach theorem now shows that states on B^1 are exactly the restrictions of states on A^1. So the conclusion follows from Lemma 2.9. □

Definition 2.11. Let (X,μ) be a measure space that is not σ-finite. Recall that a function $f : X \to \mathbb{C}$ is locally measurable if $f^{-1}(E) \cap F$ is measurable for all Borel sets $E \subseteq \mathbb{C}$ and all subsets $F \subseteq X$ of finite measure. Two such functions are "locally a.e. equal" if they agree a.e. on any such set F. We interpret $L^\infty(X,\mu)$ as $L^\infty_{\mathrm{loc}}(X,\mu)$, the Banach space of essentially bounded locally measurable scalar functions mod local a.e. equality.

Further recall that a measure space (X,μ) is decomposable if X may be partitioned into sets X_i of finite measure for $i \in I$ such that a set F in X is measurable if and only if $F \cap X_i$ is measurable for every $i \in I$, and then $\mu(F) = \sum_{i\in I} \mu(F \cap X_i)$.

By, e.g., the corollary on page 136 in [Lacey 1974], any abstract L^p-space "is" decomposable, indeed it is isometric to a direct sum of L^p-spaces of finite measures. Thus, we may assume that all measure spaces (X,μ) are decomposable.

The following result is in the literature with extra hypotheses, such as if μ is σ-finite [Gardella and Thiel 2019, Lemma 5.2]. (See also, e.g., Theorem 4 and the remark following it in [Tam 1969], when in addition p is not an even integer.) We are not aware of a reference for the general case, but it is probably folklore.

Proposition 2.12. *Let $p \in [1,\infty) \setminus \{2\}$. Let (X,μ) be a decomposable measure space, and let $a \in B(L^p(X,\mu))$ be hermitian. Then there is a real-valued function $f \in L^\infty(X,\mu)$ such that a is multiplication by f, and such that $|f(x)| \le \|a\|$ for all $x \in X$.*

Proof. Let $X = \coprod_{i\in I} X_i$ be a partition of X into sets of finite measure as in the discussion of decomposability above. For $i \in I$ let $e_i \in B(L^p(X,\mu))$ be multiplication by χ_{X_i}. Since hermitian elements have numerical range contained in $\mathbb{R}$, we can apply Theorem 6 of [Payá-Albert 1982] (see the beginning of [Payá-Albert 1982] for the definitions and notation), to see that a commutes with e_i for all $i \in I$. One easily checks that $h = e_i a e_i$ is a hermitian element of $B(L^p(X_i,\mu))$. By the finite measure case of our result ([Gardella and Thiel 2019, Lemma 5.2]), there is a real-valued function $f_i \in L^\infty(X_i,\mu)$ such that h is multiplication by f_i.

We can clearly assume that f_i is bounded by $\|e_i a e_i\| \le \|a\|$. Now define $f : X \to \mathbb{R}$ by $f(x) = f_i(x)$ when $i \in I$ and $x \in X_i$. Then f is bounded by $\|a\|$, and is measurable by the choice of the partition of X. For $i \in I$ and $\xi \in L^p(X_i,\mu)$ we clearly have $a\xi = f\xi$. It follows from density of the linear span of the subspaces $L^p(X_i,\mu)$ that a is multiplication by f. $\square$

The σ-finite case is deduced in [Gardella and Thiel 2019] from the finite measure case of Lamperti's theorem [Fleming and Jamison 2003, Theorem 3.2.5] by considering the invertible isometries e^{ith} for $t \in [0,1]$. We mention another approach when p is not an even integer. It is known ([Delbaen et al. 1998, Corollary 1.8]; we thank Gideon Schechtman for this reference) that l^p doesn't contain a two-dimensional

Hilbert space, and so Theorem 4 of [Tam 1969] implies our conclusion. Lemma 11 of [Tam 1969] also proves the result in the case that μ has no atomic part in X_i.

Definition 2.13. Let A be a unital Banach algebra. Let $a \in A$. We say that a is *accretive* or *real positive* if the numerical range of a is contained in the closed right half plane. That is, $\mathrm{Re}(\varphi(a)) \geq 0$ for all states φ of A.

If instead A is approximately unital, we define the real positive elements of A to be the elements in A which are real positive in the multiplier unitization A^1.

In both cases, we denote the set of real positive elements of A by $\mathfrak{r}_A$.

Following page 8 of [Blecher and Ozawa 2015], we further define

$$\mathfrak{c}_{A^*} = \{\varphi \in A^* : \mathrm{Re}(\varphi(a)) \geq 0 \text{ for all } a \in \mathfrak{r}_A\}.$$

The elements of $\mathfrak{c}_{A^*}$ are called *real positive functionals* on A.

For other equivalent conditions for real positivity, see for example [Blecher 2016, Lemma 2.4 and Proposition 6.6].

We warn the reader that $\mathfrak{r}_{A^{**}}$ is defined after Lemma 2.5 of [Blecher and Ozawa 2015] to be a proper subset of the real positive elements in A^{**}, the set of elements of A^{**} which are real positive with respect to $(A^1)^{**}$. One should be careful with this ambiguity; fortunately it only pertains to second duals and seldom arises. (Also see Proposition 4.26.)

Lemma 2.14. *Let A be an approximately unital Banach algebra, and let $B \subseteq A$ be a closed subalgebra which contains a cai for A. Let $a \in B$. Then a is real positive as an element of B if and only if a is real positive as an element of A.*

Proof. The proof is the same as that of Lemma 2.10, using Definition 2.13 in place of Lemma 2.9. □

Lemma 2.15. *Let $p \in [1, \infty) \setminus \{2\}$, let A be an approximately unital L^p-operator algebra, and assume that the multiplier unitization A^1 is again an L^p-operator algebra. Let $a \in A$ be hermitian. Then there exist $b, c \in A$, each of which is both hermitian and real positive, such that*

$$a = b - c, \quad bc = cb = 0, \quad \|b\| \leq \|a\|, \quad \text{and} \quad \|c\| \leq \|a\|. \tag{2-1}$$

By Lemma 2.24, the hypothesis that A^1 be an L^p-operator algebra is automatic for $p \neq 1$.

It seems unlikely that Lemma 2.15 holds for a general Banach algebra.

Proof of Lemma 2.15. We may assume (using, e.g., the corollary on page 136 in [Lacey 1974]) that (X, μ) is a decomposable measure space and A^1 is a unital subalgebra of $B(L^p(X, \mu))$. Since a is hermitian in A^1, Lemma 2.10 implies that a is hermitian in $B(L^p(X, \mu))$. Proposition 2.12 provides $f \in L^\infty(X, \mu)$ such that a is multiplication by f, and such that $|f(x)| \leq \|a\|$ for all $x \in X$.

Choose a sequence $(r_n)_{n\in\mathbb{N}}$ of polynomials with real coefficients such that $r_n(\lambda) \to \lambda^{1/4}$ uniformly on $[0, \|a\|^2]$. Adjusting by constants and scaling, we may assume that $r_n(0) = 0$ and $|r_n(\lambda)| \leq \|a\|^{1/2}$ for $\lambda \in [0, \|a\|^2]$. Set $s_n(\lambda) = r_n(\lambda^2)^2$ for $\lambda \in [-\|a\|, \|a\|]$. Then $(s_n)_{n\in\mathbb{N}}$ is a sequence of polynomials with real coefficients such that $r_n(\lambda) \to |\lambda|$ uniformly on $[-\|a\|, \|a\|]$. Moreover, for all $n \in \mathbb{N}$ we have $s_n(0) = 0$ and $0 \leq s_n(\lambda) \leq \|a\|$ for all $\lambda \in [-\|a\|, \|a\|]$. In particular, $s_n \circ f \to |f|$ uniformly on X.

For $n \in \mathbb{N}$, define $d_n = s_n(a)$, which is the multiplication operator by the function $s_n \circ f$, and let d be the multiplication operator by $|f|$. Then $d_n \in A$ for all $n \in \mathbb{N}$ and $\|d_n - d\| \to 0$, so $d \in A$ and $\|d\| \leq \|a\|$. Therefore also

$$b = \tfrac{1}{2}(d + a) \quad \text{and} \quad c = \tfrac{1}{2}(d - a)$$

are in A. The conditions (2-1) are clearly satisfied.

The multiplication operator map from $L^\infty(X, \mu)$ to $B(L^p(X, \mu))$ is an isometric unital homomorphism. (Recall the convention that we are using $L^\infty_{\mathrm{loc}}(X, \mu)$ here.) The functions $\frac{1}{2}(|f| + f)$ and $\frac{1}{2}(|f| - f)$ are nonnegative, hence both hermitian and real positive in $L^\infty(X, \mu)$ (because $L^\infty(X, \mu)$ is a C^*-algebra). Lemmas 2.10 and 2.14 therefore imply that their multiplication operators b and c are both hermitian and real positive in $B(L^p(X, \mu))$. A second application of these lemmas shows that the same holds in A^1. By definition, this is also true in A. $\square$

Definition 2.16. Let A be a unital or approximately unital Banach algebra. Taking 1 to be the identity of A^1 in the approximately unital case, we define

$$\mathfrak{F}_A = \{a \in A : \|1 - a\| \leq 1\}.$$

Proposition 2.17 [Blecher and Ozawa 2015, Proposition 3.5]. *Let A be a unital or approximately unital Banach algebra. Then, in the notation of Definitions 2.13 and 2.16, we have $\mathfrak{r}_A = \overline{\mathbb{R}_+ \mathfrak{F}_A}$.*

We recall some facts about roots of elements of $\mathfrak{r}_A$.

Definition 2.18. Let A be a unital or approximately unital Banach algebra, let $b \in \mathfrak{r}_A$, and let $t \in (0, 1)$. If A is unital, we denote by b^t the element b_t constructed in [Li et al. 2003, Theorem 1.2]. If A is approximately unital, let A^1 be the multiplier unitization, recall that $b \in \mathfrak{r}_{A^1}$ by definition, and define b^t to be as above but evaluated in A^1.

The conditions required in [Li et al. 2003, Theorem 1.2] for the existence of b^t are weaker than what we require in Definition 2.18, but the case in Definition 2.18, is all we need. Such noninteger powers, for the special case $\|b - 1\| < 1$ and when A is commutative, seem to have first appeared in Definition 2.3 of [Esterle 1978]. A discussion relating this definition to others, and giving a number of properties, is contained in [Blecher and Ozawa 2015], from Proposition 3.3 through Lemma 3.8 there. In particular, $(b^{1/n})^n = b$ and $t \mapsto b^t$ is continuous. For later use, we recall several of these properties and state a few other facts not given explicitly in [Blecher and Ozawa 2015].

Proposition 2.19. *Let A be a unital or approximately unital Banach algebra, and let $a \in \mathfrak{r}_A$.*

(1) *If $t \in (0, 1)$ and $\|b - 1\| \leq 1$ (that is, $b \in \mathfrak{F}_A$), then*

$$b^t = 1 + \sum_{k=1}^{\infty} \frac{t(t-1)(t-2)\cdots(t-k+1)}{k!}(-1)^k(1-b)^k,$$

with absolute convergence.

(2) *If $t \in (0, 1)$ and $\lambda \in (0, \infty)$ then $(\lambda x)^t = \lambda^t x^t$.*

(3) *For all $t \in (0, 1)$, $\|a^t\| \leq 2\|a\|^t/(1-t)$.*

(4) *For all $t \in (0, 1)$, a^t is a norm limit of polynomials in a with no constant term.*

(5) *For all $t \in (0, 1)$, $a^t a = a a^t$.*

(6) $\lim_{n\to 0} \|a^{1/n}a - a\| = \lim_{n\to 0} \|aa^{1/n} - a\| = 0$.

(7) *If $a \in \mathfrak{F}_A$ and $t \in (0, 1)$, then $\|1 - a^t\| \leq 1$.*

Proof. For part (1), see the proof of [Blecher and Ozawa 2015, Proposition 3.3] and the discussion in and before the remark before [Blecher and Ozawa 2015, Lemma 3.6].

For (2), see the discussion after [Blecher and Ozawa 2015, Proposition 3.5].

Part (3) is a slight weakening of the second estimate in Lemma 3.6 of [Blecher and Ozawa 2015].

Part (4) holds for $a \in \mathfrak{F}_A$ by the proof of Proposition 3.3 of [Blecher and Ozawa 2015]. By (2), it holds for $a \in \mathbb{R}_+ \mathfrak{F}_A$. By continuity (Corollary 1.3 of [Li et al. 2003]), it holds for $a \in \overline{\mathbb{R}_+ \mathfrak{F}_A}$. Apply Proposition 2.17.

Part (5) is immediate from Part (4). Part (6) is Lemma 3.7 of [Blecher and Ozawa 2015].

For (7), use (1), together with

$$\frac{t(t-1)(t-2)\cdots(t-k+1)}{n!}(-1)^k < 0$$

for $k = 1, 2, \ldots$ and

$$\sum_{k=1}^{\infty} \frac{t(t-1)(t-2)\cdots(t-k+1)}{k!}(-1)^k = -1.$$

This completes the proof. □

Lemma 2.20. *Suppose that A is a closed subalgebra of an approximately unital Banach algebra B, and suppose that A has a cai. Then $\mathfrak{F}_B \cap A \subseteq \mathfrak{F}_A$ and $\mathfrak{r}_B \cap A \subset \mathfrak{r}_A$.*

Proof. The first statement follows easily from Lemma 1.10. The second follows from the first and the relations $\mathfrak{r}_A = \overline{\mathbb{R}_+ \mathfrak{F}_A}$ and $\mathfrak{r}_B = \overline{\mathbb{R}_+ \mathfrak{F}_B}$ (Proposition 2.17). □

Proposition 2.21. *Let B be a nonunital approximately unital Banach algebra, and let $A \subseteq B$ be a closed subalgebra which contains a cai for B. Then:*

(1) *$A^1 \subseteq B^1$ isometrically.*

(2) *$\mathfrak{F}_A = \mathfrak{F}_B \cap A$ and $\mathfrak{r}_A = \mathfrak{r}_B \cap A$.*

(3) *Every state or quasistate on A may be extended to a state or quasistate on B.*

Proof. Part (1) is Lemma 1.11. That $\mathfrak{F}_A = \mathfrak{F}_B \cap A$ is immediate from (1), and now $\mathfrak{r}_A = \mathfrak{r}_B \cap A$ by, e.g., Proposition 2.17. Part (3) is obvious from (1), Definition 2.6, and the Hahn–Banach theorem. □

Lemma 2.22. *Suppose that an Arens regular Banach algebra A has a cai and also has a real positive approximate identity. Then A has a cai in $\mathfrak{F}_A$. If in addition A has a countable bounded approximate identity, then A has a cai in $\mathfrak{F}_A$ which is a sequence.*

Proof. Corollary 3.9 of [Blecher and Ozawa 2015] implies that A has an approximate identity in $\mathfrak{F}_A$. Since $\mathfrak{F}_A$ is bounded, one may then use the argument in the second paragraph of the proof of [Blecher 2016, Proposition 6.13] to see that A has a cai $(e_t)_{t \in \Lambda}$ in $\mathfrak{F}_A$. If in addition A has a countable bounded approximate identity, then one can use Corollary 32.24 of [Hewitt and Ross 1970] and its analog on the right (see also Theorem 4.4 of [Blecher and Ozawa 2015]) to find $x, y \in A$ with $A = \overline{xA} = \overline{Ay}$. Choose $t_1, t_2, \ldots \in \Lambda$ with $t_1 < t_2 < \cdots$ and $\| f_{t_k} x - x \| + \| y f_{t_k} - y \| < 2^{-k}$; then (f_{t_k}) is a countable cai in $\mathfrak{F}_A$. □

Corollary 2.23. *Suppose that A is an approximately unital Arens regular Banach algebra. If $1_{A^{**}}$ is a weak* limit of a bounded net of real positive elements in A, then A has a real positive cai.*

Proof. By a standard convexity argument, or, e.g., [Blecher and Ozawa 2015, Lemma 2.1], A has a real positive bounded approximate identity. It follows from Lemma 2.22 that A has a cai in $\mathfrak{F}_A$. □

The hypothesis in the last result about $1_{A^{**}}$ being a weak* limit holds if A has one of the Kaplansky density type properties, e.g., properties (1)–(3) in Proposition 7.1. See also the proof of Proposition 6.4 of [Blecher and Ozawa 2015].

2C. ***More on the multiplier unitization.*** The multiplier unitization was defined in Definition 1.8.

Lemma 2.24. *Let E be a Banach space. Suppose that A is a nonunital closed approximately unital subalgebra of $B(E)$ which acts nondegenerately on E. Then the multiplier unitization of A is isometrically isomorphic to $A + \mathbb{C}\, 1_E$, where 1_E is the identity operator on E.*

Proof. For $a, c \in A$ and $\lambda \in \mathbb{C}$, we clearly have

$$\|ac + \lambda c\| = \|(a + \lambda 1_E)c\| \leq \|a + \lambda 1_E\| \|c\|.$$

So $\|a + \lambda 1\|_{A^1} \leq \|a + \lambda 1_E\|$. The reverse inequality follows from the fact that if $(e_t)_{t \in \Lambda}$ is a cai for A, then $ae_t + \lambda e_t \to a + \lambda 1_E$ in the strong operator topology on $B(E)$. □

Lemma 2.25. *Suppose that A is an approximately unital Arens regular Banach algebra, and let $\mathfrak{e} = (e_t)_{t \in \Lambda}$ be a cai for A. Then*:

(1) *The multiplier unitization of A is isometrically isomorphic to $A + \mathbb{C}\, 1_{A^{**}}$ in A^{**}.*

(2) *With $S_{\mathfrak{e}}(A)$ as defined in Definition 2.6, and identifying A^* with the weak* continuous functionals on A^{**}, we have*

$$S_{\mathfrak{e}}(A) = \{\omega \in S(A^{**}) : \omega \text{ is weak* continuous}\}$$

(the normal state space of A^{**}).

(3) *$S_{\mathfrak{e}}(A)$ and $S(A)$ both span A^*, and both separate the points of A.*

(4) *In the notation found before Lemma* 2.6 *of* [*Blecher and Ozawa 2015*] *and in Definition 2.13, we have*

$$\mathfrak{r}_A^{\mathfrak{e}} = \mathfrak{r}_A \quad \textit{and} \quad \mathfrak{c}_{A^*}^{\mathfrak{e}} = \mathfrak{c}_{A^*}.$$

(5) *If A is also nonunital then $\{\varphi|_A : \varphi \in S(A^1)\}$ is the weak* closure in A^* of any one of the following sets in Definition 2.6: $S(A)$, $S_{\mathfrak{e}}(A)$, $Q(A)$, or $Q_{\mathfrak{e}}(A)$.*

Proof. The proof of (1) is essentially the same as the proof of Lemma 2.24: for $a, c \in A$ and $\lambda \in \mathbb{C}$, clearly

$$\|ac + \lambda c\| = \|(a + \lambda 1_{A^{**}})c\| \leq \|a + \lambda 1_{A^{**}}\| \|c\|.$$

So $\|a + \lambda 1\|_{A^1} \leq \|a + \lambda 1_{A^{**}}\|$. The reverse inequality follows from the fact that if $(e_t)_{t \in \Lambda}$ is a cai, then Lemma 1.14 implies that $ae_t + \lambda e_t \to a + \lambda 1_{A^{**}}$ weak*.

For (2), since $e_t \to 1$ weak* in A^{**} by Lemma 1.14, it is clear that weak* continuous states on A^{**} restrict to elements of $S_{\mathfrak{e}}(A)$. For the reverse inclusion, let $\omega \in S_{\mathfrak{e}}(A)$. Then ω^{**} is a weak* continuous functional on A^{**} and $\|\omega^{**}\| = 1$. That $\omega^{**}(1) = 1$ follows from weak* continuity of ω^{**} and the weak* convergence $e_t \to 1$.

The assertion about $S_{\mathfrak{e}}(A)$ in (3) follows from part (2) and Theorem 2.2 of [Magajna 2009], according to which the normal state space of A^{**} spans A^* and separates the points of A. The second assertion in (3) follows from the first assertion and the inclusion $S_{\mathfrak{e}}(A) \subseteq S(A)$, which is in Lemma 2.2 of [Blecher and Ozawa 2015].

We prove (4). We need only prove $\mathfrak{r}_A^{\mathfrak{e}} \subseteq \mathfrak{r}_A$, since the reverse inclusion holds by definition, and equality implies $\mathfrak{c}_{A^*} = \mathfrak{c}_{A^*}^{\mathfrak{e}}$ by definition. So let $a \in \mathfrak{r}_A^{\mathfrak{e}}$ and let $\omega \in S(A)$.

By definition, ω extends to a state ω^1 on A^1. By part (1) we have $A^1 \subseteq A^{**}$, so the Hahn–Banach theorem provides an extension of ω^1 to a state φ on A^{**}. Use weak* density of the normal states in $S(A^{**})$ (which follows from Theorem 2.2 of [Magajna 2009]) to find a net $(\varphi_t)_{t\in\Lambda}$ in the normal state space of A^{**} which converges weak* to φ. Now $\mathrm{Re}(\omega(a)) = \lim_t \mathrm{Re}(\varphi_t(a)) \geq 0$. So $a \in \mathfrak{r}_A$.

Finally, we prove (5).

It follows from [Blecher and Ozawa 2015, Lemma 2.6] that, with overlines denoting weak* closures, we have

$$\overline{S(A)} = \overline{Q(A)} \subseteq \{\varphi|_A : \varphi \in S(A^1)\}.$$

Also, $\{\varphi|_A : \varphi \in S(A^1)\}$ is shown to be weak* closed in the proof of that lemma.

Now suppose that $\varphi \in S(A^1)$ and set $\psi = \varphi|_A$. Use the Hahn–Banach theorem to extend φ to a state ρ on A^{**}. Use again weak* density of the normal states in $S(A^{**})$ to find a net $(\psi_t)_{t\in\Lambda}$ in the normal state space of A^{**} which converges weak* to ρ. Set $\varphi_t = \psi_t|_A$ for $t \in \Lambda$. For $a \in A$ we then have

$$\varphi_t(a) = \psi_t(a) \to \psi(a) = \varphi(a).$$

By part (2), this shows that ψ is in the weak* closure of $S_{\mathfrak{e}}(A)$. Since

$$S_{\mathfrak{e}}(A) \subseteq S(A) \subseteq Q(A) \quad \text{and} \quad S_{\mathfrak{e}}(A) \subseteq Q_{\mathfrak{e}}(A),$$

the assertion follows. □

The set $\mathfrak{r}_{A^{**}}$, as defined on page 11 of [Blecher and Ozawa 2015], may be a proper subset of the accretive elements in A^{**}, even for approximately unital L^p-operator algebras. In fact, the identity e of A^{**} is certainly accretive in A^{**}, but need not be accretive in $(A^1)^{**}$. (Equivalently, by Lemma 2.29 (4), we need not have $\|1 - e\| \leq 1$.) This happens for $A = \mathbb{K}(L^p([0, 1]))$, by Proposition 3.10. However, it follows from the later result Proposition 4.26 (and Proposition 4.24 (2)) that $\mathfrak{r}_{A^{**}}$, as defined on page 11 of [Blecher and Ozawa 2015], equals the accretive elements in A^{**} if A is a scaled approximately unital L^p-operator algebra.

Remark 2.26. The sets $S_{\mathfrak{e}}(A)$ and $Q_{\mathfrak{e}}(A)$ are easily seen to be convex in A^*. We do not know whether $S(A)$ and $Q(A)$ are necessarily convex if A is a general approximately unital Arens regular Banach algebra, since convex combinations of norm 1 functionals may have norm strictly less than 1. However they are convex if A is an approximately unital L^p-operator algebra, since Corollary 4.25 (1) implies convexity of $S(A)$, and this implies convexity of $Q(A)$.

Proposition 2.27. *Let $p \in (1, \infty)$. The multiplier unitization of an approximately unital L^p-operator algebra is an L^p-operator algebra.*

Proof. This follows from Lemma 2.25 (1) and the fact (Lemma 2.1 (3)) that biduals of L^p-operator algebras are L^p-operator algebras (or from Lemmas 2.24 and 2.33). □

Similarly, for $p \in (1, \infty)$ the multiplier unitization of an approximately unital SQ_p-operator algebra is an SQ_p-operator algebra.

The multiplier algebra $M(A)$, and the left and right multiplier algebras $LM(A)$ and $RM(A)$, of an approximately L^p-operator algebra may be defined to be subsets of A^{**} just as in the operator algebra case. Then the multiplier unitization A^1 is contained in $M(A)$ isometrically and unitally. If A is represented isometrically and nondegenerately on $L^p(X)$ then, just as in the operator algebra case, $M(A)$, $LM(A)$, and $RM(A)$ may be identified isometrically as Banach algebras with the usual subalgebras of $B(L^p(X))$. See Theorem 3.19 of [Gardella and Thiel 2019], and the discussion in that paper. One can also, for example, copy the proof of Theorem 2.6.2 of [Blecher and Le Merdy 2004] for $LM(A)$, and later results in Section 2.6 of [Blecher and Le Merdy 2004] for $RM(A)$ and $M(A)$.

In particular, $M(A)$, $LM(A)$, and $RM(A)$ are all unital L^p-operator algebras. Similarly, $LM(A)$ can be identified with the algebra of bounded right A-module endomorphisms of A, as usual. One may also check that the useful principle in [Blecher and Le Merdy 2004, Proposition 2.6.12] holds for approximately L^p-operator algebras, with the same proof. (Also see Theorem 3.17 of [Gardella and Thiel 2019].)

2D. *Idempotents.*

Definition 2.28. We recall that if A is a unital Banach algebra, then an idempotent $e \in A$ is called *bicontractive* if $\|e\| \leq 1$ and $\|1 - e\| \leq 1$. We say that an element s of a unital Banach algebra A is an *invertible isometry* if s is invertible, $\|s\| = 1$, and $\|s^{-1}\| = 1$.

We collect some standard facts related to bicontractive idempotents.

Lemma 2.29. (1) *Let A be a unital Banach algebra and let $e \in A$ be a hermitian idempotent. Then $1 - 2e$ is an invertible isometry of order 2.*

(2) *Let A be a unital Banach algebra. Then every hermitian idempotent in A is bicontractive.*

(3) *Let $p \in [1, \infty)$, let (X, μ) be a measure space, and let $e \in B(L^p(X, \mu))$ be an idempotent. Then e is bicontractive if and only if $1 - 2e$ is an invertible isometry.*

(4) *Let A be a unital Banach algebra and let $e \in A$ be an idempotent. Then e is real positive if and only if $1 - e$ is contractive* ($\|1 - e\| \leq 1$).

The converse of (2) is false, even in L^p-operator algebras. See Lemma 6.11 of [Phillips and Viola 2017], which is just the idempotent e_2 of Example 3.2 for $p \neq 2$.

Part (3) fails in general unital Banach algebras. This failure is well known, and our Example 4.7 contains an explicit counterexample.

Proof of Lemma 2.29. For (1), by definition we have

$$\|1 + [\exp(i\lambda) - 1]e\| = \|\exp(i\lambda e)\| \le 1$$

for all $\lambda \in \mathbb{R}$. Setting $\lambda = \pi$ gives $\|1 - 2e\| \le 1$. One checks immediately that $(1 - 2e)^2 = 1$, so in fact $\|1 - 2e\| = 1$. The rest of (1) follows easily.

Part (2) follows from Lemma 6.6 of [Phillips and Viola 2017].

We prove (3). The forward direction follows from [Bernau and Lacey 1977, Theorem 2.1] (or, when $\mu(X) = 1$, from the corollary on page 11 of [Byrne and Sullivan 1972]). Conversely, if $\|1 - 2e\| \le 1$ then

$$\|e\| = \left\|\tfrac{1}{2}[1 - (1 - 2e)]\right\| \le \tfrac{1}{2}(\|1\| + \|1 - 2e\|) \le 1,$$

and the proof that $\|1 - e\| \le 1$ is similar.

Part (4) is [Blecher and Ozawa 2015, Lemma 3.12]. □

Definition 2.30. We define two order relations on idempotents e, f in a Banach algebra A. We write $e \le_{\mathrm{r}} f$ if $fe = e$ and $e \le f$ if $ef = fe = e$.

If A is a subalgebra of $B(E)$ then, viewing these idempotents as operators on E, then $e \le_{\mathrm{r}} f$ simply says that $\mathrm{Ran}(e) \subseteq \mathrm{Ran}(f)$. The second relation is the ordering considered in, e.g., [Phillips and Viola 2017, Section 6].

Clearly $e \le f$ and $f \le e$ imply $e = f$. This isn't true for the relation $\le_{\mathrm{r}}$.

Lemma 2.31. *Let $p \in (1, \infty)$, and let A be an approximately unital L^p-operator algebra. Let $e, f \in A$ be idempotents. Assume that e and f are both contractive or both real positive. Then*:

(1) *$fe = e$ if and only if $ef = e$.*

(2) *$e \le_{\mathrm{r}} f$ if and only if $e \le f$.*

Proof. Part (2) is immediate from part (1), so we just prove part (1).

By definition (see Definition 2.13), we may work in the multiplier unitization A^1, which is a unital L^p-operator algebra by Proposition 2.27. So we can assume that there is a measure space (X, μ) such that A is a unital subalgebra of $B(L^p(X, \mu))$.

First suppose that e and f are contractive. Assume that $fe = e$. Then ef is necessarily an idempotent, and is clearly contractive. Clearly $\mathrm{Ran}(ef) \subseteq \mathrm{Ran}(e)$. Since $efe = e^2 = e$, we have $\mathrm{Ran}(e) \subseteq \mathrm{Ran}(ef)$. By [Cohen and Sullivan 1970, Theorem 6], the range of a contractive idempotent on a smooth space determines the idempotent. So $ef = e$, as desired.

Next assume that $ef = e$. Let $q \in (1, \infty)$ satisfy $\frac{1}{p} + \frac{1}{q} = 1$. Then $e^*, f^* \in B(L^q(X, \mu))$ are contractive idempotents such that $f^* e^* = e^*$. The case already considered implies $e^* f^* = e^*$, whence $fe = e$.

Now suppose that e and f are real positive. Then $1 - e$ and $1 - f$ are contractive idempotents by Lemma 2.29 (4). So $(1 - e)(1 - f) = 1 - f$ if and only if

$(1-f)(1-e) = 1-f$ by the contractive case. Expanding and rearranging, we get $fe = e$ if and only if $ef = e$. ☐

2E. *Representations.* We say a few words on representations.

Lemma 2.32. *Let $p \in (1, \infty)$, let A be an L^p-operator algebra, let X be a measure space, let M be a weak* closed subalgebra of $B(L^p(X))$, and let $\pi : A \to M$ be a contractive homomorphism. Then there exists a unique weak* continuous contractive homomorphism $\widetilde{\pi} : A^{**} \to M$ which extends π.*

Proof. The proof is the same as for the operator algebra case (2.5.5 in [Blecher and Le Merdy 2004], but without the matrix norms) and using Lemma 2.1. ☐

Let $\pi : A \to B(L^p(X))$ be a contractive representation of an approximately unital L^p-operator algebra. Then $E = \overline{\operatorname{span}}(\pi(A)(L^p(X)))$ may not be an L^p-space on a subset of X. Indeed, in Example 3.2, $\operatorname{Ran}(e_2)$ is not an L^p-space on a subset. However it is isometric to an L^p-space, as we will see next.

Some of the following follows from [Johnson 1972, Proposition 1.8] (we thank Eusebio Gardella for this reference) and [Gardella and Thiel 2019, Theorem 3.12, Corollary 3.13] (see also [Phillips and Viola 2017, Section 2]), but for completeness we give a self-contained proof.

Lemma 2.33. *Let $p \in (1, \infty)$, let A be an approximately unital Banach algebra, and let $\pi : A \to B(L^p(X))$ be a contractive representation. Set $E = \overline{\operatorname{span}}(\pi(A)(L^p(X)))$. Then there exists a unique contractive idempotent $f \in B(L^p(X))$ whose range is E. Moreover, E and f have the following properties.*

(1) *For every cai $(e_t)_{t\in\Lambda}$ for A, the net $(\pi(e_t))_{t\in\Lambda}$ converges to f in both the weak* topology and the strong operator topology on $B(L^p(X))$.*

(2) *For all $a \in A$ we have $\pi(a) = f\pi(a)f$.*

(3) *The compression of π to E is a contractive representation, which is isometric if π is isometric.*

(4) *The compression of π to E is nondegenerate.*

(5) *E is linearly isometric to an L^p-space.*

Proof. Let $q \in (1, \infty)$ satisfy $\frac{1}{p} + \frac{1}{q} = 1$.

We claim that if $(e_t)_{t\in\Lambda}$ is a cai in A such that $(\pi(e_t))_{t\in\Lambda}$ converges weak* to some $f \in B(L^p(X))$, then f is a contractive idempotent whose range is E. Assume the claim has been proved. Since $L^p(X)$ is a smooth space, such an idempotent is unique by [Cohen and Sullivan 1970, Theorem 6]. The argument of Lemma 1.14, with this uniqueness statement in place of uniqueness of the identity in A^{**}, shows that such an idempotent f exists and that for any cai $(e_t)_{t\in\Lambda}$ in A, we have $\pi(e_t) \to f$ weak*.

We prove the claim. We have $\|f\| \leq 1$ and $\langle f\pi(a)\xi,\, \eta\rangle = \langle \pi(a)\xi,\, \eta\rangle$ for all $a \in A$, $\xi \in L^p(X)$, and $\eta \in L^q(X)$. It follows that $f\xi = \xi$ for all $\xi \in E$. So $E \subseteq \mathrm{Ran}(f)$. Also, if $\eta \in E^\perp \subseteq L^q(X)$, then $\langle f\xi, \eta\rangle = \lim_t \langle \pi(e_t)\xi,\, \eta\rangle = 0$. Thus $E^\perp \subseteq \mathrm{Ran}(f)^\perp$, whence $\mathrm{Ran}(f) \subseteq E$. The claim is proved. We now have the main statement, and weak* convergence in (1).

Part (5) follows from the fact (Theorem 3 in Section 17 of [Lacey 1974]; see also Theorem 4 of [Ando 1966]) that the range of a contractive idempotent on an L^p-space is isometrically isomorphic to an L^p-space.

We prove (2). We know that $f\pi(a) = \pi(a)$ for all $a \in A$, so we prove that $\pi(a)f = \pi(a)$. For $\xi \in L^p(X)$ and $\eta \in L^q(X)$, we have

$$\begin{aligned}\langle \pi(a)f\xi, \eta\rangle &= \langle f\xi,\, \pi(a)^*\eta\rangle = \lim_t \langle \pi(e_t)\xi,\, \pi(a)^*\eta\rangle \\ &= \lim_t \langle \pi(ae_t)\xi,\, \eta\rangle = \langle \pi(a)\xi, \eta\rangle.\end{aligned}$$

Thus $\pi(a)f = \pi(a)$.

Part (3) is now immediate, as is (4) since $\pi(e_t)\pi(a)\xi \to \pi(a)\xi$ for $a \in A$ and $\xi \in L^p(X)$.

We prove strong operator convergence in (1). It suffices to prove that $\pi(e_t)\xi \to f\xi$ for $\xi \in fL^p(X)$ and for $\xi \in (1-f)L^p(X)$. The first of these follows from (4). The second case is trivial: $\pi(e_t)\xi = 0$ by (2), and $f\xi = 0$. □

Remark 2.34. The last result also holds with L^p-spaces replaced by the SQ_p-spaces mentioned in the introduction, although (5) would then say that E is an SQ_p-space. The proof is essentially the same, except that (5) becomes trivial. We also need to use the fact that SQ_p-spaces are smooth for $p \in (1, \infty)$. In fact, they are also strictly convex. To see this, first observe that reflexivity of L^p-spaces implies reflexivity of SQ_p-spaces. Next, L^p-spaces are both smooth and strictly convex, so their subspaces are as well. So the duals of subspaces are both strictly convex and smooth. By reflexivity, the quotient of a subspace is the dual of a subspace of the dual, so both smooth and strictly convex.

If A is unital as a Banach algebra and also is an L^p-operator algebra then it follows that A may be viewed as a subalgebra of $B(L^p(X))$ containing the identity operator on $L^p(X)$, for some measure space X. This was proved first in Section 2 of [Phillips and Viola 2017].

Corollary 2.35. *Let $p \in (1, \infty)$. Let A be a dual unital L^p-operator algebra (Definition 2.3). Then A has an isometric unital representation on an L^p-space which is a weak* homeomorphism onto its range.*

Proof. Let $\pi : A \to B(L^p(X))$ be an isometric representation which is a weak* homeomorphism onto its range. As in Lemma 2.33, let $E = \overline{\mathrm{span}}(\pi(A)(L^p(X)))$, and let f be as there. Clearly $f = \pi(1_A)$. Define $\sigma : A \to B(E) = fB(L^p(X))f$ by $\sigma(a) = f\pi(a)f$ for $a \in A$. Lemma 2.33 implies that σ is an isometric unital representation on an L^p-space. In light of the Krein–Smulian theorem, all we need to show is that the weak* topology on $B(E)$ is the same as the restriction to $fB(L^p(X))f$ of the weak* topology on $B(L^p(X))$. The inclusion of E in $L^p(X)$ as a complemented subspace gives an inclusion of $\mathbb{K}(E)$ in $\mathbb{K}(L^p(X))$, and by Theorem 1.13 (2) the second dual of this inclusion is $B(E) \hookrightarrow B(L^p(X))$, which is therefore a weak* homeomorphism onto its image. □

In particular, applying this principle to the bidual of an approximately unital L^p-operator algebra A, we obtain a faithful normal isometric representation of A^{**} that can to some extent play the role of the enveloping von Neumann algebra coming from the universal representation of a C^*-algebra.

Corollary 2.36. *Let $p \in (1, \infty)$, and let A be an approximately unital L^p-operator algebra. Then there exists a measure space (X, μ) and a unital isometric representation $\theta : A^{**} \to B(L^p(X, \mu))$ such that*:

(1) *θ is a weak* homeomorphism onto its range.*

(2) *$\theta|_A$ acts nondegenerately on $L^p(X, \mu)$.*

(3) *For any cai $(e_t)_{t\in\Lambda}$ in A, we have $\theta(e_t) \to 1$ in the strong operator topology on $B(L^p(X, \mu))$.*

Proof. This is clear from Corollary 2.35 and Lemma 2.33. □

3. Examples

As we mentioned in the introduction, so far the study of L^p-operator algebra has been very largely example driven. Thus there is a wealth of examples in the literature, or in preprint form. (See the works of Phillips, Viola, Gardella and Thiel, and others referred to earlier.) In this section we discuss the main examples which we have used, or which seem useful but are not in the literature. We recall again that, as always, in this section $p \in (1, \infty) \setminus \{2\}$ unless stated to the contrary.

Notation 3.1. As in, for example, [Phillips and Viola 2017, Lemma 6.11], for $n \in \mathbb{N}$ and $p \in [1, \infty]$ we write l_n^p for L^p of an n point space with counting measure, and define $M_n^p = B(l_n^p)$.

Example 3.2. Let $p \in [1, \infty)$. Let $e_n \in M_n^p$ be the $n \times n$ matrix whose entries are all $\frac{1}{n}$. We will use e_n several times in this paper and so the calculations that follow will be important for us. If $p = 2$ then e_n is a rank one projection. For the rest of this example, assume $p \neq 2$, and let $q \in (1, \infty]$ satisfy $\frac{1}{p} + \frac{1}{q} = 1$.

Suppose $n = 2$. We have

$$1 - 2e_2 = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix},$$

which is an invertible isometry. So $\|e_2\| = \|1 - e_2\| = 1$ by Lemma 2.29 (3), and e_2 is real positive by Lemma 2.29 (4). However, e_2 is not hermitian, by Proposition 2.12, or by Lemma 6.11 of [Phillips and Viola 2017].

For the rest of this example, assume $n \geq 3$ (as well as $p \neq 2$). We claim that $\|e_n\| = 1$ but $\|1 - e_n\| > 1$, so that e_n is not bicontractive. Then Lemma 2.29 (4) implies that e_n is not real positive.

To see that e_n is contractive, set

$$\eta = (1, 1, \dots, 1) \in l_n^p \quad \text{and} \quad \mu = \tfrac{1}{n}(1, 1, \dots, 1) \in l_n^q.$$

Then one easily checks that for all $\xi \in l_n^p$ we have $e_n \xi = \langle \mu, \xi \rangle \eta$, so $\|e_n\| \leq \|\mu\|_q \|\eta\|_p = 1$.

To show that $\|1 - e_n\| > 1$, by Lemma 2.29 (3) it is enough to prove that $1 - 2e_n$ is not isometric. As pointed out to us by Eusebio Gardella, Lamperti's theorem [Fleming and Jamison 2003, Theorem 3.2.5] implies that the only matrices which are isometries in the L^p-operator norm are the complex permutation matrices, and clearly $1 - 2e_n$ is not of this form. However, we can give a direct proof.

Define $g : [1, \infty) \to [0, \infty)$ by

$$g(p) = \|(1 - 2e_n)(1, 0, 0, \dots, 0)\|_p^p.$$

We have

$$(1 - 2e_n)(1, 0, 0, \dots, 0) = \left(1 - \frac{2}{n}, \, -\frac{2}{n}, \, -\frac{2}{n}, \, \dots, \, -\frac{2}{n}\right),$$

so

$$g(p) = \left(1 - \frac{2}{n}\right)^p + (n-1)\left(\frac{2}{n}\right)^p$$

for $p \in [1, \infty)$. One further has $g(2) = 1$ and

$$g'(p) = \left(1 - \frac{2}{n}\right)^p \log\left(1 - \frac{2}{n}\right) + (n-1)\left(\frac{2}{n}\right)^p \log\left(\frac{2}{n}\right)$$

for all $p \in [1, \infty)$. Both the logarithm terms are strictly negative, so $g'(p) < 0$. Therefore,

$$\|(1 - 2e_n)(1, 0, 0, \dots, 0)\|_p \neq 1$$

for all $p \in [1, \infty) \setminus 2$. Thus $\|1 - e_n\| > 1$.

One can see easily that $\|1 - e_n\| < 2$ (this follows for example from a lemma in the sequel paper), but we will not use this here.

Lemma 2.29 (4) implies that $1 - e_n$ is real positive. It follows also that the "support idempotent" $s(1 - e_n)$ of $1 - e_n$ (see Definition 4.12) is not contractive, unlike support idempotents for real positive Hilbert space operators (see, e.g., Corollary 3.4 of [Blecher and Read 2013]). In turn this shows that, unlike the Hilbert space operator case, the limit $\lim_{m \to \infty} \|x^{1/m}\|$ need not equal 1 for real positive elements in an L^p-operator algebra A (or even for elements of $\mathfrak{F}_A$). We are using the m-th root in Definition 2.18 and the discussions after it. We also see that, unlike the Hilbert space operator case in Proposition 2.3 of [Blecher and Read 2011], $\frac{1}{2}\mathfrak{F}_A$ is not closed under n-th roots. Indeed,

$$\tfrac{1}{2}(1-e_n) \in \tfrac{1}{2}\mathfrak{F}_A \subseteq \mathrm{Ball}(A)$$

but

$$\lim_{m\to\infty} \left(\tfrac{1}{2}(1-e_n)\right)^{1/m} = s(1-e_n) = 1-e_n \notin \mathrm{Ball}(A).$$

Nonetheless it is true that $\mathfrak{F}_A$ is closed under n-th roots, by Proposition 2.19 (7).

Another example of bicontractive idempotents, related to the case of M_2^p discussed above, appears in the group L^p-operator algebra of a discrete group containing elements of order 2. (See, e.g., [Phillips 2013a; Gardella and Thiel 2015a; 2015b].) These elements give projections in the group C^*-algebra, which are actually in the purely algebraic group algebra. The corresponding idempotents in the group L^p-operator algebra are bicontractive, and “look like” the bicontractive idempotents in M_2^p. Since we make little use of group L^p-operator algebras in this paper, we omit the details. As described below, however, they motivate Example 3.3.

Let E be a Banach space of the form $L^p(X, \mu)$ for some measure space (X, μ) and some $p \in (1, \infty)$. Let $e, f \in B(E)$ be commuting contractive idempotents. It is very tempting to conjecture that, as in the Hilbert space operator case, $e + f - ef$, which is an idempotent with range $\mathrm{Ran}(e) + \mathrm{Ran}(f)$, is also contractive. This conjecture is false, as we will see in Example 3.3, even if e and f are bicontractive. Thus, the lattice theoretic properties of (even commuting) bicontractive idempotents on L^p-spaces are deficient. Indeed we shall see that there is a disappointing comparison between the structure of the lattice of idempotents in $B(L^p(X))$ and the beautiful and fundamental behavior of projections in von Neumann algebras. Our example also does two other things. It shows that the product of two commuting real positive idempotents need not be real positive. And it shows that on L^p, there are commuting accretive operators whose geometric mean exists but is not accretive. This shows that [Blecher and Wang 2016, Lemma 5.8] fails with Hilbert spaces replaced by L^p-spaces.

The construction of the example is motivated as follows. Fix $p \in (1, \infty) \setminus \{2\}$. By Lemma 2.29 (3), commuting pairs of bicontractive idempotents in $B(L^p(X, \mu))$ are in one-to-one correspondence with pairs of commuting invertible isometries of order 2 in $B(L^p(X, \mu))$, and therefore with representations of $(\mathbb{Z}/2\mathbb{Z})^2$ on $L^p(X, \mu)$ via isometries. In particular, the conjecture in the previous paragraph holds for all (X, μ) (for our given value of p) if and only if it holds for the pair of bicontractive idempotents coming from the universal isometric L^p representation of $(\mathbb{Z}/2\mathbb{Z})^2$. Since $(\mathbb{Z}/2\mathbb{Z})^2$ is amenable, this will be true if and only if it holds for the left regular representation of $(\mathbb{Z}/2\mathbb{Z})^2$ on

$$l^p((\mathbb{Z}/2\mathbb{Z})^2) \cong l_4^p.$$

Example 3.3. Fix $p \in (1, \infty) \setminus \{2\}$. There is a finite-dimensional unital L^p-operator algebra (specifically M_4^p) which contains the following:

(1) Two commuting bicontractive idempotents whose product is not bicontractive.

(2) Two commuting real positive idempotents whose product is not real positive.

(3) Two commuting accretive operators whose geometric mean exists but is not accretive.

We work throughout in M_4^p. Define

$$s = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \in M_4^p \quad \text{and} \quad t = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \in M_4^p.$$

One checks that these are commuting isometries of order 2. Next, define

$$e = \tfrac{1}{2}(1+s) \quad \text{and} \quad f = \tfrac{1}{2}(1+t).$$

These are commuting idempotents, and they are bicontractive by Lemma 2.29 (3). Then one checks that ef is the idempotent e_4 of Example 3.2, and that $e+f-ef$ is an idempotent. We claim that it is not contractive. First, we look at $1-(e+f-ef)$, getting

$$1-(e+f-ef) = \frac{1}{4}\begin{bmatrix} 1 & -1 & -1 & 1 \\ -1 & 1 & 1 & -1 \\ -1 & 1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix}.$$

Define $w = \operatorname{diag}(1, -1, -1, 1)$, which is an invertible isometry in M_4^p. Then one checks that $w[1-(e+f-ef)]w^{-1} = e_4$ in the language of Example 3.2. In that example we showed that this idempotent is contractive, and also showed that $1 - w[1-(e+f-ef)]w^{-1}$ is not contractive. Therefore also

$$e+f-ef = w^{-1}(1 - w[1-(e+f-ef)]w^{-1})w$$

is not contractive. This yields (1) for the bicontractive idempotents $1-e$ and $1-f$.

Now define $e_0 = 1-e$ and $f_0 = 1-f$. We have seen that e and f are contractive, so e_0 and f_0 are real positive by Lemma 2.29 (4). However, $1 - e_0 f_0 = e+f-ef$ is not contractive, so $e_0 f_0$ is not real positive, again by Lemma 2.29 (4). This is (2).

We turn to (3). We want invertible elements. Neither e nor f is invertible, but this is easily fixed by adding $\varepsilon 1$ to each of them, which does not change the fact that they commute. We recall the well-known Ando et al. list of properties that a "good" geometric mean should possess (see, e.g., page 306 of [Ando et al. 2004]). One of these is that the geometric mean of a and b should be $a^{1/2} b^{1/2}$ (as in Definition 2.18) whenever a and b commute. One also needs to assume in our case that these principal square roots exist.

Suppose that $(\varepsilon 1+e)^{1/2}(\varepsilon 1+f)^{1/2}$ is accretive for all $\varepsilon > 0$. Using the Macaev–Palant formula $\|a^{1/2}-b^{1/2}\| \leq K\|a-b\|^{1/2}$ (see Lemma 2.4 and the discussion which precedes it in [Blecher and Wang 2016]; the proof is the same as Theorem 1 of [Macaev and Palant 1962], which is referenced there), letting $\varepsilon \to 0$ implies that $e^{1/2}f^{1/2}$ is accretive. We have $e^{1/2}=e$ and $f^{1/2}=f$ by, e.g., Proposition 2.19 (1). So ef is accretive, a contradiction.

Example 3.4. Let $p \in [1,\infty)$. Given a closed linear subspace $E \subseteq B(L^p(X))$, define $\mathcal{U}(E) \subseteq B(L^p(X) \oplus^p L^p(X))$ to be the set of operators which have the 2×2 matrix form

$$\begin{bmatrix} \lambda & x \\ 0 & \mu \end{bmatrix} \tag{3-1}$$

with $\lambda,\mu \in \mathbb{C}$ and $x \in E$. Then $\mathcal{U}(E)$ is a unital L^p-operator algebra. Moreover, if $F \subseteq L^p(Y)$ and $u : E \to F$ is linear, then the map $\mathcal{U}(u) : \mathcal{U}(E) \to \mathcal{U}(F)$, defined by

$$\mathcal{U}(u)\left(\begin{bmatrix} \lambda & x \\ 0 & \mu \end{bmatrix}\right) = \begin{bmatrix} \lambda & u(x) \\ 0 & \mu \end{bmatrix}$$

for $\lambda,\mu \in \mathbb{C}$ and $x \in E$, is a unital homomorphism. We will show that if u is contractive or isometric, then so is $\mathcal{U}(u)$.

To begin, we claim that if $\lambda,\mu \in \mathbb{C}$ and $x \in B(L^p(X))$, then

$$\left\|\begin{bmatrix} \lambda & x \\ 0 & \mu \end{bmatrix}\right\| = \left\|\begin{bmatrix} |\lambda| & \|x\| \\ 0 & |\mu| \end{bmatrix}\right\|, \tag{3-2}$$

with the norm on the right-hand side being taken in M_2^p. Hence the norm on $\mathcal{U}(E)$ only depends on the norms of elements in E, not the elements themselves.

We prove the claim. Let $\lambda,\mu \in \mathbb{C}$ and let $x \in B(L^p(X))$. Define

$$a = \begin{bmatrix} \lambda & x \\ 0 & \mu \end{bmatrix} \in B(L^p(X) \oplus^p L^p(X)) \quad \text{and} \quad c = \begin{bmatrix} |\lambda| & \|x\| \\ 0 & |\mu| \end{bmatrix} \in M_2^p.$$

We have

$$\|a\| = \sup\Big(\big\{(\|\lambda\eta + x\xi\|_p^p + \|\mu\xi\|_p^p)^{1/p} : \eta,\xi \in L^p(X),\ \|\eta\|_p^p + \|\xi\|_p^p \leq 1\big\}\Big). \tag{3-3}$$

The quantity inside the supremum is dominated by

$$\big[(|\lambda|\|\eta\|_p + \|x\|\|\xi\|_p)^p + (|\mu|\|\xi\|_p)^p\big]^{1/p} = \|c(\|\eta\|_p,\ \|\xi\|_p)\|_p \leq \|c\|.$$

So $\|a\| \leq \|c\|$. To see the other direction we may assume that $x \neq 0$. Choose scalars α,β with $|\alpha|^p + |\beta|^p \leq 1$ such that the norm of c is achieved at (α,β). Multiplying α and β by a complex number of absolute value 1, we may assume that $\beta \geq 0$.

Since $c(\alpha, \beta) = (\alpha|\lambda| + \beta\|x\|,\ \beta|\mu|)$, we see that $\|c(\alpha, \beta)\|_p \leq \|c(|\alpha|, \beta)\|_p$, so we may also assume that $\alpha \geq 0$. If $\beta = 0$ then

$$\|c\| = \|c(\alpha, \beta)\|_p = |\alpha\lambda| \leq |\lambda| \leq \|a\|.$$

Otherwise, let $\varepsilon > 0$. Choose $\delta > 0$ such that

$$\delta < \beta\|x\| \quad \text{and} \quad \big(\big||\lambda|\alpha + \beta\|x\|\big| - \delta\big)^p > \big||\lambda|\alpha + \beta\|x\|\big|^p - \varepsilon.$$

Choose $\xi \in L^p(X)$ of norm β so that $|\,\|x\xi\|_p - \beta\|x\|\,| < \delta$. Then $x\xi \neq 0$. Choose $\zeta \in \mathbb{C}$ such that $|\zeta| = 1$ and $\zeta\lambda = |\lambda|$. Define $\eta = \zeta\alpha\|x\xi\|_p^{-1}x\xi \in L^p(X)$. Then η has norm α, so that $\|\eta\|_p^p + \|\xi\|_p^p \leq 1$. Now

$$\begin{aligned}
\|a(\eta, \xi)\|^p = \|\lambda\eta + x\xi\|_p^p + \|\mu\xi\|_p^p &= \left(\left|\frac{\lambda\zeta\alpha}{\|x\xi\|_p} + 1\right|\|x\xi\|_p\right)^p + |\mu\beta|^p \\
&= \big||\lambda|\alpha + \|x\xi\|_p\big|^p + |\mu\beta|^p > \big(\big||\lambda|\alpha + \beta\|x\|\big| - \delta\big)^p + |\mu\beta|^p \\
&> \big||\lambda|\alpha + \beta\|x\|\big|^p - \varepsilon + |\mu\beta|^p \\
&= \|c(\alpha, \beta)\|_p^p - \varepsilon = \|c\|^p - \varepsilon.
\end{aligned}$$

Since $\varepsilon > 0$ is arbitrary, the claim follows.

It follows that if $u : E \to F$ as above is isometric, then so is $\mathcal{U}(u)$.

We claim that if $u : E \to F$ is a linear contraction, then $\mathcal{U}(u)$ is also contractive. By the previous claim, it suffices to prove that if $\lambda, \mu, \rho, \sigma \in [0, \infty)$ and $\rho \leq \sigma$, then

$$\left\|\begin{bmatrix}\lambda & \rho \\ 0 & \mu\end{bmatrix}\right\| \leq \left\|\begin{bmatrix}\lambda & \sigma \\ 0 & \mu\end{bmatrix}\right\|. \tag{3-4}$$

We apply (3-3) to these matrices. For $\alpha, \beta \in \mathbb{C}$ we have $\|(|\alpha|, |\beta|)\|_p = \|(\alpha, \beta)\|_p$. Since $\lambda, \rho \geq 0$, the expression $|\lambda\alpha + \rho\beta|^p + |\mu\beta|^p$ becomes no smaller if α and β are replaced by $|\alpha|$ and $|\beta|$, and similarly with σ in place of ρ. Therefore the norms of the matrices in (3-4) are $N(\rho)$ and $N(\sigma)$, with N given by

$$N(\tau) = \sup\big(\big\{((\lambda\alpha + \tau\beta)^p + (\mu\beta)^p)^{1/p} : \alpha, \beta \in [0, \infty) \text{ satisfy } \alpha^p + \beta^p \leq 1\big\}\big)$$

for $\tau \in [0, \infty)$. Since all the variables are nonnegative, clearly $\rho \leq \sigma$ implies $N(\rho) \leq N(\sigma)$. This yields (3-4). The claim is proved.

Example 3.4 is often useful for counterexamples because it can convert a bad linear subspace of $B(L^p(X))$ into a suitably badly behaved L^p-operator algebra. Note that if E is weak* closed in $B(L^p(X))$ then $\mathcal{U}(E)$ is a dual L^p-operator algebra in the sense of Definition 2.3. This follows just as in Lemma 2.7.7 (1) of [Blecher and Le Merdy 2004], but using the characterization of weak* convergent nets in $B(L^p(X))$ given after Corollary 2.2.

Example 3.5. Let $p \in [1, \infty)$. The set of continuous functions $f : [0, 1] \to M_2^p$ is a unital L^p-operator algebra. We may view this as the canonical copy of $C([0, 1]) \otimes M_2^p$ inside the bounded operators on

$$L^p([0, 1]) \otimes l_2^p \cong l_2^p(L^p([0, 1])) \cong L^p([0, 1]) \oplus^p L^p([0, 1]).$$

The subalgebra consisting of functions with $f(1)$ diagonal is also a unital L^p-operator algebra. The subalgebras consisting of functions f with $f(0) = 0$, or with $f(0) = 0$ and $f(1)$ diagonal, are approximately unital L^p-operator algebras. Indeed, if $(e_n)_{n\in\mathbb{N}}$ is a cai for $C_0((0, 1])$, then, using tensor notation, $(e_n \otimes 1_2)_{n\in\mathbb{N}}$ is a cai for these algebras.

Example 3.6. Let $p \in (1, \infty)$. Let (X, μ) be a measure space, and, to avoid trivialities, assume that $L^p(X, \mu)$ is not separable. Let $A \subseteq B(L^p(X, \mu))$ be the ideal of operators on $L^p(X)$ with separable range, which is known to be a closed ideal. We claim that A is an L^p-operator algebra with a cai, and, if X is a discrete space with counting measure, even a cai consisting of hermitian and real positive idempotents.

We prove the first part of the claim. If $E \subseteq L^p(X)$ is any separable subspace, it follows by Theorem 6 in Section 16 on page 146 of [Lacey 1974] and Lemma 2 in Section 17 on page 153 of [Lacey 1974] (see also Proposition 1.25 in [Phillips 2013a]), that E is contained in the range of a contractive idempotent with separable range. (Spaces are assumed to be real in [Lacey 1974, Section 16], however the complex case is no doubt well known to Banach space experts. Indeed by the just cited results or their proofs, a separable subspace of $L^p(X)$ is contained in a separable closed sublattice F. Since the norm on F is p-additive, F is an abstract L^p-space (see page 131 of [Lacey 1974] for definitions of these terms), so by Theorem 3 in both Sections 15 and 17 of [Lacey 1974], F is contractively complemented.)

Also, it is well known and an exercise that an operator x on a reflexive space has separable range if and only if x^* has separable range. Taking $q \in (1, \infty)$ to satisfy $\frac{1}{p} + \frac{1}{q} = 1$, we see that A^* is the collection of operators on $L^q(X, \mu)$ with separable range. For any $x_1, x_2, \ldots, x_n \in A$, the closure of the linear span of their ranges is separable by standard arguments. It follows that there exist contractive idempotents e and f with separable ranges such that $x_k = ex_k = x_k f$ for $k = 1, 2, \ldots, n$. Thus A has a cai $(e_t)_{t\in\Lambda}$, indeed a cai consisting of contractive idempotents and such that for any finite set $F \subseteq A$ there is $t \in \Lambda$ such that $e_t x = x e_t = x$ for all $x \in F$. Indeed take Λ to be the collection of such finite subsets of A.

Now take X to be a set I with counting measure, so $L^p(X) = l^p(I)$. For any $J \subseteq I$ let e_J be the canonical hermitian (diagonal) projection e_J onto the image of $l^p(J)$ in $l^p(I)$. Suppose $x_1, x_2, \ldots, x_n \in B(l^p(I))$ have separable ranges. Then, as above, the closure E of the joint span of their ranges is separable. So there exists a countable subset J of I (the union of the supports of elements in a countable dense set in E) such that all elements of E are supported on J. As in the last paragraph, the net (e_J), indexed by the countable subsets J of I ordered by inclusion, is a real positive hermitian cai consisting of bicontractive idempotents (since $1 - e_J = e_{I \setminus J}$ is contractive).

Example 3.7. Let G be a locally compact group which is not discrete, with Haar measure μ. Then $L^1(G)$ is approximately unital, and by Wendel's theorem, its multiplier algebra is $M(G)$, the measure algebra on G. In particular, $M(G)$ in an L^1-operator algebra. The identity of $M(G)$ is δ_1, the Dirac measure at 1_G. Hence the multiplier unitization of $L^1(G)$ is $L^1(G) + \mathbb{C}\delta_1 \subseteq M(G) \subseteq B(L^1(G))$. If $f \in L^1(G)$ and $\lambda \in \mathbb{C}$ then

$$\|f + \lambda\delta_1\| = \sup\left(\left\{\left|\int_G fg\,d\mu + \lambda g(1)\right| : g \in \mathrm{Ball}(C_0(G))\right\}\right).$$

We claim that the multiplier unitization of $L^1(G)$ is $L^1(G) \oplus^1 \mathbb{C}$. Fix $f \in L^1(G)$ and $\lambda \in \mathbb{C}$; it is enough to prove that $\|f + \lambda\delta_1\|_{M(G)} \geq \|f\|_1 + |\lambda|$. Given $\varepsilon > 0$, choose $h \in \mathrm{Ball}(C_0(G))$ with $\left|\int_G fh\,d\mu\right| > \|f\|_1 - \varepsilon$. Replacing h by $e^{i\beta}h$ for suitable $\beta \in \mathbb{R}$, we may assume that $\int_G fh\,d\mu \geq 0$. We have $\mu(\{1\}) = 0$ since G is not discrete. Choose by regularity a neighborhood U of 1 such that $\int_U |f|\,d\mu < \varepsilon$. By Urysohn's lemma there is a continuous function $k_1 : G \to [0, 1]$ with compact support K contained in U and taking the value 1 at 1_G. There is also a continuous function $k_2 : G \to [0, 1]$ which is 1 on $G \setminus U$ and is 0 on K. Choose $\theta \in \mathbb{R}$ such that $e^{i\theta}\lambda = |\lambda|$, and let $g = hk_2 + e^{i\theta}k_1$. Thus we have $g \in \mathrm{Ball}(C_0(G))$ with $\lambda g(1) = |\lambda|$, and $g = h$ on $G \setminus U$. So

$$\left|\int_G fg\,d\mu - \int_G fh\,d\mu\right| \leq 2\int_U |f|\,d\mu < 2\varepsilon.$$

Using $\int_G fh\,d\mu \geq 0$ and $\lambda g(1) = |\lambda| \geq 0$, we have

$$\begin{aligned}\|f + \lambda\delta_1\| &\geq \left|\int_G fg\,d\mu + \lambda g(1)\right| > \left|\int_G fh\,d\mu + \lambda g(1)\right| - 2\varepsilon \\ &= \int_G fh\,d\mu + |\lambda| - 2\varepsilon > \|f\|_1 + |\lambda| - 3\varepsilon.\end{aligned}$$

Since $\varepsilon > 0$ is arbitrary, the claim is proved.

It follows (see Definition 2.16 and Proposition 2.17) that $\mathfrak{F}_{L^1(G)} = \mathfrak{r}_{L^1(G)} = \{0\}$. By Lemma 2.15, $L^1(G)$ also has no nonzero hermitian elements. In particular, $L^1(G)$ has no hermitian or real positive cai.

Example 3.8. A good example of an L^p-operator algebra with a real positive cai but no hermitian cai is the set A of functions in the disk algebra vanishing at 1, represented on L^p of the circle as multiplication operators. The disk algebra contains no nontrivial hermitian elements, since the latter would be real-valued functions. However, A is approximately unital. One way to see this is to combine Example I.1.4 (b) of [Harmand et al. 1993] (after Lemma I.1.5 there) with Theorem 4.8.5 (1) of [Blecher and Le Merdy 2004], realizing the disk algebra as an operator algebra by representing it on L^2 of the circle (instead of L^p) as multiplication operators.

Example 3.9. Let $p \in [1, \infty) \setminus \{2\}$. We consider the algebras $\mathbb{K}(L^p(X, \mu))$ for $X = \mathbb{N}$ with counting measure and $X = [0, 1]$ with Lebesgue measure. The first has a cai consisting of real positive, in fact, hermitian, idempotents. The second has a cai, but contains no nonzero real positive elements, and in particular no nonzero hermitian elements.

A hermitian element in $B(L^p(X, \mu))$ is "multiplication by an essentially bounded real-valued locally measurable function" (Proposition 2.12). Thus the hermitian elements in $B(l^p)$ are the infinite diagonal matrices with bounded real entries. Therefore the canonical approximate identity in $\mathbb{K}(l^p)$ is a cai consisting of real positive and hermitian elements. (Also see the discussion in [Phillips and Viola 2017, Section 6].)

Abbreviate $A = \mathbb{K}(L^p([0, 1]))$. This algebra is approximately unital by, e.g., Theorem 2 of [Palmer 1985]. We can in fact give a formula for cai $(e_n)_{n=0,1,\dots}$ consisting of contractive finite rank idempotents which is increasing in the order $\leq$ in Definition 2.30. For $n = 0, 1, \dots,$ for

$$\xi \in L^p([0, 1]), \qquad k = 1, 2, \dots, 2^n, \quad \text{and} \quad x \in \left[\frac{k-1}{2^n}, \frac{k}{2^n}\right),$$

define

$$(e_n \xi)(x) = 2^n \int_{(k-1)/2^n}^{k/2^n} \xi(t)\, dt.$$

One easily checks that $(e_n)_{n=1,2,\dots}$ has the properties claimed for it.

Assume now that $p \in (1, \infty) \setminus \{2\}$. It is known (see Theorem 2 of [Benyamini and Lin 1985]) there is no nonzero $a \in A$ with $\|1 - a\| \leq 1$. It follows from Proposition 2.17 that $\mathfrak{r}_A = \{0\}$. That is, for $p \in (1, \infty) \setminus \{2\}$, there are no nonzero real positive elements in A in the main sense of [Blecher and Ozawa 2015]. Hence by Lemma 2.25 (4) and Lemma 2.1 (1), for every cai $\mathfrak{e}$, we have $\mathfrak{r}_A^{\mathfrak{e}} = \{0\}$. (This set was defined before Lemma 2.6 in [Blecher and Ozawa 2015]. In our present case, by Lemma 2.25 (4) and Definition 2.13, $\mathfrak{r}_A^{\mathfrak{e}}$ is the set of elements $x \in A$ with $\mathrm{Re}(\varphi(x)) \geq 0$ for all $\varphi \in S(A)$.) In particular, for $p \in (1, \infty) \setminus \{2\}$, A has no real positive cai. So, by Lemma 2.15 and Proposition 2.27, A has no hermitian cai.

It is easy to see directly that $\mathbb{K}(L^p([0, 1]))$ has no nonzero hermitian elements. Indeed, Proposition 2.12 implies that a hermitian element in $B(L^p([0, 1]))$ is the multiplication operator M_f by a bounded measurable real-valued function f. If the range of such an operator M_f is nonzero then it contains $L^p(E)$ for some non-null $E \subseteq [0, 1]$. Indeed there is $\varepsilon > 0$ such that $E = \{x \in [0, 1] : |f(x)| > \varepsilon\}$ has strictly positive measure. So $L^p(E)$ is contained in the range of multiplication by f. Since the measure has no atoms, $L^p(E)$ is infinite-dimensional. This cannot be if M_f is compact, since in that case its restriction to $L^p(E)$ is compact and bounded below.

Proposition 3.10. *Let $p \in (1, \infty) \setminus \{2\}$. Set $A = \mathbb{K}(L^p([0, 1]))$. If e is the identity of A^{**}, viewed as an element of $(A^1)^{**}$, then $\|1 - e\| > 1$.*

Proof. Suppose that $\|1-e\| \le 1$. Then by Goldstine's theorem there are nets $(a_t)_{t\in\Lambda}$ in A and $(\lambda_t)_{t\in\Lambda}$ in $\mathbb{C}$ such that $\|\lambda_t 1 + a_t\| \le 1$ for all $t \in \Lambda$ and $\lambda_t 1 + a_t \to 1 - e$ weak*. Applying the character annihilating A we see that $\lambda_t \to 1$. Hence $a_t \to -e$ weak*. Theorem 2 of [Benyamini and Lin 1985] provides $\delta > 0$ such that whenever $b \in A$ satisfies $\|b\| \ge \frac{1}{2}$ then $\|1 - b\| > 1 + \delta$. Choose $t_0 \in \Lambda$ such that $|1 - \lambda_t| < \frac{\delta}{2}$ for $t \in \Lambda$ with $t \ge t_0$. There is $t_1 \in \Lambda$ such that $t_1 \ge t_0$ and $\|a_{t_1}\| > \|-e\| - \frac{1}{2}$ (for otherwise $\|a_t\| \le \|-e\| - \frac{1}{2}$ for $t \ge t_0$, giving the contradiction $\|-e\| \le \|-e\| - \frac{1}{2}$). Clearly $\|-e\| \ge 1$. So $\|a_{t_1}\| > \frac{1}{2}$, whence $\|1 + a_{t_1}\| > 1 + \delta$. But

$$\|1 + a_{t_1}\| \le |1 - \lambda_{t_1}| + \|\lambda_{t_1} + a_{t_1}\| < \frac{\delta}{2} + 1.$$

This contradiction shows that $\|1 - e\| \le 1$ is impossible. $\square$

4. Miscellaneous results on L^p-operator algebras

4A. *Quotients and bi-approximately unital algebras.*

Definition 4.1. Let A be an L^p-operator algebra and let $J \subseteq A$ be a closed ideal. We say that J is a *bi-approximately unital ideal* in A (or is *bi-approximately unital in* A) if J is approximately unital and if there is an L^p-operator unitization B of A (as in Definition 1.7) such that identity e of the bidual J^{**} is a bicontractive idempotent in B^{**}.

Definition 4.2. Let A be an approximately unital Arens regular Banach algebra. We say that A is *bi-approximately unital* if in the bidual $(A^1)^{**}$ of its multiplier unitization A^1 the identity e of A^{**} is a bicontractive idempotent.

The next lemma shows that the terminology is consistent.

Lemma 4.3. *Let A be an approximately unital L^p-operator algebra. Then A is bi-approximately unital in the sense of Definition 4.2 if and only if A is bi-approximately unital as an ideal in itself in the sense of Definition 4.1.*

Recall from Lemma 2.1 (1) that L^p-operator algebras are automatically Arens regular.

Proof of Lemma 4.3. If A is bi-approximately unital in the sense of Definition 4.2, we can take the L^p-operator unitization required in Definition 4.1 to be A^1, recalling from Proposition 2.27 that A^1 is an L^p-operator algebra. If A is bi-approximately unital as an ideal in itself, let B be an L^p-operator unitization as required in Definition 4.1, and let e be as there. The obvious homomorphism $\varphi : B \to A^1$ is contractive, by Remark 1.9 (4), so $\varphi^{**} : B^{**} \to (A^1)^{**}$ is contractive. Thus $\|\varphi^{**}(e)\| \leq \|e\| \leq 1$ and $\|1 - \varphi^{**}(e)\| \leq \|1 - e\| \leq 1$. Since $\varphi^{**}(e)$ is the identity of A^{**} as in Definition 4.2, we have shown that A is bi-approximately unital. □

The algebra $\mathbb{K}(L^p([0, 1]))$ is an approximately unital L^p-operator algebra which is not bi-approximately unital. See Example 3.9 and Proposition 3.10.

By Lemma 2.29 (3), A is bi-approximately unital if and only if A is a u-ideal in A^1 as defined at the beginning of Section 3 of [Godefroy et al. 1993], that is, that $\|1 - 2e\| \leq 1$ where e is the identity of $A^{\perp\perp}$ in $(A^1)^{**}$.

Lemma 4.4. *Let A be an approximately unital Arens regular Banach algebra. If A has a real positive bounded approximate identity, then A is bi-approximately unital in the sense of Definition 4.2.*

Proof. Lemma 2.22 implies that A has a cai in $\mathfrak{F}_A$. This cai converges weak* to the identity e of A^{**} by Lemma 1.14. Since norm closed balls are weak* closed, we get $\|e\| \leq 1$ and $\|1 - e\| \leq 1$. Hence e is bicontractive. □

We conjecture that the converse of Lemma 4.4 is always true for L^p-operator algebras, namely that a bi-approximately unital L^p-operator algebra A has a real positive cai. Corollary 2.23 may be helpful for this question.

In [Gardella and Thiel 2016] it is shown that quotients of L^p-operator algebras by closed ideals need not be L^p-operator algebras, giving a negative solution to Problem 3.8 in [Le Merdy 1996]. Things are better if the ideal is approximately unital.

Lemma 4.5. *Let $p \in (1, \infty)$, let A be an L^p-operator algebra, and let $J \subseteq A$ be a closed ideal.*

(1) *If J is a bi-approximately unital ideal in A then A/J is an L^p-operator algebra.*

(2) *If J is approximately unital then there is a continuous bijective homomorphism from A/J to an L^p-operator algebra whose inverse is also continuous.*

Proof. We may suppose that A is unital with identity 1. Recall from Lemma 2.1 (2) that multiplication on A^{**} is separately weak* continuous. Also, the weak* closure of J in A^{**} is $J^{\perp\perp}$.

Let $(e_t)_{t\in\Lambda}$ be a cai for J. Since J is Arens regular (Lemma 2.1 (2)), Lemma 1.14 shows that there is $e \in J^{**}$ which is an identity for J^{**} and such that $(e_t)_{t\in\Lambda}$ converges weak* to e. Clearly $\|e\| \leq 1$.

We claim that $eA^{**} = J^{\perp\perp}$ and $A^{**}e = J^{\perp\perp}$. The proofs are the same, so we do only the first. We have $J^{\perp\perp} \subseteq eA^{**}$ since e is an identity for $J^{\perp\perp}$. Also, if $a \in A$

then $e_t a \in J$ for all $t \in \Lambda$, and $e_t a \to ea$ weak*, so ea is in the weak* closure of J in A^{**}, which is $J^{\perp\perp}$. Thus $eA \subseteq J^{\perp\perp}$. Since multiplication on A^{**} is separately weak* continuous, it follows that $eA^{**} \subseteq J^{\perp\perp}$. The claim is proved.

For $a \in A^{**}$, since $ae, ea \in J^{\perp\perp}$ and e is an identity for $J^{\perp\perp}$, we get $(ea)e = ea$ and $e(ae) = ae$. So e is central in A^{**}.

Since e is an idempotent, we have an algebra homeomorphism (not necessarily isometric) $A^{**}/eA^{**} \cong (1-e)A^{**}$. If J is bi-approximately unital, then $\|1-e\| = 1$, and this isomorphism is isometric. Therefore we have algebras homomorphisms

$$A/J \hookrightarrow A^{**}/J^{\perp\perp} = A^{**}/eA^{**} \to (1-e)A^{**} \hookrightarrow A^{**}.$$

All maps are isometric except possibly the third, which is a homeomorphism in general and is isometric if J is bi-approximately unital. Since A^{**} is an L^p-operator algebra by Lemma 2.1 (2), we are done. □

Remark 4.6. (1) Using an ultrapower argument, Charles Read showed in an unfinished personal communication that the quotient $B(l^p)/\mathbb{K}(l^p)$ is isometrically an L^p-operator algebra. This fact is also contained in Theorem 2.1 and Remark 2 of [Boedihardjo and Johnson 2015], combined with the fact (Theorem 3.3 (ii) of [Heinrich 1980]) that ultrapowers of L^p-spaces are L^p-spaces. This result also follows from Lemma 4.5 (1), since the canonical cai for $\mathbb{K}(l^p)$ is bicontractive and hence so is its weak* limit.

Read was also working on whether $B(L^p)/\mathbb{K}(L^p)$ is an L^p-operator algebra. The results of [Boedihardjo and Johnson 2015] quoted above show that it is at least isomorphic to one, a fact which also follows from Lemma 4.5 (2). We are studying Read's unfinished proof of the latter in hopes of answering this question.

(2) We remind the reader of an example from [Gardella and Thiel 2016]: the p variant of the Toeplitz algebra quotiented by $\mathbb{K}(l^p)$ is isomorphic to $F^p(\mathbb{Z})$, the norm closed subalgebra of $B(l^l(\mathbb{Z}))$ generated by the bilateral shift and its inverse. (This is the full group L^p-operator algebra of $\mathbb{Z}$ as defined in [Phillips 2013a]; see Definition 3.3 and the discussion before Proposition 3.14 there.) In particular, it is not $C(\mathbb{T})$.

Example 4.7. We exhibit $p \in (1, \infty) \setminus \{2\}$ and an L^p-operator algebra A with a closed approximately unital ideal J such that A/J is not isometrically isomorphic to an L^p-operator algebra. This shows that Lemma 4.5 (2) can't be improved. In our example, A is commutative and three dimensional, and J has an identity e which is central in A and with $\|e\| = 1$ (but $\|1-e\| > 1$).

Fix $n \in \{2, 3, \ldots\}$. (We will later take $n = 3$.) Let e_n be as in Example 3.2. Define $\zeta = e^{2\pi i/n}$ and $s = \operatorname{diag}(1, \zeta, \zeta^2, \ldots, \zeta^{n-1})$. For $k = 0, 1, \ldots, n-1$ set $f_k = s^k e_n s^{-k}$. We claim that:

(1) f_k is a contractive idempotent for $k = 0, 1, \ldots, n-1$.

(2) $f_0, f_1, \ldots, f_{n-1}$ are orthogonal, that is, $f_j f_k = 0$ if $j \neq k$.

(3) $\sum_{k=0}^{n-1} f_k = 1_{M_n}$, the $n \times n$ identity matrix.

For (1), recall from Example 3.2 that $\|e_n\| = 1$, and use $\|f_k\| \leq \|s\|^k \|e_n\| \|s^{-1}\|^k$. For (2) and (3), let $u \in M_n$ be the matrix whose k-th column (starting the count at 0 instead of 1) is

$$\frac{1}{\sqrt{n}} s^k (1, 1, \ldots, 1) = \frac{1}{\sqrt{n}} (1, \zeta^k, \zeta^{2k}, \ldots, \zeta^{(n-1)k}).$$

Computations show that u is unitary (in the $p = 2$ sense), and that

$$u^* e_n u = \operatorname{diag}(1, 0, 0, \ldots, 0) \quad \text{and} \quad u^* s u = \begin{bmatrix} 0 & 0 & \cdots & 0 & 1 \\ 1 & 0 & \cdots & \cdots & 0 \\ 0 & 1 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & 1 & 0 \end{bmatrix}.$$

For $k = 0, 1, \ldots, n-1$, it follows that $u^* f_k u = (u^* s u)^k (u^* e_n u)(u^* s u)^{-k}$ is the orthogonal projection (in the $p = 2$ sense) to the span of the k-th standard basis vector (starting the count at 0 instead of 1). Parts (2) and (3) of the claim now follow immediately.

Set $n = 3$ and let A be the subalgebra of M_3^p spanned by f_0, f_1, and f_2. This contains 1_{M_3}. Let $J = \mathbb{C} e_3$, an ideal in A with an identity of norm 1. We claim that if

$$p > \frac{\log(4)}{\log(4) - \log(3)} \tag{4-1}$$

then A/J is not isometric to an L^p-operator algebra. (This is presumably true for all $p \in [1, \infty) \setminus \{2\}$.) Indeed, the image f of f_1 in A/J is a contractive idempotent. It is actually bicontractive since

$$\begin{aligned} \|1 - f\| &= \inf\{\|1 - f_1 + \lambda f_0\| : \lambda \in \mathbb{C}\} \\ &\leq \|1 - f_1 - f_0\| = \|f_2\| \leq 1. \end{aligned}$$

We claim that if p is as in (4-1) then $\|1 - 2f\| > 1$. If we can prove this claim then A/J cannot be an L^p-operator algebra by Lemma 2.29 (3).

To prove the last claim note first that since

$$1 - 2f_1 + \lambda f_0 = s_1 (1 - 2e_3 + \lambda s_1^{-1} f_0 s_1) s_1^{-1},$$

we have

$$\begin{aligned} \|1 - 2f\| &= \inf\{\|1 - 2f_1 + \lambda f_0\| : \lambda \in \mathbb{C}\} \\ &= \inf\{\|1 - 2e_3 + \lambda s_1^{-1} f_0 s_1\| : \lambda \in \mathbb{C}\}. \end{aligned}$$

With $\frac{1}{p}+\frac{1}{q}=1$, the norm of $1-2e_3+\lambda s_1^{-1} f_0 s_1$ dominates the q-norm of the first row of $1-2e_3+\lambda s_1^{-1} f_0 s_1$. This first row is

$$\left(\tfrac{1}{3},\ -\tfrac{2}{3},\ -\tfrac{2}{3}\right)-\tfrac{1}{3}\lambda\,(1\,,\ \zeta\,,\ \zeta^2)=\tfrac{1}{3}(1-\lambda\,,\ -2-\lambda\zeta\,,\ -2-\lambda\zeta^2). \tag{4-2}$$

We estimate the minimum of

$$|1-\lambda|^q+|2+\lambda\zeta|^q+|2+\lambda\zeta^2|^q=|1-\lambda|^q+|2\overline{\zeta}+\lambda|^q+|2\overline{\zeta}^2+\lambda|^q.$$

Write $\lambda=x+iy$ for real x and y. Then

$$2\overline{\zeta}+\lambda=-1+x+i(y-\sqrt{3}) \quad \text{and} \quad 2\overline{\zeta}^2+\lambda=-1+x+i(y+\sqrt{3}).$$

Thus we are minimizing

$$G(x,y)=((1-x)^2+y^2)^{q/2}+((1-x)^2+(y-\sqrt{3})^2)^{q/2}+((1-x)^2+(y+\sqrt{3})^2)^{q/2}.$$

Clearly $G(x,y)\geq G(1,y)$ for all $x,y\in\mathbb{R}$. So we must minimize the function

$$g_c(y)=|y|^q+|y-c|^q+|y+c|^q$$

for $c=\sqrt{3}$. For any $c>0$, this function is continuous, even, and clearly strictly increasing on $[c,\infty)$. For $y\in(0,c)$ we have

$$g_c'(y)=q\left(y^{q-1}+(c+y)^{q-1}-(c-y)^{q-1}\right).$$

Since $q-1\geq 0$ and $c+y>c-y>0$, it follows that $g_c'(y)>0$. By symmetry, the minimum value of g_c occurs at $y=0$. So, for all $x,y\in\mathbb{R}$, we have $G(x,y)\geq G(1,0)=2\cdot 3^{q/2}$.

Applying this estimate to the q-norm of the right-hand side of (4-2), we get

$$\|1-2f\|^q\geq\frac{2\cdot 3^{q/2}}{3^q}=2\cdot 3^{-q/2}.$$

If $q<2\log(2)/\log(3)$, this quantity is greater than 1, and this happens exactly when (4-1) holds. The claim is proved.

4B. ***Unitization of nonunital L^p-operator algebras.*** Unfortunately Meyer's beautiful unitization theorem (see [Blecher and Le Merdy 2004, Corollary 2.1.15]) for operator algebras on Hilbert spaces fails badly for L^p-operator algebras. That is, unitizations of nonunital L^p-operator algebras are not unique isometrically (Examples 4.8 and 4.9 below). However if two approximately unital L^p-operator algebras A_1 and A_2 are isometrically isomorphic and they each act nondegenerately on the L^p-spaces on which they act, then $A_1+\mathbb{C}\,1$ is isometrically isomorphic to $A_2+\mathbb{C}\,1$. Indeed, for $j=1,2$, the algebra $A_j+\mathbb{C}\,1$ is isometrically isomorphic to the multiplier unitization of A_j by Lemma 2.24.

We now illustrate the failure of Meyer's theorem, even in the case of approximately unital L^p-operator algebras. We give two versions. In the first, the algebras are finite-dimensional and already unital, but degenerately represented. In the second, the algebras are genuinely nonunital.

Example 4.8. Let $M_2^p = B(l_2^p)$ be as in Notation 3.1. Let $e = e_2$ be as in Example 3.2, and let $f = e_{1,1}$, the $(1, 1)$ standard matrix unit. Let $1 = 1_{M_2}$ be the 2×2 identity matrix. Then $\mathbb{C}\, e \cong \mathbb{C}\, f$ isometrically. We claim that $\mathbb{C}\, e + \mathbb{C}\, 1$ is not isometric to $\mathbb{C}\, f + \mathbb{C}\, 1$, so that Meyer's unitization theorem fails. The idempotents in $\mathbb{C}\, f + \mathbb{C}\, 1$ are 0, f, $1 - f$, and 1, all of which are clearly hermitian. By Example 3.2, however, e is a nonhermitian idempotent in $\mathbb{C}\, e + \mathbb{C}\, 1$. The claim follows.

Example 4.9. We continue with the notation in Example 4.8, to produce a nonunital example where Meyer's unitization theorem fails. Set $A = c_0 \oplus \mathbb{C}\, e$ and $B = c_0 \oplus \mathbb{C}\, f$, both viewed as subalgebras of $B(l^p(\mathbb{N}) \oplus^p l_2^p)$. These are isometrically isomorphic L^p-operator algebras, which are approximately unital. Indeed, they have obvious increasing approximate identities consisting of hermitian idempotents. Write 1 for the identity of $B(l^p(\mathbb{N}) \oplus^p l_2^p)$. We claim that $A + \mathbb{C}\, 1$ is not isometrically isomorphic to $B + \mathbb{C}\, 1$. To see this, first observe that all elements of $B + \mathbb{C}\, 1$ are multiplication operators on $l^p(\mathbb{N}) \oplus^p l_2^p = l^p(\mathbb{N} \amalg \{0, 1\})$. It is immediate that all idempotents in this algebra are hermitian. On the other hand, there is a canonical restriction homomorphism $\rho : A + \mathbb{C}\, 1 \to B(l_2^p)$, which is a unital contractive surjection to $\mathbb{C}\, e + \mathbb{C}\, 1_{M_2}$, namely "compression" to the subspace l_2^p of $l^p(\mathbb{N}) \oplus^p l_2^p$. As we said in Example 4.8, $e \in \mathbb{C}\, e + \mathbb{C}\, 1_{M_2}$ is a nonhermitian idempotent. However, $g = (0, e) \in A \subseteq A + \mathbb{C}\, 1$ is an idempotent such that $\rho(g) = e$. If g were hermitian, then e would be too, by [Phillips and Viola 2017, Lemma 6.7]. So $A + \mathbb{C}\, 1$ contains a nonhermitian idempotent.

In Example 4.9, one can show that the algebra $B + \mathbb{C}\, 1$ is a spatial L^p AF algebra in the sense of Definition 9.1 of [Phillips and Viola 2017], while $A + \mathbb{C}\, 1$ isn't.

We remark that [Phillips and Viola 2017, Proposition 9.9] gives conditions which force uniqueness of the unitization of an L^p-operator algebra. The fact that Meyer's theorem fails for $\mathbb{C}\, e$ and $\mathbb{C}\, f$ in Example 4.8 shows, by Meyer's proof (see [Blecher and Le Merdy 2004, 2.1.14]), that, even in $M_2^p = B(l_2^p)$, some of the basic properties of the Cayley transform for Hilbert space operators must fail for $p \neq 2$. We turn to this next.

4C. ***The Cayley and $\mathfrak{F}$ transforms.*** The Cayley transform $\kappa(x) = (x - 1)(x + 1)^{-1}$ is an important tool for operator algebras on a Hilbert space, as is the fact that in that setting $\kappa(x)$ is a contraction for accretive x. In [Blecher and Read 2013; 2014] the associated transform

$$\mathfrak{F}(x) = x(x + 1)^{-1} = \tfrac{1}{2}(1 + \kappa(x))$$

is used. For L^2-operator algebras it takes $\mathfrak{r}_A$ onto the strict contractions in $\frac{1}{2}\mathfrak{F}_A$.

This all fails in full generality for L^p-operator algebras, which means that many of the general results in [Blecher and Ozawa 2015] do not improve for L^p-operator algebras.

Here are two things which do work. First, if A is an approximately unital L^p-operator algebra then the $\mathfrak{F}$ transform does map $\mathfrak{r}_A$ into $\mathfrak{F}_A$. (By Lemma 3.4 of [Blecher and Ozawa 2015], this is true for arbitrary approximately unital Banach algebras.) Second, if A is any unital Banach algebra and $x \in \mathfrak{F}_A$, then $\|\kappa(x)\| = \|1 - 2\mathfrak{F}(x)\| \leq 1$. Indeed, with $y = x - 1$, we have $\|y\| \leq 1$, so that

$$\|\kappa(x)\| = \left\| \left(1 + \tfrac{1}{2} y\right)^{-1} \left(\tfrac{1}{2} y\right) \right\| \leq \left\| \tfrac{1}{2} y \right\| \sum_{k=0}^{\infty} \left\| \tfrac{1}{2} y \right\|^k \leq 1.$$

Example 4.10. We prove the existence of $\delta > 0$ such that for all $p \in [1, 1 + \delta)$ there is a unital finite dimensional L^p-operator algebra containing a real positive element x for which $\|\kappa(x)\| > 1$. Presumably this happens for all $p \in [1, \infty) \setminus \{2\}$, but proving this may require more work.

Indeed, in M_2^p (Notation 3.1) consider

$$x = \begin{bmatrix} 1 - i & 1 \\ 1 & 1 - i \end{bmatrix} \quad \text{and} \quad \kappa(x) = \frac{1}{5} \begin{bmatrix} 1 - 3i & 1 + 2i \\ 1 + 2i & 1 - 3i \end{bmatrix}.$$

Since $x = 2e_2 - i\,1_{M_2}$ in the notation of Example 3.2, it follows from considerations in that example that x is real positive in M_2^p. However $\kappa(x)$ applied to the unit vector $(1, 0)$ has p-norm $\frac{1}{5}(10^{p/2} + 5^{p/2})^{1/p}$, which exceeds 1 for $p \in [1, \delta)$, for some fixed $\delta > 0$.

One may also arrive at this same example by modifying the L^1-operator algebra example given in Example 3.14 in [Blecher and Ozawa 2015]. It was stated there that the convolution algebra $l^1(\mathbb{Z}_2)$ contains real positive elements x for which $\|\kappa(x)\| > 1$. An explicit example of such an element was not given there though. Let $F_{\mathrm{r}}^p(\mathbb{Z}_2)$ be the reduced group L^p-operator algebra of the two element group (as defined in [Phillips 2013a]). This is isometric, via the regular representation of $\mathbb{Z}_2$ on $l^p(\mathbb{Z}_2)$, to the unital subalgebra of M_2^p generated by the idempotent

$$e = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

(called e_2 in Example 3.2). This latter algebra contains our element x above. The regular representation of $\mathbb{Z}_2$ on $l^p(\mathbb{Z}_2)$ sends the nontrivial group element to

$$s = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},$$

and we have the relations $e = \frac{1}{2}(s + 1)$ and $s = 2e - 1$.

Moreover, $F^1_{\mathrm{r}}(\mathbb{Z}_2) \cong l^1(\mathbb{Z}_2)$ isometrically. Via these considerations, a real positive element w in Example 3.14 in [Blecher and Ozawa 2015] corresponds to a real positive element a in $F^1_{\mathrm{r}}(\mathbb{Z}_2)$ and a real positive matrix x in M^1_2. Moreover, $\|\kappa(w)\| > 1$ if and only if $\|\kappa(a)\| > 1$, in turn if and only if $\|\kappa(x)\| > 1$. Since the map $F^1_{\mathrm{r}}(\mathbb{Z}_2) \to F^p_{\mathrm{r}}(\mathbb{Z}_2)$ is unital and contractive for $p \in [1, \infty)$, it follows easily that a (resp. x) is also real positive in $F^p_{\mathrm{r}}(\mathbb{Z}_2)$ (resp. M^p_2). By "continuity in p", the Cayley transform of x in M^p_2 is not contractive for p close to 1. A specific example of this of course is the matrix x in the second paragraph of the present example.

4D. ***Support idempotents.*** There is some improvement over [Blecher and Ozawa 2015] in the theory of support idempotents.

Proposition 4.11. *Let A be an approximately unital Arens regular Banach algebra, and let $x \in \mathfrak{r}_A$. Then, using the notation of Definition 2.18, the sequence $(x^{1/n})_{n\in\mathbb{N}}$ has a weak* limit $s(x) \in A^{**}$. Moreover*:

(1) *$s(x)$ is an idempotent.*

(2) *$s(x)$ is an identity for the second dual of the closed subalgebra of A generated by x.*

(3) $s(x)x = xs(x) = x$.

(4) *With $\mathfrak{F}$ as in Section 4C, we have $s(\mathfrak{F}(x)) = s(x)$.*

(5) $\|1 - s(x)\| \leq 1$.

(6) *$s(x)$ is a real positive idempotent in A^{**}.*

Definition 4.12. Let A and $x \in A$ be as in Proposition 4.11. We call $s(x)$ the *support idempotent* of x.

Proposition 4.11 is proved in the discussion after Proposition 3.17 of [Blecher and Ozawa 2015] (see also the discussion after Corollary 6.20 in [Blecher 2016]). Our advantage here over the situation in those papers is that the weak* limit of $x^{1/n}$ exists (it equals the identity for the second dual in (2) above), and so the support idempotent $s(x)$ is unique.

The support idempotent of x is minimal in several senses related to the orderings in Definition 2.30.

Corollary 4.13. *Under the hypotheses of Proposition 4.11, we furthermore have*:

(1) *If $f \in A^{**}$ is any idempotent with $fx = x$, then $fs(x) = s(x)$, that is, $s(x) \leq_{\mathrm{r}} f$ in the sense of Definition 2.30.*

(2) *If $f \in A^{**}$ is any idempotent with $xf = x$, then $s(x)f = s(x)$.*

(3) *If $f \in A^{**}$ is any idempotent with $fx = x$ and $xf = x$, then $s(x) \leq f$ in the sense of Definition 2.30.*

Proof. By Proposition 2.19 (4), in part (1) we have $fx^{1/n} = x^{1/n}$. Hence (1) follows from $x^{1/n} \to s(x)$ weak* and separate weak* continuity of multiplication ([Blecher and Le Merdy 2004, 2.5.3]). Similarly for (2). Part (3) is now obvious. □

Thus $s(x)$ is the smallest idempotent in A^{**} with $fx = x$, in the ordering $\leq_{\mathrm{r}}$ (or with $fx = x$ and $xf = x$, in the ordering $\leq$). Recall from Corollary 2.4 that if A is an L^p-operator algebra then so is A^{**}, and so by Lemma 2.31 (2) we see that $\leq$ coincides with $\leq_{\mathrm{r}}$ on real positive idempotents in A^{**}. Hence in this case $s(x)$ is the smallest idempotent in A^{**} with $fx = x$ (or with $xf = x$), in the ordering $\leq$.

In the case of a subalgebra of $B(L^p(X))$, we also get a support idempotent acting on $L^p(X)$.

Proposition 4.14. *Let $p \in (1, \infty)$, let $A \subseteq B(L^p(X))$ be an approximately unital closed subalgebra, and let $x \in \mathfrak{r}_A$. Let $s(x)$ be as in Proposition 4.11. Let $\varphi : A^{**} \to B(L^p(X))$ be the contractive homomorphism obtained from the identity representation of A as in Lemma 2.32, and set $e = \varphi(s(x))$. Then:*

(1) *e is an idempotent with range $\overline{xL^p(X)}$, and e is real positive if A is nondegenerate.*

(2) *$ex = xe = x$.*

(3) *$\overline{xL^p(X)}$ is a complemented subspace of $L^p(X)$.*

(4) *Using the notation of Definition 2.18, $x^{1/n} \to e$ in the strong operator topology on $B(L^p(X))$.*

(5) *If A is nondegenerate and $f \in B(L^p(X))$ is any real positive idempotent with $fx = x$ or $xf = x$, then $e \leq f$ in the sense of Definition 2.30.*

Nondegeneracy is probably needed for real positivity in (1) and for (5). Otherwise, letting f be as in Lemma 2.33, our proof below only yields a real positive idempotent in $B(fL^p(X))$.

Proof of Proposition 4.14. Let $E \subseteq L^p(X)$ and the idempotent $f \in B(L^p(X))$ be as in Lemma 2.33. We first claim that $\varphi(1) = f$. Indeed, this is always the case in the situation of Lemma 2.33 provided that A is Arens regular, by the following simple argument. Let $(e_t)_{t \in \Lambda}$ be a cai for A. Then $e_t \to 1$ weak* in A^{**} by Lemma 1.14. Therefore $e_t \to \varphi(1)$ weak* in $B(L^p(X))$ by weak* to weak* continuity of φ. Also $e_t \to f$ weak* in $B(L^p(X))$ by Lemma 2.33 (1). The claim is proved.

We have $x^{1/n} \to e$ weak* in $B(L^p(X))$. Since φ is a homomorphism, e is an idempotent satisfying $ex = xe = x$, which is (2). Using Proposition 4.11 (5) and $\varphi(1) = f$, we get $\|f - e\| \leq \|\varphi\| \|f - s(x)\| \leq 1$. If A is nondegenerate, then $f = 1$, so e is real positive by Lemma 2.29 (4). Since $ex = x$, we clearly have $xL^p(X) \subseteq eL^p(X)$. So $\overline{xL^p(X)} \subseteq eL^p(X)$. Since $x^{1/n}\eta \to e\eta$ weakly for $\eta \in L^p(X)$, it follows that $xL^p(X)$ is weakly, hence norm, dense in $eL^p(X)$. Thus $eL^p(X) = \overline{xL^p(X)}$ and we now have all of (1), as well as (3).

For $\eta \in L^p(X)$ we have $x^{1/n} x\eta \to x\eta$ in norm. Since $(x^{1/n})_{n\in\mathbb{N}}$ is a bounded sequence (using Proposition 2.19 (3)), it follows that $x^{1/n} e\xi \to e\xi$ for all $\xi \in L^p(X)$. Clearly $x^{1/n}(1-e)\xi = 0 \to e(1-e)\xi$ also, using (2) and Proposition 2.19 (4). Thus we have (4).

For (5), note that $fx = x$ if and only if $fe = e$ as in the proof of Corollary 4.13, and similarly $xf = x$ if and only if $ef = e$. Since $fe = e$ if and only if $ef = e$ by Lemma 2.31 (1), the proof of (5) is clear (as in the proof of Corollary 4.13). □

It is shown in [Blecher and Ozawa 2015, Corollary 3.19] that if $x, y \in \mathfrak{r}_A$ then $\overline{xA} \subseteq \overline{yA}$ if and only if $s(y)s(x) = s(x)$.

Lemma 4.15. *Let $p \in (1, \infty)$. Let A be an approximately unital L^p-operator algebra, and let $x, y \in \mathfrak{r}_A$. Then $\overline{xA} = \overline{yA}$ if and only if $s(x) = s(y)$.*

Proof. If $s(x) = s(y)$ then $\overline{xA} = \overline{yA}$ by [Blecher and Ozawa 2015, Corollary 3.18]. Conversely, if $\overline{xA} = \overline{yA}$ then by [Blecher and Ozawa 2015, Corollary 3.18] we have $s(x)A^{**} = s(y)A^{**}$. It follows that $s(x)s(y) = s(y)$ and $s(y)s(x) = s(x)$. By Proposition 4.11 (6) and Lemma 2.31 (2), the second equation implies $s(x)s(y) = s(x)$. So $s(x) = s(y)$. □

Unlike the L^2-operator algebra case (see, for example, [Blecher and Read 2011, Lemma 2.5]), if $x \in \frac{1}{2}\mathfrak{F}_A$ (that is, if $\|1 - 2x\| \le 1$), then $s(x)$ need not be contractive. An example is $x = \frac{1}{2}(1 - e_3)$, for e_3 as in Example 3.2.

4E. *Some consequences of strict convexity of L^p-spaces.*

Lemma 4.16. *Let E be a strictly convex Banach space, and let $f \in B(E)$ be a contractive idempotent. Let $\xi \in E$ satisfy $\|f\xi\| = \|\xi\|$. Then $f\xi = \xi$.*

Proof. This is well known. Suppose that $\xi \neq f\xi$. Set $\eta = \frac{1}{2}(\xi + f\xi)$. Then $\|\eta\| < \|f\xi\|$, giving the contradiction $\|f\xi\| = \|f\eta\| \le \|\eta\| < \|f\xi\|$. □

Lemma 4.17. *Let $p \in (1, \infty)$, let E and F be Banach spaces, and let $S \subseteq B(E, F)$ be a linear subspace. Define matrix norms on $B(E, F)$ by interpreting elements of $M_n(B(E, F))$ as linear maps from the l^p direct sum of n copies of E to the l^p direct sum of n copies of F. Then any $\varphi \in \mathrm{Ball}(S^*)$ is p-completely contractive in the sense of* [*Pisier 1990*].

Proof. This follows by essentially the argument in the L^2-operator space case, and no doubt this is well known. By the usual argument (see, e.g., the proof of [Daws 2010, Lemma 4.2]), we have to show that

$$\left\| \sum_{j,k=1}^{n} \beta_j x_{j,k} \alpha_k \right\| \le \sup\left(\left\{ \left(\sum_{j=1}^{n} \left\| \sum_{k=1}^{n} x_{j,k} \xi_k \right\|^p \right)^{1/p} : \sum_{k=1}^{n} \|\xi_k\|^p \le 1 \right\} \right),$$

where $n \in \mathbb{N}$, $\beta = (\beta_1, \beta_2, \ldots, \beta_n) \in \mathrm{Ball}(l_n^q)$, $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_n) \in \mathrm{Ball}(l_n^p)$,

$\xi_1, \xi_2, \ldots, \xi_n \in E$, and $x_{j,k} \in S$ for $j, k = 1, 2, \ldots, n$. However the latter supremum may be written as

$$\sup\left(\left\{\left|\sum_{j=1}^{n} \psi_j\left(\sum_{k=1}^{n} x_{j,k}\xi_k\right)\right| : \sum_{k} \|\xi_k\|^p \le 1, \ \sum_{j=1}^{n} \|\psi_j\|^q \le 1\right\}\right),$$

where $\xi_1, \xi_2, \ldots, \xi_n \in E$ and $\psi_1, \psi_2, \ldots, \psi_n \in F^*$. This supremum clearly dominates

$$\sup\left(\left\{\left|\sum_{j,k=1}^{n} \beta_j \psi(x_{j,k}\alpha_k \xi)\right| : \psi \in \mathrm{Ball}(F^*), \ \xi \in \mathrm{Ball}(E)\right\}\right),$$

since $\sum_{j=1}^{n} \|\beta_j \psi\|^q \le 1$ and $\sum_{k=1}^{n} \|\alpha_k \xi\|^p \le 1$. This last supremum is equal to $\left\|\sum_{j,k=1}^{n} \beta_j x_{j,k} \alpha_k\right\|$. □

Both the following lemmas apply in particular to hermitian idempotents, by parts (2) and (4) of Lemma 2.29.

Lemma 4.18. *Let E be a Banach space, let $\omega \in \mathrm{Ball}(E^*)$, and let $\xi \in \mathrm{Ball}(E)$. Let φ be the vector state on $B(E)$ given by $\varphi(a) = \langle \omega, a\xi \rangle$ for all $a \in B(E)$. Let $e \in B(E)$ be a real positive idempotent, and suppose $\varphi(e) = 0$.*

(1) *If E is strictly convex then $\varphi(ae) = 0$ for all $a \in A$.*

(2) *If E^* is strictly convex then $\varphi(ea) = 0$ for all $a \in A$.*

Proof. From $\varphi(e) = 0$ we get $\varphi(1 - e) = 1$. Also $\|1 - e\| \le 1$ by Lemma 2.29 (4).

Suppose E is strictly convex. We have

$$\|(1 - e)\xi\| \ge |\varphi(1 - e)| = 1 = \|\xi\|.$$

So $\xi = (1 - e)\xi$ by Lemma 4.16. For $a \in B(E)$ we then have $\varphi(ae) = \langle \omega, ae\xi \rangle = 0$.

Now suppose E^* is strictly convex. We have $\|(1 - e)^*\| = \|1 - e\| \le 1$, and $\varphi(a) = \langle a^*\omega, \xi \rangle$ for all $a \in B(E)$, so

$$\|(1 - e)^*\omega\| \ge |\varphi(1 - e)| = 1 = \|\omega\|.$$

So $\omega = (1 - e)^*\omega$ by Lemma 4.16, and for $a \in B(E)$ we then have $\varphi(ea) = \langle e^*\omega, a\xi \rangle = 0$. □

Lemma 4.19. *Let $p \in (1, \infty)$, and let A be a unital L^p-operator algebra. Let φ be a state on A and let $e \in A$ be a real positive idempotent. If $\varphi(e) = 0$ then $\varphi(ae) = \varphi(ea) = 0$ for all $a \in A$.*

Proof. We may assume that A is a unital subalgebra of $B(L^p(X))$ for some X. By Lemma 4.17, φ is p-completely contractive in the sense of [Pisier 1990]. So by Theorem 2.1 of that paper and the remark after it, and using the fact that ultraproducts of L^p-spaces are L^p-spaces (Theorem 3.3 (ii) of [Heinrich 1980]), there exist an SQ_p-space E, $\xi \in \mathrm{Ball}(E)$, $\omega \in \mathrm{Ball}(E^*)$, and a p-completely contractive map $\pi : A \to B(E)$ such that $\varphi(a) = \langle \omega, \pi(a)\xi \rangle$ for all $a \in A$. It is easy to see and no doubt well known that π may be taken to be a unital homomorphism. Then $\pi(e)$ is an idempotent, and $\|1 - \pi(e)\| \le 1$. As explained in Remark 2.34, SQ_p-spaces are both smooth and strictly convex. So their duals are also strictly convex. We may therefore apply Lemma 4.18 to the vector state $\langle \omega, \cdot\, \xi \rangle$ on $B(E)$. Thus for all $a \in E$ we have

$$\varphi(ae) = \langle \omega, \pi(a)\pi(e)\xi \rangle = 0 \quad \text{and} \quad \varphi(ea) = \langle \omega, \pi(e)\pi(a)\xi \rangle = 0. \qquad \square$$

Remark 4.20. (1) Lemma 4.19 holds if A is a unital SQ_p-operator algebra. The proof is the same too, but with L^p replaced by SQ_p throughout. For further details on the construction of π in this case see [Pisier 1990, Theorem 2.1] and, e.g., [Daws 2010, Theorem 4.1].

(2) Lemma 4.19 holds for an approximately unital L^p- (or SQ_p-) operator algebra A, and indeed holds for restrictions of states on any L^p- (or SQ_p-) operator algebra unitization of A. This follows by applying the unital case to the extending state on the unitization of A.

Corollary 4.21. *Let $p \in (1, \infty)$. Let A be an approximately unital L^p-operator algebra. If $x \in \mathfrak{r}_A$ and $\varphi \in S(A)$ with $\varphi(s(x)) = 0$, then $\varphi(x) = 0$. Conversely, if further $x \in \mathfrak{F}_A$ and $\varphi(x) = 0$ then $\varphi(s(x)) = 0$.*

Proof. We may work in A^1 by extending φ to a state there, and we may thus assume that A is unital.

The idempotent $s(x)$ is real positive by Proposition 4.11 (6). Using Lemma 4.19, Proposition 4.11 (3), and $\varphi(s(x)) = 0$, we get $\varphi(x) = 0$.

On the other hand, if $x \in \mathfrak{F}_A$ and $\varphi(x) = 0$ then $\varphi(1 - x) = 1$. As in the proof of Lemma 4.19, there are an SQ_p-space F, a contractive unital homomorphism $\pi : A^1 \to B(F)$, $\xi \in \mathrm{Ball}(F)$, and $\eta \in \mathrm{Ball}(F^*)$, such that $\varphi = \langle \pi(\cdot)\xi, \eta \rangle$ for all $a \in A^1$. Then

$$1 = \varphi(1 - x) = \langle \omega, (1 - \pi(x))\xi \rangle \le \|\pi(1 - x)\xi\| \le 1.$$

Therefore, with $\frac{1}{p} + \frac{1}{q} = 1$, both ξ and $(1 - \pi(x))\xi$ define norm one linear functionals on $L^q(X)$ which take ω to 1. Strict convexity of $L^q(X)$ implies $(1 - \pi(x))\xi = \xi$. So $\pi(x)\xi = 0$. Proposition 2.19 (4) now implies that $\pi(x^{1/n})\xi = 0$ for all $n \in \mathbb{N}$. Hence $\varphi(x^{1/n}) = 0$. In the limit $\varphi(s(x)) = 0$. $\square$

Lemma 4.22 is a generalization of part of [Blecher and Read 2011, Lemma 2.10], with a similar proof but using Corollary 4.21.

Lemma 4.22. *Let $p \in (1, \infty)$. Let A be an approximately unital L^p-operator algebra, and let $x \in \mathfrak{F}_A$. The following are equivalent:*

(1) $s(x) = 1$.

(2) $\varphi(x) \neq 0$ *for all* $\varphi \in S(A)$.

(3) $\mathrm{Re}(\varphi(x)) > 0$ *for all* $\varphi \in S(A)$.

If $x \in \mathfrak{r}_A$ *then* (3) *implies* (2) *and* (2) *implies* (1).

Proof. Let $x \in \mathfrak{r}_A$. Then (3) implies (2) trivially. To show that (2) implies (1), suppose (1) fails. Represent A^{**} as a unital subalgebra of $B(L^p(X))$ for some X by Corollary 2.36. Choose $\xi \in \mathrm{Ball}(L^p(X))$ in the range of the idempotent $1 - s(x)$, and choose $\eta \in \mathrm{Ball}(L^p(X)^*)$ with $\langle \xi, \eta \rangle = 1$. Then $\varphi(x) = \langle x\xi, \eta \rangle$ defines a state on A with $\varphi(1 - s(x)) = 1$. Since $\varphi(s(x)) = 0$, Corollary 4.21 implies $\varphi(x) = 0$.

If $x \in \mathfrak{F}_A$ then (1) implies (2) by Corollary 4.21. For (2) implies (3), follow part of the proof of [Blecher and Read 2011, Lemma 2.10]: $|1 - \varphi(x)| \leq 1$ is not compatible with both $\varphi(x) \neq 0$ and $\mathrm{Re}(\varphi(x)) \leq 0$. □

4F. *Hahn–Banach smoothness of L^p-operator algebras.*

Definition 4.23. Let E be a Banach space and let $M \subseteq E$ be a closed subspace. We say that M is *Hahn–Banach smooth* in E if for every $\omega_0 \in M^*$ there is a unique $\omega \in E^*$ with $\|\omega\| = \|\omega_0\|$ and $\omega|_M = \omega_0$,

Existence of ω is just the Hahn–Banach theorem. When verifying this property, we need only consider the case $\|\omega_0\| = 1$.

Proposition 2.1.18 in [Blecher and Le Merdy 2004] works for L^p-operator algebras.

Proposition 4.24. *Let* $p \in (1, \infty)$. *Let A be an approximately unital L^p-operator algebra and denote the identity of A^1 by* 1.

(1) *Let* $(e_t)_{t \in \Lambda}$ *be a cai in A. If* $\psi : A^1 \to \mathbb{C}$ *is a functional on* A^1, *then* $\lim_t \psi(e_t) = \psi(1)$ *if and only if* $\|\psi\| = \|\psi|_A\|$.

(2) *A is Hahn–Banach smooth in A^1 (Definition 4.23).*

Proof. We may assume that A is nonunital (the case of unital algebras being easy).

The forward direction of (1) is just as in the proof of [Blecher and Le Merdy 2004, Proposition 2.1.18].

For the other direction suppose that $\psi : A^1 \to \mathbb{C}$ with $\|\psi\| = \|\psi|_A\| = 1$. As in the proof of Lemma 4.19, there are an SQ_p-space F, a contractive unital homomorphism $\pi : A^1 \to B(F)$, $\xi \in \mathrm{Ball}(F)$, and $\eta \in \mathrm{Ball}(F^*)$, such that $\psi = \langle \pi(\cdot)\xi, \eta \rangle$ for all $a \in A^1$.

Apply the extension of Lemma 2.33 given in Remark 2.34 to the representation $\pi|_A$. Let $E \subseteq F$ and the idempotent $f \in B(F)$ be as there. The extensions of parts (1) and (3) of Lemma 2.33 imply that $\pi(e_t) \to f$ weak* in $B(F)$ and $\pi(a) = \pi(a) f$ for all $a \in A$. Thus, for all $a \in A$,

$$\left|\langle \pi(a)\xi, \eta \rangle\right| = \left|\langle \pi(a) f\xi, \eta \rangle\right| \leq \|a\| \|f\xi\|.$$

This shows that $\|\psi|_A\| \leq \|f\xi\|$. Hence, by hypothesis, $\|f\xi\| = \|\xi\| = 1$. Since E is strictly convex (see Remark 2.34), Lemma 4.16 implies $f\xi = \xi$, that is, $\xi \in \overline{\operatorname{span}}(\pi(A)E)$. Now, since $\pi(e_t) \to f$ weak* we have

$$\langle \pi(e_t)\xi, \eta\rangle \to \langle f\xi, \eta\rangle = \langle \xi, \eta\rangle,$$

which says that $\psi(e_t) \to \psi(1)$.

For the deduction of (2) from (1), let $\varphi \in A^*$ satisfy $\|\varphi\| = 1$. Proceed as in the proof of [Blecher and Le Merdy 2004, Proposition 2.1.18], but beginning by writing $\varphi \in A^*$ as $\varphi = \langle \pi(\cdot)\zeta, \eta\rangle$ for E as above, and for a contractive homomorphism $\pi : A \to B(E)$, $\zeta \in \operatorname{Ball}(E)$, and $\eta \in \operatorname{Ball}(E^*)$. This may be done for example by considering a Hahn–Banach extension of φ to A^1 and using the unital case above. □

Corollary 4.25. *Let $p \in (1, \infty)$, and let A be a nonunital approximately unital L^p-operator algebra.*

(1) *Let $\varphi \in A^*$ satisfy $\|\varphi\| = 1$. Then the following are equivalent*:
   - (a) *φ is a state on A, that is (see Definition 2.6), φ extends to a state on A^1.*
   - (b) *$\varphi(e_t) \to 1$ for every cai $(e_t)_{t\in\Lambda}$ for A.*
   - (c) *$\varphi(e_t) \to 1$ for some cai $(e_t)_{t\in\Lambda}$ for A.*
   - (d) *$\varphi(1_{A^{**}}) = 1$.*

(2) *Every state on A has a unique extension to a state on A^1.*

Proof. Everything is immediate from Proposition 4.24. □

Part (1) says that states on such algebras may be defined by any one of the equivalent conditions in Lemma 2.2 of [Blecher and Ozawa 2015]. The change in the statement of the last condition is justified by Lemma 1.14.

In the notation of Definition 2.6 (taken from [Blecher and Ozawa 2015]), for any cai $\mathfrak{e} = (e_t)_{t\in\Lambda}$ of A we have $S_{\mathfrak{e}}(A) = S(A)$. That is, states on an approximately unital L^p-operator algebra are the contractive functionals φ with $\varphi(e_t) \to 1$, or equivalently have norm 1 and extend to a state on A^1 (or on A^{**}).

We remark that the last several results hold (beginning with Lemma 4.19) if A is an approximately unital SQ_p-operator algebra. The proofs are almost identical, but with the kinds of emendations prescribed in the proof of Lemma 2.1 for SQ_p-spaces, Remark 4.20, and Remark 2.34.

The definition of a scaled Banach algebra, used in the next proposition, is stated in the introduction (see also the beginning of Section 6 below).

Proposition 4.26. *Suppose that A is an approximately unital scaled Banach algebra, that A is Hahn–Banach smooth in A^1 (Definition 4.23), and that A^{**} is unital. Then $\mathfrak{r}_{A^{**}}$ as defined in [Blecher and Ozawa 2015] (after Lemma 2.5 there) agrees with the set of accretive elements of the unital Banach algebra A^{**}.*

We are ignoring the statement in [Blecher and Ozawa 2015] that the definition there is only to be applied when A^{**} is not unital.

To be explicit, let R_0 be the set of accretive elements of A^{**}, where A^{**} is thought of as a unital Banach algebra in its own right, and let R_1 be the analogous subset of $(A^1)^{**}$. Then the assertion of the proposition is that $R_1 \cap A^{**} = R_0$.

Proof of Proposition 4.26. We may assume that A is nonunital (the case of unital algebras being easy). To avoid confusion, we use the notation R_0 and R_1 above.

We show $R_1 \cap A^{**} \subseteq R_0$. Proposition 2.11 of [Blecher and Ozawa 2015] (which works also when A^{**} is unital) implies that the weak* closure of $\mathfrak{r}_A$ is $R_1 \cap A^{**}$. So we need to show that $\mathfrak{r}_A \subseteq R_0$ and that R_0 is weak* closed. The second part is, e.g., Theorem 2.2 of [Magajna 2009]; the set $D_{A^{**}}$ (following the notation there) is $\{-a : a \in R_0\}$. One way to see the first part is that part of the proof of Lemma 1.14 shows that every cai for A converges weak* to $1_{A^{**}}$. Given this, the argument for Lemma 2.25 (1) shows that the subalgebra $A + \mathbb{C} \cdot 1_{A^{**}} \subseteq A^{**}$ is isometrically isomorphic to A^1. Thus, if $a \in \mathfrak{r}_A$, then $a \in \mathfrak{r}_{A^1}$ by Definition 2.13, so $a \in R_0$ by Lemma 2.14.

It remains to show that $R_0 \subseteq R_1$. Let $a \in R_0$, and let φ be a state on $(A^1)^{**}$. By weak* density of the normal states in $S((A^1)^{**})$ (which follows from Theorem 2.2 of [Magajna 2009]) there is a net $(\psi_t)_{t \in \Lambda}$ in $S(A^1)$ such that $\psi_t \to \varphi$ weak*. For $t \in \Lambda$, since A is scaled, there are $\lambda \in [0, 1]$ and $\omega \in S(A)$ such that $\psi_t = \lambda\omega$. Since A is Hahn–Banach smooth in A^1, [Blecher and Ozawa 2015, Lemma 2.2] implies that the canonical weak* continuous extension of ω is a state on A^{**}. So $\mathrm{Re}(\omega(a)) \geq 0$, whence $\mathrm{Re}(\psi_t(a)) \geq 0$. Then $\mathrm{Re}(\varphi(a)) = \lim_t \mathrm{Re}(\psi_t(a)) \geq 0$. So $a \in R_1$. $\square$

5. *M*-ideals

We recall the definitions of M-ideals and M-summands, together with some elementary facts. See, for example, Definition I.1.1 of [Harmand et al. 1993] and the discussion afterwards. If E is a Banach space and $P \in B(E)$ is an idempotent, then P is called an *L-projection* if $\|\xi\| = \|P\xi\| + \|(1 - P)\xi\|$ for all $\xi \in E$, and an *M-projection* if $\|\xi\| = \max(\|P\xi\|, \|(1 - P)\xi\|)$ for all $\xi \in E$. The ranges of L-projections and M-projections are called *L-summands* and *M-summands*. The idempotent P is an M-projection if and only if P^* is an L-projection, and is an L-projection if and only if P^* is an M-projection. Finally, a subspace $J \subseteq E$ is an *M-ideal* if $J^{\perp}$ is an L-summand in E^*, equivalently (using [Harmand et al. 1993, Theorem I.1.9]), $J^{\perp\perp}$ is an M-summand in E^{**}. By [Harmand et al. 1993, Proposition I.1.2 (a)], if J is an M-summand, then there is exactly one contractive idempotent with range J, namely the M-projection used in the definition.

Smith and Ward [1978] showed that the M-ideals in a C^*-algebra are exactly the closed ideals in the usual sense (Theorem 5.3), that an M-ideal in a unital Banach algebra must be a subalgebra (Theorem 3.6), and that M-ideals in Banach algebras are often ideals (see, for example, Theorem 3.8). Example 4.1 of [Smith and Ward 1978] shows that there are M-ideals in $B(l_2^1)$ which are subalgebras but not ideals and do not have cais.

The following definition is from the introduction to [Blecher and Ozawa 2015].

Definition 5.1. Let A be a Banach algebra. We say that A is *M-approximately unital* if A is an M-ideal in the multiplier unitization A^1.

As in the introduction to [Blecher and Ozawa 2015], an M-approximately unital Banach algebra is approximately unital. The papers [Blecher and Ozawa 2015; Blecher 2016] give a number of properties of M-approximately unital Banach algebras. For example, an M-approximately unital Banach algebra has a real positive cai $(e_t)_{t\in\Lambda}$ satisfying $\|1-2e_t\| \leq 1$ for all $t \in \Lambda$ ([Blecher and Ozawa 2015, Theorem 5.2]), is Hahn–Banach smooth in its multiplier unitization (Proposition I.1.12 of [Harmand et al. 1993]), and has the Kaplansky density properties given in [Blecher and Ozawa 2015, Theorem 5.2 and Proposition 6.4].

Proposition 5.2. *Let $p \in (1,\infty) \setminus \{2\}$ and let (X,μ) be a measure space. Then $\mathbb{K}(L^p(X,\mu))$ is M-approximately unital if and only if μ is purely atomic.*

Proof. Theorem 11 of [Lima 1979] states that $\mathbb{K}(L^p(X,\mu))$ is an M-ideal in $B(L^p(X,\mu))$ if and only if μ is purely atomic. By Theorem VI.4.17 in [Harmand et al. 1993], $\mathbb{K}(L^p(X,\mu))$ is an M-ideal in $B(L^p(X,\mu))$ if and only if it is an M-ideal in $\mathbb{K}(L^p(X,\mu)) + \mathbb{C}\,1$, where 1 is the identity operator on $L^p(X,\mu)$. By Lemma 2.24, $\mathbb{K}(L^p(X,\mu)) + \mathbb{C}\,1$ is the multiplier unitization of $\mathbb{K}(L^p(X,\mu))$. □

Lemma 5.3. *Let A be an approximately unital Arens regular Banach algebra, and let $J \subseteq A$ be an M-ideal in A, with associated M-projection $P : A^{**} \to J^{\perp\perp}$. Then J is an approximately unital closed ideal if and only if $P(1)$ is central in A^{**}.*

Proof. By the discussion before Proposition 8.1 of [Blecher and Ozawa 2015], centrality of $P(1)$ implies that J is an approximately unital closed ideal.

If J is an approximately unital closed ideal then, as in the proof of Lemma 4.5, there is a central idempotent e such that $J^{\perp\perp} = eA^{**} = A^{**}e$. The uniqueness of projections onto an M-summand implies that P is multiplication by e. So $P(1) = e$ is central. □

Theorem 5.4. *Let $p \in (1,\infty)$ and let A be an L^p-operator algebra.*

(1) *Suppose that A is approximately unital. Then every M-ideal in A is an approximately unital closed ideal.*

(2) *Suppose that A is unital. Then $J \subseteq A$ is an M-summand if and only if there is a central hermitian idempotent $z \in A$ such that $J = Az$. In this case, multiplication by z is an M-projection with range J.*

(3) *Suppose that A is M-approximately unital (Definition 5.1). Then*:
   (a) *Every M-ideal in A is M-approximately unital.*
   (b) *The intersection of finitely many M-ideals in A is an M-ideal in A.*
   (c) *The closed ideal generated by any collection of M-ideals in A is an M-ideal in A.*

Proof. We prove (2). We may assume (by the discussion above Proposition 2.12, or the corollary on page 136 in [Lacey 1974]) that there is a decomposable measure space X such that A is a unital subalgebra of $B(L^p(X, \mu))$.

Suppose that $z \in A$ is a central hermitian idempotent. Then z is a hermitian idempotent in $B(L^p(X, \mu))$. It follows from Proposition 2.12 that z is multiplication by the characteristic function of a locally measurable subset E of X. Thus for $x, y \in A$ (with suitable interpretation of the integrals below if E is only locally measurable),

$$\begin{aligned}
&\|zxz + (1-z)y(1-z)\|^p \\
&\quad = \sup\left(\left\{ \int_E |xz\xi|^p \, d\mu + \int_{X\setminus E} |y(1-z)\xi|^p \, d\mu : \xi \in \operatorname{Ball}(L^p(X)) \right\}\right) \\
&\quad \leq \max(\|x\|, \|y\|)^p \, \sup\left(\left\{ \int_E |\xi|^p \, d\mu + \int_{X\setminus E} |\xi|^p \, d\mu : \xi \in \operatorname{Ball}(L^p(X)) \right\}\right) \\
&\quad = \max(\|x\|, \|y\|)^p.
\end{aligned}$$

So multiplication by z is an M-projection on A and zA is an M-summand.

Conversely, let P be an M-projection on A, and let $z = P(1)$. By [Smith and Ward 1978, Proposition 3.1], z is a hermitian idempotent. Also, P^* is an L-projection, so for any state φ on A, if $P^*(\varphi) \neq 0$ then $\psi = \|P^*(\varphi)\|^{-1} P^*(\varphi)$ is a state with $\psi(z) = 1$ as in the proof of 4.8.5 in [Blecher and Le Merdy 2004]. It follows from Lemma 4.19 that

$$\psi((1-z)A) = \psi(A(1-z)) = 0.$$

So

$$\varphi(P((1-z)A)) = \varphi(P(A(1-z))) = 0$$

for any state φ on A. Thus

$$P((1-z)A) = P(A(1-z)) = 0$$

by Lemma 2.25 (3). A similar argument applied to $1 - P$ shows that

$$(1-P)(zA) = (1-P)(Az) = 0.$$

So $zA + Az \subseteq P(A)$. Thus

$$P(a) = P(za + (1-z)a) = P(za) = za,$$

for all $a \in A$, and similarly $P(a) = az$. So z is central and $P(A) = Az$. This completes the proof of (2).

We prove (1). Let $J \subseteq A$ be an M-ideal. Since $J^{\perp\perp}$ is an M-ideal in A^{**}, since A is Arens regular (Lemma 2.1 (1)), and since A^{**} is an L^p-operator algebra (Lemma 2.1 (3)), we can apply part (2) and Lemma 5.3.

Part (3)(a) follows from [Blecher and Ozawa 2015, Proposition 3.2(3)] and part (1), and (3)(b) and (3)(c) now follow from [Blecher and Ozawa 2015, Theorem 8.3]. □

Remark 5.5. Let A be an approximately unital L^p-operator algebra. The proof of Theorem 5.4 shows that the h-ideals, as defined at the beginning of Section 3 of [Godefroy et al. 1993], are exactly the M-ideals. One may ask if these are also the u-ideals as defined before our Lemma 4.4. This is not true: the idempotent e_2 in Example 3.2 gives a u-projection which is not an M-projection, since as we said there e_2 is not hermitian. Suppose that A is a u-ideal in its multiplier unitization A^1, or, equivalently, as pointed out before Lemma 4.4, that A is bi-approximately unital. One may ask whether it follows that A is an M-ideal in A^1. As we will see in Corollary 6.2, the latter is equivalent to being scaled. Recall from Lemma 4.4 that an approximately unital L^p-operator algebra A with a real positive bounded approximate identity is bi-approximately unital. (We conjectured after Lemma 4.4 that the converse is true.)

6. Scaled L^p-operator algebras

In the Introduction we said that an approximately unital Banach algebra A is *scaled* if the set of restrictions to A of states on A^1 equals the quasistate space $Q(A)$ of A. Equivalently, (see [Blecher and Ozawa 2015], before Lemma 2.7 there) an approximately unital Banach algebra is scaled if every real positive functional (see Definition 2.13) is a nonnegative multiple of a state. That is, in the notation of Definitions 2.6 and 2.13, we have $\mathfrak{c}_{A^*} = \mathbb{R}_+ S(A)$, or, equivalently, $\mathfrak{c}_{A^*} \cap \mathrm{Ball}(A^*) = Q(A)$.

Unital Banach algebras are scaled (this is a special case of [Blecher and Ozawa 2015, Proposition 6.2]), and all C^*-algebras are well known to be scaled.

If A is a nonunital approximately unital Arens regular Banach algebra, then the support idempotent of A in $(A^1)^{**}$ is the weak* limit in $(A^1)^{**}$ of any cai in A. This exists and is an identity for A^{**} by the argument of Lemma 1.14. Clearly it is central in $(A^1)^{**}$.

Lemma 6.1. *Suppose that A is a nonunital scaled approximately unital Arens regular Banach algebra. Then the support idempotent of A in $(A^1)^{**}$ is hermitian.*

Proof. Suppose that A is scaled and $(e_t)_{t\in\Lambda}$ is a cai for A. Then, as above, $(e_t)_{t\in\Lambda}$ converges weak* to a central idempotent $e \in (A^1)^{**}$ which is an identity for A^{**}.

If φ is a state on A^1 then $\varphi|_A$ is a nonnegative multiple, r say, of a state on A, so that $\varphi(e) = \lim_t \varphi(e_t) = r \geq 0$. So every weak* continuous state on $(A^1)^{**}$ is nonnegative on e. Since the weak* continuous states on a dual Banach algebra are weak* dense in the states by [Magajna 2009, Theorem 2.2], it follows from Lemma 2.9 that e is hermitian. □

The last result says that scaled approximately unital Arens regular Banach algebras are h-ideals in their multiplier unitizations as defined at the beginning of Section 3 of [Godefroy et al. 1993].

Corollary 6.2. *Suppose that A is an approximately unital Arens regular Banach algebra with the property that whenever $e \in (A^1)^{**}$ is a hermitian idempotent and $x, y \in A$, then $\|exe + (1-e)y(1-e)\| \leq \max(\|x\|, \|y\|)$. Then A is scaled if and only if A is M-approximately unital.*

Proof. Since unital algebras are both scaled and approximately unital, we may assume that A is nonunital. If A is M-approximately unital then A is scaled by [Blecher and Ozawa 2015, Proposition 6.2]. For the other direction, by Lemma 6.1 and the hypothesis, the support idempotent e of A in $(A^1)^{**}$ satisfies

$$\|ex + (1-e)y\| \leq \max(\|x\|, \|y\|) \quad \text{for } x, y \in A.$$

By Goldstine's theorem and separate weak* continuity of multiplication ([Blecher and Le Merdy 2004, 2.5.3]), this inequality holds for all $x, y \in A^{**}$. So multiplication by e is an M-projection on $(A^1)^{**}$. Therefore A is an M-ideal in A^1. □

Corollary 6.3. *Let A be an approximately unital L^p-operator algebra. Then A is scaled if and only if A is M-approximately unital.*

Proof. Use Corollary 6.2 and a computation in the proof of Theorem 5.4 (2). □

Corollary 6.4. *Let $p \in (1, \infty)$ and let A be a nonunital approximately unital L^p-operator algebra. Then the following are equivalent*:

(1) *A is scaled.*

(2) *The support idempotent e of A in $(A^1)^{**}$* (*as defined at the beginning of the section*) *is hermitian.*

(3) *The quasistate space $Q(A)$ is weak* compact.*

If these hold then, by Corollary 6.3, A has all the properties of M-approximately unital algebras described after Definition 5.1.

Proof of Corollary 6.4. The implication from (1) to (2) is Lemma 6.1. For the reverse, if e is hermitian then multiplication by e is an M-projection from $(A^1)^{**}$ to A^{**} by Theorem 5.4 (2), so A is M-approximately unital. Apply Corollary 6.3.

For the equivalence with (3), first, $Q(A)$ is weak* compact if and only if it is weak* closed. Also, Corollary 4.25 (1) implies convexity of $Q(A)$, as explained in Remark 2.26. Apply Lemma 2.7 (2) in [Blecher and Ozawa 2015]. □

The following answers the open question from [Blecher and Ozawa 2015] as to whether all approximately unital Banach algebras are scaled.

Corollary 6.5. *If $p \in (1, \infty) \setminus \{2\}$ then $\mathbb{K}(L^p([0, 1]))$ is an approximately unital L^p-operator algebra which is not scaled.*

Proof. That $\mathbb{K}(L^p([0, 1]))$ has a cai is observed in Example 3.9. This algebra is not M-approximately unital by Proposition 5.2, and so is not scaled by Corollary 6.3. ☐

Corollary 6.6. *The algebra $\mathbb{K}(l^p)$ is scaled.*

Proof. This algebra is M-approximately unital by Proposition 5.2, hence scaled by Corollary 6.3. ☐

The last result can also be deduced from Proposition 6.7.

Proposition 6.7. *Let $p \in (1, \infty)$. Suppose that an L^p-operator algebra A has a cai $(e_t)_{t\in\Lambda}$ consisting of hermitian elements of A^1. Then A is scaled.*

Proof. Since unital algebras are scaled, we may assume that A is nonunital. With $e_t \to e$ as usual, it follows as in the proof of Lemma 2.25 (4) (using the fact that normal states are weak* dense) that e is hermitian and central in $(A^1)^{**}$. It follows from Theorem 5.4 or Corollary 6.4 that A is M-approximately unital and scaled. ☐

Proposition 6.7 may suggest that one requirement for a nonunital L^p-operator algebra to be "C^*-like" is that it have a hermitian cai. The canonical cai for $\mathbb{K}(l^p)$ is a real positive hermitian cai as we said in Example 3.9. On the other hand the cai for $\mathbb{K}(L^p([0, 1]))$ in Example 3.9 seems, perhaps surprisingly, to have no good "positivity" properties. Indeed as we said in Example 3.9, $A = \mathbb{K}(L^p([0, 1]))$ has no real positive cai. Of course for any approximately unital L^p-operator algebra the identity e of A^{**} is real positive in A^{**}. However e need not be real positive (accretive) in $(A^1)^{**}$, and certainly is not hermitian, as we said after the proof of Lemma 2.25. Example 3.8 shows that the converse of Proposition 6.7 is false.

Proposition 6.8. *Let $p \in (1, \infty)$. Suppose that A is a closed subalgebra of a scaled L^p-operator algebra B, with a common cai. Then A is scaled.*

Proof. We may assume that A is nonunital (unital algebras are scaled). We may view $A^1 \subseteq B^1$. Any state φ of A^1 extends to a state of B^1, and the restriction of this extension to B equals $\lambda\psi$ for some $\lambda \in [0, 1]$ and $\psi \in S(B)$. However $\psi|_A \in S(A)$ since Corollary 4.25 (1) implies that $\psi(e_t) \to 1$, where $(e_t)_{t\in\Lambda}$ is the common cai. Since $\varphi|_A = \lambda\psi|_A$ we are done. ☐

Remark 6.9. Approximately unital ideals in a scaled L^p-operator algebra A need not be scaled, for example $\mathbb{K}(L^p([0, 1]))$ in $B(L^p([0, 1]))$. (The latter is scaled as is any unital Banach algebra, and we showed above that $\mathbb{K}(L^p([0, 1]))$ is not scaled.) However if the approximately unital ideal is also an M-ideal in A, then it is scaled by Theorem 5.4.

7. Kaplansky density

One may ask if in an approximately unital L^p-operator algebra there are Kaplansky density theorems analogous to the ones established by Blecher and Read for approximately unital L^2-operator algebras. See, e.g., [Blecher and Ozawa 2015, Theorem 5.2 and Proposition 6.4] for a more general variant of the latter. As we said in the introduction, the usual Kaplansky density theorem variants for C^*-algebras can be shown to follow easily from the weak* density of the subset of interest in A within the matching set in A^{**}; and our Kaplansky density theorems have this flavor.

In the following result, for an approximately unital L^p-operator algebra A we take $\mathfrak{r}_{A^{**}}$ to be the accretive elements in the unital Banach algebra A^{**}. This is different from the definition after Lemma 2.5 in [Blecher and Ozawa 2015]. The two definitions do coincide if also A is scaled, by Proposition 4.26 and Proposition 4.24 (2).

Proposition 7.1. *Let $p \in (1, \infty)$ and let A be an approximately unital L^p-operator algebra. The following are equivalent*:

(1) $\mathfrak{r}_A$ *is weak* dense in* $\mathfrak{r}_{A^{**}}$.

(2) $\mathfrak{r}_A \cap \mathrm{Ball}(A)$ *is weak* dense in* $\mathfrak{r}_{A^{**}} \cap \mathrm{Ball}(A^{**})$.

(3) $\mathfrak{F}_A$ *is weak* dense in* $\mathfrak{F}_{A^{**}}$.

(4) *A is scaled.*

Proof. Since the definition of $\mathfrak{r}_{A^{**}}$ in [Blecher and Ozawa 2015] coincides with ours when A is scaled (as pointed out above), that (4) implies (1) follows from Proposition 2.11 of [Blecher and Ozawa 2015]. The proof of Lemma 6.4 of [Blecher and Ozawa 2015] works just as well for our version of $\mathfrak{r}_{A^{**}}$ as for the one there, and thus shows that (1) implies (2). By our Corollary 6.3 and by Theorem 5.2 of [Blecher and Ozawa 2015] it follows that (4) implies (3). That (3) implies (1) follows easily from Proposition 2.17.

Assuming (2) we will prove (4) by showing that every nontrivial real positive functional φ (see Definition 2.13) is a nonnegative multiple of a state. We may assume that A is nonunital. The canonical weak* continuous extension $\widetilde{\varphi}$ of φ to A^{**} is real positive by our assumption (2) and a standard approximation argument. Since A^{**} is unital it is scaled, so that $\widetilde{\varphi} = t\psi$ for a state ψ on A^{**} and some $t > 0$. Thus $\varphi = t\psi|_A$. The span of A and the identity of A^{**} is the multiplier unitization of A by the last paragraph of Section 1 of [Blecher and Ozawa 2015]. Hence $\psi|_A$ is a state on A. □

These hold in particular if A is unital. Such results also hold if A has the following property: with 1 being the identity of some unitization of A, given $\varepsilon > 0$ there exists $\delta > 0$ such that if $y \in A$ with $\|1 - y\| < 1 + \delta$ then there is $z \in A$ with $\|1 - z\| = 1$ and $\|y - z\| < \varepsilon$. This follows from [Blecher and Ozawa 2015, Proposition 6.4] and the proof of [Blecher and Ozawa 2015, Theorem 5.2]. It may be interesting to ascertain which L^p-operator algebras have this property.

We end by mentioning some of what seem to us to be the most important open questions related to the approach of this paper. See the "Remarks added in proof" section below for the solution to several of these.

(1) Is there a Kaplansky density type theorem for a nonscaled approximately unital L^p-operator algebra A? (See Proposition 7.1 for the scaled case.) For example, one may ask if $\mathfrak{r}_A$ is weak* dense in $\mathfrak{r}_{(A^1)^{**}} \cap A^{**}$.

(2) Is every approximately unital subalgebra of $B(l^p)$ scaled?

(3) Let A be an approximately unital L^p-operator algebra. Is $\mathfrak{r}_A - \mathfrak{r}_A$ always a subalgebra?

(4) Is every bi-approximately unital L^p-operator algebra scaled? Does it have a real positive cai? More drastically, if an L^p-operator algebra possesses a real positive cai, then is it scaled?

8. Index

For the readers' convenience we list, alphabetically but compactly, some of the main definitions in this paper and where they may be found (the definition number, which is usually their first occurrence).

Accretive: 2.13; approximately unital Banach algebra: 1.4; Arens products, Arens regular: 1.12; bi-approximately unital algebra: 4.2; bi-approximately unital ideal: 4.1; bicontractive idempotent: 2.28; $\mathfrak{c}_{A^*}$: 2.13; cai: 1.4; decomposable: 2.11; dual L^p-operator algebra: 2.3; $\mathfrak{F}_A$: 2.16; Hahn–Banach smooth: 4.23; hermitian: 2.8; invertible isometry: 2.28; locally measurable, locally a.e.: 2.11; L^p-operator algebra: 1.6; M-approximately unital: 5.1; M-ideal, M-projection, M-summand: beginning of Section 5; multiplier unitization A^1: 1.8; order on idempotents $e \leq_{\mathrm{r}} f$, $e \leq f$: 2.30; powers and roots b^t: 2.18; quasistate space $Q(A)$: 2.6; $\mathfrak{r}_A$: 2.13; real positive: 2.13; scaled: beginning of Section 6; smooth: 1.5; SQ_p-algebra, SQ_p-space: the introduction; state space $S(A)$: 2.6; strictly convex: 1.5; support idempotent $s(x)$: 4.12; unital Banach algebra: 1.3; unitization: 1.7.

Other definitions may be found in the introduction, or in the sections where they first appear (often at the start of the section), but are not specifically numbered.

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Remarks added in proof

We are indebted to an anonymous reviewer of a different paper who referred us to the paper [Berkson 1972], which contains somewhat of a systematic study of hermitian idempotents on general Banach spaces, and which is well worth studying. There is not much overlap with that paper but some of the motifs are similar. For example Theorem 2.25 in Berkson's paper is our Lemma 4.16, but as we said there, this result is well known. Also, that paper has some nice examples in general Banach spaces complementing some of the examples which we give.

The paper [Phillips and Viola 2017] is in the process of revision, and this will change the section and result numbering. The references to that paper here refer to the arXiv version 2, as linked to in our bibliography.

Finally, question (2) at the end of Section 7 and the first and third questions stated in (4) there, have negative solutions. A counterexample to all three is the set of continuous functions from [0, 1] to M_2^p with $f(0) \in \mathbb{C}\, e_2$. We give full details elsewhere.

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THE CENTER OF A GREEN BISET FUNCTOR

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For a Green biset functor A, we define the commutant and the center of A and we study some of their properties and their relationship. This leads in particular to the main application of these constructions: the possibility of splitting the category of A-modules as a direct product of smaller abelian categories. We give explicit examples of such decompositions for some classical shifted representation functors. These constructions are inspired by similar ones for Mackey functors for a fixed finite group.

Introduction

This paper is devoted to the construction of two analogues of the center of a ring in the realm of Green biset functors, that is "biset functors with a compatible ring structure". For a Green biset functor A, we present *the commutant* CA of A, defined from a commutation property, and *the center* ZA of A, defined from the structure of the category of A-modules. Both CA and ZA are again Green biset functors. These constructions are inspired by similar ones for Mackey functors for a fixed finite group made in Chapter 12 of [Bouc 1997].

The commutant CA is always a Green biset subfunctor of A, and we say that A is *commutative* if $CA = A$. Most of the classical representation functors are commutative in that sense. One of them plays a fundamental — we should say *initial* — role, namely the Burnside biset functor B, as biset functors are nothing but *modules* over the Burnside functor. An important feature of the category B-Mod is its monoidal structure: given two biset functors M and N, one can build their tensor product $M \otimes N$, which is again a biset functor. For this tensor product, the category B-Mod becomes a symmetric monoidal category, and a Green biset functor A is a *monoid object* in B-Mod.

More generally, for any Green biset functor A, we consider the category A-Mod of A-modules. We will make a heavy use of the equivalence of categories between A-Mod and the category of linear representations of the category $\mathcal{P}_A$ introduced in Chapter 8 of [Bouc 2010] (see also Definition 9 below), which has finite groups as objects, and in which the set of morphisms from G to H is equal to $A(H \times G)$.

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The category $\mathcal{P}_B$ associated to the Burnside functor is precisely the *biset category* of finite groups. It is a symmetric monoidal category (for the product given by the direct product of groups), and this monoidal structure induces via Day convolution ([Day 1970]) the monoidal structure of B-Mod mentioned before.

A natural question is then to know when the cartesian product of groups endows the category $\mathcal{P}_A$ with a symmetric monoidal structure, and we show that this is the case precisely when A is commutative. In this case the category A-Mod also becomes a symmetric monoidal category.

Even though the definition of the center ZA of a Green biset functor A is fairly natural, showing that it is endowed with a Green biset functor structure (even showing that $ZA(G)$ is indeed a set!) is not an easy task; it requires several sometimes rather nasty computations. On the other hand, one of the rewarding consequences of this laborious process is that we obtain a description of $ZA(G)$ in terms also of a commutation condition, this time on the morphisms of $\mathcal{P}_A$. Once we have that ZA is indeed a Green biset functor, we show some nice properties of it, for instance that there is an injective morphism of Green biset functors from CA to ZA. This implies in particular that ZA is a CA-module. We show also that in the case where A is commutative, it is a direct summand of ZA as A-modules.

In the last section, we work within $ZA(1)$, which, as we will see, coincides with the center of the category A-Mod. Any decomposition of the identity element of $ZA(1)$ as a sum of orthogonal idempotents, fulfilling certain finiteness conditions, allows us to decompose A-Mod as a direct product of smaller abelian categories. Moreover, since $CA(1)$ is generally easier to compute than $ZA(1)$, we can also use similar decompositions of the identity element of $CA(1)$ instead, thanks to the inclusion $CA \hookrightarrow ZA$. We give then a series of explicit examples. The first one is the Burnside p-biset functor $A = RB_p$ over a ring R where the prime p is invertible. In this case, we obtain an infinite series of orthogonal idempotents in $ZA(1)$, and this shows in particular that ZA can be much bigger than CA. Next we consider some classical representation functors, shifted by some fixed finite group L via the *Yoneda–Dress functor*. In this series of examples, we will see that the smaller abelian categories obtained in the decomposition are also module categories for Green biset functors arising from the functor A, the shifting group L, and the above-mentioned idempotents.

1. Preliminaries

Throughout the paper, we fix a commutative unital ring R. All referred groups will be finite. The center of a ring S will be denoted by $Z(S)$.

1.1. ***Green biset functors.*** The biset category over R will be denoted by $R\mathcal{C}$. Recall that its objects are all finite groups, and that for finite groups G and H, the hom-set

$\mathrm{Hom}_{R\mathcal{C}}(G, H)$ is $RB(H, G) = R \otimes_{\mathbb{Z}} B(H, G)$, where $B(H, G)$ is the Grothendieck group of the category of finite (H, G)-bisets. The composition of morphisms in $R\mathcal{C}$ is induced by R-bilinearity from the composition of bisets, which will be denoted by $\circ$.

We fix a nonempty class $\mathcal{D}$ of finite groups closed under subquotients and cartesian products, and a set $\boldsymbol{D}$ of representatives of isomorphism classes of groups in $\mathcal{D}$. We denote by $R\mathcal{D}$ the full subcategory of $R\mathcal{C}$ consisting of groups in $\mathcal{D}$, so in particular $R\mathcal{D}$ is a *replete subcategory* of $R\mathcal{C}$, in the sense of [Bouc 2010, Definition 4.1.7]. The category of biset functors, i.e., the category of R-linear functors from $R\mathcal{C}$ to the category R-Mod of all R-modules, will be denoted by Fun_R. The category $\mathrm{Fun}_{\mathcal{D},R}$ of *$\mathcal{D}$-biset functors* is the category of R-linear functors from $R\mathcal{D}$ to R-Mod.

A Green $\mathcal{D}$-biset functor is defined as a monoid in $\mathrm{Fun}_{\mathcal{D},R}$ (see Definition 8.5.1 in [Bouc 2010]). This is equivalent to the following definition:

Definition 1. A $\mathcal{D}$-biset functor A is a Green $\mathcal{D}$-biset functor if it is equipped with bilinear products $A(G) \times A(H) \to A(G \times H)$ denoted by $(a, b) \mapsto a \times b$, for groups G, H in $\mathcal{D}$, and an identity element $\varepsilon_A \in A(1)$, satisfying the following conditions:

1. Associativity: Let G, H and K be groups in $\mathcal{D}$. If we consider the canonical isomorphism from $G \times (H \times K)$ to $(G \times H) \times K$, then for any $a \in A(G)$, $b \in A(H)$ and $c \in A(K)$,
$$(a \times b) \times c = A\big(\mathrm{Iso}_{G\times(H\times K)}^{(G\times H)\times K}\big)(a \times (b \times c)).$$
2. Identity element: Let G be a group in $\mathcal{D}$ and consider the canonical isomorphisms $1 \times G \to G$ and $G \times 1 \to G$. Then for any $a \in A(G)$,
$$a = A\big(\mathrm{Iso}_{1\times G}^{G}\big)(\varepsilon_A \times a) = A\big(\mathrm{Iso}_{G\times 1}^{G}\big)(a \times \varepsilon_A).$$
3. Functoriality: If $\varphi : G \to G'$ and $\psi : H \to H'$ are morphisms in $R\mathcal{D}$, then for any $a \in A(G)$ and $b \in A(H)$,
$$A(\varphi \times \psi)(a \times b) = A(\varphi)(a) \times A(\psi)(b).$$

The identity element of A will be denoted simply by ε if there is no risk of confusion.

If A and C are Green $\mathcal{D}$-biset functors, a morphism of Green $\mathcal{D}$-biset functors from A to C is a natural transformation $f : A \to C$ such that $f_{H\times K}(a\times b) = f_H(a)\times f_K(b)$ for any groups H and K in $\mathcal{D}$ and any $a \in A(H)$, $b \in A(K)$, and such that $f_1(\varepsilon_A) = \varepsilon_C$. We will denote by $\mathrm{Green}_{\mathcal{D},R}$ the category of Green $\mathcal{D}$-biset functors with morphisms given in this way.

There is an equivalent way of defining a Green biset functor; see Lemma 3.

Definition 2. A $\mathcal{D}$-biset functor A is a Green $\mathcal{D}$-biset functor provided that for each group H in $\mathcal{D}$, the R-module $A(H)$ is an R-algebra with unity that satisfies the following. If K and G are groups in $\mathcal{D}$ and $K \to G$ is a group homomorphism, then:

1. For the (K, G)-biset G, which we denote by G_r, the morphism $A(G_r)$ is a ring homomorphism.
2. For the (G, K)-biset G, denoted by G_l, the morphism $A(G_l)$ satisfies the Frobenius identities
$$A(G_l)(a) \cdot b = A(G_l)(a \cdot A(G_r)(b)),$$
$$b \cdot A(G_l)(a) = A(G_l)(A(G_r)(b) \cdot a)$$
for all $b \in A(G)$ and $a \in A(K)$, where $\cdot$ denotes the ring product on $A(G)$ and $A(K)$, respectively.

Lemma 3 [Romero 2011, Lema 4.2.3]. *Definitions 1 and 2 are equivalent. Starting with Definition 1, the ring structure of $A(H)$ is given by*
$$a \cdot b = A\big(\mathrm{Iso}^{H}_{\Delta(H)} \circ \mathrm{Res}^{H\times H}_{\Delta(H)}\big)(a \times b)$$
for a and b in $A(H)$, with the unity given by $A(\mathrm{Inf}^{H}_{1})(\varepsilon)$. Conversely, starting with Definition 2, the product of $A(G) \times A(H) \to A(G \times H)$ is given by
$$a \times b = A\big(\mathrm{Inf}^{G\times H}_{G}\big)(a) \cdot A\big(\mathrm{Inf}^{G\times H}_{H}\big)(b)$$
for $a \in A(G)$ and $b \in A(H)$, with the identity element given by the unity of $A(1)$.

In what follows, the ring structure on $A(G)$ will be understood as $(A(G), \cdot)$.

Observe that in the case of $A(1)$, the product $\times : A(1) \times A(1) \to A(1)$ coincides with the ring product $\cdot : A(1) \times A(1) \to A(1)$, up to identification of 1×1 with 1, and the unity coincides with the identity element.

Remark 4. A morphism of Green $\mathcal{D}$-biset functors $f : A \to C$ induces, in each component G, a unital ring homomorphism $f_G : A(G) \to C(G)$. Conversely, a morphism of biset functors $f : A \to C$ such that f_G is a unital ring homomorphism for every G in $\mathcal{D}$, is a morphism of Green $\mathcal{D}$-biset functors.

Example 5. Classical examples of Green biset functors are the following:

• The Burnside functor B. The Burnside group of a finite group G is known to define a biset functor. The cross product of sets defines the bilinear products $B(G) \times B(H) \to B(G \times H)$ that make B a Green biset functor. The functor B can also be considered with coefficients in R, and denoted by $RB = R \otimes_{\mathbb{Z}} B(\_)$. It is shown in Proposition 8.6.1 of [Bouc 2010] that RB is an initial object in $\mathrm{Green}_{\mathcal{D},R}$. More precisely, for a Green $\mathcal{D}$-biset functor A, the unique morphism of Green functors $\upsilon_A : RB \to A$ is defined at $G \in \mathcal{D}$ as the linear map $\upsilon_{A,G}$ sending a G-set X to $A({}_G X_1)(\varepsilon_A)$, where ${}_G X_1$ is the set X viewed as a $(G, 1)$-biset.

• The functor of $\mathbb{K}$-linear representations, $R_{\mathbb{K}}$, where $\mathbb{K}$ is a field of characteristic 0. That is, the functor which sends a finite group G to the Grothendieck group $R_{\mathbb{K}}(G)$ of the category of finitely generated $\mathbb{K}G$-modules. Also known to be a biset functor, it has a Green biset functor structure given by the tensor product over $\mathbb{K}$. We will consider the scalar extension $\mathbb{F}R_{\mathbb{K}} = \mathbb{F} \otimes_{\mathbb{Z}} R_{\mathbb{K}}(\_)$, where $\mathbb{F}$ is a field of characteristic 0.

• The functor of p-permutation representations pp_k, for k an algebraically closed field of positive characteristic p. This is the functor sending a finite group G to the Grothendieck group $pp_k(G)$ of the category of finitely generated p-permutation kG-modules (also known as trivial source modules), for relations given by direct sum decompositions. The biset functor pp_k is a Green biset functor with products given by the tensor product over the field k. When considering coefficients for this functor, we will assume that $\mathbb{F}$ is a field of characteristic 0 containing all the p'-roots of unity, and we write $\mathbb{F}pp_k = \mathbb{F} \otimes_{\mathbb{Z}} pp_k(\_)$.

In Section 5.2 we will focus on the above examples only, but there are many other important examples of Green biset functors, e.g., the monomial Burnside functor — also called the fibred Burnside functor — which gives rise to fibred biset functors (see [Barker 2004; Romero 2013; Boltje and Coşkun 2018]), or the slice Burnside functor (see [Bouc 2012; Tounkara 2018a; 2018b]).

When p is a prime number, and $\mathcal{D}$ is the full subcategory of $\mathcal{C}$ consisting of finite p-groups, the $\mathcal{D}$-biset functors are simply called *p-biset functors*, and their category is denoted by $\mathrm{Fun}_{p,R}$. Similarly, the Green $\mathcal{D}$-biset functors will be called *Green p-biset functors*, and their category will be denoted by $\mathrm{Green}_{p,R}$.

An important element in what follows will be the Yoneda–Dress construction. We recall some of the basic results about it, more details can be found in [Bouc 2010, Section 8.2]. If G is a fixed group in $\mathcal{D}$ and F is a $\mathcal{D}$-biset functor, then the Yoneda–Dress construction of F at G is the $\mathcal{D}$-biset functor F_G that sends each group K in $\mathcal{D}$ to $F(K \times G)$. The morphism $F_G(\varphi) : F(H \times G) \to F(K \times G)$ associated to an element φ in $RB(K, H)$ is defined as $F(\varphi \times G)$. In turn, $F(\varphi \times G)$ is defined by R-bilinearity from the case where φ is represented by a (K, H)-biset U: in this case, $\varphi \times G$ denotes the cartesian product $U \times G$, endowed with its obvious $(K \times G, H \times G)$-biset structure. We also call F_G the functor *shifted* by G.

If $f : F \to T$ is a morphism of $\mathcal{D}$-biset functors, then $f_G : F_G \to T_G$ is defined in its component K as $(f_G)_K = f_{K\times G}$. It is shown in Proposition 8.2.7 of [Bouc 2010] that this construction is a self-adjoint exact R-linear endofunctor of $\mathrm{Fun}_{D,R}$.

When A is a Green $\mathcal{D}$-biset functor, the particular shifted functor A_G is also a Green $\mathcal{D}$-biset functor (Lemma 4.4 in [Romero 2012]) with product given by

$$A_G(H) \times A_G(K) \to A_G(H \times K), \quad (a, b) \mapsto A(\alpha)(a \times b),$$

where α is the biset $\mathrm{Iso}_D^{H\times K\times G}\mathrm{Res}_D^{H\times G\times K\times G}$ and $D \cong H \times K \times G$ is the subgroup of $H \times G \times K \times G$ consisting of elements of the form (h, g, k, g). Usually, by an abuse of notation, we will denote this biset simply by $\mathrm{Res}^{H\times G\times K\times G}_{H\times K\times\Delta(G)}$. To avoid confusion with the product $\times$ of A we denote the product of A_G by $\times^d$, where the exponent d stands for *diagonal*.

Remark 6. It is not hard to show that the ring structure of Lemma 3 in $A_G(H)$ induced by the product $\times^d$ of A_G coincides with the ring structure of $A(H \times G)$ induced by the product $\times$ of A. So there is no risk of confusion when talking about *the ring* $A_G(H)$, since the ring structure we are considering is unique. In particular, the isomorphism $A_G(1) \cong A(G)$ is an isomorphism of rings.

1.2. *A-modules.*

Definition 7 [Bouc 2010, Definition 8.5.5]. Given a Green $\mathcal{D}$-biset functor A, a left A-module M is defined as a $\mathcal{D}$-biset functor, together with bilinear products

$$\_ \times \_ : A(G) \times M(H) \to M(G \times H)$$

for every pair of groups G and H in $\mathcal{D}$, that satisfy analogous conditions to those of Definition 1. The notion of right A-module is defined similarly, from bilinear products $M(G) \times A(H) \to M(G \times H)$.

We use the same notation $\times$ for the product of A and the action of A on A-modules, as long as there is no risk of confusion.

If M and N are A-modules, a *morphism of A-modules* is defined as a morphism of $\mathcal{D}$-biset functors $f : M \to N$ such that $f_{G\times H}(a \times m) = a \times f_H(m)$ for all groups G and H in $\mathcal{D}$, $a \in A(G)$ and $m \in M(H)$. With these morphisms, the A-modules form a category, denoted by A-Mod. The category A-Mod is an abelian subcategory of $\mathrm{Fun}_{\mathcal{D},R}$. Actually, the direct sum of biset functors is also the direct sum of A-modules. Furthermore, the kernel, the image and the cokernel of a morphism of A-modules are A-modules. Basic results on modules over a ring can be stated for A-modules.

In particular, a left (resp. right) ideal of a Green $\mathcal{D}$-biset functor A is an A-submodule of the left (resp. right) A-module A. A two-sided ideal of A is a left ideal which is also a right ideal.

Example 8. If A is the Burnside functor RB, then an A-module is nothing but a biset functor with values in R-Mod.

From Proposition 8.6.1 of [Bouc 2010], or Proposition 2.11 of [Romero 2012], an equivalent way of defining an A-module is as an R-linear functor from the category $\mathcal{P}_A$ to R-Mod, where the category $\mathcal{P}_A$ is defined next.

Definition 9. Let A be a Green $\mathcal{D}$-biset functor over R. The category $\mathcal{P}_A$ is defined in the following way:

- The objects of $\mathcal{P}_A$ are all finite groups in $\mathcal{D}$.
- If G and H are groups in $\mathcal{D}$, then $\mathrm{Hom}_{\mathcal{P}_A}(H, G) = A(G \times H)$.
- Let H, G and K be groups in $\mathcal{D}$. The composition of $\beta \in A(H \times G)$ and $\alpha \in A(G \times K)$ in $\mathcal{P}_A$ is

$$\beta \circ \alpha = A\big(\mathrm{Def}^{H\times\Delta(G)\times K}_{H\times K} \circ \mathrm{Res}^{H\times G\times G\times K}_{H\times\Delta(G)\times K}\big)(\beta \times \alpha).$$

- For a group G in $\mathcal{D}$, the identity morphism ε_G of G in $\mathcal{P}_A$ is

$$A\big(\mathrm{Ind}^{G\times G}_{\Delta(G)} \circ \mathrm{Inf}^{\Delta(G)}_{1}\big)(\varepsilon).$$

Observe that the biset $\mathrm{Def}^{H\times\Delta(G)\times K}_{H\times K} \circ \mathrm{Res}^{H\times G\times G\times K}_{H\times\Delta(G)\times K}$ can also be written as

$$H \times \big(\mathrm{Def}^{\Delta(G)}_{1} \circ \mathrm{Res}^{G\times G}_{\Delta(G)}\big) \times K.$$

Another way of denoting the $(1, G \times G)$-biset $\mathrm{Def}^{\Delta(G)}_{1} \circ \mathrm{Res}^{G\times G}_{\Delta(G)}$ is as $\overleftarrow{G}$. In some cases it will be more convenient to use this notation.

The category $\mathcal{P}_A$ is essentially small, as it has a skeleton consisting of our chosen set $\boldsymbol{D}$ of representatives of isomorphism classes of groups in $\mathcal{D}$. Hence, the category $\mathrm{Fun}_R(\mathcal{P}_A, R\text{-Mod})$ of R-linear functors is an abelian category. The above-mentioned equivalence of categories between A-Mod and $\mathrm{Fun}_R(\mathcal{P}_A, R\text{-Mod})$ is built as follows:

- If M is an A-module, let $\widetilde{M} \in \mathrm{Fun}_R(\mathcal{P}_A, R\text{-Mod})$ be the functor defined by:
  (1) For $G \in \mathcal{D}$, we have $\widetilde{M}(G) = M(G)$.
  (2) For $G, H \in \mathcal{D}$ and a morphism $\alpha \in A(H \times G)$ from G to H in $\mathcal{P}_A$, the map $\tilde{\alpha} : \widetilde{M}(G) \to \widetilde{M}(H)$ is the map sending

$$m \in M(G) \mapsto M(H \times \overleftarrow{G})(\alpha \times m).$$

- Conversely if $F \in \mathrm{Fun}_R(\mathcal{P}_A, R\text{-Mod})$, let $\widehat{F}$ be the A-module defined by:
  (1) If $G \in \mathcal{D}$, then $\widehat{F}(G) = F(G)$.
  (2) For $G, H \in \mathcal{D}$, $a \in A(G)$ and $m \in F(H)$, set

$$a \times m = F\Big(A\big(\mathrm{Ind}^{G\times H\times H}_{G\times\Delta(H)}\,\mathrm{Inf}^{G\times H}_{G}\big)(a)\Big)(m) \in F(G \times H),$$

  where $A\big(\mathrm{Ind}^{G\times H\times H}_{G\times\Delta(H)}\,\mathrm{Inf}^{G\times H}_{G}\big)(a) \in A(G\times H\times H)$ is viewed as a morphism from H to $G \times H$ in the category $\mathcal{P}_A$.

Then $M \mapsto \widetilde{M}$ and $F \mapsto \widehat{F}$ are well-defined equivalences of categories between A-Mod and $\mathrm{Fun}_R(\mathcal{P}_A, R\text{-Mod})$, inverse to each other.

Finally, we extend to A-modules our previous definition of the Yoneda–Dress construction.

Definition 10. Let A be a Green $\mathcal{D}$-biset functor. For $L \in \mathcal{D}$, consider the assignment $\rho_L = - \times L$ defined for objects G, H of $\mathcal{P}_A$ and morphisms $\alpha \in \mathrm{Hom}_{\mathcal{P}_A}(G, H) = A(H \times G)$ by

$$\begin{cases} \rho_L(G) = G \times L, \\ \rho_L(\alpha) = \alpha \times L := \mathrm{Iso}_{H\times G\times L\times L}^{H\times L\times G\times L}(\alpha \times \upsilon_{A,L\times L}(L)), \end{cases}$$

where $\upsilon_{A,L\times L}(L)$ is the image in $A(L \times L)$ of the identity (L, L)-biset L under the canonical morphism $\upsilon_{A,L\times L}$, and the isomorphism $H\times G\times L\times L \to H\times L\times G\times L$ maps (h, g, l_1, l_2) to (h, l_1, g, l_2).

A straightforward computation shows that

$$\rho_L(\alpha) = A\big(\mathrm{Ind}_{H\times G\times L}^{H\times L\times G\times L} \mathrm{Inf}_{H\times G}^{H\times G\times L}\big)(\alpha),$$

and this form may be more convenient for calculations. Here $H \times G \times L$ embeds into $H \times L \times G \times L$ via the map $(h, g, l) \mapsto (h, l, g, l)$, and maps surjectively onto $H \times G$ via $(h, g, l) \mapsto (h, g)$.

It is easy to check that ρ_L is in fact an endofunctor of $\mathcal{P}_A$, called the (*right*) *L-shift*. It induces by precomposition an endofunctor of the category $\mathrm{Fun}_R(\mathcal{P}_A, R\text{-Mod})$, that is, up to the above equivalence of categories, an endofunctor of the category A-Mod, which can be described as follows. It maps an A-module M to the shifted $\mathcal{D}$-biset functor M_L, endowed with the following product: for $G, H \in \mathcal{D}$, $\alpha \in A(H)$ and $m \in M_L(G) = M(G \times L)$, the element $\alpha \times m$ of $M_L(H \times G) = M(H \times G \times L)$ is simply the element $\alpha \times m$ obtained from the A-module structure of M.

This endofunctor $M \mapsto M_L$ of the category A-Mod will be denoted by Id_L. It is the Yoneda–Dress construction for A-modules.

Remark 11. For $L \in \mathcal{D}$, there is another obvious endofunctor $\lambda_L = L \times -$ of $\mathcal{P}_A$ defined for objects G, H of $\mathcal{P}_A$ and morphisms $\alpha \in \mathrm{Hom}_{\mathcal{P}_A}(G, H) = A(H \times G)$ by

$$\begin{cases} \lambda_L(G) = L \times G, \\ \lambda_L(\alpha) = L \times \alpha := \mathrm{Iso}_{L\times L\times H\times G}^{L\times H\times L\times G}(\upsilon_{A,L\times L}(L) \times \alpha), \end{cases}$$

where the isomorphism $L \times L \times H \times G \to L \times H \times L \times G$ maps (l_1, l_2, h, g) to (l_1, h, l_2, g). As before, it is easy to see that $L\times\alpha = A\big(\mathrm{Ind}_{L\times H\times G}^{L\times H\times L\times G} \mathrm{Inf}_{H\times G}^{L\times H\times G}\big)(\alpha)$.

It is then natural to ask if the assignment $\times : \mathcal{P}_A \times \mathcal{P}_A \to \mathcal{P}_A$ sending (G, K) to $G\times K$ and $(\alpha, \beta) \in A(H\times G)\times A(L\times K)$ to $(\alpha\times L)\circ(G\times\beta) \in A(H\times L\times G\times K)$ is a functor. We will answer this question at the end of Section 3 (Corollary 26).

2. Adjoint functors

Let A and C be Green $\mathcal{D}$-biset functors. A morphism $f : A \to C$ of Green $\mathcal{D}$-biset functors induces an obvious functor $\mathcal{P}_f : \mathcal{P}_A \to \mathcal{P}_C$, which is the identity on objects, and maps $\alpha \in \mathrm{Hom}_{\mathcal{P}_A}(G, H) = A(H \times G)$ to $f_{H\times G}(\alpha) \in C(H \times G) = \mathrm{Hom}_{\mathcal{P}_C}(G, H)$.

Let L be a fixed group in $\mathcal{D}$. The *inflation* morphism $\mathrm{Inf}_L : A \to A_L$, introduced in [García 2018], is the morphism of Green biset functors defined for each $G \in \mathcal{D}$ and each $\alpha \in A(G)$ by $\mathrm{Inf}_L(\alpha) = A(\mathrm{Inf}_G^{G\times L})(\alpha) \in A(G \times L) = A_L(G)$, where G is identified with $(G \times L)/(\{1\} \times L)$. The corresponding functor $\mathcal{P}_A \to \mathcal{P}_{A_L}$ will be denoted by ψ_L. Explicitly, for each $G \in \mathcal{D}$, we have $\psi_L(G) = G$, and for a morphism $\alpha \in A(H \times G)$, we have

$$\begin{aligned}\psi_L(\alpha) &= A\big(\mathrm{Inf}_{H\times G}^{H\times G\times L}\big)(\alpha) \in A(H \times G \times L)\\ &= A_L(H \times G) = \mathrm{Hom}_{\mathcal{P}_{A_L}}(\psi_L(G), \psi_L(H)).\end{aligned}$$

We introduce another functor $\theta_L : \mathcal{P}_{A_L} \to \mathcal{P}_A$, defined as follows: for an object G of $\mathcal{P}_{A_L}$, we set $\theta_L(G) = G \times L$, viewed as an object of $\mathcal{P}_A$. For a morphism $\alpha \in \mathrm{Hom}_{\mathcal{P}_{A_L}}(G, H) = A_L(H \times G) = A(H \times G \times L)$, we define

$$\theta_L(\alpha) = A\big(\mathrm{Ind}_{H\times G\times L}^{H\times L\times G\times L}\big)(\alpha) \in A(H \times L \times G \times L) = \mathrm{Hom}_{\mathcal{P}_A}(\theta_L(G), \theta_L(H)),$$

where $H \times G \times L$ is viewed as a subgroup of $H \times L \times G \times L$ via the injective group homomorphism $(h, g, l) \in H \times G \times L \mapsto (h, l, g, l) \in H \times L \times G \times L$.

Notation 12. In what follows, we will use a convenient abuse of notation, and generally drop the symbols $\times$ of cartesian products of groups, writing, e.g., $HLGL$ instead of $H \times L \times G \times L$.

Theorem 13. (1) *ψ_L is an R-linear functor from $\mathcal{P}_A$ to $\mathcal{P}_{A_L}$.*

(2) *θ_L is an R-linear functor from $\mathcal{P}_{A_L}$ to $\mathcal{P}_A$.*

(3) *The functors ψ_L and θ_L are left- and right-adjoint to one another. In other words, for any G and H in $\mathcal{D}$, there are R-module isomorphisms*

$$\begin{aligned}\mathrm{Hom}_{\mathcal{P}_{A_L}}(G, \psi_L(H)) &\cong \mathrm{Hom}_{\mathcal{P}_A}(\theta_L(G), H),\\ \mathrm{Hom}_{\mathcal{P}_{A_L}}(\psi_L(G), H) &\cong \mathrm{Hom}_{\mathcal{P}_A}(G, \theta_L(H))\end{aligned}$$

which are natural in G and H.

Proof. Assertion (1) is clear, since the functor ψ_L is built from a morphism of Green biset functors $\mathrm{Inf}_L : A \to A_L$.

To prove assertion (2), let $G, H, K \in \mathcal{D}$. If $\alpha \in A_L(HG)$ and $\beta \in A_L(KH)$, then

$$\begin{aligned}&\theta_L(\beta) \circ \theta_L(\alpha)\\ &\qquad = A\big(\mathrm{Def}_{KLGL}^{KLHLGL}\,\mathrm{Res}_{KLHLGL}^{KLHLHLGL}\big)\big(A\big(\mathrm{Ind}_{KHL}^{KLHL}\big)(\beta) \times A\big(\mathrm{Ind}_{HGL}^{HLGL}\big)(\alpha)\big)\\ &\qquad = A\big(\mathrm{Def}_{KLGL}^{KLHLGL}\,\mathrm{Res}_{KLHLGL}^{KLHLHLGL}\mathrm{Ind}_{KHLHGL}^{KLHLHLGL}\big)(\beta \times \alpha).\end{aligned}$$

In the restriction $\mathrm{Res}^{KLHLHLGL}_{KLHLGL}$, the group $KLHLGL$ maps into $KLHLHLGL$ via

$$f:(k,l_1,h,l_2,g,l_3)\in KLHLGL\mapsto(k,l_1,h,l_2,h,l_2,g,l_3)\in KLHLHLGL,$$

and in the induction $\mathrm{Ind}^{KLHLHLGL}_{KHLHGL}$, the group $KHLHGL$ maps into $KLHLHLGL$ via

$$f':(k',h'_1,l'_1,h'_2,g,l'_2)\in KHLHGL\mapsto(k',l'_1,h'_1,l'_1,h'_2,l'_2,g',l'_2)\in KLHLHLGL.$$

Then one checks easily that $\mathrm{Im}(f)\mathrm{Im}(f')=KLHLHLGL$, and that $\mathrm{Im}(f)\cap\mathrm{Im}(f')$ is isomorphic to $KHGL$. Hence by the Mackey formula, there is an isomorphism of bisets

$$\mathrm{Res}^{KLHLHLGL}_{KLHLGL}\mathrm{Ind}^{KLHLHLGL}_{KHLHGL}\cong\mathrm{Ind}^{KLHLGL}_{KHGL}\mathrm{Res}^{KHLHGL}_{KHGL},$$

where in $\mathrm{Ind}^{KLHLGL}_{KHGL}$, the inclusion $KHGL\hookrightarrow KLHLGL$ is

$$(k,h,g,l)\mapsto(k,l,h,l,g,l),$$

and in $\mathrm{Res}^{KHLHGL}_{KHGL}$, the inclusion $KHGL\hookrightarrow KHLHGL$ is

$$(k,h,g,l)\mapsto(k,h,l,h,g,l).$$

Now in the deflation $\mathrm{Def}^{KLHLGL}_{KLGL}$, the group $KLHLGL$ maps onto $KLGL$ via $(k,l_1,h,l_2,g,l_3)\mapsto(k,l_1,g,l_3)$. It follows that there is an isomorphism of bisets

$$\mathrm{Def}^{KLHLGL}_{KLGL}\,\mathrm{Ind}^{KLHLGL}_{KHGL}\cong\mathrm{Ind}^{KLGL}_{KGL}\,\mathrm{Def}^{KHGL}_{KGL},$$

which gives

$$\begin{aligned}\theta_L(\beta)\circ\theta_L(\alpha)&=A\big(\mathrm{Ind}^{KLGL}_{KGL}\big)A\big(\mathrm{Def}^{KHGL}_{KGL}\,\mathrm{Res}^{KHLHGL}_{KHGL}\big)(\beta\times\alpha)\\&=A\big(\mathrm{Ind}^{KLGL}_{KGL}\big)A_L\big(\mathrm{Def}^{KHG}_{KG}\,\mathrm{Res}^{KHHG}_{KHG}\big)A\big(\mathrm{Res}^{KHLHGL}_{KHHGL}\big)(\beta\times\alpha)\\&=A\big(\mathrm{Ind}^{KLGL}_{KGL}\big)A_L\big(\mathrm{Def}^{KHG}_{KG}\,\mathrm{Res}^{KHHG}_{KHG}\big)(\beta\times^d\alpha)\\&=A\big(\mathrm{Ind}^{KLGL}_{KGL}\big)(\beta\circ^d\alpha)\\&=\theta_L(\beta\circ^d\alpha),\end{aligned}$$

where $\circ^d$ denotes the composition in the category $\mathcal{P}_{A_L}$. This shows that θ_L is compatible with composition of morphisms. A straightforward computation shows that it maps identity morphisms to identity morphisms. This completes the proof of assertion (2), since θ_L is obviously R-linear.

The complete proof of assertion (3) demands the verification of many technical details, so we only include the full proof that θ_L is left-adjoint to ψ_L. We next simply give the description of the bijection involved in the other direction, and leave the corresponding verifications to the reader.

For G and H in $\mathcal{D}$, we have

$$\mathrm{Hom}_{\mathcal{P}_{A_L}}(G, \psi_L(H)) = A_L(\psi_L(H)G) = A(HGL),$$

and

$$\mathrm{Hom}_{\mathcal{P}_A}(\theta_L(G), H) = A(HGL),$$

so the identity map of $A(HGL)$ is an obvious candidate for an isomorphism $\mathrm{Hom}_{\mathcal{P}_{A_L}}(G, \psi_L(H)) \to \mathrm{Hom}_{\mathcal{P}_A}(\theta_L(G), H)$. For $\alpha \in \mathrm{Hom}_{\mathcal{P}_{A_L}}(G, \psi_L(H))$, we denote by $\tilde{\alpha}$ the element α viewed as an element of $\mathrm{Hom}_{\mathcal{P}_A}(\theta_L(G), H)$, to avoid confusion.

We now check that the map $\alpha \mapsto \tilde{\alpha}$ is natural in G and H. For naturality in G, if $G' \in \mathcal{D}$ and $u \in \mathrm{Hom}_{A_L}(G', G)$, we have the diagrams

$$\begin{tikzcd} G \arrow[r, "\alpha"] & \psi_L(H) \\ G' \arrow[u, "u"] \arrow[ur, "\alpha u"'] & \end{tikzcd} \qquad \begin{tikzcd} \theta_L(G) \arrow[r, "\tilde{\alpha}"] & H \\ \theta_L(G') \arrow[u, "\theta_L(u)"] \arrow[ur, "\widetilde{\alpha \circ^d u}"'] & \end{tikzcd}$$

and we have to show that the right-hand side diagram is commutative, i.e., that

$$\widetilde{\alpha \circ^d u} = \tilde{\alpha} \circ \theta_L(u).$$

But

$$\begin{aligned} \tilde{\alpha} \circ \theta_L(u) &= \alpha \circ A\big(\mathrm{Ind}_{GG'L}^{GLG'L}\big)(u) \\ &= A\big(\mathrm{Def}_{HG'L}^{HGLG'L}\,\mathrm{Res}_{HGLG'L}^{HGLGLG'L}\big)\big(\alpha \times A\big(\mathrm{Ind}_{GG'L}^{GLG'L}\big)(u)\big) \\ &= A\big(\mathrm{Def}_{HG'L}^{HGLG'L}\,\mathrm{Res}_{HGLG'L}^{HGLGLG'L}\mathrm{Ind}_{HGLGG'L}^{HGLGLG'L}\big)(\alpha \times u). \end{aligned}$$

In the restriction $\mathrm{Res}_{HGLG'L}^{HGLGLG'L}$, the inclusion $HGLG'L \hookrightarrow HGLGLG'L$ is the map

$$f : (h, g, l_1, g', l_2) \in HGLG'L \mapsto (h, g, l_1, g, l_1, g', l_2) \in HGLGLG'L,$$

and in the induction $\mathrm{Ind}_{HGLGG'L}^{HGLGLG'L}$, the inclusion $HGLGG'L \hookrightarrow HGLGLG'L$ is the map

$$f' : (\eta, \gamma_1, \lambda_1, \gamma_2, \gamma', \lambda_2) \in HGLGG'L \mapsto (\eta, \gamma_1, \lambda_1, \gamma_2, \lambda_2, \gamma', \lambda_2) \in HGLGLG'L.$$

Then clearly $\mathrm{Im}(f)\mathrm{Im}(f') = HGLGLG'L$, and $\mathrm{Im}(f) \cap \mathrm{Im}(f') \cong HGG'L$. By the Mackey formula, this gives an isomorphism of bisets

$$\mathrm{Res}_{HGLG'L}^{HGLGLG'L}\mathrm{Ind}_{HGLGG'L}^{HGLGLG'L} \cong \mathrm{Ind}_{HGG'L}^{HGLG'L}\mathrm{Res}_{HGG'L}^{HGLGG'L},$$

where, in $\mathrm{Ind}_{HGG'L}^{HGLG'L}$, the inclusion $HGG'L \hookrightarrow HGLG'L$ is

$$(h, g, g', l) \mapsto (h, g, l, g', l),$$

and in $\mathrm{Res}^{HGLGG'L}_{HGG'L}$, the inclusion $HGG'L \hookrightarrow HGLGG'L$ is

$$(h, g, g', l) \mapsto (h, g, l, g, g', l).$$

Now in $\mathrm{Def}^{HGLG'L}_{HG'L}$, the quotient map $HGLG'L \to HG'L$ sends (h, g, l_1, g', l_2) to (h, g', l_2), so the image of the subgroup $HGG'L$ is the whole of $HG'L$. It follows that there is an isomorphism of bisets

$$\mathrm{Def}^{HGLG'L}_{HG'L}\,\mathrm{Ind}^{HGLG'L}_{HGG'L} \cong \mathrm{Def}^{HGG'L}_{HG'L},$$

which gives finally

$$\begin{aligned}
\tilde{\alpha} \circ \theta_L(u) &= A\big(\mathrm{Def}^{HGG'L}_{HG'L}\,\mathrm{Res}^{HGLGG'L}_{HGG'L}\big)(\alpha \times u)\\
&= A_L\big(\mathrm{Def}^{HGG'}_{HG'}\big)A_L\big(\mathrm{Res}^{HGGG'}_{HGG'}\big)A\big(\mathrm{Res}^{HGLGG'L}_{HGGG'L}\big)(\alpha \times u)\\
&= A_L\big(\mathrm{Def}^{HGG'}_{HG'}\big)A_L\big(\mathrm{Res}^{HGGG'}_{HGG'}\big)(\alpha \times^d u)\\
&= \alpha \circ^d u,
\end{aligned}$$

as was to be shown.

We check that the map $\alpha \mapsto \tilde{\alpha}$ is natural in H. If $H' \in \mathcal{D}$ and $v \in \mathrm{Hom}_{\mathcal{P}_A}(H, H') = A(H'H)$, we have the diagrams

$$\begin{tikzcd}
A \arrow[r, "\alpha"] \arrow[dr, "\psi_L(v)\circ^d\alpha"'] & \psi_L(H) \arrow[d, "\psi_L(v)"] \\
& \psi_L(H')
\end{tikzcd}
\qquad
\begin{tikzcd}
\theta_L(G) \arrow[r, "\tilde{\alpha}"] \arrow[dr, "\widetilde{\psi_L(v)\circ^d\alpha}"'] & H \arrow[d, "v"] \\
& H'
\end{tikzcd}$$

and we have to show that the right-hand side diagram is commutative, i.e., that

$$\widetilde{\psi_L(v)\circ^d\alpha} = v \circ \tilde{\alpha}.$$

But

$$\begin{aligned}
\psi_L(v) \circ^d \alpha &= A\big(\mathrm{Inf}^{H'HL}_{H'H}\big)(v) \circ^d \alpha\\
&= A_L\big(\mathrm{Def}^{H'HG}_{H'G}\,\mathrm{Res}^{H'HHG}_{H'HG}\big)\big(A\big(\mathrm{Inf}^{H'HL}_{H'H}\big)(v) \times^d \alpha\big)\\
&= A\big(\mathrm{Def}^{H'HGL}_{H'GL}\,\mathrm{Res}^{H'HHGL}_{H'HGL}\big)A\big(\mathrm{Res}^{H'HLHGL}_{H'HHGL}\,\mathrm{Inf}^{H'HLHGL}_{H'HHGL}\big)(v \times \alpha)\\
&= A\big(\mathrm{Def}^{H'HGL}_{H'GL}\,\mathrm{Res}^{H'HLHGL}_{H'HGL}\,\mathrm{Inf}^{H'HLHGL}_{H'HHGL}\big)(v \times \alpha).
\end{aligned}$$

In $\mathrm{Res}^{H'HLHGL}_{H'HGL}$, the inclusion $H'HGL \hookrightarrow H'HLHGL$ is

$$(h', h, g, l) \mapsto (h', h, l, h, g, l),$$

and in $\mathrm{Inf}^{H'HLHGL}_{H'HHGL}$, the quotient map $H'HLHGL \to H'HHGL$ is

$$(h', h_1, l_1, h_2, g, l_2) \mapsto (h', h_1, h_2, g, l_2).$$

The composition of these two maps sends (h', h, g, l) to (h', h, h, g, l), hence it is injective. This gives an isomorphism of bisets

$$\mathrm{Res}^{H'HLHGL}_{H'HGL}\,\mathrm{Inf}^{H'HLHGL}_{H'HHGL} \cong \mathrm{Res}^{H'HHGL}_{H'HGL},$$

from which we get

$$\psi_L(v) \circ^d \alpha = A\big(\mathrm{Def}^{H'HGL}_{H'GL}\,\mathrm{Res}^{H'HHGL}_{H'HGL}\big)(v \times \alpha) = v \circ \tilde{\alpha},$$

as was to be shown.

Hence the isomorphism $\alpha \in \mathrm{Hom}_{\mathcal{P}_{A_L}}(G, \psi_L(H)) \mapsto \tilde{\alpha} \in \mathrm{Hom}_{\mathcal{P}_A}(\theta_L(G), H)$ is natural in G and H, so θ_L is left-adjoint to ψ_L.

We now describe the bijection implying that θ_L is also right-adjoint to ψ_L. So, for $G, H \in \mathcal{D}$, we have to build an isomorphism

$$\alpha \in \mathrm{Hom}_{\mathcal{P}_{A_L}}(\psi_L(G), H) \mapsto \widehat{\alpha} \in \mathrm{Hom}_{\mathcal{P}_A}(G, \theta_L(H))$$

of R-modules, natural in G and H. But

$$\mathrm{Hom}_{\mathcal{P}_{A_L}}(\psi_L(G), H) = A_L(HG) = A(HGL) \quad \text{and} \quad \mathrm{Hom}_{\mathcal{P}_A}(G, \theta_L(H)) = A(HLG),$$

so an obvious candidate for the above isomorphism is to set $\widehat{\alpha} = A(\mathrm{Iso}^{HLG}_{HGL})(\alpha)$. The verification that this isomorphism is functorial in G and H is similar to the proof of the first adjunction, and we omit it. □

Definition 14. Let A be a Green $\mathcal{D}$-biset functor and $L \in \mathcal{D}$. We denote by

$$\Psi_L : \mathrm{Fun}_R(\mathcal{P}_{A_L}, R\text{-Mod}) \to \mathrm{Fun}_R(\mathcal{P}_A, R\text{-Mod})$$

the functor induced by precomposition with ψ_L, and by

$$\Theta_L : \mathrm{Fun}_R(\mathcal{P}_A, R\text{-Mod}) \to \mathrm{Fun}_R(\mathcal{P}_{A_L}, R\text{-Mod})$$

the functor induced by precomposition with θ_L.

Proposition 15. *The functors Ψ_L and Θ_L are mutual left- and right-adjoint functors between $\mathrm{Fun}_R(\mathcal{P}_{A_L}, R\text{-Mod})$ and $\mathrm{Fun}_R(\mathcal{P}_A, R\text{-Mod})$.*

Proof. This follows from Theorem 13, by standard category theory. □

Remark 16. Using the above equivalences of categories between $\mathrm{Fun}_R(\mathcal{P}_A, R\text{-Mod})$ and A-Mod, and $\mathrm{Fun}_R(\mathcal{P}_{A_L}, R\text{-Mod})$ and A_L-Mod, we will consider Ψ_L as a functor from A_L-Mod to A-Mod and Θ_L as a functor from A-Mod to A_L-Mod. One can check that, from this point of view, if N is an A_L-module, then $\Psi_L(N)$ is the A-module defined as follows:

- If $G \in \mathcal{D}$, then $\Psi_L(N)(G) = N(G)$.

- If $G, H \in \mathcal{D}$, $a \in A(G)$ and $v \in N(H)$, then
$$a \times v = A\big(\mathrm{Inf}_G^{G\times L}\big)(a) \times^d v$$
where $\times^d$ denotes the action of A_L on N, and $A(\mathrm{Inf}_G^{G\times L})(a) \in A(G \times L)$ is viewed as an element of $A_L(G)$.

Conversely, if M is an A-module, then $\Theta_L(M)$ is the A_L-module defined as follows:

- If $G \in \mathcal{D}$, then $\Theta_L(M)(G) = M(G \times L)$.
- If $G, H \in \mathcal{D}$, $a \in A_L(G)$ and $m \in M(H \times L)$, then
$$a \times^d m = M\big(\mathrm{Res}_{G\times H\times L}^{G\times L\times H\times L}\big)(a \times m),$$
where $a \times m$ is the product of $a \in A(G \times L)$ and $m \in M(H \times L)$, and $H \times G \times L$ is viewed as a subgroup of $G \times L \times H \times L$ via the map $(g, h, l) \mapsto (g, l, h, l)$.

Theorem 17. *Let A be a Green $\mathcal{D}$-biset functor, and $L \in \mathcal{D}$. The endofunctor ρ_L of $\mathcal{P}_A$ is isomorphic to $\theta_L \circ \psi_L$ and so the endofunctor $\Psi_L \circ \Theta_L$ of A-*Mod *is isomorphic to the Yoneda–Dress functor* Id_L. *In particular,* Id_L *is self-adjoint.*

Proof. One checks readily that ρ_L is isomorphic to the composition $\theta_L \circ \psi_L$. The other assertions follow by Theorem 13, as the Yoneda–Dress functor Id_L is obtained by precomposition with $\rho_L = - \times L$. □

We observe that the L-shift of the A-module A is the representable functor $A(-, L)$ of the category $\mathcal{P}_A$, so it is projective. More generally, the L-shift of the representable functor $A(-, X)$ is the representable functor $A(-, L \times X)$. Hence the Yoneda–Dress construction maps a representable functor to a representable functor.

3. The commutant

Definition 18. Let A be a Green $\mathcal{D}$-biset functor.

(1) For $G, H \in \mathcal{D}$, we say that an element $a \in A(G)$ and an element $b \in A(H)$ *commute* if
$$a \times b = A\big(\mathrm{Iso}_{H\times G}^{G\times H}\big)(b \times a).$$

(2) For a group G in $\mathcal{D}$, we denote by $CA(G)$ the set of elements of $A(G)$ which commute with any element of $A(H)$, for any $H \in \mathcal{D}$, i.e.,
$$\big\{a \in A(G) \mid \text{for all } H \in \mathcal{D} \text{ and all } b \in A(H),\ a \times b = A\big(\mathrm{Iso}_{H\times G}^{G\times H}\big)(b \times a)\big\},$$
and call it *the commutant* of A at G.

Observe that $CA(G)$ is an R-submodule of $A(G)$, since the product $\times$ is bilinear.

Lemma 19. *Let A be a Green $\mathcal{D}$-biset functor. Then the commutant of A is a Green $\mathcal{D}$-biset subfunctor of A.*

Proof. To see it is a biset functor, let Y be a (K, G)-biset for groups K and G in $\mathcal{D}$, and let a be in $CA(G)$. If b is in $A(H)$ for a given group H in $\mathcal{D}$, we have

$$A(Y)(a) \times b = A\big((Y \times H) \circ \mathrm{Iso}_{H\times G}^{G\times H}\big)(b \times a),$$

where $Y \times H$ is seen as a $(K \times H, G \times H)$-biset. If we show that $(Y \times H) \circ \mathrm{Iso}_{H\times G}^{G\times H}$ is isomorphic to $\mathrm{Iso}_{H\times K}^{K\times H} \circ (H \times Y)$, where $H \times Y$ is seen as a $(H \times K, H \times G)$-biset, the right-hand side of the equality above will be equal to

$$A\big(\mathrm{Iso}_{H\times K}^{K\times H}\big)(b \times A(Y)(a)),$$

which is what we want. Now, $\mathrm{Iso}_{H\times G}^{G\times H}$ is the group $H \times G$, seen as a $(G \times H, H \times G)$-biset, and $\mathrm{Iso}_{H\times K}^{K\times H}$ is the group $H \times K$, seen as a $(K \times H, H \times K)$-biset. So, it is not hard to see that $(Y \times H) \circ \mathrm{Iso}_{H\times G}^{G\times H}$ is isomorphic to $Y \times H$ as a $(K \times H, H \times G)$-biset, where the right action of $H \times G$ is given by $(y, h)(h_1, g_1) = (yg_1, hh_1)$. Similarly, $\mathrm{Iso}_{H\times K}^{K\times H} \circ (H \times Y)$ is isomorphic to $H \times Y$ as a $(K \times H, H \times G)$-set, where the left action of $K \times H$ is given by $(k_1, h_1)(h, y) = (h_1 h, k_1 y)$. Hence, it is easy to verify that the map $Y \times H \to H \times Y$ sending (y, h) to (h, y) defines an isomorphism between these two bisets.

To see that CA is closed under the product $\times$, let a be in $CA(G)$, b be in $CA(H)$ and c be in $A(K)$. We have

$$a \times (b \times c) = a \times A\big(\mathrm{Iso}_{K\times H}^{H\times K}\big)(c \times b),$$

which is clearly equal to $A\big(\mathrm{Iso}_{G\times K\times H}^{G\times H\times K}\big)(a \times c \times b)$. Similarly,

$$(a \times c) \times b = A\big(\mathrm{Iso}_{K\times G\times H}^{G\times K\times H}\big)(c \times a \times b).$$

Finally, clearly we have

$$\mathrm{Iso}_{G\times K\times H}^{G\times H\times K} \circ \mathrm{Iso}_{K\times G\times H}^{G\times K\times H} = \mathrm{Iso}_{K\times G\times H}^{G\times H\times K},$$

which yields the first equality

$$(a \times b) \times c = A\big(\mathrm{Iso}_{K\times G\times H}^{G\times H\times K}\big)(c \times (a \times b)).$$

To finish the proof, it is clear that the identity element $\varepsilon \in A(1)$ belongs to $CA(1)$. □

Corollary 20. *Let A be a Green $\mathcal{D}$-biset functor. Then the image of the unique Green biset functor morphism $\upsilon_A : RB \to A$ is contained in CA.*

Proof. Indeed, by uniqueness of υ_A and υ_{CA}, the diagram

$$\begin{tikzcd} & CA \arrow[dr, hook] & \\ RB \arrow[ur, "\upsilon_{CA}"] \arrow[rr, "\upsilon_A"'] & & A \end{tikzcd}$$

is commutative. □

Definition 21. We will say that a Green $\mathcal{D}$-biset functor A is *commutative* if $A = CA$.

It is easy to see that CA is commutative. All the examples considered in Example 5 are commutative Green biset functors.

If A is commutative, then clearly A_G is commutative for any G. More generally, we have the following result.

Proposition 22. *Let A be a Green $\mathcal{D}$-biset functor and $G \in \mathcal{D}$. Then $CA_G = (CA)_G$.*

Proof. Observe that CA_G and $(CA)_G$ are both Green $\mathcal{D}$-biset subfunctors of A_G, so to prove they are equal as Green $\mathcal{D}$-biset functors, it suffices to prove that for every group $H \in \mathcal{D}$, we have $(CA)_G(H)$=$CA_G(H)$.

To prove that $(CA)_G(H) \subseteq CA_G(H)$, we choose a group K in $\mathcal{D}$, and elements $a \in (CA)_G(H)$ and $b \in A_G(K)$. We must prove that

$$a \times^d b = A_G\big(\mathrm{Iso}_{K\times H}^{H\times K}\big)(b \times^d a).$$

We have

$$a \times^d b = A\big(\mathrm{Res}_{H\times K\times\Delta(G)}^{H\times G\times K\times G}\big)(a \times b) \quad \text{and} \quad b \times^d a = A\big(\mathrm{Res}_{K\times H\times\Delta(G)}^{K\times G\times H\times G}\big)(b \times a).$$

Now, by definition $(CA)_G(H) = CA(H \times G)$, so the element a satisfies

$$a \times b = A\big(\mathrm{Iso}_{K\times G\times H\times G}^{H\times G\times K\times G}\big)(b \times a).$$

Substituting this in the above equation on the left we easily obtain what we wanted.

To prove the reverse inclusion $CA_G(H) \subseteq (CA)_G(H)$, we now let $a \in CA_G(H)$ and $b \in A(K)$, and consider $c = A(\mathrm{Inf}_K^{K\times G})(b)$. Then we have

$$a \times^d c = A_G\big(\mathrm{Iso}_{K\times H}^{H\times K}\big)(c \times^d a),$$

and clearly

$$a \times^d c = A\big(\mathrm{Res}_{H\times K\times\Delta(G)}^{H\times G\times K\times G} \circ \mathrm{Inf}_{H\times G\times K}^{H\times G\times K\times G}\big)(a \times b).$$

But it is easy to see (for example from Section 1.1.3 of [Bouc 2010]) that

$$\mathrm{Res}_{H\times K\times\Delta(G)}^{H\times G\times K\times G} \circ \mathrm{Inf}_{H\times G\times K}^{H\times G\times K\times G} \cong \mathrm{Iso}_{H\times G\times K}^{H\times K\times\Delta(G)}.$$

By doing a similar transformation with $c \times^d a$, and applying the corresponding isomorphisms, we easily obtain what we wanted. □

Lemma 23. *Let A be a Green $\mathcal{D}$-biset functor. Then for any group G in $\mathcal{D}$, the commutant $CA(G)$ is a subring of $Z(A(G))$.*

Proof. Take $a \in CA(G)$ and $b \in A(G)$, then

$$\begin{aligned} a \cdot b = A\big(\mathrm{Iso}_{\Delta(G)}^{G} \circ \mathrm{Res}_{\Delta(G)}^{G\times G}\big)(a \times b) &= A\big(\mathrm{Iso}_{\Delta(G)}^{G} \circ \mathrm{Res}_{\Delta(G)}^{G\times G} \circ \mathrm{Iso}(\sigma_G)\big)(b \times a) \\ &= A\big(\mathrm{Iso}_{\Delta(G)}^{G} \circ \mathrm{Res}_{\Delta(G)}^{G\times G}\big)(b \times a) = b \cdot a, \end{aligned}$$

where σ_G is the automorphism of $G \times G$ switching the components. Since $CA(G)$

and $Z(A(G))$ have the same ring structure, inherited from the Green $\mathcal{D}$-biset functor structure of A, this shows that $CA(G)$ is a subring of $Z(A(G))$. $\square$

Remark 24. It is not hard to see then that A is a commutative Green biset functor if and only if for every group G, the ring $A(G)$ is a commutative ring.

We now answer the question raised in Remark 11.

Proposition 25. *Let A be a Green $\mathcal{D}$-biset functor, and $G, H, K, L \in \mathcal{D}$. Let $\alpha \in A(HG)$ and $\beta \in A(LK)$. Then the square*

$$\begin{array}{ccc} G \times K & \xrightarrow{G\times\beta} & G \times L \\ {\scriptstyle \alpha\times K}\Big\downarrow & & \Big\downarrow{\scriptstyle \alpha\times L} \\ H \times K & \xrightarrow[H\times\beta]{} & H \times L \end{array}$$

commutes in $\mathcal{P}_A$ if and only if α and β commute.

Proof. Let $u = (\alpha \times L) \circ (G \times \beta)$. By definition

$$\begin{aligned} u &= A\big(\mathrm{Ind}_{HGL}^{HLGL}\,\mathrm{Inf}_{HG}^{HGL}\big)(\alpha) \circ A\big(\mathrm{Ind}_{GLK}^{GLGK}\,\mathrm{Inf}_{LK}^{GLK}\big)(\beta) \\ &= A\big(\mathrm{Def}_{HLGK}^{HL\underline{GL}GK}\,\mathrm{Res}_{HL\underline{GL}GK}^{HL\underline{GLGL}GK}\big) \\ &\qquad\qquad \times\big(A\big(\mathrm{Ind}_{HG\underline{L}}^{H\underline{L}G\underline{L}}\,\mathrm{Inf}_{HG}^{HG\underline{L}}\big)(\alpha) \times A\big(\mathrm{Ind}_{\underline{G}LK}^{\underline{G}L\underline{G}K}\,\mathrm{Inf}_{LK}^{\underline{G}LK}\big)(\beta)\big), \end{aligned}$$

where the notation $\mathrm{Def}_{HLGK}^{HL\underline{GL}GK}$ means the deflation with respect to the underlined normal subgroup, and $\mathrm{Res}_{HL\underline{GL}GK}^{HL\underline{GLGL}GK}$ means that the underlined GL in the subscript embeds diagonally in the underlined $GLGL$ in the superscript. Similarly, in $\mathrm{Ind}_{HG\underline{L}}^{H\underline{L}G\underline{L}}$, the group L in the subscript embeds diagonally in the two underlined copies of L in the superscript, and in $\mathrm{Inf}_{HG}^{HG\underline{L}}$, inflation is relative to the underlined L in the superscript. Thus,

$$u = A\big(\mathrm{Def}_{HLGK}^{HL\underline{GL}GK}\,\mathrm{Res}_{HL\underline{GL}GK}^{HL\underline{GLGL}GK}\,\mathrm{Ind}_{HG\underline{LG}LK}^{H\underline{L}G\underline{LG}L\underline{G}K}\,\mathrm{Inf}_{HGLK}^{HG\underline{LG}LK}\big)(\alpha \times \beta).$$

Standard relations in the composition of bisets (see Section 1.1.3 and Lemma 2.3.26 of [Bouc 2010]) and some tedious but straightforward calculations finally give

$$u = (\alpha \times L) \circ (G \times \beta) = A\big(\mathrm{Iso}_{HGLK}^{HLGK}\big)(\alpha \times \beta).$$

Similar calculations show that

$$(H \times \beta) \circ (\alpha \times K) = A\big(\mathrm{Iso}_{LKHG}^{HLGK}\big)(\beta \times \alpha).$$

So $(H \times \beta) \circ (\alpha \times K) = (\alpha \times L) \circ (G \times \beta)$ if and only if

$$\beta \times \alpha = A\big(\mathrm{Iso}_{HLGK}^{LKHG}\mathrm{Iso}_{HGLK}^{HLGK}\big)(\alpha \times \beta) = A\big(\mathrm{Iso}_{HGLK}^{LKHG}\big)(\alpha \times \beta),$$

that is, if α and β commute. $\square$

Corollary 26. *The assignment* $\times : \mathcal{P}_A \times \mathcal{P}_A \to \mathcal{P}_A$ *sending* (G, K) *to* $G \times K$ *and* $(\alpha, \beta) \in A(H \times G) \times A(L \times K)$ *to* $(\alpha \times L) \circ (G \times \beta) \in A(H \times L \times G \times K)$ *is a functor if and only if* A *is commutative. In particular, when* A *is commutative, this functor* $\times$ *endows* $\mathcal{P}_A$ *with a structure of a* ***symmetric monoidal category****.*

4. The center

Definition 27. Let A be a Green $\mathcal{D}$-biset functor. For a group L in $\mathcal{D}$, we denote by $ZA(L)$ the family of all natural transformations $\mathrm{Id} \to \mathrm{Id}_L$ from the identity functor $\mathrm{Id} : A\text{-Mod} \to A\text{-Mod}$ to the functor Id_L. We call it *the center* of A at L.

When L is trivial, the functor Id_L is isomorphic to the identity functor, hence $ZA(1)$ is the family of natural endotransformations of the identity functor. So our definition is analogous to that of the center of a category (see for example [Hoffmann 1975] for arbitrary categories, or Section 19 of [Butler and Horrocks 1961] for abelian categories). Nonetheless, we want to regard this center as a Green $\mathcal{D}$-biset functor, and see its relation with the commutant CA. Our construction is inspired by an analogous construction for Green functors over a fixed finite group in [Bouc 1997, Section 12.2].

4.1. ***The center as a Green biset functor.*** Our goal is to show that for each Green $\mathcal{D}$-biset functor A, the assignment $L \mapsto ZA(L)$ is itself a Green $\mathcal{D}$-biset functor. For this, we will first give an equivalent description of $ZA(L)$, and then build a Green functor structure on ZA.

Proposition 28. *Let* A *be a Green* $\mathcal{D}$*-biset functor, and* $L \in \mathcal{D}$*. Then* $ZA(L)$ *is isomorphic to the family* $ZA'(L)$ *of natural transformations from the identity functor of* $\mathcal{P}_A$ *to* ρ_L*.*

Proof. Consider the Yoneda embedding $\mathcal{Y}_A : \mathcal{P}_A \to A$-Mod sending $L \in \mathcal{D}$ to the functor $A(-, L)$. Since Id_L preserves the image of $\mathcal{Y}_A$, which is a fully faithful functor, we have $\mathrm{Id}_L \circ \mathcal{Y}_A = \mathcal{Y}_A \circ \rho_L$, and it follows that each element of $ZA(L)$ induces a natural transformation from the identity functor of $\mathcal{P}_A$, denoted by ρ_1, to ρ_L. In this way, we get a linear map $f_L : ZA(L) \to ZA'(L)$. Conversely, each natural transformation $\rho_1 \to \rho_L$ induces a natural transformation $\mathcal{Y}_A \to \mathrm{Id}_L \circ \mathcal{Y}_A$. Since the image of $\mathcal{Y}_A$ generates A-Mod, such a natural transformation extends to a natural transformation from the identity functor of A-Mod to Id_L. This gives a linear map $g_L : ZA'(L) \to ZA(L)$. Clearly f_L and g_L are inverse to one another. □

We will now use the previous identification to get a better understanding of $ZA(L)$. Indeed, a natural transformation t from the identity functor of $\mathcal{P}_A$ to the functor $\rho_L = - \times L = \theta_L \psi_L$ consists, for each $G \in \mathcal{D}$, of a morphism $t_G : G \to G \times L$ in $\mathcal{P}_A$, i.e., $t_G \in A(G \times L \times G)$, such that for any $H \in \mathcal{D}$ and any $\alpha \in A(H \times G)$, the diagram

(1)
$$\begin{tikzcd} G \arrow[r, "t_G"] \arrow[d, "\alpha"'] & G \times L \arrow[d, "\alpha\times L=\theta_L\psi_L(\alpha)"] \\ H \arrow[r, "t_H"] & H \times L \end{tikzcd}$$

is commutative in $\mathcal{P}_A$.

Lemma 29. *Let $G, H \in \mathcal{D}$, and $\alpha \in A(H \times G) = \mathrm{Hom}_{\mathcal{P}_A}(G, H)$. For an element u of $A(H \times L \times G) = \mathrm{Hom}_{\mathcal{P}_A}(G, H \times L)$, let $u^\natural$ denote the element u, viewed as a morphism from $L \times G$ to H in $\mathcal{P}_A$. Then, for any $t \in A(G \times L \times G)$,*

$$(\theta_L\psi_L(\alpha) \circ t)^\natural = \alpha \circ t^\natural \quad \text{in } A(H \times L \times G).$$

Proof. The functor ρ_L is a self-adjoint R-linear endofunctor of $\mathcal{P}_A$. It follows from the proof of Theorem 13 that for any $G, H \in \mathcal{P}_A$, the natural bijection given by this adjunction

$$v \in \mathrm{Hom}_{\mathcal{P}_A}(G, \rho_L(H)) = A(HLG) \to v^\sharp \in \mathrm{Hom}_{\mathcal{P}_A}(\rho_L(G), H) = A(HGL)$$

is induced by the isomorphism $HLG \to HGL$ switching the components L and G. By adjunction we have commutative diagrams

$$\begin{tikzcd} G \arrow[r, "t"] \arrow[dr, "\rho_L(\alpha)\circ t"'] & \rho_L(G) \arrow[d, "\rho_L(\alpha)"] \\ & \rho_L(H) \end{tikzcd} \qquad \begin{tikzcd} \rho_L(G) \arrow[r, "t^\sharp"] \arrow[dr, "(\rho_L(\alpha)\circ t)^\sharp"'] & G \arrow[d, "\alpha"] \\ & H \end{tikzcd}$$

so $(\rho_L(\alpha) \circ t)^\sharp = \alpha \circ t^\sharp$. Since $t^\natural = t^\sharp \circ \tau_{L,G}$, where $\tau_{G,L} : LG \to GL$ is the isomorphism switching G and L, the lemma follows by right composition of the previous equality with $\tau_{G,L}$. ☐

Since v and $v^\natural$ are actually the same element of $A(HLG)$, for any $v \in A(HLG)$, the commutativity in diagram (1) can be simply written as

(2)
$$\alpha \circ_G t_G = t_H \circ_H \alpha,$$

where $\circ_G$ is the composition $A(HG) \times A(GLG) \to A(HLG)$, and $\circ_H$ is the composition $A(HLH) \times A(HG) \to A(HLG)$. Thus:

Proposition 30. *Let A be a Green $\mathcal{D}$-biset functor, and $L \in \mathcal{D}$. Then an element t of $ZA(L)$ consists of a family of elements $t_G \in A(GLG)$, for every $G \in \mathcal{D}$, such that $\alpha \circ_G t_G = t_H \circ_H \alpha$, for any G, H in $\mathcal{D}$ and $\alpha \in A(HG)$. In particular $ZA(L)$ is a set.*

Proof. It remains to see that $ZA(L)$ is a set. This is clear, since an element t of $ZA(L)$ is determined by its components t_G, where G runs through our chosen set $\boldsymbol{D}$ of representatives of isomorphism classes of groups in $\mathcal{D}$. More precisely, $ZA(L)$ is in one-to-one correspondence with the set $Cr_A(L)$ of sequences of elements $(t_G)_{G\in\boldsymbol{D}} \in \prod_{G\in\boldsymbol{D}} A(GLG)$ such that the above condition (2) holds for any $G, H \in \boldsymbol{D}$ and any $\alpha \in A(HG)$. $\square$

Proposition 31. (1) *Let $K, L \in \mathcal{D}$, and $\beta \in CA(LK)$. Then the family of morphisms $\lambda_G(\beta) = G \times \beta : G \times K \to G \times L$, for $G \in \mathcal{D}$, define a natural transformation of functors ρ_β from ρ_K to ρ_L.*

(2) *Let $\mathrm{End}_R(\mathcal{P}_A)$ denote the category of R-linear endofunctors of $\mathcal{P}_A$, where morphisms are natural transformations of functors. Then the assignment*

$$\begin{cases} K \in \mathcal{D} \mapsto \rho_K \in \mathrm{End}_R(\mathcal{P}_A), \\ \beta \in CA(LK) \mapsto (\rho_\beta : \rho_K \to \rho_L) \end{cases}$$

is a faithful R-linear functor ρ_{CA} from $\mathcal{P}_{CA}$ to $\mathrm{End}_R(\mathcal{P}_A)$.

Proof. (1) This follows from Proposition 25.

(2) We have to check that if $G, J, K, L \in \mathcal{D}$, if $\alpha \in A(KJ)$ and $\beta \in A(LK)$, then $(G\times\beta)\circ(G\times\alpha) = G\times(\beta\circ\alpha)$ in $A(GLGJ)$, and that if β is the identity element of $CA(KK)$, then $G \times \beta$ is the identity morphism of $G \times K$ in $\mathcal{P}_A$. This follows from the fact that λ_G is a functor.

So we get a functor $\rho_{CA} : \mathcal{P}_{CA} \to \mathrm{End}_R(\mathcal{P}_A)$. Seeing that this functor is faithful amounts to seeing that if $\beta \in CA(LK)$, then $\rho_\beta = 0$ if and only if $\beta = 0$. But the component $1 \times \beta$ of ρ_β is clearly equal to β, after identification of $1 \times K$ with K and $1 \times L$ with L. $\square$

Remark 32. In particular, it follows from assertion (2) that an isomorphism of groups $K \to K'$ induces an isomorphism of functors $\rho_K \to \rho'_K$: indeed, a group isomorphism $\varphi : K \to K'$ is represented by a (K', K)-biset $U_\varphi \in RB(K'K)$, and hence by an element $\beta_\varphi = \upsilon_{K'K}(U_\varphi) \in CA(K'K)$, by Corollary 20. The corresponding natural transformation ρ_{β_φ} is an isomorphism $\rho_K \to \rho'_K$, with inverse $\rho_{\beta_{\varphi^{-1}}}$.

Lemma 33. *Let A be a Green $\mathcal{D}$-biset functor and $K, L \in \mathcal{D}$.*

(1) *The endofunctors $\rho_L \circ \rho_K$ and ρ_{KL} of $\mathcal{P}_A$ are naturally isomorphic.*

(2) *Let $s \in ZA(LK)$, given by the family of elements $s_G \in A(GLKG)$, for $G \in \mathcal{D}$. Then the natural transformation $s^o : \rho_K \to \rho_L$ deduced from $s : \mathrm{Id} \to \rho_K\rho_L$ by adjunction, is defined by the family of morphisms*

$$s^o_G = \mathrm{Iso}^{GLGK}_{GLKG}(s_G) \in A(GLGK) = \mathrm{Hom}_{\mathcal{P}_A}(GK, GL).$$

(3) *The map $s \mapsto s^o$ is an isomorphism of R-modules,*

$$ZA(LK) \to \mathrm{Hom}_{\mathrm{End}_R(\mathcal{P}_A)}(\rho_K, \rho_L).$$

Proof. (1) This follows from a straightforward verification.

(2) By the proof of Theorem 13, for each $G \in \mathcal{D}$, the morphism $s_G \in A(GLKG)$,

$$s_G : G \to GLK = \rho_K \rho_L(G) = \theta_K \psi_K \rho_L(G),$$

in $\mathcal{P}_A$ gives by adjunction the morphism

$$u : \psi_K(G) \to \psi_K \rho_L(G)$$

in $\mathcal{P}_{A_K}$, defined as the element

$$u = A\big(\mathrm{Iso}_{GLKG}^{GLGK}\big)(s_G) \in A_K(GLG) = A(GLGK).$$

This element u gives in turn the morphism

$$v : \theta_K \psi_K(G) = \rho_K(G) \to \rho_L(G)$$

equal to $u \in A(GLGK)$, but viewed as a morphism in $\mathcal{P}_A$ from GK to GL.

(3) This is clear, by adjunction. □

Proposition 34. *The center of A is a $\mathcal{D}$-biset functor.*

Proof. First, $ZA(L)$ is obviously an R-module, for any $L \in \mathcal{D}$. Let $K \in \mathcal{D}$ and $t \in ZA(K)$, i.e., let t be a natural transformation $\mathrm{Id} \to \rho_K$ of endofunctors of the category $\mathcal{P}_A$. If $L \in \mathcal{D}$ and $u \in RB(LK)$, let $u_A = \upsilon_{LK}(u) \in A(LK)$ be the image of u under the unique morphism of Green functor $\upsilon : RB \to A$. Since $u_A \in CA(LK)$, by Corollary 20, we can compose t with the natural transformation $\rho_{u_A} : \rho_K \to \rho_L$ from Proposition 31, to get a natural transformation $\rho_{u_A} \circ t : \mathrm{Id} \to \rho_L$, i.e., an element of $ZA(L)$. Hence we get a linear map

$$u \in RB(LK) \mapsto (t \mapsto \rho_{u_A} \circ t \in \mathrm{Hom}_R(ZA(K), ZA(L))),$$

and assertion (2) of Proposition 31 shows that this endows ZA with a structure of biset functor. □

We now build a product on ZA, to make it a Green biset functor. For $K, L \in \mathcal{D}$, let $s \in ZA(K)$ and $t \in ZA(L)$. Since s is a natural transformation $\mathrm{Id} \to \rho_K$, we get, by adjunction, a natural transformation $s^o : \rho_K \to \mathrm{Id}$. By composition with $t : \mathrm{Id} \to \rho_L$, we obtain a natural transformation $t \circ s^o : \rho_K \to \rho_L$, which in turn, by adjunction again, gives a natural transformation ${}^o(t \circ s^o) : \mathrm{Id} \to (\rho_L)_K \cong \rho_{LK}$, i.e., an element of $ZA(LK)$. So we set

(3) $\quad t \times s = {}^o(t \circ s^o) \in ZA(LK) \quad$ for all $s \in ZA(K)$ and all $t \in ZA(L)$.

Translating this in the terms of Proposition 30 gives:

Lemma 35. *Let $s \in ZA(K)$ and $t \in ZA(L)$ be defined, respectively, by families of elements $s_G \in A(GKG)$ and $t_G \in A(GLG)$, for $G \in \mathcal{D}$. Then $t \times s$ is the element of $ZA(LK)$ defined by the family $(t \times s)_G = t_G \circ s_G \in A(GLKG)$, for $G \in \mathcal{D}$.*

Proof. As the adjunction $s \mapsto s^o$ amounts to switching the last two components of GKG, the element $t \times s = {}^o(t \circ s^o)$ is defined by the family

$$\begin{aligned}(t \times s)_G &= A\big(\mathrm{Iso}_{GLGK}^{GLKG}\big)\big(t_G \circ A\big(\mathrm{Iso}_{GKG}^{GGK}\big)(s_G)\big) \\ &= A\big(\mathrm{Iso}_{GLGK}^{GLKG}\big)A\big(\mathrm{Def}_{GL\underline{G}K}^{GL\underline{GG}K}\,\mathrm{Res}_{GL\underline{G}GK}^{GL\underline{GG}GK}\big)\big(t_G \times A\big(\mathrm{Iso}_{GKG}^{GGK}\big)(s_G)\big),\end{aligned}$$

where the notation $\mathrm{Def}_{GL\underline{G}K}^{GL\underline{GG}K}$ indicates that we take deflation with respect to the underlined factor, and $\mathrm{Res}_{GL\underline{G}GK}^{GL\underline{GG}GK}$ means that the underlined G in the subscript embeds diagonally in the underlined group GG in the superscript. It follows that

$$\begin{aligned}(t \times s)_G &= A\big(\mathrm{Def}_{GLKG}^{GL\underline{G}KG}\,\mathrm{Iso}_{GLGGK}^{GLGKG}\mathrm{Res}_{GL\underline{G}GK}^{GL\underline{GG}GK}\,\mathrm{Iso}_{GLGGKG}^{GLGGGK}\big)(t_G \times s_G) \\ &= A\big(\mathrm{Def}_{GLKG}^{GL\underline{G}KG}\,\mathrm{Res}_{GL\underline{G}KG}^{GL\underline{GG}KG}\big)(t_G \times s_G) \\ &= t_G \circ s_G \in A(GLKG). \qquad \square\end{aligned}$$

Notation 36. Let A be a Green $\mathcal{D}$-biset functor, and $G, H, K, L \in \mathcal{D}$. For morphisms in $\mathcal{P}_A$, namely $\alpha : G \to H$ in $A(HG)$ and $\beta : K \to L$ in $A(LK)$, we denote by $\alpha \boxtimes \beta : GK \to HL$ the morphism defined by

$$\alpha \boxtimes \beta = A\big(\mathrm{Iso}_{HGLK}^{HLGK}\big)(\alpha \times \beta) \in A(HLGK).$$

Proposition 37. *Let A be a Green $\mathcal{D}$-biset functor, and $G, H, K, L \in \mathcal{D}$. Let, moreover, $\alpha \in CA(HG)$ and $\beta \in CA(LK)$. Then for any $s \in ZA(G)$ and $t \in ZA(K)$, and for any $X \in \mathcal{D}$,*

$$(\rho_\alpha \circ s)_X \circ (\rho_\beta \circ t)_X = (\rho_{\alpha\boxtimes\beta} \circ (s \times t))_X.$$

Proof. The proof amounts to rather lengthy but straightforward calculations on bisets, similar to those we have already done several times above, e.g., in the proof of Theorem 13. We leave it as an exercise. $\square$

Theorem 38. *Let A be a Green $\mathcal{D}$-biset functor. Then ZA, endowed with the product defined in (3), is a Green $\mathcal{D}$-biset functor.*

Proof. It is clear from Lemma 35 and Proposition 30 that the product on ZA is associative. Moreover the identity transformation from the identity functor to $\rho_1 = \mathrm{Id}_{\mathcal{P}_A}$ is obviously an identity element for the product on ZA. This product is also R-bilinear by construction. Finally, the equality $ZA(U)(s) \times ZA(V)(t) = ZA(U \boxtimes V)(s \times t)$ for bisets U and V is a special case of Proposition 37. $\square$

4.2. *Relations between the commutant and the center.*

Proposition 39. *Let A be a Green $\mathcal{D}$-biset functor.*

(1) *The maps sending $\alpha \in CA(L)$ to $\rho_\alpha \in ZA(L)$, for $L \in \mathcal{D}$, define a morphism of Green biset functors $\iota_A : CA \to ZA$.*

(2) *The maps sending $t \in Cr_A(L) \cong ZA(L)$ to $t_1 \in A(L)$, for $L \in \mathcal{D}$, define a morphism of Green biset functors $\pi_A : ZA \to A$. The image of this morphism in the component* 1 *lies in $Z(A(1))$, hence there is a morphism of rings $\pi_{A,1}$: $ZA(1) \to Z(A(1))$.*

(3) *The composition*

$$CA \overset{\iota_A}{\hookrightarrow} ZA \xrightarrow{\pi_A} A$$

is equal to the inclusion $CA \hookrightarrow A$. In particular, ι_A is injective.

Proof. For assertion (1), let $\alpha \in CA(K)$, for $K \in \mathcal{D}$. Then the element ρ_α of $ZA(K)$ corresponds to the family of elements $\rho_{\alpha,G} \in A(GKG)$, for $G \in \mathcal{D}$, defined by

$$\rho_{\alpha,G} = A\big(\mathrm{Ind}_{KG}^{GKG}\,\mathrm{Inf}_K^{KG}\big)(\alpha).$$

Similarly, if $L \in \mathcal{D}$ and $\beta \in CA(L)$, the element ρ_β of $ZA(L)$ corresponds to the family $\rho_{\beta,G} = A\big(\mathrm{Ind}_{LG}^{GLG}\,\mathrm{Inf}_L^{LG}\big)(\beta)$. By Lemma 35, the product $q = \rho_\alpha \times \rho_\beta$ in $ZA(KL)$ corresponds to the family

$$\begin{aligned}
q_G &= \rho_{\alpha,G} \circ \rho_{\beta,G} \\
&= A\big(\mathrm{Ind}_{KG}^{GKG}\,\mathrm{Inf}_K^{KG}\big)(\alpha) \circ A\big(\mathrm{Ind}_{LG}^{GLG}\,\mathrm{Inf}_L^{LG}\big)(\beta) \\
&= A\big(\mathrm{Def}_{GKLG}^{GK\underline{G}LG}\,\mathrm{Res}_{GK\underline{G}LG}^{GK\underline{GG}LG}\big)\big(A\big(\mathrm{Ind}_{KG}^{GKG}\,\mathrm{Inf}_K^{KG}\big)(\alpha) \times A\big(\mathrm{Ind}_{LG}^{GLG}\,\mathrm{Inf}_L^{LG}\big)(\beta)\big) \\
&= A\big(\mathrm{Def}_{GKLG}^{GK\underline{G}LG}\,\mathrm{Res}_{GK\underline{G}LG}^{GK\underline{GG}LG}\mathrm{Ind}_{KGLG}^{GKGGLG}\,\mathrm{Inf}_{KL}^{KGLG}\big)(\alpha \times \beta).
\end{aligned}$$

Standard relations in the composition of bisets then show that

$$q_G = A\big(\mathrm{Ind}_{KLG}^{GKLG}\,\mathrm{Inf}_{KL}^{KLG}\big)(\alpha \times \beta),$$

and it follows that $q = \rho_{\alpha\times\beta}$. In other words $\iota_A(\alpha \times \beta) = \iota_A(\alpha) \times \iota_A(\beta)$. Moreover, the identity element $\varepsilon_A \in CA(1)$ is mapped by ι_A to the element of $ZA(1)$ defined by the family of elements $A\big(\mathrm{Ind}_G^{GG}\,\mathrm{Inf}_1^G\big)(\varepsilon_A)$, for $G \in \mathcal{D}$, that is, the identity element of ZA. So ι_A is a morphism of Green $\mathcal{D}$-biset functors.

The first part of assertion (2) is a consequence of Lemma 35. Indeed, if $K, L \in \mathcal{D}$, if $s \in ZA(K)$ corresponds to the family $s_G \in Cr_A(K)$, and if $t \in ZA(L)$ corresponds to the family $\beta_G \in Cr_A(L)$, for $G \in \mathcal{D}$, then the product $u = s \times t$ is the element of $ZA(KL)$ corresponding to the family $u_G = s_G \circ t_G$. In particular, for $G = 1$,

$$u_1 = s_1 \circ t_1 = s_1 \times t_1.$$

This shows that the maps sending $t \in ZA(L)$ to $t_1 \in A(L)$, for $L \in \mathcal{D}$, is a morphism of Green $\mathcal{D}$-biset functors $\pi : ZA \to A$.

Since composition $\circ : A(1) \times A(1) \to A(1)$ coincides with the product of $A(1)$ as a ring, the commutativity property defining the series of $Cr_A(1)$ shows that $\pi_{A,1}$ has image in $Z(A(1))$. This completes the proof of assertion (2).

For assertion (3), we start with an element $\alpha \in CA(L)$, for $L \in \mathcal{D}$. It is sent by ι_A to the element $t \in ZA(L)$ corresponding to the family $t_G = A\big(\mathrm{Ind}_{LG}^{GLG} \mathrm{Inf}_L^{LG}\big)(\alpha)$, for $G \in \mathcal{D}$, in $Cr_A(L)$. In particular $t_1 = A\big(\mathrm{Ind}_L^L \mathrm{Inf}_L^L\big)(\alpha) = \alpha$, so $\pi_A \circ \iota_A$ is equal to the inclusion $CA \hookrightarrow A$. □

The morphism ι_A of the previous proposition allows us to give a CA-module structure to ZA. With this structure, (the image under ι_A of) CA is a CA-submodule of ZA. In the particular case where A is commutative, Proposition 39 tells us more.

Corollary 40. *If A is a commutative Green $\mathcal{D}$-biset functor, then A is isomorphic to a direct summand of ZA in the category A-Mod.*

Proof. This follows from the fact that ι_A and π_A are morphisms of Green $\mathcal{D}$-biset functors, and thus, in particular, are morphisms of A-modules. Moreover, the composition $\pi_A \circ \iota_A$ is equal to the identity when A is commutative. □

Proposition 41. *Let A be a Green $\mathcal{D}$-biset functor. Let $\mathrm{End}_R(\mathcal{P}_A)$ be the category of R-linear endofunctors of $\mathcal{P}_A$.*

(1) *The assignment*

$$\begin{cases} K \in \mathcal{D} \mapsto \rho_K \in \mathrm{End}_R(\mathcal{P}_A), \\ t \in ZA(LK) \mapsto t^o \in \mathrm{Hom}_{\mathrm{End}_R(\mathcal{P}_A)}(\rho_K, \rho_L) \end{cases}$$

is a fully faithful R-linear functor ρ_{ZA} from $\mathcal{P}_{ZA}$ to $\mathrm{End}_R(\mathcal{P}_A)$.

(2) *The assignment μ_A,*

$$\begin{cases} K \in \mathcal{D} \mapsto K \in \mathcal{D}, \\ \alpha \in CA(LK) \mapsto {}^o\rho_\alpha \in ZA(LK), \end{cases}$$

is equal to the functor $\mathcal{P}_{\iota_A}$ from $\mathcal{P}_{CA}$ to $\mathcal{P}_{ZA}$, induced by $\iota_A : CA \to ZA$. In particular μ_A is faithful, and such that

$$\rho_{ZA} \circ \mu_A = \rho_{CA}.$$

(3) *The assignment ν_A,*

$$\begin{cases} K \in \mathcal{D} \mapsto K \in \mathcal{D}, \\ s \in ZA(LK) \mapsto s_1 \in A(LK), \end{cases}$$

is equal to the functor $\mathcal{P}_{\pi_A}$ from $\mathcal{P}_{ZA}$ to $\mathcal{P}_A$ induced by the morphism of Green biset functors $\pi_A : ZA \to A$. The composition $\nu_A \circ \mu_A$ is equal to the inclusion functor $\mathcal{P}_{CA} \to \mathcal{P}_A$.

Proof. All the assertions are straightforward consequences of Proposition 39. □

To conclude this section, we will show that the isomorphism $CA_L \cong (CA)_L$ of Proposition 22 only extends to an injection $ZA_L \hookrightarrow (ZA)_L$.

Lemma 42. *Let A be a Green $\mathcal{D}$-biset functor. For $L \in \mathcal{D}$, let $\psi_L^A : \mathcal{P}_A \to \mathcal{P}_{A_L}$ be the functor ψ_L of Theorem 13. If $K \in \mathcal{D}$, let $\psi_K^{A_L} : \mathcal{P}_{A_L} \to \mathcal{P}_{(A_L)_K}$ be the similar functor built from A_L and K. Then the diagram*

$$\begin{tikzcd} \mathcal{P}_A \arrow[r, "\psi_L^A"] \arrow[drr, "\psi_{KL}^A"'] & \mathcal{P}_{A_L} \arrow[r, "\psi_K^{A_L}"] & \mathcal{P}_{(A_L)_K} \arrow[d, "e_{K,L}"', "\cong"] \\ & & \mathcal{P}_{A_{KL}} \end{tikzcd}$$

of categories and functors, is commutative, where $e_{K,L}$ is the natural equivalence of categories $\mathcal{P}_{(A_L)_K} \to \mathcal{P}_{A_{KL}}$ provided by the canonical isomorphism of Green $\mathcal{D}$-biset functors $(A_L)_K \cong A_{KL}$.

Proof. Indeed, all the functors involved are the identity on objects. And for a morphism $\alpha : G \to H$ in $\mathcal{P}_A$, i.e., an element α of $A(HG)$, we have

$$\begin{aligned} \psi_K^{A_L}\psi_L^A(\alpha) &= \psi_K^{A_L} A\big(\mathrm{Inf}_{HG}^{HGL}\big)(\alpha) = A_L\big(\mathrm{Inf}_{HG}^{HGK}\big)A\big(\mathrm{Inf}_{HG}^{HGL}\big)(\alpha) \\ &= A\big(\mathrm{Inf}_{HGL}^{HGKL}\big)A\big(\mathrm{Inf}_{HG}^{HGL}\big)(\alpha) \\ &= A\big(\mathrm{Inf}_{HG}^{HGKL}\big)(\alpha) = \psi_{KL}^A(\alpha). \end{aligned}$$

□

Proposition 43. *Let A be a Green biset functor and $L \in \mathcal{D}$. Then there is an injective morphism of Green $\mathcal{D}$-biset functors from ZA_L to $(ZA)_L$.*

Proof. Let $K, L \in \mathcal{D}$, and $t \in ZA_L(K)$, i.e., a natural transformation,

$$t : \mathrm{Id}_{\mathcal{P}_{A_L}} \to \rho_K^{A_L},$$

from the identity functor of $\mathcal{P}_{A_L}$ to the functor $\rho_K^{A_L} = \theta_K^{A_L}\psi_K^{A_L}$, where $\theta_K^{A_L}$ is the functor $\mathcal{P}_{(A_L)_K} \to \mathcal{P}_{A_L}$ of Theorem 13 built from A_L and K. By precomposition of this natural transformation with the functor ψ_L^A, we get a natural transformation,

$$\psi_L^A \to \theta_K^{A_L}\psi_K^{A_L}\psi_L^A,$$

which by adjunction, gives a natural transformation,

$$\mathrm{Id}_{\mathcal{P}_A} \to \theta_L^A\theta_K^{A_L}\psi_K^{A_L}\psi_L^A.$$

By Lemma 42, the functor $\psi_K^{A_L}\psi_L^A$ is isomorphic to ψ_{KL}^A. By Theorem 13, the functor $\theta_K^{A_L}$ is left- and right-adjoint to the functor $\psi_K^{A_L}$, and θ_L^A is left- and right-adjoint to ψ_L^A. It follows that the functor $\theta_L^A\theta_K^{A_L}$ is isomorphic to the adjoint θ_{KL}^A of ψ_{KL}^A. Hence we have a natural transformation,

$$T : \mathrm{Id}_{\mathcal{P}_A} \to \theta_{KL}^A\psi_{KL}^A = \rho_{KL}^A,$$

that is an element of $ZA(KL) = (ZA)_L(K)$.

So we have a map $j_{L,K} : t \in ZA_L(K) \mapsto T \in (ZA)_L(K)$, which is obviously R-linear. Lengthy but straightforward calculations show that the family of these maps, for $K \in \mathcal{D}$, form a morphism of Green biset functors from ZA_L to $(ZA)_L$. $\square$

5. Application: some equivalences of categories

5.1. ***General setting.*** We begin by recalling some well-known folklore facts on the decomposition of a category $\mathcal{F}_{\mathcal{P}}$ of functors from a small R-linear category $\mathcal{P}$ to R-Mod, using an orthogonal decomposition of the identity in the center $Z\mathcal{P}$ of $\mathcal{P}$.

Since $\mathcal{P}$ is R-linear, its center $Z\mathcal{P}$ is a commutative R-algebra. Suppose we have a family $(\gamma_i)_{i\in I}$ of elements of $Z\mathcal{P}$ indexed by a set I, with the following properties:

(1) For $i, j \in I$, the product $\gamma_i\gamma_j$ is equal to 0 if $i \neq j$, and to γ_i if $i = j$.

(2) For any object G of $\mathcal{P}$, there is only a finite number of elements $i \in I$ such that $\gamma_{i,G} \neq 0$. Then, for each object $G \in \mathcal{P}$, we can consider the (finite) sum $\sum_{i\in I} \gamma_{i,G}$, which is a well-defined endomorphism of G. We assume that this endomorphism is the identity of G, for any $G \in \mathcal{P}$.

If F is an R-linear functor from $\mathcal{P}$ to R-Mod, and $i \in I$, we denote by $F\gamma_i$ the functor that in an object G of $\mathcal{P}$ is defined as the image of $F(\gamma_{i,G})$, that is,

$$(F\gamma_i)(G) = \mathrm{Im}(F(\gamma_{i,G}) : F(G) \to F(G)),$$

which is an R-submodule of $F(G)$. For a morphism $\alpha : G \to H$, we denote by $(F\gamma_i)(\alpha)$ the restriction of $F(\alpha)$ to $(F\gamma_i)(G)$. The image of $(F\gamma_i)(\alpha)$ is contained in $F\gamma_i(H)$, because the square

$$\begin{tikzcd} G \arrow[r, "\gamma_{i,G}"] \arrow[d, "\alpha"'] & G \arrow[d, "\alpha"] \\ H \arrow[r, "\gamma_{i,H}"'] & H \end{tikzcd}$$

is commutative in $\mathcal{P}$, and hence also its image by F.

It is easy to check that $F\gamma_i$ is an R-linear functor from $\mathcal{P}$ to R-Mod, which is a subfunctor of F. Moreover, the assignment $F \mapsto F\gamma_i$ is an endofunctor Γ_i of the category $\mathcal{F}_{\mathcal{P}}$. The image of this functor consists of those functors $F \in \mathcal{F}_{\mathcal{P}}$ such that the subfunctor $F\gamma_i$ is equal to F. Let $\mathcal{F}_{\mathcal{P}}\gamma_i$ be the full subcategory of $\mathcal{F}_{\mathcal{P}}$ consisting of such functors. It is an abelian subcategory of $\mathcal{F}_{\mathcal{P}}$.

For each $G \in \mathcal{P}$, the direct sum $\bigoplus_{i\in I} F\gamma_i(G)$ is actually finite, and our assumptions ensure that it is equal to $F(G)$. This shows that the functor sending $F \in \mathcal{F}_{\mathcal{P}}$ to the family of functors $F\gamma_i$ is an equivalence between $\mathcal{F}_{\mathcal{P}}$ and the product of the categories $\mathcal{F}_{\mathcal{P}}\gamma_i$.

A particular case of the previous situation is when the identity element $\varepsilon \in A(1)$ of a Green biset functor A has a decomposition in orthogonal idempotents $\varepsilon = \sum_{i=1}^{n} e_i$ in the ring $CA(1)$. Each e_i induces a natural transformation $E^i : \mathrm{Id} \to \mathrm{Id}_1$, defined at an A-module M and a group $H \in \mathcal{D}$ as

$$E^i_{M,H} : M(H) \to M_1(H), \quad m \mapsto M(\mathrm{Iso}^{H\times 1}_{1\times H})(e_i \times m).$$

For simplicity, we will think of this natural transformation as sending m simply to $e_i \times m$, and we will denote by $e_i M$ the A-submodule of M given by the image of E^i_M.

Since the morphism from $CA(1)$ to $ZA(1)$ is a ring homomorphism, we have that the natural transformations E^i satisfy $E^i \circ E^i = E^i$, $E^i \circ E^j = 0$ if $i \neq j$ and that the identity natural transformation, $\mathbf{1}$, is equal to $\sum_{i=1}^{n} E^i$. By Proposition 28, we have then the hypothesis assumed at the beginning of the section, and so we obtain the equivalence of categories mentioned above. In this case, we can give a more precise description of this equivalence.

Lemma 44. *The A-module $e_i A$ is a Green $\mathcal{D}$-biset functor, and for every A-module M, the functor $e_i M$ is an $e_i A$-module. Furthermore $A \cong \bigoplus_{i=1}^{n} e_i A$ as Green $\mathcal{D}$-biset functors.*

Proof. As we have said, $e_i A$ is an A-module, in particular it is a biset functor. We claim that it is a Green biset functor with the product

$$e_i A(G) \times e_i A(K) \to e_i A(G \times K), \quad (e_i \times a) \times (e_i \times b) = e_i \times a \times b.$$

Observe that since all the $\times$ represent the product of A, then $(e_i \times a) \times (e_i \times b)$ is isomorphic to $a \times e_i \times e_i \times b$, because $e_i \in CA(1)$. But the product $\times$ coincides with the ring product in $A(1)$, hence this element is isomorphic to $a \times e_i \times b$ and then to $e_i \times a \times b$. This implies immediately that the product is associative; the identity element in $e_i A(1)$ is of course $e_i \times \varepsilon$. Next, notice that since E^i_A is a morphism of A-modules, if $L, G \in \mathcal{D}$ and X is an (L, G)-biset, then $A(X)(e_i \times a) \cong e_i \times A(X)(a)$ for all $a \in A(G)$. With this, one can easily show the functoriality of the product.

Similar arguments show that $e_i M$ is an $e_i A$-module with the product

$$e_i A(G) \times e_i M(K) \to e_i M(G \times K), \quad (e_i \times a) \times (e_i \times m) = e_i \times a \times m.$$

For the final statement, first it is an easy exercise to verify that given Green biset functors $A_1, \ldots, A_r$, then their direct sum $\bigoplus_{i=1}^{r} A_i$ in the category of biset functors is again a Green biset functor, with the product given component-wise. With this, it is straightforward to see that the isomorphism of biset functors $A \cong \bigoplus_{i=1}^{n} e_i A$ is an isomorphism of Green biset functors. $\square$

All these observations give us the following result.

Theorem 45. *Let A be a Green $\mathcal{D}$-biset functor as above. Then the category A-*Mod *is equivalent to the product category*

$$\prod_{i=1}^{n} e_i A\text{-Mod}.$$

Moreover, for each indecomposable A-module M, there exists only one e_i such that $e_i M \neq 0$, and hence $e_i M \cong M$.

When considering the shifted functor A_H, if we have an idempotent $e \in CA_H(1)$ as before, then the evaluation of eA_H at a group G can be seen as follows. Since $eA_H(G) = e \times^d A_H(G)$, then for $a \in A_H(G)$ it is easy to see that

$$e \times^d a = A\big(\mathrm{Res}^{1\times H\times G\times H}_{G\times\Delta(H)}\big)(e \times a) = A\big(\mathrm{Inf}^{G\times H}_{H}\big)(e) \cdot a,$$

where the product $\cdot$ indicates the ring structure in $A(G \times H)$. The last equality follows from Lemma 3 and the properties of restriction and inflation. So, the evaluation of eA_H at a given group depends on how inflation of A acts on the idempotents of $CA(H)$.

5.2. *Some examples.*

5.2.1. *p-biset functors.* Let p be a prime, and RB_p denote the restriction to finite p-groups of the Burnside functor RB of Example 5. When p is invertible in the ring R, a family of orthogonal idempotents in the center of the Green biset functor RB_p of Example 5 was introduced in [Bouc 2018]. These idempotents $\widehat{b_L}$ are indexed by *atoric* p-groups L up to isomorphism, i.e., finite p-groups which cannot be decomposed as a direct product $Q \times C_p$ of a finite p-group Q and a group C_p of order p.

More precisely, for each such atoric p-group L and each finite p-group P, a specific idempotent b_L^P of $RB_p(P, P)$ was introduced (cf. [Bouc 2018, Theorem 7.4]), with the property that

$$a \circ b_L^P = b_L^Q \circ a$$

for any finite p-groups P and Q, and any $a \in RB(Q, P)$. In other words, the family $b_L = (b_L^P)_P$ is an element of the center of the biset category $R\mathcal{C}_p$ of finite p-groups. The elements $\widehat{b_L}$ of the center of the category of p-biset functors over R — i.e., the category RB_p-Mod — are deduced from the elements b_L in [Bouc 2018, Corollary 7.5].

Let $[\mathcal{A}t_p]$ denote a set of representatives of isomorphism classes of atoric p-groups. The idempotents b_L^P have the following additional properties:

(1) If L and L' are isomorphic atoric p-groups, then $b_L^P = b_{L'}^P$.

(2) If L and L' are nonisomorphic atoric p-groups, then $b_L^P b_{L'}^P = 0$.

(3) For a given finite p-group P, there are only a finite number of atoric p-groups L, up to isomorphism, such that $b_L^P \neq 0$.

(4) The sum $\sum_{L\in[\mathcal{A}t_p]} b_L^P$, which is a finite sum by the previous property, is equal to the identity element of $RB(P, P)$.

It follows that one can consider the sum $\sum_{L\in[\mathcal{A}t_p]} \widehat{b}_L$ in $Z(RB_p)(1)$, and that this sum is equal to the identity element of $Z(RB_p)(1)$. So we obtain a *locally finite* decomposition of the identity element of $Z(RB_p)(1)$ as a sum of orthogonal idempotents, which allows for a splitting of the category of p-biset functors over R as a direct product of abelian subcategories (cf. [Bouc 2018, Corollary 7.5]). As a consequence, for each indecomposable p-biset functor F over R, there is an atoric p-group L, unique up to isomorphism, such that $\widehat{b}_L$ acts as the identity of F (or equivalently, does not act by zero on F). This group L is called the *vertex* of F (cf. [Bouc 2018, Definition 9.2]).

Remark 46. This example shows in particular that ZA can be much bigger than CA: indeed, for $A = RB_p$, when R is a field of characteristic different from p, we see that $ZA(1)$ is an infinite-dimensional R-vector space, whereas $CA(1) \cong R$ is one-dimensional.

5.2.2. *Shifted representation functors.* Now we apply the results of Section 5.1 to some shifted classical representation functors, with coefficients in a field $\mathbb{F}$ of characteristic 0. In each case we will begin with a commutative Green biset functor C such that for each group H, the $\mathbb{F}$-algebra $C(H)$ is split semisimple. In particular, taking $A = C_H$, in $A(1) = C(H)$ we will have a family of orthogonal idempotents $\{e_i^H\}_{i=1}^{n_H}$ such that $\varepsilon = \sum_{i=1}^{n_H} e_i^H$. As we said in Section 5.1, the evaluation $e_i^H A(G)$ is given as

$$e_i^H \times^d a = A\big(\mathrm{Inf}_1^G\big)(e_i^H)\cdot a = C\big(\mathrm{Inf}_H^{G\times H}\big)(e_i^H)\cdot a$$

for $a \in A(G)$. Now, since inflation is a ring homomorphism, $A(\mathrm{Inf}_1^G)(e_i^H)$ is equal to $\sum_{j\in J} e_j^{G\times H}$ for some $J \subseteq \{1, \dots, n_{G\times H}\}$ depending on e_i^H and G. On the other hand, we also have

$$a = \sum_{i=1}^{n_{G\times H}} \alpha_i(a) e_i^{G\times H}$$

for some $\alpha_i(a) \in \mathbb{F}$. This implies that the idempotents appearing in the evaluation $e_i^H A(G)$ depend only on the set $\{e_j^{G\times H}\}_{j\in J}$.

Shifted Burnside functors. We consider the Burnside functor $\mathbb{F}B$ over $\mathbb{F}$. We fix a finite group H, and consider the shifted functor $A = \mathbb{F}B_H$. Then the algebra $A(1)$ is isomorphic to $\mathbb{F}B(H)$; hence it is split semisimple. Its primitive idempotents e_K^H are indexed by subgroups K of H, up to conjugation, and explicitly given (see [Gluck 1981; Yoshida 1983]) by

$$e_K^H = \frac{1}{|N_H(K)|}\sum_{L\le K}|K|\mu(L,K)\,[H/L],$$

where μ is the Möbius function of the poset of subgroups of H and $[H/L]\in B(H)$ is the class of the transitive H-set H/L.

By Theorem 45, we get a decomposition of the category A-Mod as a product $\prod_{K\in[s_H]} e_K^H A$-Mod, where $[s_H]$ is a set of representatives of conjugacy classes of subgroups of H. From the action of inflation on the primitive idempotents of Burnside rings (see [Bouc 2010, Theorem 5.2.4]), it is easy to see that for $K\le H$, the value $e_K^H A(G)$ of the Green functor $e_K^H A$ at a finite group G is equal to the set of linear combinations of idempotents $e_L^{G\times H}$ of $\mathbb{F}B(G\times H)$ indexed by subgroups L of $(G\times H)$ for which the second projection $p_2(L)$ is conjugate to K in H. Also, for each indecomposable A-module M, there exists a unique $K\le H$, up to conjugation, such that $e_K^H M\ne 0$, and then $e_K^H M = M$.

Shifted functors of linear representations. Next, we consider the functor $\mathbb{F}R_{\mathbb{K}}$ of linear representations over $\mathbb{K}$, a field of characteristic 0. As before, we fix a finite group H and consider the shifted functor $A=(\mathbb{F}R_{\mathbb{K}})_H$. This is a commutative Green biset functor, and $A(1)$ is isomorphic to the split semisimple $\mathbb{F}$-algebra $\mathbb{F}R_{\mathbb{K}}(H)$. If $|H|=n$, it is shown in [García 2018, Section 3.3.1] (and slightly differently in [García 2019]) that $\mathbb{F}R_{\mathbb{K}}(H)$ has a complete family of orthogonal primitive idempotents e_D^H indexed by the E-conjugacy classes of H, where E is certain subgroup of $(\mathbb{Z}/n\mathbb{Z})^\times$. By E-conjugacy we mean that two elements $x, y\in H$ are E-conjugated if there exist $[i]\in E$ such that $x =_H y^i$. This defines an equivalence relation on H and the set of E-conjugacy classes is denoted by $\mathrm{Cl}_E(H)$. The group E is built in the following way: First we fix an algebraically closed field $\mathbb{L}$, which is an extension of $\mathbb{F}$ and $\mathbb{K}$, and then we take the intersection $\mathbb{E}=\mathbb{F}\cap\mathbb{K}$ in $\mathbb{L}$. By adding an n-th primitive root of unity, ω, to $\mathbb{E}$, we obtain E as the group isomorphic to $\mathrm{Gal}(\mathbb{E}[\omega]/\mathbb{E})$ in $(\mathbb{Z}/n\mathbb{Z})^\times$. Observe that, as a group, E depends only on $\mathbb{F}$, $\mathbb{K}$ and n, and not on the choice of $\mathbb{L}$. Then, by Theorem 45, we get a decomposition of the category A-Mod as a product

$$\prod_{D\in\mathrm{Cl}_E(H)} e_D^H A\text{-Mod}.$$

Also, for each indecomposable A-module M, there exists a unique E-conjugacy class D of H such that $e_D^H M\ne 0$ and so $e_D^H M = M$. On the other hand, in Corollary 3.3.14 of [García 2018] it is shown that $e_D^H A$ is a simple A-module and hence that A is a semisimple A-module, since $A=\sum_D e_D^H A$.

Finally, using Lemma 3.3.10 in [García 2018], we see that the idempotents $e_C^{G\times H}$, for C an E-class of $G\times H$, appearing in the evaluation $A(\mathrm{Inf}_1^G)(e_D^H)$ are those for which $\pi_H(C)$, the projection of C on H, is equal to D.

Shifted p-permutation functors. Let k be an algebraically closed field of positive characteristic p. In this case we assume also that $\mathbb{F}$ contains all the p'-roots of unity, and consider the functor $\mathbb{F}pp_k$. Then $\mathbb{F}pp_k$ is a commutative Green biset functor, and the category $\mathbb{F}pp_k$-Mod has been considered in particular in [Ducellier 2015] (when $\mathbb{F}$ is algebraically closed).

We fix a finite group H, and consider the shifted functor $A = (\mathbb{F}pp_k)_H$. Then the algebra $A(1)$ is isomorphic to the algebra $\mathbb{F}pp_k(H)$. This algebra is split semisimple, and its primitive idempotents $F^H_{Q,s}$ have been determined in [Bouc and Thévenaz 2010]: they are indexed by (conjugacy classes of) pairs (Q, s) consisting of a p-subgroup Q of H, and a p'-element s of $N_H(Q)/Q$. We denote by $\mathcal{Q}_{H,p}$ the set of such pairs, and by $[\mathcal{Q}_{H,p}]$ a set of representatives of orbits of H for its action on $\mathcal{Q}_{H,p}$ by conjugation.

If $(Q, s) \in \mathcal{Q}_{H,p}$ and $u \in \mathbb{F}pp_k(H)$, then $F^H_{Q,s}u = \tau^H_{Q,s}(u)F^H_{Q,s}$, where $\tau^H_{Q,s}(u) \in \mathbb{F}$. The maps $u \mapsto \tau^H_{Q,s}(u)$, for $(Q, s) \in [\mathcal{Q}_{H,p}]$ are the distinct algebra homomorphisms (the species) from $\mathbb{F}pp_k(H)$ to $\mathbb{F}$ (see, e.g., [Bouc and Thévenaz 2010, Proposition 2.18]). Moreover, the map $\tau^H_{Q,s}$ is determined by the fact that for any p-permutation kH-module M, the scalar $\tau^H_{Q,s}(M)$ is equal to the value at s of the Brauer character of the Brauer quotient $M[Q]$ of M at Q.

It follows that if $N \trianglelefteq H$, and $v \in \mathbb{F}pp_k(H/N)$, then $\tau^H_{Q,s}(\mathrm{Inf}^H_{H/N}\, v) = \tau^{H/N}_{\overline{Q},\overline{s}}(v)$, where $\overline{Q} = QN/N$, and $\overline{s} \in N_{H/N}(\overline{Q})/\overline{Q}$ is the projection of s to H/N. As a consequence, if $(R, t) \in \mathcal{Q}_{H/N,p}$, then $\mathrm{Inf}^H_{H/N}(F^{H/N}_{R,t})$ is equal to the sum of the idempotents $F^H_{Q,s}$ for those elements $(Q, s) \in [\mathcal{Q}_{H,p}]$ for which $(\overline{Q}, \overline{s})$ is conjugate to (R, t) in H/N.

Now by Theorem 45, we get a decomposition of the category A-Mod as a product $\prod_{(Q,s)\in[\mathcal{Q}_{H,p}]} F^H_{Q,s}A$-Mod. Let G be a finite group. It follows from the previous discussion on inflation that the evaluation $F^H_{Q,s}A(G)$ of A at G is equal to the set of linear combinations of primitive idempotents $F^{G\times H}_{L,t}$, for $(L, t) \in \mathcal{Q}_{G\times H,p}$, such that the pair $(p_2(L), p_2(t))$ is conjugate to (Q, s) in H, where $p_2 : G \times H \to H$ is the second projection. Also, for each indecomposable A-module M, there exists a unique $(Q, s) \in [\mathcal{Q}_{H,p}]$ such that $F^H_{Q,s}M \neq 0$, and then $F^H_{Q,s}M = M$.

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ON THE BOUNDEDNESS OF MULTILINEAR FRACTIONAL STRONG MAXIMAL OPERATORS WITH MULTIPLE WEIGHTS

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We investigate the boundedness of multilinear fractional strong maximal operator $\mathcal{M}_{\mathcal{R},\alpha}$ associated with rectangles or related to more general basis with multiple weights $A_{(\vec{p},q),\mathcal{R}}$. In the rectangular setting, we first give an end-point estimate of $\mathcal{M}_{\mathcal{R},\alpha}$, which not only extends the famous linear result of Jessen, Marcinkiewicz and Zygmund, but also extends the multilinear result of Grafakos, Liu, Pérez and Torres ($\alpha = 0$) to the case $0 < \alpha < mn$. Then, in the one weight case, we give several equivalent characterizations between $\mathcal{M}_{\mathcal{R},\alpha}$ and $A_{(\vec{p},q),\mathcal{R}}$. Based on the Carleson embedding theorem regarding dyadic rectangles, we obtain a multilinear Fefferman–Stein type inequality, which is new even in the linear case. We present a sufficient condition for the two weighted norm inequality of $\mathcal{M}_{\mathcal{R},\alpha}$ and establish a version of the vector-valued two weighted inequality for the strong maximal operator when $m = 1$. In the general basis setting, we study the properties of the multiple weight $A_{(\vec{p},q),\mathcal{R}}$ conditions, including the equivalent characterizations and monotonic properties, which essentially extends previous understanding. Finally, a survey on multiple strong Muckenhoupt weights is given, which demonstrates the properties of multiple weights related to rectangles systematically.

1. Introduction

The study of multiparameter operators originated in the works of Fefferman and Stein [1982] on two-parameter singular integral operators. Journé [1985] gave a multiparameter version of the $T1$ theorem on product spaces. A new type of the $T1$ theorem on product spaces was formulated by Pott and Villarroya [2011].

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Martikainen [2012] demonstrated a two-parameter representation of singular integrals in expression of the dyadic shifts, which was extended in the famous result of Hytönen [2017] for the one-parameter case. More recently, using the probabilistic methods and the techniques of dyadic analysis, Hytönen and Martikainen [2014] gave a two-parameter version of the $T1$ theorem in spaces of nonhomogeneous type. A two-parameter version of the Tb theorem on product Lebesgue spaces was obtained by Ou [2015], where b is a tensor product of two pseudoaccretive functions.

It is also well known that the most prototypical representative of the multiparameter operators is the following strong maximal operator $M_{\mathcal{R}}$:

$$M_{\mathcal{R}} f(x) := \sup_{\substack{R \ni x \\ R \in \mathcal{R}}} \frac{1}{|R|} \int_R |f(y)|\, dy, \quad x \in \mathbb{R}^n,$$

where $\mathcal{R}$ is the collection of all rectangles $R \subset \mathbb{R}^n$ with sides parallel to the coordinate axes. It can be seen as a geometric maximal operator which commutes with a full n-parameter group of dilations $(x_1, \dots, x_n) \to (\delta_1 x_1, \dots, \delta_n x_n)$. The strong $L^p(\mathbb{R}^n)(1 < p < \infty)$ boundedness of $M_{\mathcal{R}}$ was given by García-Cuerva and Rubio de Francia [1985, p.456]. A maximal theorem was given by Jessen, Marcinkiewicz and Zygmund in [Jessen et al. 1935]. They pointed out that unlike the classical Hardy–Littlewood maximal operator, the strong maximal function is not of weak type (1, 1). Moreover, they studied the end-point behavior of $M_{\mathcal{R}}$ and obtained the inequality

$$|\{x \in \mathbb{R}^n : M_{\mathcal{R}} f(x) > \lambda\}| \lesssim_n \int_{\mathbb{R}^n} \frac{|f(x)|}{\lambda} \left(1 + \left(\log^+ \frac{|f(x)|}{\lambda}\right)^{n-1}\right) dx. \tag{1-1}$$

Córdoba and Fefferman [1975] gave a geometric proof of (1-1) and established a covering lemma for rectangles. Their covering lemma is quite useful because it overcomes the failure of the Besicovitch covering argument for rectangles with arbitrary eccentricities. The selection algorithm given by Córdoba and Fefferman was used many times to gain end-point estimates for $M_{\mathcal{R}}$, as demonstrated in [Córdoba 1976; Fefferman 1981; Grafakos et al. 2011; Hagelstein and Parissis 2018; Liu and Luque 2014; Long and Shen 1988; Luque and Parissis 2014; Mitsis 2006].

The corresponding weighted version of (1-1) with $w \in A_{1,\mathcal{R}}$ was shown by Bagby and Kurtz [1984]. In addition, the weighted weak type and strong type norm inequalities for vector-valued strong maximal operators were obtained in [Capri and Gutiérrez 1988]. It is worth pointing out that this was the first time that the Córdoba–Fefferman covering lemma was not used in obtaining the end-point estimate of $M_{\mathcal{R}}$. Subsequently, the above weighted results were improved by enlarging the range of weights class in [Luque and Parissis 2014; Mitsis 2006]. Luque and Parissis [2014] formulated a weighted version of the Córdoba–Fefferman covering lemma and showed the weighted version of (1-1) for any $n \geq 2$ and $w \in A_{\infty,\mathcal{R}}$. For $n = 2$, the weighted endpoint estimate was first proved in [Mitsis 2006] for $w \in A_{p,\mathcal{R}}$ and $1 < p < \infty$. Unfortunately, the combinatorics of two-dimensional rectangles used there are not available in higher dimensions. To overcome this obstacle, Luque and Parissis [2014] adopted a different approach, relying heavily on the best constant of the weighted estimates of the strong maximal operator [Long and Shen 1988].

Grafakos et al. [2011] first introduced the multilinear version of the strong maximal operator $\mathcal{M}_{\mathcal{R}}$. Later, it was improved by Cao, Xue and Yabuta [Cao et al. 2017] to the multilinear fractional strong maximal operator $\mathcal{M}_{\mathcal{R},\alpha}$

$$\mathcal{M}_{\mathcal{R},\alpha}(\vec{f})(x) := \sup_{\substack{R\ni x\\ R\in\mathcal{R}}} \prod_{i=1}^{m} \frac{1}{|R|^{1-\alpha/(mn)}} \int_R |f_i(y)|\,dy, \tag{1-2}$$

where $0 \le \alpha < mn$. Similarly, one can define the multilinear maximal function $\mathcal{M}_{\mathscr{B}}$ on a general basis $\mathscr{B}$ if $\mathcal{R}$ is replaced by $\mathscr{B}$ in (1-2). In [Grafakos et al. 2011], it is also proved that for a Muckenhoupt basis $\mathscr{B}$, the multilinear maximal operator $\mathcal{M}_{\mathscr{B}}$ is bounded from $L^{p_1}(w_1) \times \cdots \times L^{p_m}(w_m)$ to $L^{p,\infty}(v)$ provided that $(\vec{w}, v)$ are weights satisfying $v \in A_{\infty,\mathscr{B}}$ and the power bump condition for some $r > 1$,

$$\sup_{B\in\mathscr{B}} \left(\frac{1}{|B|}\int_B v\,dx\right) \prod_{i=1}^{m} \left(\frac{1}{|B|}\int_B w_i^{(1-p_i')r}\,dx\right)^{p/p_i'r} < \infty. \tag{1-3}$$

It is also worth mentioning that the authors of [Grafakos et al. 2011] established the sharp multilinear version of the endpoint inequality for $\mathcal{M}_{\mathcal{R}}$. Subsequently, under a weaker condition (Tauberian condition) than $v \in A_{\infty,\mathscr{B}}$, Liu and Luque [2014] investigated the strong boundedness of the two-weighted inequality for the maximal operator $\mathcal{M}_{\mathscr{B}}$. They showed that if the maximal operator $M_{\mathscr{B}}$ satisfies the Tauberian condition (called condition (A) in [Hagelstein et al. 2015; Jawerth 1986; Pérez 1993]) then $\mathcal{M}_{\mathscr{B}}$ enjoys the strong-type boundedness. Recently, Hagelstein et al. [2015] discussed the relationship between the boundedness of $M_{\mathscr{B}}$, the Tauberian condition $(A_{\mathscr{B},\gamma,\mu})$ and the weighted Tauberian condition. Furthermore, Hagelstein and Parissis [2018] proved that the asymptotic estimate for weighted Tauberian constant associated to rectangles is equivalent to $w \in A_{\infty,\mathcal{R}}$, which gives a new characterization of the class $A_{\infty,\mathcal{R}}$.

Inspired by [Grafakos et al. 2011], the authors [Cao et al. 2017] studied the relationship between the multilinear fractional strong maximal operator $\mathcal{M}_{\mathcal{R},\alpha}$ and multiple weights $A_{(\vec{p},q),\mathcal{R}}$ associated with rectangles defined by

$$[\vec{w}, v]_{A_{(\vec{p},q),\mathcal{R}}} := \sup_{R\in\mathcal{R}} |R|^{\frac{\alpha}{n}+\frac{1}{q}-\frac{1}{p}} \left(\frac{1}{|R|}\int_R v\,dx\right)^{\frac{1}{q}} \prod_{i=1}^{m} \left(\frac{1}{|R|}\int_R w_i^{1-p_i'}\,dx\right)^{\frac{1}{p_i'}} < \infty.$$

The dyadic reverse doubling condition associated with rectangles, which is weaker than $A_{\infty,\mathcal{R}}$, was also introduced. It was shown that if each $w_i^{1-p_i'}$ satisfies the dyadic reverse doubling condition, then the two-weight boundedness of $\mathcal{M}_{\mathcal{R},\alpha}$ is equivalent to $(\vec{w}, v) \in A_{(\vec{p},q),\mathcal{R}}$. Significantly, a Carleson embedding theorem regarding dyadic rectangles was established and was the core of the proof.

Motivated by [Cao et al. 2017; Grafakos et al. 2011; Liu and Luque 2014], here we continue to investigate the boundedness of multilinear strong and fractional strong maximal operators in the setting of rectangles and in the setting of a more general basis. We are mainly concerned with the end-point behavior, characterizations of two weighted norm inequalities and vector-valued norm inequalities. We will also give a survey on multiple strong Muckenhoupt weights, which demonstrates the properties of multiple weights associated with rectangles systematically.

2. Definitions and main results

Rectangular setting. We now formulate the main results of the maximal operators related to rectangles. The first result is concerned with the end-point behavior of $\mathcal{M}_{\mathcal{R},\alpha}$.

Theorem 2.1. *Let $n \geq 1$, $m \geq 1$ and $0 \leq \alpha < mn$. Then for any $\lambda > 0$, the following endpoint estimate holds*:

$$\left|\left\{x \in \mathbb{R}^n ; \mathcal{M}_{\mathcal{R},\alpha}(\vec{f})(x) > \lambda^m\right\}\right|^{m-\alpha/n}$$
$$\lesssim_{m,n,\alpha} \prod_{i=1}^m \left[1+\left(\frac{\alpha}{mn}\log^+ \prod_{j=1}^m \int_{\mathbb{R}^n} \Phi_n^{(m)}\left(\frac{|f_j(y)|}{\lambda}\right) dy\right)^{n-1}\right]^m \int_{\mathbb{R}^n} \Phi_n^{(m)}\left(\frac{|f_i(y)|}{\lambda}\right) dy,$$

where $\Phi_n(t) := t[1+(\log^+ t)^{n-1}]$ and $\Phi_n^{(m)} = \overbrace{\Phi_n \circ \cdots \circ \Phi_n}^{m}$. Moreover, the exponent is sharp in the sense that we cannot replace $\Phi_n^{(m)}$ by $\Phi_n^{(k)}$ for $k \leq m-1$.

Remark 2.2. If $m = 1$ and $\alpha = 0$, then the above inequality in Theorem 2.1 coincides with the inequality (1-1). In the multilinear setting, if $\alpha = 0$, Theorem 2.1 recovers the corresponding inequality in [Grafakos et al. 2011]. Therefore, Theorem 2.1 extends not only the linear result given by Jessen, Marcinkiewicz and Zygmund [Jessen et al. 1935] but also extends the multilinear result proved by Grafakos et al. [2011]. Even in the linear setting, Theorem 2.1 is completely new for $0 < \alpha < n$.

In order to state the other results, we need to introduce one more definition:

Definition 2.3 [Liu and Luque 2014]. Let $1 < p < \infty$. A Young function Φ is said to satisfy the B_p^* condition, written $\Phi \in B_p^*$, if there is a positive constant c such that

$$\int_c^\infty \frac{\Phi_n(\Phi(t))}{t^p} \frac{dt}{t} < \infty,$$

where $\Phi_n(t) := t[1+(\log^+ t)^{n-1}]$ for all $t > 0$.

We obtain the two weighted, vector-valued estimate of $M_{\mathcal{R}}$ as follows:

Theorem 2.4. *Let $1 < q < p < \infty$, $r = p/q$. Assume that A and B are Young functions such that their complementary Young functions $\bar{A}$ and $\bar{B}$ satisfy $\bar{A} \in B^*_{r'}$ and $\bar{B} \in B^*_q$, respectively. Let (w, v) be a couple of weights such that*

$$\sup_{R\in\mathcal{R}} \|w^q\|^{1/q}_{A,R} \|v^{-1}\|_{B,R} < \infty. \tag{2-1}$$

For some fixed $\gamma \in (0, 1)$ and for any nonnegative function $h \in L^{r'}(\mathbb{R}^n)$ with $\|h\|_{L^{r'}(\mathbb{R}^n)} = 1$, assume that $M_{\mathcal{R}}$ satisfies the $(A_{\mathcal{R},\gamma,h})$ condition and the $(A_{\mathcal{R},\gamma,w^q h})$ condition. Then, the two weight vector-valued inequality holds for $M_{\mathcal{R}}$,

$$\|M_{\mathcal{R}} f\|_{L^p(\ell^q,w^p)} \lesssim \|f\|_{L^p(\ell^q,v^p)}.$$

Remark 2.5. Theorem 2.4 was shown by Pérez [2000], whenever the family of rectangles $\mathcal{R}$ is replaced by cubes. Moreover, in the scalar-valued case, Theorem 2.4 was proved by Liu and Luque [2014].

In order to establish the boundedness of the multilinear fractional strong maximal operator $\mathcal{M}_{\mathcal{R},\alpha}$, we give the definition of the corresponding multiple weights.

Definition 2.6 (class of $A_{(\vec{p},q),\mathcal{R}}$, [Cao et al. 2017]). Let $1 < p_1, \dots, p_m < \infty$, $\frac{1}{p} = \frac{1}{p_1} + \cdots + \frac{1}{p_m}$, and $q > 0$. Suppose that $\vec{w} = (w_1, \dots, w_m)$ and each w_i is a nonnegative locally integrable function on $\mathbb{R}^n$. We say that $\vec{w}$ satisfies the $A_{(\vec{p},q),\mathcal{R}}$ condition or $\vec{w} \in A_{(\vec{p},q),\mathcal{R}}$ if it satisfies

$$[\vec{w}]_{A_{(\vec{p},q),\mathcal{R}}} := \sup_R \left(\frac{1}{|R|}\int_R \nu_{\vec{w}}^q \, dx\right)^{1/q} \prod_{i=1}^m \left(\frac{1}{|R|}\int_R w_i^{-p_i'} \, dx\right)^{1/p_i'} < \infty,$$

where $\nu_{\vec{w}} = \prod_{i=1}^m w_i$. If $p_i = 1$, $\left(\frac{1}{R}\int_R w_i^{1-p_i'}\right)^{1/p_i'}$ is understood as $(\inf_R w_i)^{-1}$.

We formulate the weighted results of $\mathcal{M}_{\mathcal{R},\alpha}$ in the following characterizations:

Theorem 2.7. *Let $k \in \mathbb{N}$, $0 \le \alpha < mn$, $\frac{1}{p} = \frac{1}{p_1} + \cdots + \frac{1}{p_m}$ with $1 < p_1, \dots, p_m < \infty$, and $0 < p \le q < \infty$ satisfying $\frac{1}{q} = \frac{1}{p} - \frac{\alpha}{n}$. Then the following are equivalent:*

$$\vec{w} \in A_{(\vec{p},q),\mathcal{R}}; \tag{2-2}$$

$$\vec{w}^r \in A_{(\vec{p}/r,\,q/r),\mathcal{R}} \quad \textit{for some } r > 1; \tag{2-3}$$

$$\mathcal{M}_{\mathcal{R},\alpha} : L^{p_1}(w_1^{p_1}) \times \cdots \times L^{p_m}(w_m^{p_m}) \to L^q(\nu_{\vec{w}}^q); \tag{2-4}$$

$$\mathcal{M}_{\mathcal{R},\alpha,\Phi_{k+1}} : L^{p_1}(w_1^{p_1}) \times \cdots \times L^{p_m}(w_m^{p_m}) \to L^q(\nu_{\vec{w}}^q). \tag{2-5}$$

Remark 2.8. Although the fact that (2-2) is equivalent to (2-4) was given in [Cao et al. 2017], we here present some new ingredients. In addition, Theorem 2.7 tells us that the weight class $A_{(\vec{p},q),\mathcal{R}}$ not only implies the boundedness of $\mathcal{M}_{\mathcal{R},\alpha}$, but that it also characterizes much bigger operators $\mathcal{M}_{\mathcal{R},\alpha,\Phi_{k+1}}$.

Furthermore, we obtain the following result:

Theorem 2.9. *Let* $0 \le \alpha < mn$, $\frac{1}{p} = \frac{1}{p_1} + \cdots + \frac{1}{p_m}$ *with* $1 < p_1, \ldots, p_m < \infty$, *and* $0 < p \le q < \infty$. *If* $(\vec{w}, v)$ *are weights such that* $v \in A_{\infty,\mathcal{R}}$ *and the power bump condition holds for some* $r > 1$,

$$\sup_{R \in \mathcal{R}} |R|^{\frac{\alpha}{n}+\frac{1}{q}-\frac{1}{p}} \biggl(\frac{1}{|R|} \int_R v \, dx \biggr)^{\frac{1}{q}} \prod_{i=1}^m \biggl(\frac{1}{|R|} \int_R w_i^{(1-p_i')r} dx \biggr)^{\frac{1}{rp_i'}} < \infty, \tag{2-6}$$

then $\mathcal{M}_{\mathcal{R},\alpha} : L^{p_1}(w_1) \times \cdots \times L^{p_m}(w_m) \to L^q(v)$.

Corollary 2.10. *Suppose that* $0 \le \alpha < mn$ *and that* $\frac{1}{p} = \frac{1}{p_1} + \cdots + \frac{1}{p_m}$ *with* $1 < p_1, \ldots, p_m < mn/\alpha$. *Let each* u_i *be a nonnegative locally integrable function. Then* $\vec{u} \in A_{\vec{p},\mathcal{R}}$ *implies that*

$$\|\mathcal{M}_{\mathcal{R},\alpha}(\vec{f})\|_{L^p(v^p)} \le C \prod_{i=1}^m \|f_i\|_{L^{p_i}(w_i^{p_i})},$$

where $v = \prod_{i=1}^m u_i^{1/p_i}$ *and* $w_i = M_{\alpha p_i/m}(u_i)$.

Finally, we end this subsection with a multilinear Fefferman–Stein type inequality.

Theorem 2.11. *Let* $0 \le \alpha < mn$, $\frac{1}{p} = \frac{1}{p_1} + \cdots + \frac{1}{p_m}$ *with* $1 < p_1, \ldots, p_m < \infty$, *and* $0 < p \le q < \infty$ *satisfying* $\frac{1}{q} = \frac{1}{p} - \frac{\alpha}{n}$. *Then, for any weights* $\vec{\omega}$ *on* $\mathbb{R}^n$ *and* $\nu = \prod_{i=1}^m \omega_i^{1/m}$, *we have that*

$$\|\mathcal{M}_{\mathcal{R},\alpha}(\vec{f})\|_{L^q(\nu)} \le C \prod_{i=1}^m \|f_i\|_{L^{p_i}((M_{\mathcal{R}} w_i)^{p_i/mq})},$$

where the constant C *is independent of the weights* $\vec{\omega}$ *and* $\vec{f}$.

The general basis and two weight norm inequalities. In this subsection, we will present some general results for the maximal operator defined on the general basis. We start by introducing some definitions and notations, which will be used later.

By a basis $\mathscr{B}$ in $\mathbb{R}^n$ we mean a collection of open sets in $\mathbb{R}^n$. We say that w is a weight associated with the basis $\mathscr{B}$ if w is a nonnegative measurable function in $\mathbb{R}^n$ such that $w(B) = \int_B w(x)\,dx < \infty$ for each $B \in \mathscr{B}$. Moreover, $w \in A_{p,\mathscr{B}}$ means that

$$\sup_{B \in \mathscr{B}} \biggl(\frac{1}{|B|} \int_B w \, dx \biggr) \biggl(\frac{1}{|B|} \int_B w^{1-p'} dx \biggr)^{p/p'} < \infty.$$

We say that $\mathscr{B}$ is a Muckenhoupt basis if $M_{\mathscr{B}} : L^p(w) \to L^p(w)$ for any $1 < p < \infty$ and for any $w \in A_{p,\mathscr{B}}$.

We also need some basic property of Orlicz spaces. More details can be found in [Rao and Ren 1991]. A Young function is a continuous, convex, increasing function

$\Phi : [0, \infty) \to [0, \infty)$ with $\Phi(0) = 0$ and such that $\Phi(t)/t \to \infty$ as $t \to \infty$. The Φ-norm of a function f over a set E with finite measure is defined by

$$\|f\|_{\Phi,E} = \inf\left\{\lambda > 0;\, \frac{1}{|E|}\int_E \Phi\left(\frac{|f(x)|}{\lambda}\right) dx \le 1\right\}. \tag{2-7}$$

For a given Young function Φ, one can define a complementary function

$$\overline{\Phi}(s) = \sup_{t>0}\{st - \Phi(t)\}, \quad s \ge 0.$$

Moreover, the generalized Hölder inequality holds:

$$\frac{1}{|E|}\int_E |f(x)g(x)|\, dx \le 2\|f\|_{\Phi,E}\|g\|_{\overline{\Phi},E}. \tag{2-8}$$

Definition 2.12. Suppose that the function $\varphi : (0, \infty) \to (0, \infty)$ is essentially nondecreasing and $\lim_{t\to\infty} \frac{\varphi(t)}{t} = 0$. Assume that $\mathscr{B}$ is a basis and that $\{\Psi_i\}_{i=1}^m$ is a sequence of Young functions. We define the multilinear Orlicz maximal operator associated with the function φ by

$$\mathcal{M}_{\mathscr{B},\varphi,\vec{\Psi}}(\vec{f})(x) = \sup_{\substack{B\ni x\\ B\in\mathscr{B}}} \varphi(|B|)\prod_{i=1}^m \|f_i\|_{\Psi_i,B}, \quad x \in \mathbb{R}^n.$$

In particular, if $\Psi_i(t)=t,\ i=1, \dots, m$, we denote $\mathcal{M}_{\mathscr{B},\varphi,\vec{\Psi}}$ by $\mathcal{M}_{\mathscr{B},\varphi}$. If $\varphi(t)=t^{\alpha/n}$, we denote $\mathcal{M}_{\mathscr{B},\varphi,\vec{\Psi}}$ and $\mathcal{M}_{\mathscr{B},\varphi}$ by $\mathcal{M}_{\mathscr{B},\alpha,\vec{\Psi}}$ and $\mathcal{M}_{\mathscr{B},\alpha}$ respectively. When $\mathscr{B} = \mathcal{R}$, $\mathcal{M}_{\mathscr{B},\alpha}$ coincides with $\mathcal{M}_{\mathcal{R},\alpha}$.

Definition 2.13. We say that the maximal operator $M_{\mathscr{B}}$ satisfies the $(A_{\mathscr{B},\gamma,\mu})$ condition with respect to some $\gamma \in (0, 1)$ and a weight μ, if there exists a positive constant $C_{\mathscr{B},\gamma,\mu}$ such that, for all measurable sets E, it holds that

$$\mu\big(\{x \in \mathbb{R}^n : M_{\mathscr{B}}(\mathbf{1}_E)(x) > \gamma\}\big) \le C_{\mathscr{B},\gamma,\mu}\mu(E).$$

We summarize the main results as follows:

Theorem 2.14. *Let* $0 < p \le q < \infty$, $\frac{1}{p} = \frac{1}{p_1} + \cdots + \frac{1}{p_m}$ *with* $1 < p_1, \dots, p_m < \infty$. *Let* $\mathcal{A}_i$, $\mathcal{B}_i$ *and* $\mathcal{C}_i$ $(i = 1, \dots, m)$ *be Young functions such that* $\mathcal{A}_i^{-1}(t)\mathcal{C}_i^{-1}(t) \le \mathcal{B}_i^{-1}(t)$, $t > 0$ *for each* $i = 1, \dots, m$. *Assume that* $\mathscr{B}$ *is a basis and* $\{\mathcal{C}_i\}_{i=1}^m$ *is a sequence of Young functions satisfying*

$$\mathcal{M}_{\mathscr{B},\vec{\mathcal{C}}} : L^{p_1}(\mathbb{R}^n) \times \cdots \times L^{p_m}(\mathbb{R}^n) \to L^p(\mathbb{R}^n).$$

If $(\vec{w}, v)$ *are weights such that* $\mathcal{M}_{\mathscr{B},\varphi,\vec{\mathcal{B}}}$ *satisfies the* $(A_{\mathscr{B},\gamma,v^q})$ *condition and*

$$\sup_{B\in\mathscr{B}} \varphi(|B|)|B|^{\frac{1}{q}-\frac{1}{p}}\left(\frac{1}{|B|}\int_B v^q\, dx\right)^{\frac{1}{q}} \prod_{i=1}^m \|w_i^{-1}\|_{\mathcal{A}_i,B} < \infty, \tag{2-9}$$

then $\mathcal{M}_{\mathscr{B},\varphi,\vec{\mathcal{B}}} : L^{p_1}(w_1^{p_1}) \times \cdots \times L^{p_m}(w_m^{p_m}) \to L^q(v^q)$.

Corollary 2.15. *Let $0 \leq \alpha < mn$, $\frac{1}{p} = \frac{1}{p_1} + \cdots + \frac{1}{p_m}$ with $1 < p_1, \dots, p_m < \infty$, and $0 < p \leq q < \infty$. Assume that $\mathscr{B}$ is a Muckenhoupt basis. If $(\vec{w}, v)$ are weights such that $\mathcal{M}_{\mathscr{B},\alpha}$ satisfies the $(A_{\mathscr{B},\gamma,v})$ condition and the power bump condition*

$$\sup_{B\in\mathscr{B}} |B|^{\frac{\alpha}{n}+\frac{1}{q}-\frac{1}{p}} \left(\frac{1}{|B|}\int_B v\,dx\right)^{\frac{1}{q}} \times \prod_{i=1}^m \left(\frac{1}{|B|}\int_B w_i^{(1-p_i')r}\,dx\right)^{\frac{1}{rp_i'}} < \infty \quad \text{for some } r > 1, \tag{2-10}$$

then $\mathcal{M}_{\mathscr{B},\alpha} : L^{p_1}(w_1) \times \cdots \times L^{p_m}(w_m) \to L^q(v)$.

Remark 2.16. It is easy to see that our Corollary 2.15 extends Theorem 2.3 of [Grafakos et al. 2011]. Indeed, under the same assumptions, the authors [Grafakos et al. 2011] only achieved boundedness from $L^{p_1}(w_1) \times \cdots \times L^{p_m}(w_m)$ to $L^{p,\infty}(v)$. On the other hand, we enlarge the range of α from $\alpha = 0$ to $0 \leq \alpha < mn$.

Finally, we present a two weighted norm inequality in the more general context of Banach function spaces.

Theorem 2.17. *Let $\frac{1}{p} = \frac{1}{p_1} + \cdots + \frac{1}{p_m}$ with $1 < p_1, \dots, p_m < \infty$, and $0 < p \leq q < \infty$. Let φ be a function as in Definition 2.12. Suppose that $Y_1, \dots, Y_m$ are Banach function spaces such that*

$$\mathcal{M}_{\vec{Y}'} : L^{p_1}(\mathbb{R}^n) \times \cdots \times L^{p_m}(\mathbb{R}^n) \to L^p(\mathbb{R}^n).$$

If $(\vec{w}, v)$ are weights such that $\mathcal{M}_{\vec{Y}'}$ satisfies the $(A_{\mathscr{B},\gamma,v^q})$ condition and

$$\sup_{B\in\mathscr{B}} \varphi(|B|)|B|^{\frac{1}{q}-\frac{1}{p}} \left(\frac{1}{|B|}\int_B v^q\,dx\right)^{\frac{1}{q}} \prod_{i=1}^m \|w_i^{-1}\|_{Y_i,B} < \infty, \tag{2-11}$$

then $\mathcal{M}_{\mathscr{B},\varphi} : L^{p_1}(w_1^{p_1}) \times \cdots \times L^{p_m}(w_m^{p_m}) \to L^q(v^q)$.

This article is organized as follows. In Section 3, some important properties of multiple weight $A_{(\vec{p},q),\mathcal{R}}$ will be given. In Section 4, we shall prove Theorems 2.1 and 2.7. Section 5 is devoted to proving Theorem 2.11. As for the rest of the theorems, we will complete their proofs in Section 6.

3. A survey on multiple strong Muckenhoupt weights

In this section, our goal is to study the properties of multiple weights related to rectangles systematically. We first recall the definition of $A_{\vec{p},\mathcal{R}}$ which was introduced in [Grafakos et al. 2011].

Definition 3.1. Let $1 \le p_1, \dots, p_m < \infty$. We say that m-tuple of weights $\vec{w}$ satisfies the $A_{\vec{p},\mathcal{R}}$ condition (or $\vec{w} \in A_{\vec{p},\mathcal{R}}$) if

$$[\vec{w}]_{A_{\vec{p},\mathcal{R}}} := \sup_{R\in\mathcal{R}} \left(\frac{1}{|R|}\int_R \hat{\nu}_{\vec{w}}\,dx\right) \prod_{i=1}^m \left(\frac{1}{|R|}\int_R w_i^{1-p_i'}\,dx\right)^{p/p_i'} < \infty,$$

where $\hat{\nu}_{\vec{w}} = \prod_{i=1}^m w_i^{p/p_i}$. If $p_i = 1$, $\left(\frac{1}{R}\int_R w_i^{1-p_i'}\right)^{1/p_i'}$ is understood as $(\inf_R w_i)^{-1}$.

The characterizations of multiple weights are as follows.

Theorem 3.2. *Let* $1 \le p_1, \dots, p_m < \infty$, $\frac{1}{p} = \frac{1}{p_1} + \cdots + \frac{1}{p_m}$ *and* $p_0 = \min\{p_i\}_i$. *Then the following statements hold*:

(1) $A_{r_1\vec{p},\mathcal{R}} \subsetneqq A_{r_2\vec{p},\mathcal{R}}$ *for any* $1/p_0 \le r_1 < r_2 < \infty$.

(2) $A_{\vec{p},\mathcal{R}} = \bigcup_{1/p_0 \le r < 1} A_{r\vec{p},\mathcal{R}}$.

(3) $\vec{w} \in A_{\vec{p},\mathcal{R}}$ *if and only if*

$$\hat{\nu}_{\vec{w}} \in A_{mp,\mathcal{R}} \quad \textit{and} \quad w_i^{1-p_i'} \in A_{mp_i',\mathcal{R}},\ i = 1, \dots, m,$$

where $w_i^{1-p_i'} \in A_{mp_i',\mathcal{R}}$ *is understood as* $w_i^{1/m} \in A_{1,\mathcal{R}}$ *if* $p_i = 1$.

Theorem 3.3. *Let* $1 \le p_1, \dots, p_m < \infty$, $\frac{1}{p} = \frac{1}{p_1} + \cdots + \frac{1}{p_m}$ *and* $\frac{1}{m} \le p \le q < \infty$. *Then, it holds that*

(i) $\vec{w} \in A_{(\vec{p},q),\mathcal{R}}$ *if and only if*

$$\nu_{\vec{w}}{}^q \subset A_{mq,\mathcal{R}} \quad \textit{and} \quad w_i^{-p_i'} \in A_{mp_i',\mathcal{R}},\ i = 1, \dots, m.$$

When $p_i = 1$, $w_i^{-p_i'}$ *is understood as* $w_i^{1/m} \in A_{1,\mathcal{R}}$.

(ii) *Assume that* $0 < \alpha < mn$, $p_1, \dots, p_m < \frac{mn}{\alpha}$ *and* $\frac{1}{q} = \frac{1}{p} - \frac{\alpha}{n}$. *Then* $\vec{w} \in A_{(\vec{p},q),\mathcal{R}}$ *if and only if*

$$\nu_{\vec{w}}{}^q \in A_{q(m-\alpha/n),\mathcal{R}} \quad \textit{and} \quad w_i^{-p_i'} \in A_{p_i'(m-\alpha/n),\mathcal{R}},\ i = 1, \dots, m.$$

When $p_i = 1$, $w_i^{-p_i'} \in A_{p_i'(m-\alpha/n),\mathcal{R}}$ *is understood as* $w_i^{n/(mn-\alpha)} \in A_{1,\mathcal{R}}$.

Theorem 3.4. *Let* $1 < p_1, \dots, p_m < \infty$, $\frac{1}{p} = \frac{1}{p_1} + \cdots + \frac{1}{p_m}$, $\frac{1}{m} < p \le q < \infty$ *and* $p_0 = \min\{p_i\}_i$. *It holds that*

(a) $A_{(\vec{p},q,r_2),\mathcal{R}} \subsetneqq A_{(\vec{p},q,r_1),\mathcal{R}}$, *whenever* $1 \le r_1 < r_2 < p_0$.

(b) *For any* $1 \le r_1 < p_0$,

$$A_{(\vec{p},q,r_1),\mathcal{R}} = \bigcup_{r_1 < r < p_0} A_{(\vec{p},q,r),\mathcal{R}},$$

where $A_{(\vec{p},q,s),\mathcal{R}} := \left\{\vec{w};\ \vec{w}^s = (w_1^s, \dots, w_m^s) \in A_{(\vec{p}/s,\,q/s),\mathcal{R}}\right\}$ *for any* $s \ge 1$.

Proofs of Theorems 3.2–3.4. The argument used in [Chen et al. 2014, Theorems 2.4 and 3.11] relies only on the use of Hölder's inequality, and doesn't involve any geometric property of cubes or rectangles. Hence we may also use the method in [Chen et al. 2014] to complete our proof. Since the main ideas are almost the same, we omit the proof here. It is worth mentioning that when considering the strict inclusion relation in Theorem 3.2 (1) and Theorem 3.4 (a), we need the characterization of $|x|^\alpha \in A_{p,\mathcal{R}}$, which will be shown in Proposition 3.7 below. $\square$

Definition 3.5. We say that a nonnegative measurable function ω satisfies the dyadic reverse doubling condition, or $\omega \in RD^{(\beta)}$, if ω is locally integrable on $\mathbb{R}^n$ and there is a constant $\beta > 1$ such that $\beta\omega(I) \le \omega(J)$ for any $I, J \in \mathcal{DR}$, where $I \subset J$ and $|I| = 2^{-1}|J|$.

Proposition 3.6. *$A_{\infty,\mathcal{R}}(\mathbb{R}^n) \subsetneqq RD^{(\beta)}(\mathbb{R}^n)$, for any $\beta > 1$ and $n \ge 2$.*

Proof. The inclusion relation $A_{\infty,\mathcal{R}}(\mathbb{R}^n) \subset RD^{(\beta)}(\mathbb{R}^n)$ has been proved in [Cao et al. 2017, Proposition 4.2]. Thus, it suffices to show that there exists some weight $w \in RD^{(\beta)}(\mathbb{R}^n) \setminus \bigcup_{1 \le p < \infty} A_{p,\mathcal{R}}$. This follows from the following fact.

Let $\omega_0(t)$ be an even function on $(-\infty, \infty)$, which is defined for $t > 0$ by

$$\omega_0(t) = (1-t)\mathbf{1}_{[0,1)} + \sum_{k=1}^{\infty}[1 - 2^{-k+1}(t - 2^{k-1})]\,\mathbf{1}_{[2^{k-1},2^k)}.$$

Then ω_0 satisfies the dyadic reverse doubling condition with $\beta = \frac{4}{3}$, but $\omega_0 \notin A_\infty(\mathbb{R})$. Moreover, if we define

$$\omega_j(x) := \omega_0(x_j)dx_1 \cdots dx_n, \qquad j = 1, \ldots, n,$$

then it holds that $\omega_j \in RD^{(\beta^*)} \setminus A_{\infty,\mathcal{R}}(\mathbb{R}^n)$, where $\beta^* = \max\{\beta, 2\}$.

Let us begin by showing $\omega_0 \notin A_\infty(\mathbb{R})$. For $j \in \mathbb{N}$, we get

$$\int_{1-j^{-2}}^{1+j^{-3}} \omega_0(t)\,dt = \int_{1-j^{-2}}^{1} \omega_0(t)\,dt + \int_{1}^{1+j^{-3}} \omega_0(t)\,dt = \frac{1}{2j^4} + \left(\frac{1}{j^3} - \frac{1}{2j^6}\right),$$

and so

$$\frac{\omega_0([1, 1+j^{-3}))}{\omega_0([1-j^{-2}, 1+j^{-3}))} = \frac{\frac{1}{j^3} - \frac{1}{2j^6}}{\frac{1}{2j^4} + \frac{1}{j^3} - \frac{1}{2j^6}} = \frac{1 - \frac{1}{2j^3}}{1 + \frac{1}{2j} - \frac{1}{2j^3}} \to 1 \text{ as } j \to \infty,$$

and

$$\frac{|[1, 1+j^{-3})|}{|[1-j^{-2}, 1+j^{-3})|} = \frac{1}{j+1} \to 0 \text{ as } j \to \infty.$$

From this we see that $\omega_0 \notin A_\infty(\mathbb{R})$.

A direct proof that $\omega_0 \notin A_\infty(\mathbb{R})$. For $0 < a < 1$ and $p > 2$ we have

$$\begin{aligned}\int_{1-a^2}^{1+a^3} \omega_0(t)\,dt &= \int_{1-a^2}^{1} (1-t)\ dt + \int_1^{1+a^3} (2-t)\,dt \\ &= \frac{a^4}{2} + a^3 - \frac{a^6}{2} \geq \frac{a^3}{2} + \frac{a^4}{2},\end{aligned}$$

$$\begin{aligned}\int_{1-a^2}^{1+a^3} \omega_0(t)^{1-p'}\,dt &= \int_{1-a^2}^{1} (1-t)^{1-p'}\,dt + \int_1^{1+a^3} (2-t)^{1-p'}\,dt \\ &= \frac{1}{2-p'}[a^{2(2-p')} + 1 - (1-a^3)^{2-p'}] \geq \frac{a^{2(2-p')}}{2-p'}.\end{aligned}$$

Hence for $I_a = [1-a^2, 1+a^3)$ we get

$$\begin{aligned}&\left(\frac{1}{|I_a|}\int_{-a^2}^{a^3} \omega_0(t)\,dt\right)\left(\frac{1}{|I_a|}\int_{-a^2}^{a^3} \omega_0(t)^{1-p'}\,dt\right)^{p-1} \\ &\qquad \geq \frac{1}{a^2+a^3}\left(\frac{a^3}{2}+\frac{a^4}{2}\right)\left(\frac{1}{a^2+a^3}\frac{a^{2(2-p')}}{2-p'}\right)^{p-1} \\ &\qquad \gtrsim a \times \left(\frac{a^{2(2-p')}}{a^2}\right)^{p-1} = a \times a^{2(1-p')(p-1)} = a^{-1}.\end{aligned}$$

This shows

$$\sup_{I:\text{intervals}} \left(\frac{1}{|I|}\int_I \omega_0(t)\,dt\right)\left(\frac{1}{|I|}\int_I \omega_0(t)^{1-p'}\,dt\right)^{p-1} = \infty,$$

Hence $\omega_0 \notin A_\infty(\mathbb{R})$.

Next, we demonstrate $\omega_0 \in RD^{(\beta)}$ with $\beta = \frac{4}{3}$.

Let $I \subset \mathbb{R}$ be a dyadic interval, with I_- and I_+ the left and right children of I, respectively. Set $I = [m2^k, (m+1)2^k),\ m, k \in \mathbb{Z}$. Since ω_0 is even, it suffices to consider $m \geq 0$.

Case 1: $m = 0$, $k \geq 1$. In this case, we have

$$\begin{aligned}\omega_0(I) &= \int_0^{2^k} \omega_0(t)\,dt = \int_0^1 \omega_0(t)\,dt + \sum_{j=1}^{k} \int_{2^{j-1}}^{2^j} \omega_0(t)\,dt \\ &= \frac{1}{2} + \sum_{j=1}^{k} 2^{j-2} = 2^{k-1},\end{aligned} \tag{3-1}$$

and

$$\omega_0(I_-) = \int_0^{2^{k-1}} \omega_0(t)\,dt = 2^{k-2}, \quad \omega_0(I_+) = \int_{2^{k-1}}^{2^k} \omega_0(t)\,dt = 2^{k-2}. \tag{3-2}$$

Thus, it holds that

$$2\omega_0(I_+) = 2\omega_0(I_-) = \omega_0(I). \tag{3-3}$$

Case 2: $m = 0$, $k \leq 0$. It is easy to get $I = [0, 2^k) \subset [0, 1)$. Then we obtain

$$\frac{1}{4} \leq \frac{\omega_0(I_-)}{\omega_0(I)} = \frac{2^{k-1}(1-2^{k-2})}{2^k(1-2^{k-1})} = \frac{1}{2}\left(\frac{1}{2} + \frac{1}{2-2^k}\right) \leq \frac{1}{2} \times \left(\frac{1}{2}+1\right) = \frac{3}{4},$$

and hence,

$$\tfrac{4}{3}\omega_0(I_-) \leq \omega_0(I), \quad \tfrac{4}{3}\omega_0(I_+) \leq \omega_0(I). \tag{3-4}$$

Case 3: $m \geq 1$, $m \cdot 2^k < 1$. We have $0 < m < 2^{-k} \in \mathbb{Z}_+$, and so $0 < m \leq 2^{-k} - 1$. Hence $I = [m2^k, (m+1)2^k) \subset (0, 1)$. So, we also have (3-4)

Case 4: $m \geq 1$, $m \cdot 2^k \geq 1$. There exists some $\ell \in \{0, 1, 2, 3, \dots\}$ such that $m2^k \in [2^\ell, 2^{\ell+1})$. Then it follows that $2^{\ell-k} \leq m < 2^{\ell-k+1}$, which, together with the fact that $m \in \mathbb{Z}_+$, implies that $\ell \geq k$. From this, we have $m + 1 \leq 2^{\ell-k+1}$, and so $(m+1)2^k \leq 2^{\ell+1}$. This means that

$$I = [m2^k, (m+1)2^k) \subset [2^\ell, 2^{\ell+1}).$$

Therefore, we deduce that

$$\begin{aligned}
\frac{1}{2} \leq \frac{\omega_0(I_-)}{\omega_0(I)} &= \frac{2^{k-1}\big[1-\big(m+\frac{1}{4}\big)2^{k-\ell}\big]}{2^k\big[1-\big(m+\frac{1}{2}\big)2^{k-\ell}\big]} \\
&= \frac{1}{2}\left(1 + \frac{2^{k-\ell}/4}{1-\big(m+\frac{1}{2}\big)2^{k-\ell}}\right) \\
&\leq \frac{1}{2} \times \left(1+\frac{1}{2}\right) = \frac{3}{4},
\end{aligned}$$

and

$$\frac{1}{4} \leq \frac{\omega_0(I_+)}{\omega_0(I)} = 1 - \frac{\omega_0(I_-)}{\omega_0(I)} \leq \frac{1}{2}.$$

This implies that in this setting, the inequality (3-4) holds as well.

From Cases 1–4, we see that ω_0 satisfies the dyadic reverse doubling condition. The proof in higher dimensions follows from the one-dimension result. □

Proposition 3.7. *Let $1 < p < \infty$. The strong Muckenhoupt weight has the characterization*: $|x|^\alpha \in A_{p,\mathcal{R}}(\mathbb{R}^n)$ *if and only if* $-1 < \alpha < p - 1$.

Although this proposition is contained in [Kurtz 1980], we here present a new proof.

Proof. The "only if" part follows from Lemma 2.2 in [Kurtz 1980, p. 239], and the following fact:

$$w(t) = (1+|t|)^\alpha \in A_p(\mathbb{R}) \text{ if and only if } -1 < \alpha < p-1. \tag{3-5}$$

Conversely, in the case $-1 < \alpha \leq 0$, we see that $t^\alpha \in A_1(\mathbb{R}_+)$ and is decreasing. So, $|x|^\alpha \in \widetilde{A}_1(\mathbb{R}_+)$, and hence by Theorem 4.4 in [Yabuta 2011] it belongs to $A_{1,\mathcal{R}}(\mathbb{R}^n) \subset A_{p,\mathcal{R}}(\mathbb{R}^n)$.

In the case $0 < \alpha < p-1$, we have $-1 < \alpha/(1-p) < 0$, and so $t^{\alpha/(1-p)} \in A_1(\mathbb{R}_+)$ and is decreasing. Hence $|x|^\alpha = (|x|^{\alpha/(1-p)})^{1-p} \in \widetilde{A}_p(\mathbb{R}_+)$, and so, as before, it belongs to $A_{p,\mathcal{R}}(\mathbb{R}^n)$.

Here,

$$\widetilde{A}_p(\mathbb{R}_+) := \{\omega(x) = \nu_1(|x|)\nu_2(|x|)^{1-p} : \nu_1, \nu_2 \in A_1(\mathbb{R}_+) \text{ are decreasing or } \nu_1^2, \nu_2^2 \in A_1(\mathbb{R}_+)\}$$

and

$$\widetilde{A}_1(\mathbb{R}_+) := \{\omega(x) = \nu_1(|x|) : \nu_1 \in A_1(\mathbb{R}_+) \text{ is decreasing or } \nu_1^2 \in A_1(\mathbb{R}_+)\},$$

which are the weight classes introduced by Duoandikoetxea [1993]. □

4. Proofs of Theorem 2.1 and Theorem 2.7

To show the endpoint estimate of $\mathcal{M}_{\mathcal{R},\alpha}$, we need the following key lemma:

Lemma 4.1 [Grafakos et al. 2011]. *Let $m \in \mathbb{N}$, and E be any set. If Φ is a submultiplicative Young function, then there is a constant C such that whenever*

$$1 < \prod_{i=1}^m \|f_i\|_{\Phi,E}$$

holds, one can get

$$\prod_{i=1}^m \|f_i\|_{\Phi,E} \leq C \prod_{i=1}^m \frac{1}{|E|} \int_E \Phi^{(m)}(|f_i(x)|)\,dx.$$

Proof of Theorem 2.1. Denote $E = \{x \in \mathbb{R}^n : \mathcal{M}_{\mathcal{R},\alpha} f(x) > \lambda^m\}$. Then there exists a compact set K such that $K \subset E$ and

$$|K| \leq |E| \leq 2|K|.$$

By the compactness of K, one can find a finite collection of rectangles $\{R_j\}_{j=1}^N$ such that

$$K \subset \bigcup_{j=1}^N R_j \quad \text{and} \quad \lambda^m < \prod_{i=1}^m \frac{1}{|R_j|^{1-\alpha/(mn)}} \int_{R_j} |f_i(y)|\,dy, \qquad j = 1, \dots, N. \tag{4-1}$$

According to the Córdoba–Fefferman rectangle covering lemma [1975], there are positive constants δ, c depending only on n and a subfamily $\{\widetilde{R}_j\}_{j=1}^{\ell}$ of $\{R_j\}_{j=1}^{N}$ satisfying

$$\Big|\bigcup_{j=1}^{N} R_j\Big| \le c\Big|\bigcup_{j=1}^{\ell} \widetilde{R}_j\Big|, \tag{4-2}$$

and

$$\int_{\bigcup_{j=1}^{\ell} \widetilde{R}_j} \exp\Big(\delta \sum_{j=1}^{\ell} \mathbf{1}_{\widetilde{R}_j}(x)\Big)^{\frac{1}{n-1}} dx \le 2\Big|\bigcup_{j=1}^{\ell} \widetilde{R}_j\Big|. \tag{4-3}$$

For convenience, we introduce the following notation: $\widetilde{E} = \bigcup_{j=1}^{\ell} \widetilde{R}_j$ and $\Psi_n(t) = \exp(t^{1/(n-1)}) - 1$. Then the inequality (4-3) is the same as

$$\frac{1}{|\widetilde{E}|} \int_{\widetilde{E}} \Psi_n\Big(\delta \sum_{j=1}^{\ell} \mathbf{1}_{\widetilde{R}_j}(x)\Big) dx \le 1.$$

Furthermore, using the fact that

$$\|f\|_{\Phi,E} \le 1 \Leftrightarrow \frac{1}{|E|} \int_E \Phi(|f(x)|)\, dx \le 1, \quad \text{for any set } |E| < \infty, \tag{4-4}$$

one can obtain

$$\Big\|\sum_{j=1}^{\ell} \mathbf{1}_{\widetilde{R}_j}\Big\|_{\Psi_n,\widetilde{E}} \le \delta^{-1}. \tag{4-5}$$

Therefore, in all, combining the inequalities (4-1) and (4-2), we have

$$\begin{aligned}
|\widetilde{E}|^{1-\alpha/(mn)} &= \Big|\bigcup_{j=1}^{\ell} \widetilde{R}_j\Big|^{1-\alpha/(mn)} \\
&\le \sum_{j=1}^{\ell} |\widetilde{R}_j|^{1-\alpha/(mn)} \Big(\frac{1}{\lambda^m} \prod_{i=1}^{m} \frac{1}{|\widetilde{R}_j|^{1-\alpha/(mn)}} \int_{\widetilde{R}_j} |f_i(y)|\, dy\Big)^{1/m} \\
&= \sum_{j=1}^{\ell} \Big(\prod_{i=1}^{m} \int_{\widetilde{R}_j} \frac{|f_i(y)|}{\lambda}\, dy\Big)^{1/m} \\
&\le \Big(\prod_{i=1}^{m} \sum_{j=1}^{\ell} \int_{\widetilde{R}_j} \frac{|f_i(y)|}{\lambda}\, dy\Big)^{1/m} \\
&= \Big(\prod_{i=1}^{m} \int_{\widetilde{E}} \sum_{j=1}^{\ell} \mathbf{1}_{\widetilde{R}_j}(y) \frac{|f_i(y)|}{\lambda}\, dy\Big)^{1/m}.
\end{aligned}$$

Hence, from the Hölder's inequalities (2-8) and (4-5), it now follows that

$$\begin{aligned}1 &\le \prod_{i=1}^{m} \frac{1}{|\widetilde{E}|} \int_{\widetilde{E}} \sum_{j=1}^{\ell} \mathbf{1}_{\widetilde{R}_j}(y) \cdot |\widetilde{E}|^{\alpha/(mn)} \frac{|f_i(y)|}{\lambda}\, dy \\ &\le \prod_{i=1}^{m} \Big\| \sum_{j=1}^{\ell} \mathbf{1}_{\widetilde{R}_j} \Big\|_{\Psi_n, \widetilde{E}} \Big\| |\widetilde{E}|^{\alpha/(mn)} \frac{f_i}{\lambda} \Big\|_{\Phi_n, \widetilde{E}} \\ &\le \prod_{i=1}^{m} \delta^{-1} \Big\| |\widetilde{E}|^{\alpha/(mn)} \frac{f_i}{\lambda} \Big\|_{\Phi_n, \widetilde{E}} = \prod_{i=1}^{m} \Big\| \delta^{-1} |\widetilde{E}|^{\alpha/(mn)} \frac{f_i}{\lambda} \Big\|_{\Phi_n, \widetilde{E}}.\end{aligned}$$

Applying Lemma 4.1, we deduce that

$$1 \le \prod_{i=1}^{m} \frac{1}{|\widetilde{E}|} \int_{\widetilde{E}} \Phi_n^{(m)}\Big(\delta^{-1} |\widetilde{E}|^{\alpha/(mn)} \frac{|f_i(y)|}{\lambda} \Big)\, dy.$$

Notice that the function $\Phi_n^{(m)}$ is submultiplicative. Accordingly, we get

$$\begin{aligned}1 &\lesssim \prod_{i=1}^{m} \frac{1}{|\widetilde{E}|} \int_{\widetilde{E}} \Phi_n^{(m)}(|\widetilde{E}|^{\alpha/(mn)}) \Phi_n^{(m)}\Big(\frac{|f_i(y)|}{\lambda} \Big)\, dy \\ &\lesssim \prod_{i=1}^{m} \frac{1}{|\widetilde{E}|^{1-\alpha/(mn)}} \big[1 + (\log^+ |\widetilde{E}|^{\alpha/(mn)})^{n-1}\big]^m \int_{\widetilde{E}} \Phi_n^{(m)}\Big(\frac{|f_i(y)|}{\lambda} \Big)\, dy,\end{aligned} \tag{4-6}$$

where we have used the fact that $\Phi_n^{(m)}(t) \lesssim t[1 + (\log^+ t)^{n-1}]^m$. Moreover, (4-6) implies that

$$|\widetilde{E}|^{m-\alpha/n} \lesssim \prod_{i=1}^{m} \big[1 + (\log^+ |\widetilde{E}|^{\alpha/(mn)})^{n-1}\big]^m \int_{\mathbb{R}^n} \Phi_n^{(m)}\Big(\frac{|f_i(y)|}{\lambda} \Big)\, dy. \tag{4-7}$$

In order to get a further estimate, we need a basic fact: if $\theta \in (0, 1)$, then there exists a constant $C_0 > 1$ and β small enough such that

$$0 < \beta < \frac{1-\theta}{mn}, \quad 1 + \log^+ t^\theta \le t^\beta, \text{ if } t > C_0. \tag{4-8}$$

If $|\widetilde{E}| > C_0$, then by the inequalities (4-7) and (4-8) we have

$$|\widetilde{E}|^{m-\alpha/n} \lesssim |\widetilde{E}|^{m^2(n-1)\beta} \prod_{i=1}^{m} \int_{\mathbb{R}^n} \Phi_n^{(m)}\Big(\frac{|f_i(y)|}{\lambda} \Big)\, dy,$$

and hence

$$|\widetilde{E}|^{m-\alpha/n-m^2(n-1)\beta} \lesssim \prod_{i=1}^{m} \int_{\widetilde{E}} \Phi_n^{(m)}\Big(\frac{|f(x)|}{\lambda} \Big)\, dx.$$

Therefore,

$$\log^+ |\widetilde{E}|^{\alpha/(mn)} \lesssim \frac{\alpha}{mn} \log^+ \prod_{i=1}^m \int_{\mathbb{R}^n} \Phi_n^{(m)}\left(\frac{|f_i(y)|}{\lambda}\right) dy.$$

From this inequality and (4-7), we obtain

$$|\widetilde{E}|^{m-\alpha/n} \lesssim \prod_{i=1}^m \Biggl[1 + \left(\frac{\alpha}{mn} \log^+ \prod_{j=1}^m \int_{\mathbb{R}^n} \Phi_n^{(m)}\left(\frac{|f_j(y)|}{\lambda}\right) dy\right)^{n-1}\Biggr]^m \times \int_{\mathbb{R}^n} \Phi_n^{(m)}\left(\frac{|f_i(y)|}{\lambda}\right) dy. \tag{4-9}$$

On the other hand, if $|\widetilde{E}| \le C_0$, then

$$1 + (\log^+ |\widetilde{E}|^{\alpha/(mn)})^{n-1} \lesssim 1.$$

Hence,

$$|\widetilde{E}|^{m-\alpha/n} \lesssim \prod_{i=1}^m \int_{\mathbb{R}^n} \Phi_n^{(m)}\left(\frac{|f_i(y)|}{\lambda}\right) dy. \tag{4-10}$$

Consequently, combining (4-9), (4-10) with the fact that $|E| \lesssim |\widetilde{E}|$, we deduce the desired result. □

Next, we will demonstrate Theorem 2.7. The proof will be based on Theorem 2.14, which will be proved in Section 6. First we recall the definition of the generalized Hölder's inequality on Orlicz spaces due to O'Neil [1965].

Lemma 4.2. *If $\mathcal{A}$, $\mathcal{B}$ and $\mathcal{C}$ are Young functions satisfying*

$$\mathcal{A}^{-1}(t)\mathcal{C}^{-1}(t) \le \mathcal{B}^{-1}(t) \quad \textit{for any } t > 0,$$

then for all functions f, g and any measurable set $E \subset \mathbb{R}^n$, the following inequality holds:

$$\|fg\|_{\mathcal{B},E} \le 2\|f\|_{\mathcal{A},E}\|g\|_{\mathcal{C},E}. \tag{4-11}$$

Proof of Theorem 2.7. The process of our proof is (2-3) $\Leftrightarrow$ (2-2) $\Rightarrow$ (2-5) $\Rightarrow$ (2-4) $\Rightarrow$ (2-2). In fact, (2-3) $\Leftrightarrow$ (2-2) is contained in [Cao et al. 2017, Theorem 2.2]. From Lemma 4.2, it follows that $\mathcal{M}_{\mathcal{R},\alpha}(\vec{f}) \le \mathcal{M}_{\mathcal{R},\alpha,\Phi_{k+1}}(\vec{f})$. This shows (2-5) $\Rightarrow$ (2-4). Moreover, taking $f_i = w_i^{-p_i'}\chi_R$ for a given rectangle R, we may obtain (2-4) $\Rightarrow$ (2-2). Hence, it remains to prove (2-2) $\Rightarrow$ (2-5).

By Theorem 3.3 and [García-Cuerva and Rubio de Francia 1985, Theorem 6.7, p. 458], it is easy to see that $\nu_{\vec{w}}^q$ satisfies the condition (A) and $w_i^{-p_i'}$ satisfies the reverse Hölder inequality. Thus, there exist constants $c_i > 0$, $r_i > 1$ $(i = 1, \dots, m)$ such that

$$\left(\frac{1}{|R|}\int_R w_i^{-p_i' r_i}\,dx\right)^{\frac{1}{r_i}} \le \frac{c_i}{|R|}\int_R w_i^{-p_i'}\,dx \quad \text{for any rectangle } R. \tag{4-12}$$

For fixed $k \in \mathbb{N}$, we introduce the notation

$$\mathcal{A}_i(t) = t^{r_i p_i'}, \quad \mathcal{C}_i(t) = [t(1+\log^+ t)^k]^{(r_i p_i')'}.$$

Thus, we can obtain that

$$\mathcal{A}_i^{-1}(t) = t^{1/(r_i p_i')} \quad \text{and} \quad \mathcal{A}_i^{-1}(t)\mathcal{C}_i^{-1}(t) \approx \Phi_{k+1}^{-1}(t).$$

Notice that $\mathcal{C}_i \in B_{p_i}^*$ and $\mathcal{C}_i$ is submultiplicative. From [Liu and Luque 2014, Proposition 2.2], it now follows that

$$M_{\mathcal{R},\mathcal{C}_i} : L^{p_i}(\mathbb{R}^n) \to L^{p_i}(\mathbb{R}^n), \quad i = 1, \dots, m.$$

This yields immediately that

$$\mathcal{M}_{\mathcal{R},\vec{\mathcal{C}}} : L^{p_1}(\mathbb{R}^n) \times \cdots \times L^{p_m}(\mathbb{R}^n) \to L^p(\mathbb{R}^n).$$

In addition, for a given rectangle R, (4-12) yields that

$$\begin{aligned}
|R|^{\frac{\alpha}{n}+\frac{1}{q}-\frac{1}{p}}&\left(\frac{1}{|R|}\int_R \nu_{\vec{w}}^q\,dx\right)^{\frac{1}{q}}\prod_{i=1}^m \|w_i^{-1}\|_{\mathcal{A}_i,R} \\
&= \left(\frac{1}{|R|}\int_R \nu_{\vec{w}}^q\,dx\right)^{\frac{1}{q}}\prod_{i=1}^m\left(\frac{1}{|R|}\int_R w_i^{-r_i p_i'}\,dx\right)^{\frac{1}{r_i p_i'}} \\
&\lesssim \left(\frac{1}{|R|}\int_R \nu_{\vec{w}}^q\,dx\right)^{\frac{1}{q}}\prod_{i=1}^m\left(\frac{1}{|R|}\int_R w_i^{-p_i'}\,dx\right)^{\frac{1}{p_i'}} \\
&\le [\vec{w}]_{A_{(\vec{p},q),\mathcal{R}}} < \infty.
\end{aligned}$$

This implies that $(\vec{w}, \nu_{\vec{w}})$ satisfies the two weighted condition (2-9). By Theorem 2.14, we get

$$\mathcal{M}_{\mathcal{R},\alpha,\Phi_{k+1}} : L^{p_1}(w_1^{p_1}) \times \cdots \times L^{p_m}(w_m^{p_m}) \to L^q(\nu_{\vec{w}}^q).$$

Therefore, in all, we have completed the proof of Theorem 2.7. □

5. The multilinear Fefferman–Stein inequality

Before showing our multilinear Fefferman–Stein inequality, we present a Carleson embedding theorem regarding dyadic rectangles.

Theorem 5.1 [Cao et al. 2017]. *Let $1 < p \le q < \infty$, ω be a nonnegative locally integrable function on $\mathbb{R}^n$. Assume that $\omega^{1-p'}$ satisfies the dyadic reverse doubling condition with $\beta > 1$. Then the inequality*

$$\sum_{R\in\mathcal{DR}}\left(\int_R \omega^{1-p'}\,dx\right)^{-q/p'}\left(\int_R f(x)\,dx\right)^q \le C\left(\int_{\mathbb{R}^n} f(x)^p\omega\,dx\right)^{q/p}$$

holds for all nonnegative $f \in L^p(\omega)$, where C depends on n, p, q and β.

Proof of Theorem 2.11. It suffices to show the above result for the dyadic version of the maximal operator,

$$\mathcal{M}^d_{\mathcal{R},\alpha}(\vec{f})(x) = \sup_{\substack{R\ni x\\ R\in\mathcal{DR}}}\prod_{i=1}^m \frac{1}{|R|^{1-\alpha/(mn)}}\int_R |f_i(y_i)|\,dy_i, \quad x\in\mathbb{R}^n.$$

Adopting the policy in [Cao et al. 2017], we will obtain the general result from the dyadic setting.

Without loss of generality, we can assume that $\vec{f}$ is bounded, $\vec{f} \ge 0$ and has a compact support. Therefore, $\mathcal{M}^d_{\mathcal{R},\alpha}(\vec{f})(x) < \infty$ for all $x\in\mathbb{R}^n$.

According to the definition of $\mathcal{M}^d_{\mathcal{R},\alpha}(\vec{f})(x)$, we have that for any $x\in\mathbb{R}^n$, there exists a dyadic rectangle R such that $x\in R$ and

$$\mathcal{M}^d_{\mathcal{R},\alpha}(\vec{f})(x) \le 2\prod_{i=1}^m \frac{1}{|R|^{1-\alpha/(mn)}}\int_R f_i(y_i)\,dy_i. \tag{5-1}$$

For any dyadic rectangle R, define

$$E(R) := \{x\in\mathbb{R}^n : \text{(5-1) holds for } R \text{ but not for any proper subset of it}\}.$$

From the definition of maximal operators and the inequality (5-1), it is obvious that

$$\mathbb{R}^n = \bigcup_{R\in\mathcal{DR}} E(R).$$

Then it follows that

$$\begin{aligned}\|\mathcal{M}^d_{\mathcal{R},\alpha}(\vec{f})\|^q_{L^q(\nu)} &\le \sum_{R\in\mathcal{DR}}\int_{E(R)}\left(\mathcal{M}^d_{\mathcal{R},\alpha}(\vec{f})(x)\right)^q \nu\,dx\\ &\lesssim \sum_{R\in\mathcal{DR}}\left(\prod_{i=1}^m \frac{1}{|R|^{1-\alpha/(mn)}}\int_R f_i(y_i)\,dy_i\right)^q \nu(R).\end{aligned}$$

Note that

$$\nu(R) = \int_R \prod_{i=1}^m \omega_i(x)^{1/m}\,dx \le \prod_{i=1}^m \omega_i(R)^{1/m}.$$

Thus we have

$$\begin{aligned}\|\mathcal{M}^d_{\mathcal{R},\alpha}(\vec{f})\|^q_{L^q(\nu)} &\lesssim \sum_{R\in\mathcal{DR}} \prod_{i=1}^m \biggl(\frac{1}{|R|}\int_R f_i(y_i)\,dy_i \cdot \langle\omega_i\rangle_R^{1/mq}\biggr)^q |R|^{q/p_i} \\ &\le \sum_{R\in\mathcal{DR}} \prod_{i=1}^m \biggl(\frac{1}{|R|}\int_R f_i(y_i)\cdot M^d_{\mathcal{R}}\omega_i(y_i)^{1/mq}\,dy_i\biggr)^q |R|^{q/p_i}.\end{aligned}$$

Therefore, by Hölder's inequality $\sum_{j=1}^\infty \prod_{i=1}^m |a_{ij}| \le \prod_{i=1}^m \bigl(\sum_{j=1}^\infty |a_{ij}|^{p_i/p}\bigr)^{p/p_i}$, we further deduce that

$$\begin{aligned}\|\mathcal{M}^d_{\mathcal{R},\alpha}(\vec{f})\|^q_{L^q(\nu)} &\le \prod_{i=1}^m \biggl[\sum_{R\in\mathcal{DR}} |R|^{q/p}\biggl(\frac{1}{|R|}\int_R f_i(y_i)\cdot M^d_{\mathcal{R}}\omega_i(y_i)^{1/mq}\,dy_i\biggr)^{qp_i/p}\biggr]^{p/p_i} \\ &\lesssim \prod_{i=1}^m \|f_i\|^q_{L^{p_i}((M^d_{\mathcal{R}}\omega_i)^{p_i/mq})},\end{aligned}$$

where we used Theorem 5.1 with respect to the exponents $(p_i, qp_i/p)$ for $\omega \equiv 1$. □

6. Proofs of Theorems 2.4, 2.9, 2.14, 2.17 and Corollaries 2.10, 2.15

To prove Theorem 2.14, we first introduce the definition of the general basis and a key covering lemma.

Definition 6.1 [Jawerth 1986; Jawerth and Torchinsky 1984]. Let $\mathscr{B}$ be a basis and let $0<\alpha<1$. A finite sequence $\{A_i\}_{i=1}^N \subset \mathscr{B}$ of sets of finite dx-measure is called α-scattered with respect to the Lebesgue measure if

$$\Bigl|A_i \cap \bigcup_{s<i} A_s\Bigr| \le \alpha|A_i| \quad \text{for all } 1<i\le N.$$

Lemma 6.2 [Grafakos et al. 2011; Jawerth 1986]. *Let $\mathscr{B}$ be a basis and let w be a weight associated to this basis. Suppose further that $M_{\mathscr{B}}$ satisfies the condition $(A_{\mathscr{B},\gamma,w})$ for some $0<\gamma<1$. Then, given any finite sequence $\{A_i\}_{i=1}^N$ of sets $A_i\in\mathscr{B}$, one can find a subsequence $\{\widetilde{A}_i\}_{i\in I}$ such that*:

(a) $\{\widetilde{A}_i\}_{i\in I}$ *is γ-scattered with respect to the Lebesgue measure.*

(b) $\widetilde{A}_i = A_i,\ i\in I$.

(c) *For any $1\le i<j\le N+1$,*

$$w\Bigl(\bigcup_{s<j} A_s\Bigr) \lesssim w\Bigl(\bigcup_{s<i} A_s\Bigr) + w\Bigl(\bigcup_{i\le s<j} \widetilde{A}_s\Bigr),$$

where $\widetilde{A}_s = \varnothing$ when $s\notin I$.

Proof of Theorem 2.14. The idea of the following arguments is essentially a combination of the ideas from [Grafakos et al. 2011; Jawerth 1986; Liu and Luque 2014]. Let $N > 0$ be a large integer. We will prove the required estimate for the quantity

$$\int_{\{2^{-N}<\mathcal{M}_{\mathscr{B},\varphi,\vec{\Psi}}(\vec{f})\le 2^{N+1}\}} \mathcal{M}_{\mathscr{B},\varphi,\vec{\Psi}}(\vec{f})(x)^q v^q\,dx,$$

with a bound independent of N. We begin with the following claim.

Claim 6.3. *For each integer k with $|k| \le N$, there exists a compact set K_k and a finite sequence $b_k = \{B_r^k\}_{r\ge 1}$ of sets $B_r^k \in \mathscr{B}$ such that*

$$v^q(K_k) \le v^q(\{\mathcal{M}_{\mathscr{B},\varphi,\vec{\Psi}}(\vec{f}) > 2^k\}) \le 2v^q(K_k).$$

Moreover, $\{\bigcup_{B\in b_k} B\}_{k=-N}^{N}$ is decreasing and therefore

$$\bigcup_{B\in b_k} B \subset K_k \subset \{\mathcal{M}_{\mathscr{B},\varphi,\vec{\Psi}}(\vec{f}) > 2^k\},$$

and

$$\varphi(|B_r^k|)\prod_{j=1}^{m}\|f_j\|_{\Psi_j,B_r^k} > 2^k. \tag{6-1}$$

Proof. To see the claim, for each k we choose a compact set $\widetilde{K}_k \subset \{\mathcal{M}_{\mathscr{B},\varphi,\vec{\Psi}}(\vec{f}) > 2^k\}$ such that

$$v^q(\widetilde{K}_k) \le v^q(\{\mathcal{M}_{\mathscr{B},\varphi,\vec{\Psi}}(\vec{f}) > 2^k\})2 \le v^q(\widetilde{K}_k).$$

For this $\widetilde{K}_k$, there exists a finite sequence $b_k = \{B_r^k\}_{r\ge 1}$ of sets $B_r^k \in \mathscr{B}$ such that every B_r^k satisfies (6-1) and such that $\widetilde{K}_k \subset \bigcup_{B\in b_k} B \subset \{\mathcal{M}_{\mathscr{B},\varphi,\vec{\Psi}}(\vec{f}) > 2^k\}$. Now, we take a compact set K_k such that

$$\bigcup_{B\in b_k} B \subset K_k \subset \{\mathcal{M}_{\mathscr{B},\varphi,\vec{\Psi}}(\vec{f}) > 2^k\}.$$

Finally, to ensure that $\{\bigcup_{B\in b_k} B\}_{k=-N}^{N}$ is decreasing, we begin the above selection from $k = N$ and once a selection is done for k we do the selection for $k-1$ with the additional requirement $\widetilde{K}_{k-1} \supset K_k$. This finishes the proof of the claim. □

We continue with the proof of Theorem 2.14. Since $\{\bigcup_{B\in b_k} B\}_{k=-N}^{N}$ is a sequence of decreasing sets, we set

$$\Omega_k = \begin{cases} \bigcup_r B_r^k = \bigcup_{B\in b_k} B & \text{when } |k| \le N. \\ \varnothing & \text{otherwise.} \end{cases}$$

Observe that these sets are decreasing in k, i.e., $\Omega_{k+1} \subset \Omega_k$ when $-N < k \le N$.

We now distribute the sets in $\bigcup_k b_k$ over μ sequences $\{A_i(\ell)\}_{i\geq 1}$, $0\leq\ell\leq\mu-1$, where μ will be chosen momentarily to be an appropriately large natural number. Set $i_0(0)=1$. In the first $i_1(0)-i_0(0)$ entries of $\{A_i(0)\}_{i\geq 1}$, i.e., for

$$i_1(0)\leq i<i_1(0),$$

we place the elements of the sequence $b_N=\{B_r^N\}_{r\geq 1}$ in the order indicated by the index r. For the next $i_2(0)-i_1(0)$ entries of $\{A_i(0)\}_{i\geq 1}$, i.e., for

$$i_1(0)\leq i<i_2(0),$$

we place the elements of the sequence $b_{N-\mu}$. We continue in this way until we reach the first integer m_0 such that $N-m_0\mu\geq -N$, when we stop. For indices i satisfying

$$i_{m_0}(0)\leq i<i_{m_0+1}(0),$$

we place in the sequence $\{A_i(0)\}_{i\geq 1}$ the elements of $b_{N-m_0\mu}$. The sequences $\{A_i(\ell)\}_{i\geq 1}$, $1\leq\ell\leq\mu-1$, are defined similarly, starting from $b_{N-\ell}$ and using the families $b_{N-\ell-s\mu}$, $s=0,1,\ldots,m_l$, where m_l is chosen to be the biggest integer such that $N-l-m_l\mu\geq -N$.

Since v^q is a weight associated to $\mathscr{B}$ and it satisfies the condition (A), we can apply Lemma 6.2 to each $\{A_i(\ell)\}_{i\geq 1}$ for some fixed $0<\lambda<1$. Then we obtain sequences

$$\{\widetilde{A}_i(\ell)\}_{i\geq 1}\subset\{A_i(\ell)\}_{i\geq 1},\quad 0\leq\ell\leq\mu-1,$$

which are λ-scattered with respect to the Lebesgue measure. In view of the definition of the set k and the construction of the families $\{A_i(\ell)\}_{i\geq 1}$, we may use assertion (c) of Lemma 6.2 to show that: for any $k=N-\ell-s\mu$ with $0\leq\ell\leq\mu-1$ and $1\leq s\leq m_\ell$,

$$\begin{aligned}v^q(\Omega_k)=v^q(\Omega_{N-\ell-s\mu})&\lesssim v^q(\Omega_{k+\mu})+v^q\Biggl(\bigcup_{i_s(\ell)\leq i\leq i_{s+1}(\ell)}\widetilde{A}_i(\ell)\Biggr)\\&\leq v^q(\Omega_{k+\mu})+\sum_{i=i_s(\ell)}^{i_{s+1}(\ell)-1}v^q(\widetilde{A}_i(\ell)).\end{aligned}$$

For the case $s=0$, we have $k=N-\ell$ and

$$v^q(\Omega_k)=v^q(\Omega_{N-\ell})\lesssim\sum_{i=i_0(\ell)}^{i_1(\ell)-1}v^q(\widetilde{A}_i(\ell)).$$

Now, all these sets $\{\widetilde{A}_i(\ell)\}_{i=i_s(\ell)}^{i_{s+1}(\ell)}$ belong to b_k with $k=N-\ell-s\mu$ and so

$$\varphi(|\widetilde{A}_i(\ell)|)\prod_{j=1}^m\|f_j\|_{\Psi_j,\widetilde{A}_i(\ell)}>2^k.\tag{6-2}$$

Therefore, it now readily follows that

$$\int_{\{2^{-N}<\mathcal{M}_{\mathscr{B},\varphi,\vec{\Psi}}(\vec{f})\le 2^{N+1}\}} \mathcal{M}_{\mathscr{B},\varphi,\vec{\Psi}}(\vec{f})(x)^q v^q\,dx \lesssim \sum_{k=-N}^{N-1} 2^{kq} v^q(\Omega_k) := \Delta_1,$$

and thus, we have

$$\begin{aligned} \Delta_1 &= \sum_{\ell=0}^{\mu-1} \sum_{0\le s\le m_\ell} 2^{q(N-\ell-s\mu)} v^q(\Omega_{N-\ell-s\mu}) \\ &\lesssim \sum_{\ell=0}^{\mu-1} \sum_{0\le s\le m_\ell} 2^{q(N-\ell-s\mu)} v^q(\Omega_{N-\ell-s\mu+\mu}) \\ &\qquad + \sum_{\ell=0}^{\mu-1} \sum_{0\le s\le m_\ell} 2^{q(N-\ell-s\mu)} \sum_{i=i_s(\ell)}^{i_{s+1}(\ell)-1} v^q(\widetilde{A}_i(\ell)) \\ &:= \Delta_2 + \Delta_3. \end{aligned} \tag{6-3}$$

To analyze the contribution of Δ_2, we choose μ so large that $2^{-q\mu} \le \frac{1}{2}$. Therefore,

$$\begin{aligned} \Delta_2 &= 2^{-q\mu} \sum_{\ell=0}^{\mu-1} \sum_{0\le s\le m_{\ell-1}} 2^{q(N-\ell-s\mu)} v^q(\Omega_{N-\ell-s\mu}) \\ &\le 2^{-q\mu} \sum_{k=-N}^{N-1} 2^{kq} v^q(\Omega_k) \le \tfrac{1}{2}\Delta_1. \end{aligned} \tag{6-4}$$

Since everything involved is finite, Δ_2 can be subtracted from Δ_1. This yields that

$$\int_{\{2^{-N}<\mathcal{M}_{\mathscr{B},\varphi,\vec{\Psi}}(\vec{f})\le 2^{N+1}\}} \mathcal{M}_{\mathscr{B},\varphi,\vec{\Psi}}(\vec{f})(x)^q v^q\,dx \lesssim \Delta_1 \lesssim \Delta_3.$$

Next we consider the contribution of Δ_3. For the sake of simplicity, for each ℓ we let $I(\ell)$ be the index set of $\{\widetilde{A}_i(\ell)\}_{0\le s\le m_\ell, i_s(\ell)\le i<i_{s+1}(\ell)}$. By (6-2) and the generalized Hölder's inequality (4-11), we obtain

$$\begin{aligned} \Delta_3 &\lesssim \sum_{\ell=0}^{\mu-1} \sum_{i\in I(\ell)} v^q(\widetilde{A}_i(\ell)) \Big[\varphi(|\widetilde{A}_i(\ell)|) \prod_{i=1}^m \|f_i\|_{\Phi,\widetilde{A}_i(\ell)}\Big]^q \\ &\lesssim \sum_{l=0}^{\mu-1} \sum_{i\in I(\ell)} \Big[\prod_{j=1}^m \|f_j\|^p_{C_j,\widetilde{A}_i(\ell)} |\widetilde{A}_i(\ell)|\Big]^{q/p} \\ &\quad \times \Big[\varphi(|\widetilde{A}_i(\ell)|)|\widetilde{A}_i(\ell)|^{\frac{1}{q}-\frac{1}{p}} \Big(\frac{1}{|\widetilde{A}_i(\ell)|}\int_{\widetilde{A}_i(\ell)} v^q\,dx\Big)^{\frac{1}{q}} \prod_{j=1}^m \|w_j^{-1}\|_{A_j,\widetilde{A}_i(\ell)}\Big]^q \end{aligned} \tag{6-5}$$

$$\lesssim \sum_{\ell=0}^{\mu-1} \sum_{i\in I(\ell)} \Bigg[\prod_{j=1}^{m} \|f_j w_j\|_{C_j,\widetilde{A}_i(\ell)}^{p} |\widetilde{A}_i(\ell)|\Bigg]^{q/p}$$
$$\le \Bigg[\sum_{\ell=0}^{\mu-1} \sum_{i\in I(\ell)} \prod_{j=1}^{m} \|f_j w_j\|_{C_j,\widetilde{A}_i(\ell)}^{p} |\widetilde{A}_i(\ell)|\Bigg]^{q/p},$$

where in the third step we used the two-weight condition (2-9).

Now, we introduce the notations

$$E_1(\ell) = \widetilde{A}_i(\ell) \quad \text{and} \quad E_i(\ell) = \widetilde{A}_i(\ell) \setminus \bigcup_{s<i} \widetilde{A}_s(\ell) \quad \text{for all } i \in I(\ell). \tag{6-6}$$

Since the sequences $\{\widetilde{A}_i(\ell)\}_{i\in I(\ell)}$ are λ-scattered with respect to the Lebesgue measure, $|\widetilde{A}_i(\ell)| \le \frac{1}{1-\lambda}|E_i(\ell)|$ for each i. Then we have the following estimate for (6-5):

$$\Delta_3 \lesssim \Bigg[\frac{1}{1-\lambda} \sum_{\ell=0}^{\mu-1} \sum_{i\in I(\ell)} \prod_{j=1}^{m} \|f_j w_j\|_{C_j,\widetilde{A}_i(\ell)}^{p} |E_i(\ell)|\Bigg]^{q/p}. \tag{6-7}$$

The collection $\{E_i(\ell)\}_{i\in I(\ell)}$ is a disjoint family; we can therefore use the fact that $\mathcal{M}_{\mathscr{B},\vec{C}}$ is bounded from $L^{p_1}(\mathbb{R}^n)\times\cdots\times L^{p_m}(\mathbb{R}^n)$ to $L^p(\mathbb{R}^n)$ to estimate (6-7). Then

$$\Delta_3 \lesssim \Bigg[\sum_{\ell=0}^{\mu-1} \sum_{i\in I(\ell)} \int_{E_i(\ell)} \Big(\mathcal{M}_{\mathscr{B},\vec{C}}(f_1 w_1, \dots, f_m w_m)(x)\Big)^p dx\Bigg]^{q/p}$$
$$\lesssim \Bigg[\int_{\mathbb{R}^n} \Big(\mathcal{M}_{\mathscr{B},\vec{C}}(f_1 w_1, \dots, f_m w_m)(x)\Big)^p dx\Bigg]^{q/p}$$
$$\lesssim \prod_{i=1}^{m} \|f_i w_i\|_{L^{p_i}(\mathbb{R}^n)}^{q} = \prod_{i=1}^{m} \|f_i\|_{L^{p_i}(w_i^{p_i})}^{q}.$$

Finally, letting $N \to \infty$, we finish the proof. □

Proof of Corollary 2.15. For each $i = 1, \dots, m$, we set $\widetilde{w}_i := w_i^{1/p_i}$ and $\Psi_i(t) := t^{p_i' r}$ for any $t > 0$. Set $\tilde{v} := v^{1/q}$. Then we can rewrite the power bump condition (2-10) as

$$\sup_{B\in\mathscr{B}} |B|^{\frac{\alpha}{n}+\frac{1}{q}-\frac{1}{p}} \bigg(\frac{1}{|B|}\int_B \tilde{v}^q\, dx\bigg)^{\frac{1}{q}} \prod_{i=1}^{m} \|\widetilde{w}_i^{-1}\|_{\Psi_i,B} < \infty.$$

In this case, for all $x \in \mathbb{R}^n$,

$$M_{\mathscr{B},\bar{\Phi}_i} f(x) = \sup_{\substack{B\ni x\\ B\in\mathscr{B}}} \bigg\{\frac{1}{|B|}\int_B |f(y)|^{(p_i' r)'} dy\bigg\}^{1/(p_i' r)'}.$$

Since $\mathscr{B}$ is a Muckenhoupt basis and $(p_i'r)' < p_i$, every $M_{\mathscr{B},\overline{\Psi}_i}$ is bounded on $L^{p_i}(\mathbb{R}^n)$. It is easy to see that

$$\mathcal{M}_{\mathscr{B},\vec{\overline{\Psi}}}(\vec{f})(x) \le \prod_{i=1}^{m} M_{\mathscr{B},\overline{\Psi}_i}(f_i)(x), \quad x \in \mathbb{R}^n,$$

which implies that $\mathcal{M}_{\mathscr{B},\vec{\overline{\Psi}}}$ is bounded from $L^{p_1}(\mathbb{R}^n) \times \cdots \times L^{p_m}(\mathbb{R}^n)$ to $L^p(\mathbb{R}^n)$. Therefore, from Theorem 2.14, it follows that

$$\mathcal{M}_{\mathscr{B},\alpha} : L^{p_1}(\widetilde{w}_1^{p_1}) \times \cdots \times L^{p_m}(\widetilde{w}_m^{p_m}) \to L^q(\tilde{v}^q),$$

which completes the proof. □

Proof of Theorem 2.9. The fact that $\mathcal{R}$ is a Muckenhoupt basis can be found in [García-Cuerva and Rubio de Francia 1985, p. 454]. Moreover, for the rectangle family $\mathcal{R}$, the $A_{\infty,\mathcal{R}}$ condition is equivalent to Tauberian condition $(A_{\mathcal{R},\gamma,w})$, which was proved in [Hagelstein et al. 2015, Corollary 4.8]. Therefore, Theorem 2.9 follows from these facts and Corollary 2.15. □

Proof of Corollary 2.10. From Theorem 3.2, it follows that $v^p \in A_{mp,\mathcal{R}} \subset A_{\infty,\mathcal{R}}$. As for $v = \prod_{i=1}^m u_i^{1/p_i}$ and $w_i = M_{\alpha p_i/m}(u_i)$, it is easy to verify that $(\vec{w}, v)$ satisfies the power bump condition (2-6). Hence, it yields the desired result. □

Proof of Theorem 2.17. Theorem 2.17 follows by using similar arguments to those in the proof of Theorem 2.14. The difference lies in the boundedness of $\mathcal{M}_{\vec{Y}'}$ and the generalized Hölder's inequality

$$\int_{\mathbb{R}^n} |f(x)g(x)|\,dx \le \|f\|_X \|g\|_{X'}$$

for any Banach function space X. □

Proof of Theorem 2.4. It is well known that there exists some $h \in L^{r'}(\mathbb{R}^n)$ with norm $\|h\|_{L^{r'}(\mathbb{R}^n)} = 1$ such that

$$\begin{aligned}\|M_{\mathcal{R}} f\|_{L^p(\ell^q,w^p)}^p &= \int_{\mathbb{R}^n} \biggl(\sum_j M_{\mathcal{R}} f_j(x)^q w(x)^q\biggr)^r dx \\ &= \sum_j \int_{\mathbb{R}^n} M_{\mathcal{R}} f_j(x)^q w(x)^q h(x)\,dx.\end{aligned}$$

In order to estimate $\int_{\mathbb{R}^n} M_{\mathcal{R}} f_j(x)^q w(x)^q h(x)\,dx$ for fixed j, we adopt a similar method to that in the proof of Theorem 2.14. Since we obtained the inequality (6-4), we get for any fixed $N > 0$

$$\Lambda_{j,N} := \int_{\{2^{-N} < M_{\mathcal{R}} f_j(x) \le 2^{N+1}\}} M_{\mathcal{R}} f_j(x)^q w(x)^q h(x)\,dx$$
$$\lesssim \sum_{\ell=0}^{\mu-1} \sum_{0\le s\le m_\ell} \sum_{i=i_s(\ell)}^{i_{s+1}(\ell)-1} (w^q h)(\widetilde{A}_i(\ell)) \left(\frac{1}{|\widetilde{A}_i(\ell)|} \int_{\widetilde{A}_i(\ell)} |f_j(x)|\,dx \right)^q.$$

Making use of the Hölder inequality and two weight condition (2-1), we deduce

$$\Lambda_{j,N} \lesssim \sum_{\ell,s,i} \|w^q\|_{A,\widetilde{A}_i(\ell)} \|h\|_{\bar{A},\widetilde{A}_i(\ell)} \|f_j v\|^q_{\bar{B},\widetilde{A}_i(\ell)} \|v^{-1}\|^q_{B,\widetilde{A}_i(\ell)} |\widetilde{A}_i(\ell)|$$
$$\lesssim \sum_{\ell,s,i} \|f_j v\|^q_{\bar{B},\widetilde{A}_i(\ell)} \|h\|_{\bar{A},\widetilde{A}_i(\ell)} |\widetilde{A}_i(\ell)|.$$

Using the same notations $\{E_i(\ell)\}$ as (6-6), we have

$$\Lambda_{j,N} \lesssim \sum_{\ell,s,i} \|f_j v\|^q_{\bar{B},\widetilde{A}_i(\ell)} \|h\|_{\bar{A},\widetilde{A}_i(\ell)} |E_i(\ell)|$$
$$\le \sum_{\ell,i} \int_{E_i(\ell)} M_{\mathcal{R},\bar{B}}(f_j v)(x)^q M_{\mathcal{R},\bar{A}} h(x)\,dx$$
$$\lesssim \int_{\mathbb{R}^n} M_{\mathcal{R},\bar{B}}(f_j v)(x)^q M_{\mathcal{R},\bar{A}} h(x)\,dx.$$

Letting $N \to \infty$, we have

$$\int_{\mathbb{R}^n} M_{\mathcal{R}} f_j(x)^q w(x)^q h(x)\,dx \lesssim \int_{\mathbb{R}^n} M_{\mathcal{R},\bar{B}}(f_j v)(x)^q M_{\mathcal{R},\bar{A}} h(x)\,dx.$$

Therefore, from the Hölder inequality and Proposition 6.4, it follows that

$$\|M_{\mathcal{R}} f\|^q_{L^p(\ell^q,w^p)} \lesssim \left\| \left(\sum_{j=1} (M_{\mathcal{R},\bar{B}}(f_j v))^q \right)^{1/q} \right\|^q_{L^p(\mathbb{R}^n)} \|M_{\mathcal{R},\bar{A}} h\|_{L^{r'}(\mathbb{R}^n)}$$
$$\lesssim \left\| \left(\sum_{j=1} (f_j v)^q \right)^{1/q} \right\|^q_{L^p(\mathbb{R}^n)} \|h\|_{L^{r'}(\mathbb{R}^n)} = \|f\|^q_{L^p(\ell^q,v^p)}.$$

This completes the proof of Theorem 2.4. □

Proposition 6.4. *Let $1 < q < p < \infty$. Suppose Φ is a Young function such that $\Phi \in B_q^*$. If the $(A_{\mathcal{R},\gamma,g})$ condition holds for some fixed $\gamma \in (0,1)$ and any nonnegative function $g \in L^{r'}(\mathbb{R}^n)$ with $\|g\|_{L^{r'}(\mathbb{R}^n)} = 1$, then we have*

$$\|M_{\mathcal{R},\Phi} f\|_{L^p(\ell^q,\mathbb{R}^n)} \lesssim \|f\|_{L^p(\ell^q,\mathbb{R}^n)}.$$

Proof. Set $r = p/q$. Then, it holds that

$$\|M_{\mathcal{R},\Phi} f\|^q_{L^p(\ell^q,\mathbb{R}^n)} = \sup_{\|g\|_{L^{r'}(\mathbb{R}^n)}=1} \left| \int_{\mathbb{R}^n} \sum_j M_{\mathcal{R},\Phi} f_j(x)^q g(x) dx \right|.$$

For fixed $g \in L^{r'}(\mathbb{R}^n)$ with $\|g\|_{L^{r'}(\mathbb{R}^n)} = 1$, from the Fefferman–Stein inequality for the maximal operator $M_{\mathcal{R},\Phi}$ (see [Liu and Luque 2014, Theorem 2.1]), it follows that

$$\begin{aligned} \left| \int_{\mathbb{R}^n} \sum_j M_{\mathcal{R},\Phi} f_j(x)^q g(x)\, dx \right| &\le \sum_j \int_{\mathbb{R}^n} M_{\mathcal{R},\Phi} f_j(x)^q |g(x)|\, dx \\ &\lesssim \sum_j \int_{\mathbb{R}^n} |f_j(x)|^q M_{\mathcal{R}} g(x)\, dx \\ &\le \Big\| \sum_j |f_j|^q \Big\|_{L^r(\mathbb{R}^n)} \|M_{\mathcal{R}} g\|_{L^{r'}(\mathbb{R}^n)} \\ &\lesssim \|f\|^q_{L^p(\ell^q,\mathbb{R}^n)} \|g\|_{L^{r'}(\mathbb{R}^n)} = \|f\|^q_{L^p(\ell^q,\mathbb{R}^n)}. \end{aligned}$$ □

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EMBEDDING AND COMPACT EMBEDDING FOR WEIGHTED AND ABSTRACT SOBOLEV SPACES

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Let Ω be an open set in a metric space H, $1 \le p_0, p \le q < \infty$, $a, b, \gamma \in \mathbb{R}$, $a \ge 0$. Suppose σ, μ, w are Borel measures. Combining results from earlier work (2009) with those obtained in work with Wheeden (2011) and with Rodney and Wheeden (2013), we study embedding and compact embedding theorems of sets $\mathfrak{S} \subset L^1_{\sigma,\mathrm{loc}}(\Omega) \times L^p_w(\Omega)$ to $L^q_\mu(\Omega)$ (projection to the first component) where $\mathfrak{S}$ (abstract Sobolev space) satisfies a Poincaré-type inequality, σ satisfies certain weak doubling property and μ is absolutely continuous with respect to σ. In particular, when $H = \mathbb{R}^n$, w, μ, ρ are weights so that ρ is essentially constant on each ball deep inside in $\Omega \setminus F$, and F is a finite collection of points and hyperplanes. With the help of a simple observation, we apply our result to the study of embedding and compact embedding of $L^{p_0}_{\rho^\gamma}(\Omega) \cap E^p_{w\rho^b}(\Omega)$ and weighted fractional Sobolev spaces to $L^q_{\mu\rho^a}(\Omega)$, where $E^p_{w\rho^b}(\Omega)$ is the space of locally integrable functions in Ω such that their weak derivatives are in $L^p_{w\rho^b}(\Omega)$. In $\mathbb{R}^n$, our assumptions are mostly sharp. Besides extending numerous results in the literature, we also extend a result of Bourgain et al. (2002) on cubes to John domains.

1. Introduction

Sobolev embedding, compact embedding and Poincaré inequalities are essential tools in the study of elliptic partial differential equations (including Yamabe-type problems)

$$\nabla \cdot (A(x)|\nabla u|^{p-2}\nabla u) + \lambda |u|^{p-2}u = |u|^{q-2}u \quad (q > p > 1), \tag{1-1}$$

where q is less than the critical exponent in the Sobolev embedding and $A(x)$ is a uniformly (or at least locally) positive definite matrix valued function. However, stronger (for example weighted) Sobolev (and compact) embedding is needed if $A(x)$ fails to be uniformly positive definite or degenerate. In this direction, Caffarelli,

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Kohn and Nirenberg [Caffarelli et al. 1984] studied the following weighted Sobolev interpolation inequalities

$$\||x|^{\alpha}u\|_{L^q(\mathbb{R}^n)} \le C\big(\||x|^{\gamma}u\|_{L^r(\mathbb{R}^n)} + \||x|^{\beta}\nabla u\|_{L^p(\mathbb{R}^n)}\big).$$

It has been extended to Lipschitz (and $C^{0,\lambda}$) domains and various distant weights by Gurka and Opic [1988; 1989; 1991] and Kufner [1985] (see also Brown and Hinton [1988]). More recently, it has also been generalized to domains satisfying chain conditions (such as John domains and generalized John domains [Hajłasz and Koskela 1998; Chua 2005; 2009]).

Together with the Poincaré inequality, embedding and compact embedding on Sobolev spaces are used in the studies of elliptic [Saloff-Coste 2002; Brezis and Nirenberg 1983] and degenerate elliptic partial differential equations [Chua and Wheeden 2017; Rodney 2010; Sawyer and Wheeden 2006]. For example, boundedness and regularity of solutions can be obtained if the associate operator of equations satisfies some structure conditions [Monticelli et al. 2012; 2015] while existence of solutions can be assured by embedding and compact embedding [Chua and Wheeden 2017]. Indeed, just Sobolev embedding alone (for the associated operator) will lead to boundedness of solutions of degenerate equations [Chua 2017a]. We will study the counterpart of embedding and compact embedding on abstract Sobolev spaces which include degenerate Sobolev spaces (including weighted fractional Sobolev spaces) on irregular domains. We are able to obtain such embeddings for (Borel) measures that need not be doubling nor reverse doubling (on Ω). We will always assume a simple Poincaré-type inequality (1-4) and use it to obtain various Poincaré inequalities via a standard technique of self improving [Franchi et al. 2003; Chua and Wheeden 2008] on (weak) John domains and balls without any chain or geodesic path condition (see Remark 2.8(3)). Such inequalities are then used to obtain embedding and compact embedding on domains which are a countable union of bounded overlapping (weak) John domains with the same parameters (for example, a generalized John domain). We further provide a unified approach for weights that are essentially constant (1-21) on δ-balls (balls that are "deep" inside the domain). In particular, in case of Euclidean spaces, our assumptions turn out to be simple (and sharp) for such an embedding to hold. As applications, we extend many known results in the literature; for example, [Chanillo and Wheeden 1992; Gatto and Wheeden 1989] (see Corollary 1.6, Remark 1.7); Bourgain, Brezis and Mironescu [Bourgain et al. 2002] (that has been improved by Mazya and Shaposhnikova [2002]). For the latter, we extend it to weighted fractional Sobolev inequalities on John domains in Remark 1.7(3). Furthermore, we extend a weighted Sobolev interpolation inequality by Caffarelli, Kohn and Nirenberg [Caffarelli et al. 1984] to a weighted fractional interpolation inequality with much more complicated weights that may not be doubling (see Theorem 1.14).

In what follows, C will denote a generic positive constant while $C(\alpha, \beta, \gamma, \dots)$ will denote a constant that is depending only on $\alpha, \beta, \gamma, \dots$. When μ and w are weights (nonnegative locally integrable Borel measurable functions), by abusing the notation, $d\mu$ and dw will denote the measure $\mu\, dx$ and $w\, dx$ respectively. When Ω is a domain in the Euclidean space, $E^p_w(\Omega)$ will denote the class of locally Lebesgue integrable functions on Ω with weak derivatives in $L^p_w(\Omega)$. We will write $W^{1,p}_w(\Omega) = L^p_w(\Omega) \cap E^p_w(\Omega)$. This space could be just a normed space (it is a Banach space if $w^{-1/(p-1)}$ is locally integrable in Ω [Kufner and Opic 1984]). We will also work on (weighted) fractional Sobolev spaces ($0 < \alpha < 1$)

$$\widehat{W}^{\alpha,p}_w(\Omega) = \left\{ f \in L^1_{\mathrm{loc}}(\Omega) : \|f\|_{\widehat{W}^{\alpha,p}_w(\Omega)} = \left(\int_\Omega \int_{B(x,\rho_\Omega(x)/2)} \frac{|f(x) - f(y)|^p}{|x-y|^{n+\alpha p}}\, dy\, w(x) dx \right)^{1/p} < \infty \right\},$$

where $\rho_\Omega(x) = \inf\{|x-y| : y \in \Omega^c\}$ ($\rho_\Omega(x) = \infty$ if $\Omega^c = \varnothing$). Note that a more common (weighted) fractional Sobolev space is usually defined as

$$W^{\alpha,p}_w(\Omega) = \left\{ f \in L^1_{\mathrm{loc}}(\Omega) : \|f\|_{W^{\alpha,p}_w(\Omega)} = \left(\int_\Omega \int_\Omega \frac{|f(x) - f(y)|^p}{|x-y|^{n+\alpha p}}\, dy\, w(x) dx \right)^{1/p} < \infty \right\}.$$

While it is clear that $W^{\alpha,p}_w(\Omega) \subset \widehat{W}^{\alpha,p}_w(\Omega)$, the converse is in general not true even when $w = 1$ [Dyda et al. 2016]. In Euclidean spaces, we usually assume (Q is any ball in $\mathbb{R}^n$)

$$\frac{1}{|Q|}\|f - f_Q\|_{L^1(Q)} \le a(Q)\|\nabla^\Omega_{\alpha,p} f\|_{L^p_w(Q)}, \quad \text{where } f_Q = \int_Q f\, dx/|Q|, \tag{1-2}$$

$a(Q)$ is a ball set function and $\nabla^\Omega_{\alpha,p} f$ ($0 < \alpha \le 1$) could be either the usual gradient $|\nabla f|$ (when $\alpha = 1$) or the "fractional derivative," that is

$$\nabla_\alpha f(x) = \nabla^\Omega_{\alpha,p} f(x) = \left(\int_{B(x,\rho_\Omega(x)/2)} \frac{|f(x) - f(y)|^p}{|x-y|^{n+\alpha p}}\, dy \right)^{1/p}.$$

For example, when $5Q \subset \Omega$, (1-2) is known to hold for $w = 1$ with $a(Q) = C|Q|^{\alpha/n - 1/p}$ and hence also holds for any weight w with

$$a(Q) = C|Q|^{\alpha/n}\|w^{-1/p}\|_{L^{p'}(Q)}.$$

For $0 < \alpha < 1$, see Remark 1.2(5). The case where $\alpha = 1$ is well-known (for all balls Q).

Equation (1-2) can be used to obtain

$$\|f - f_{B'}\|_{L^q_\mu(\Omega)} \le C\|\nabla_\alpha f\|_{L^p_w(\Omega)}, \tag{1-3}$$

where B' is a "central ball" in Ω (see Theorem 1.8). Hence (if $\mu(\Omega) < \infty$)

$$\|f\|_{L^q_\mu(\Omega)} \le C\big(\|f\|_{L^1(\Omega)} + \|\nabla_\alpha f\|_{L^p_w(\Omega)}\big).$$

Moreover, as (1-3) will always imply the inequality (1-3) with $f_{B'}$ being replaced by $\int_\Omega f\, d\mu/\mu(\Omega)$, we also have

$$\|f\|_{L^q_\mu(\Omega)} \le C\big(\|f\|_{L^1_\mu(\Omega)} + \|\nabla_\alpha f\|_{L^p_w(\Omega)}\big).$$

The case where $d\mu = \operatorname{dist}(x, \Omega_0)^a\, dx$ and $dw = \operatorname{dist}(x, \Omega_0)^b\, dx$, $a \ge 0, b \in \mathbb{R}$, $\alpha = 1$, $\Omega_0 \subset \Omega^c$ has been studied in [Chua and Wheeden 2011] when Ω is an s-John domain ($s \ge 1$). See [Gurka and Opic 1988; 1989; 1991] for some other weights on $C^{0,1/s}$ domains. For negative a and $0 < \alpha < 1$, see [Chua 2016; 2017b]. In this note, we will discuss the case where Ω (an open set in a metric space) is a bounded overlapping countable union of weak John domains (see (1-7)) with a fixed parameter. This includes generalized John domains [Chua 2009, Definition 1.2] which include bounded and unbounded John domains [Väisälä 1989]. We also allow $\Omega_0 \not\subset \Omega^c$ and more complicated weights which may degenerate (0 or ∞) in Ω. Most of the previous studies assumed μ to be doubling or at least reverse doubling; see [Chua and Wheeden 2011; Hajłasz and Koskela 1998; Hurri-Syrjänen 2004]. Indeed, they considered mostly the case $a \ge 0$. Even though there were studies for the case $a < 0$, the weight μ was known to be doubling (i.e., μdx is doubling) [Chua 2009; 1995; Chua and Wheeden 2011]. For simplicity, we discuss only a few typical applications that include the case where the power a may be negative and μ may neither be δ-doubling (see below) nor reverse doubling. In order to overcome this problem, we first observe that a John domain is still John domain after a finite number of points is removed. We then see that the Sobolev space on the resulting smaller domain contains the original Sobolev space.

For simplicity, we will consider mostly metric spaces where Sobolev spaces are well studied [Cheeger 1999; Heinonen 2001; Hajłasz 1996; Keith 2004; Keith and Zhong 2008] instead of quasimetric spaces even though the technique can be extended to quasimetric spaces as in [Chua and Wheeden 2011; Chua et al. 2013; Sawyer and Wheeden 2010]. Indeed, given any quasimetric d, there exists $\varepsilon > 0$ such that d^ε is bi-Lipschitz equivalent to a metric [Heinonen 2001, Proposition 14.5]. Note that our study will also include Alexandrov spaces and Carnot–Carathéodory metric spaces.

Let $0 < \delta \le \frac{1}{2}$ and Ω be an open set in a metric space. $B(x, r)$ or $B_r(x)$ will denote the metric (or quasimetric) ball with center x and radius $r(B) = r$. Furthermore, $CB = CB(x, r)$ will denote the ball $B(x, Cr)$. We say B is a δ-ball of Ω if $B/\delta \subset \Omega$.

We say σ is a δ-doubling measure on Ω if $\sigma(2^k B\cap\Omega)\le(D_\sigma)^k\sigma(B)$ for all δ-balls B of Ω and $k\in\mathbb{N}$. Moreover, we say it is doubling on Ω if the above holds for all balls with center in Ω. We say σ is doubling if it is doubling on the whole metric space. Let w be a Borel measure on Ω and $1\le\tau\le 1/(2\delta)$. We will be interested in (abstract Sobolev space) $\mathfrak{S}\subset L^1_{\sigma,\mathrm{loc}}(\Omega)\times L^p_{w,\mathrm{loc}}(\Omega)$ (or $L^1_{\sigma,\mathrm{loc}}(\Omega)\times L^p_{w,\mathrm{loc}}(\Omega)^n$) that satisfies the following Poincaré-type inequality:

$$\text{(1-4)}\qquad \frac{1}{\sigma(Q)}\|f-f_{Q,\sigma}\|_{L^1_\sigma(Q)}\le a(Q)\|g\|_{L^p_w(\tau Q)}\qquad \text{for all } \delta\text{-balls } Q \text{ of } \Omega \text{ and } (f,g)\in\mathfrak{S},$$

where $f_{Q,\sigma}=\int_Q f\,d\sigma/\sigma(Q)$ and $a(Q)$ is a ball set function (independent of (f,g)). By $f\in L^1_{\sigma,\mathrm{loc}}(\Omega)$, we mean $f\in L^1_\sigma(B)$ for all δ-balls B. The definition will be independent of $\delta\le\frac{1}{2}$ as Ω in this note is assumed to be at most a countable union of bounded overlapping weak John domains Ω_j such that σ is δ-doubling on each Ω_j. Such a simple Poincaré inequality is known to hold in Riemannian manifolds with $g=|\nabla f|$ and Sobolev space on Carnot–Carathéodory metric spaces with Hörmander vector fields [Lu 1992b; 1996; Franchi et al. 1995] with $g=|Xf|$, where X is the "differential operator" associated to the vector field. Indeed, in the later case, it holds with $\sigma=w=1$ and $p=1$ on metric (associated to the vector field) balls. Furthermore, similar to [Chua and Wheeden 2011], for any function f, $b\in\mathbb{R}$ and $\omega>0$, we define (the truncation of $|f-b|$)

$$f_b^\omega=\min\bigl\{\max\{0,|f-b|-\omega\},\omega\bigr\}.$$

We say that $\mathfrak{S}$ satisfies (1-4) with the truncation property if for all $(f,g)\in\mathfrak{S}$, $b\in\mathbb{R}$ and $\omega>0$, there exists $g_b^\omega\in L^p_w(\Omega)$ such that (f_b^ω,g_b^ω) satisfies the inequality (1-4) and

$$\text{(1-5)}\qquad \sup_{\omega>0,b\in\mathbb{R}}\sum_{k=1}^\infty\|g_b^{2^k\omega}\|^p_{L^p_w(\Omega)}\le(c_T)^p\|g\|^p_{L^p_w(\Omega)}\quad(c_T\ge 1).$$

For example, if (1-4) holds for all Lipschitz functions u and their derivative $|\nabla u|$ on a Riemannian manifold, it will satisfy (1-4) with the truncation property. Similarly, when X is a "differential operator" and $g=|Xf|$, (1-4) also holds with the truncation property. A more subtle (and not obvious) example will be the fractional derivatives defined above; see Proposition 2.14. Note that our truncation property seems to be weaker than the truncation property introduced in [Hajłasz and Koskela 2000]. For example, fractional derivatives satisfy our truncation property while it is not clear that they satisfy that of [Hajłasz and Koskela 2000].

Following [Hajłasz and Koskela 2000, p. 39], given $0<c<1$, we say that a domain Ω in a metric space $\langle H,d\rangle$ (or quasimetric space) is a weak John domain if there is a fixed "center" $x'\in\Omega$ such that for any $x\ne x'$ in Ω, there exists

$\gamma : [0, l] \to \Omega$ such that $\gamma(0) = x,\ \gamma(l) = x'$ with

$$d(\gamma(t_1), \gamma(t_0)) \le |t_1 - t_0| \quad \text{for all } t_1, t_0 \in [0, l] \tag{1-6}$$

and γ satisfies the weak John condition

$$d(\gamma(t), \Omega^c) = \inf\{d(\gamma(t), y) : y \notin \Omega\} \ge c\, d(\gamma(t), x) \quad \text{for all } t. \tag{1-7}$$

We will write $\Omega \in J'(c)$. The corresponding definition in [Chua and Wheeden 2008; 2011] replaces (1-7) by $\rho(\gamma(t)) > ct$, which is nominally a stronger assumption since $d(x, \gamma(t)) = d(\gamma(0), \gamma(t)) \le t$ by (1-7). The weak version (1-7) was first given by Väisälä in $\mathbb{R}^n$ [Hajłasz and Koskela 2000, Theorem 9.6; Väisälä 1988, Theorem 2.18] and shown to be equivalent to the strong version in $\mathbb{R}^n$. It was extended to metric spaces in [Hajłasz and Koskela 2000; Chua and Wheeden 2015]. We do not know an example when the weak version is true and the strong version is false. In general, the weak version is easier to apply. See also [Martio and Sarvas 1979] for the definition and studies on John domains in Euclidean spaces. More properties of weak John domains can be found in Section 2 and [Chua and Wheeden 2015, Section 2]. Note also that Lipschitz continuity (1-6) could be replaced by just continuity. We now state the main theorem of this paper. The assumptions may look complicated on general metric spaces, but most of them become simple (and sharp) or redundant on Euclidean spaces.

Theorem 1.1. *Let $1 \le p < q < \infty$. Let Ω be an open set in a metric space H and let $0 < \delta \le \frac{1}{2}$, $1 \le \tau \le 1/(2\delta)$, μ, w, σ be Borel measures on H such that μ is absolutely continuous with respect to σ. Suppose there exists $0 < c < 1$ such that Ω is a countable union of sets $\Omega_j \in J'(c)$ with $\sum_j \chi_{\Omega_j} \le M$, $M \in \mathbb{N}$ and σ is δ-doubling on each Ω_j with doubling constant D_σ independent of j, i.e., $\sigma(2^k B \cap \Omega_j) \le (D_\sigma)^k \sigma(B)$ for all δ-balls B of Ω_j and $k \in \mathbb{N}$. Let $\mathfrak{S} \subset L^1_{\sigma,\mathrm{loc}}(\Omega) \times L^p_{w,\mathrm{loc}}(\Omega)$ satisfy the Poincaré inequality (1-4) with the truncation property (1-5). Suppose there exists a ball set function μ^* with $\mu(B \cap \Omega_j) \le \mu^*(B)$ for all balls B and Ω_j, and*

(i) *μ^* satisfies Condition (R) on each Ω_j* (with parameters independent of j):

Condition (R) *There exist $0 < \theta_1 < \theta_2 < 1$, $A_1, A_2 > 0$ such that for each $x \in \Omega_j$, there is a strictly decreasing sequence $\{r^x_m\}_{m\in\mathbb{N}}$ of positive real numbers such that $r^x_m \to 0$, $r^x_1 = \mathrm{diam}(\Omega_j)$, $r^x_m/2 \le r^x_{m+1} < r^x_m$ and*

$$A_1\theta_1^k \le \frac{\mu^*(B(x, r^x_{m+k}))}{\mu^*(B(x, r^x_m))} \le A_2\theta_2^k \quad \textit{for all } m, k \in \mathbb{N}. \tag{1-8}$$

(ii) *There exists $C_1 > 0$ such that for all j,*

$$\mu^*(B)^{1/q} a(Q) \le C_1 \quad \textit{for all balls } B \textit{ with center in } \Omega_j \textit{ and } Q \subset B,\ Q/\delta \subset \Omega_j \quad \textit{with } r(Q) \ge c\delta r(B)/(4\tau). \tag{1-9}$$

(iii) *There exists $V_\mu \geq 1$ such that for all j, given any collection of balls $\mathcal{B}_E = \{B_{r_x}(x) : x \in E\}$ with $E \subset \Omega_j$, it has a subfamily $\mathcal{B}'_E$ of pairwise disjoint balls such that*

$$\mu(E) \leq V_\mu \sum_{B \in \mathcal{B}'_E} \mu^*(B). \tag{1-10}$$

(We will say (μ, μ^*) satisfies the Vitali-type property on Ω_j with constant V_μ.)

(I) *Then*

$$\|f - f_{B'_j,\sigma}\|_{L^q_\mu(\Omega_j)} \leq C c_T C_1 V_\mu^{1/q} \|g\|_{L^p_w(\Omega_j)} \quad \text{for all } j \text{ and } (f, g) \in \mathfrak{S} \tag{1-11}$$

where $B'_j = B(x'_j, \delta d(x'_j, \Omega_j^c))$, x'_j is the center of Ω_j and C depends on q, p, θ_1, θ_2, A_1, A_2, c, δ, τ and D_σ.

(II)(a) *If in addition $1 \leq p_0 \leq q$ and there exists $C_2 > 0$ such that*

$$\mu(\Omega_j)^{1/q} \leq C_2 \sigma(\Omega_j)^{1/p_0} \quad \text{for all } j, \tag{1-12}$$

then

$$\|f\|_{L^q_\mu(\Omega)} \leq C\big(C_2 M^{1/p_0} \|f\|_{L^{p_0}_\sigma(\Omega)} + C_1 c_T V_\mu^{1/q} M^{1/p} \|g\|_{L^p_w(\Omega)}\big) \tag{1-13}$$

for all $(f, g) \in \mathfrak{S}$ where C depends on p_0 and all those parameters given in (I).

(b) *Furthermore, if $\mu(\Omega) < \infty$, then for every sequence $\{(f_n, g_n)\}$ in $\mathfrak{S}$ such that $\{f_n\}$ and $\{g_n\}$ are bounded in $L^{p_0}_\sigma(\Omega)$ and $L^p_w(\Omega)$ respectively, $\{f_n\}$ has a subsequence that converges in $L^{\tilde{q}}_\mu(\Omega)$ for $1 \leq \tilde{q} < q$ to a function in $L^q_\mu(\Omega)$.*

(c) *If $p_0 < q$ and instead of (1-12), we have*

$$\mu(\Omega_j)^{1/q - 1/p_0} \leq C_2 \quad \text{for all } j, \tag{1-14}$$

then (1-13) and the conclusion in (*a*) *will hold with $L^{p_0}_\sigma(\Omega)$ being replaced by $L^{p_0}_\mu(\Omega)$. Moreover, conclusion in* (*b*) *will hold with σ being replaced by μ* (*if $\mu(\Omega) < \infty$*).

Remark 1.2. (1) If $\mathfrak{S}$ only satisfies (1-4) without the truncation property and $\mu(\Omega_j) \leq C_3 < \infty$ for all j, then (1-13) holds with $\|f\|_{L^q_\mu(\Omega)}$ being replaced by $\|f\|_{L^{\tilde{q}}_\mu(\Omega)}$, $p, p_0 \leq \tilde{q} < q$. Thus, (II)(b) remains true if $\mu(\Omega) < \infty$, i.e., for every sequence $\{(f_n, g_n)\}$ in $\mathfrak{S}$ such that $\{f_n\}$ and $\{g_n\}$ are bounded in $L^{p_0}_\sigma(\Omega)$ and $L^p_w(\Omega)$ respectively, $\{f_n\}$ has a subsequence that converges in $L^{\tilde{q}}_\mu(\Omega)$. A similar conclusion holds for the case $p_0 < q$ under the assumption (1-14) for (II)(c).

(2) The case where μ is reverse doubling on $\Omega \subset \mathbb{R}^n$ has been discussed in [Chua and Wheeden 2011, Remark 1.7(3)] when Ω is an s-John domain; see also [Drelichman and Durán 2008] for 1-John domains.

(3) Condition (1-9) can often be simplified. For example, it can be simplified to

$$\mu^*(Q)^{1/q} a(Q) \le C_1 \quad \text{for all } \delta\text{-balls } Q \tag{1-15}$$

when μ^* is doubling. For more discussion, see [Chua and Wheeden 2011, Remark 1.7(4)].

(4) In particular, (1-11) holds with $\Omega_j = \Omega \in J'(c)$ when μ is δ-doubling, under the assumption (1-4) with the truncation property and $\mu(Q)^{1/q} a(Q) \le C_1$ for all δ-balls Q. Note that in this case μ will satisfy Condition (R) and (μ, μ) will satisfy Vitali-type property (1-10).

(5) In case $\Omega \subset H = \mathbb{R}^n$, $\mathfrak{S} = \{(f, \nabla^{\Omega}_{\alpha,p} f) : f \in \mathfrak{S}_\alpha(\Omega), \nabla^{\Omega}_{\alpha,p} f \in L^p_w(\Omega)\}$, where $\mathfrak{S}_\alpha(\Omega) = L^1_{\mathrm{loc}}(\Omega)$ for $0 < \alpha < 1$ and $\mathfrak{S}_1(\Omega) = \mathrm{Lip}_{\mathrm{loc}}(\Omega)$ the space of locally Lipschitz continuous functions on Ω, then (1-4) is known to hold with $d\sigma = dx$, $g = \nabla^{\Omega}_{\alpha,p} f$ (see (1-2)), w a Muckenhoupt A_p weight ($w \in A_p$) and $a(Q) = C_w r(Q)^\alpha w(Q)^{-1/p}$ ($C_w = C(w)$). Indeed, it holds for general weight w with

$$a(Q) = C r(Q)^{\alpha - n} \|w^{-1/p}\|_{L^{p'}(Q)} \quad (\text{where } 1/p + 1/p' = 1)$$

provided $\|w^{-1/p}\|_{L^{p'}(Q)} < \infty$. The case $\alpha = 1$ is well-known. For $0 < \alpha < 1$, first observe that

$$\begin{aligned} \frac{1}{|Q|}\|f - f_Q\|_{L^1(Q)} &\le \frac{1}{|Q|}\int_Q \frac{1}{|Q|}\int_Q |f(x) - f(y)|\,dy\,dx \\ &\le |Q|^{-1-1/p}\int_Q \left(\int_Q |f(x) - f(y)|^p\,dy\right)^{1/p} dx \\ &\le C|Q|^{\alpha/n - 1}\int_Q \left(\int_Q \frac{|f(x) - f(y)|^p}{|x-y|^{n+\alpha p}}\,dy\right)^{1/p} dx. \end{aligned} \tag{1-16}$$

Now if Q is any ball with $5Q \subset \Omega$, then $Q \subset B(x, \rho(x)/2)$ for all $x \in Q$. Finally, just apply Hölder's inequality again. Some other discussion on fractional Poincaré inequalities can be found in [Chua 2016; Mazya and Shaposhnikova 2002; Bourgain et al. 2002]. Moreover, if $\alpha = 1$, $w = |J_\phi|^{1-p/n}$, $1 < p < n$, where J_ϕ is the Jacobian of a quasiconformal map ϕ, (1-4) is known to be true with $d\sigma = dw$ and $a(Q) = C r(Q) w(Q)^{-1/p}$ [Heinonen et al. 1993, p. 10].

In case where $\mu = w \in A_p$ and $\alpha = 1$, compact embedding has already been discussed in [Chua et al. 2013, Theorem 2.2] when $\Omega \subset \mathbb{R}^n$ is a John domain.

(6) When X is a "differential operator" such that

$$\frac{1}{\sigma(Q)}\|f - f_{Q,\sigma}\|_{L^1_\sigma(Q)} \le a(Q)\|Xf\|_{L^p_w(\tau Q)} \tag{1-17}$$

for all $f \in \mathrm{Lip}_{\mathrm{loc}}(\Omega)$ and δ-balls Q, then Theorem 1.1 applies to any doubling measure μ such that $\mu(Q)^{1/q} a(Q) \le C$. For example, when a domain is equipped with Carnot–Carathéodory metric and X associated with a Hölmander's vector field, (1-17) is known to hold with $w = \sigma = 1$ and $p = 1$ by [Jerison 1986]; see [Franchi et al. 1995] for more literature review. Indeed, a complete study can be found in [Franchi et al. 1995] when weights are in (Muckenhaupt) A_p. We are able to reproduce all results in [Franchi et al. 1995] by Theorem 1.1 since the Carnot–Carathéodory metric balls are known to be Boman domains [Lu 1994, Lemma 3.1] and (1-17) is known to hold when $\sigma = 1$ and $w \in A_p$ with $a(Q) = Cr(Q)w(Q)^{-1/p}$. In particular, we obtain [Franchi et al. 1995, Theorem 2] with $\mu = w_2$ and $w_1 = w$. However, instead of assuming $w \in A_p$ together with the balance condition [Franchi et al. 1995, (1.5)], we only need to assume that μ is doubling and

$$\mu(Q)^{1/q} r(Q) \|w^{-1/p}\|_{L^{p'}(Q)} \leq C \quad \text{for all } \delta\text{-balls in a given ball } B.$$

On the other hand, if we take $\mu = w \in A_p$, we then obtain the compact embedding given in [Lu 1992a, Lemmas 2.6, 2.9 and Corollary 2.10], where it uses a quite complicated method involving lifting and the Ascoli theorem. Indeed, it will follow from our theorem that if $\mathcal{D}$ is a finite union of sets $\Omega_j \in J'(c)$, then the embedding $W^{1,p}_w(\mathcal{D})$ to $L^q_w(\mathcal{D})$ is compact for $1 \leq q < d/(d-1)$ (where d is the homogeneous dimension of the Carnot–Carathéodory metric) when $p = 1$ and $1 \leq q \leq dp/(d-1) + \varepsilon$ for some $\varepsilon > 0$ depending on w when $1 < p < d$. Furthermore, when $w \in A_1$, the embedding of $W^{1,p}_w(\mathcal{D})$ to $L^q_w(\mathcal{D})$ is compact for $1 \leq q < dp/(d-p)$. To see that, it suffices to note that $w \in A_1$ implies $w \in A_p$ and

$$w(\tau B) \leq C\tau^d w(B) \quad \text{for any ball } B \text{ and } \tau > 1, \tag{1-18}$$

and hence if $B_r(x)$ is a δ-ball in a John domain $\mathcal{D}$ and $R = \operatorname{diam}(\mathcal{D})$, then

$$w(B_r(x))^{1/q} r w(B_r(x))^{-1/p} \leq C w(B_R(x))^{1/q-1/p} (r/R)^{d/q-d/p} r.$$

The above is bounded if $d/q - d/p + 1 \geq 0$. The claim will now follow from Theorem 1.1. The rest of our observations can be done similarly. Furthermore, in view of our theorem, we only need w to be A_p restricted to just δ-balls in the domain and (1-18) instead of assuming $w \in A_1$. A similar conclusion can be extended to weighted fractional Poincaré inequalities (see Theorem 1.8). In particular in $\mathbb{R}^n$, taking $w = 1$, we have the classical Rellich compact embedding. Note that some studies on certain nonsmooth domains using a quasi-isometrical homeomorphism can be found in [Goldshtein and Ukhlov 2009] for A_p weights.

(7) A not so refined Condition (R) was introduced in [Chua and Wheeden 2011, (1-5)] where it was assumed without constants A_1, A_2. The present Condition (R) appears to be weaker and easier to verify than that of [Chua and Wheeden 2011]. It is easy to see that a "reverse doubling weight" (on $\mathbb{R}^n$) will induce a ball set

function that satisfies Condition (R). For more discussion, see [Chua and Wheeden 2011, Remark 1.7(2)]. Indeed, in general, μ^* satisfies Condition (R) on $\Omega \subset \mathbb{R}^n$ if $\mu^* : \Omega \times \operatorname{diam}(\Omega) \to \mathbb{R}$ (written usually as $\mu^*(B_r(x))$) is positive continuous and reverse doubling (i.e., there exists $R_C > 1$ such that $\mu^*(B_{2r}(x)) \geq R_C \mu^*(B_r(x))$ for all $r \leq \operatorname{diam}(\Omega)/2$ and $x \in \Omega$); see [Chua and Wheeden 2011, Remark 1.7(2)] when μ^* is a measure. The assumption $r_1^x = \operatorname{diam}(\Omega)$ is not essential. Indeed we need only that $\mu(\Omega) \leq C\mu^*(B(x, r_1^x))$ for all $x \in \Omega$.

(8) If μ^* satisfies Condition (R) on Ω, then for any fixed $0 < \delta \leq \frac{1}{2}$,

$$\lim_{r \to 0} \sup\bigl\{\mu^*(B_r(x)) : x \in \Omega,\, B_r(x) \text{ is a } \delta\text{-ball of } \Omega\bigr\} = 0.$$

(9) If either the Besicovitch covering property holds or μ (or μ^*) is doubling, then (μ, μ^*) will satisfy the Vitali-type property. In particular, in $\mathbb{R}^n$, (μ, μ) (and hence (μ, μ^*)) will always satisfy the Vitali-type property (with parameter depending only on n) by Besicovitch covering.

(10) In general, for any Borel measure μ, by the triangle inequality and Hölder's inequality, if $\mathcal{D}' \subset \mathcal{D}$ with $\mu(\mathcal{D}') > 0$, then (for any constant C)

$$\begin{aligned} \|f - f_{\mathcal{D}',\mu}\|_{L^q_\mu(\mathcal{D})} &\leq \|f - C\|_{L^q_\mu(\mathcal{D})} + \mu(\mathcal{D})^{1/q} |f_{\mathcal{D}',\mu} - C| \\ &\leq \|f - C\|_{L^q_\mu(\mathcal{D})} + \frac{\mu(\mathcal{D})^{1/q}}{\mu(\mathcal{D}')^{1/q}} \biggl(\int_{\mathcal{D}'} |f - C|^q \, d\mu\biggr)^{1/q} \\ &\leq \bigl(1 + (\mu(\mathcal{D})/\mu(\mathcal{D}'))^{1/q}\bigr) \|f - C\|_{L^q_\mu(\mathcal{D})}. \end{aligned} \tag{1-19}$$

Applying the above to (1-11) with $\mathcal{D} = \Omega_j$ and $C = f_{B'_j,\sigma}$, we have

$$\|f - f_{\mathcal{D}',\mu}\|_{L^q_\mu(\mathcal{D})} \leq C c_T C_1 V_\mu^{1/q} \bigl(1 + (\mu(\mathcal{D})/\mu(\mathcal{D}'))^{1/q}\bigr) \|g\|_{L^p_w(\mathcal{D})}, \tag{1-20}$$

for all $(f, g) \in \mathfrak{S}$ and $\mathcal{D}' \subset \mathcal{D}$ with $\mu(\mathcal{D}') > 0$.

Next we will consider weighted versions of Theorem 1.1. We will be interested in weights ρ being essentially constant on δ-balls of Ω, i.e., for all δ-balls of Ω,

$$\bar{\rho}(B) = \sup\{\rho(y) : y \in B\} \leq C(\rho, \delta)\rho(x) \quad \text{for all } x \in B.$$

Furthermore, as we always assume $\delta \leq \frac{1}{2}$, we have

$$\bar{\rho}(B) \leq e_\rho \rho(x) \quad \text{for all } x \in B \text{ with } 2B \subset \Omega. \tag{1-21}$$

Indeed, many weights that have been studied in the literature satisfy (1-21). Let us look at some examples.

Example 1.3. (i) (1-21) holds if $\rho(x) = \inf\{d(x, y) : y \in \Omega_0\}$, with $\Omega_0 \subset \Omega^c$. In general, it holds if

$$\rho(x) = \prod_{i=1}^{l} \eta_i(x)^{\alpha_i} \prod_{i=l+1}^{l'} \left(\frac{\eta_i(x)}{1+\eta_i(x)}\right)^{\alpha_i} \prod_{i=l'+1}^{l''} (1+\eta_i(x))^{\alpha_i}, \tag{1-22}$$

where $\eta_i(x) = d(x, S_i) = \inf\{d(x, y) : y \in S_i\}$ with $S_i \subset \Omega^c$. A special case in $\mathbb{R}^n$,

$$(1+|x|)^{\alpha_0} \prod_{i=1}^{l} \left(\frac{|x-z_i|}{1+|x-z_i|}\right)^{\alpha_i}, \quad l \in \mathbb{N},\ \alpha_i \geq 0,\ z_i \in \mathbb{R}^n, \tag{1-23}$$

has been considered in [Chanillo and Wheeden 1992; Gatto and Wheeden 1989]; see Remark 1.7.

(ii) We say $\Psi : [0, \infty) \to [0, \infty)$ is doubling if it is a monotone increasing continuous function such that there exists $C_\Psi > 1$ with $\Psi(2t) \leq C_\Psi \Psi(t)$ for all $t > 0$. Then

$$\rho(x) = \prod_{i=1}^{l} \Psi_i(\eta_i(x))^{\alpha_i}, \quad \alpha_i \in \mathbb{R},\ \alpha_i \neq 0, \tag{1-24}$$

will satisfy (1-21) if all Ψ_i are doubling and η_i are as in (1-22). In particular, when $\alpha_i > 0$ for all i in (1-24), if μ is δ-doubling on Ω with doubling constant D_μ, then $\rho d\mu$ is δ-doubling on Ω with doubling constant $C\big(\{\alpha_i, C_{\Psi_i}\}_{i=1}^{l}\big) D_\mu$. Thus, weights in (1-23) are clearly δ-doubling (indeed, they are doubling on $\mathbb{R}^n$). In general, we will let $I^- = \{i : \alpha_i < 0\}$ and I^+ be its complement. Then we know $\prod_{i \in I^+} \Psi_i(\eta_i(x))^{\alpha_i}$ is doubling on Ω.

(iii) In case $H = \mathbb{R}^n$ and S_i's are finite and disjoint (i.e., $S_i \cap S_j = \varnothing$ for $i \neq j$). Let

$$\rho(x) = \prod_{i=1}^{l} d(x, S_i)^{a_i}, \quad -n < a_i < 0 \quad \text{for all } i.$$

Then $\rho\, dx$ is δ-doubling on any bounded domain; see Proposition A.4. However, this weight is neither doubling nor reverse doubling on any unbounded domain when $\sum a_i < -n$ as $\rho(\mathbb{R}^n) = \int_{\mathbb{R}^n} \rho(x)\, dx < \infty$.

(iv) In $\mathbb{R}^n$ (or other "nice" metric spaces), we do not need to assume $\bigcup_{i=1}^{l} S_i \subset \Omega^c$ (if S_i's are finite) since we can consider $\Omega \setminus \bigcup_{i=1}^{l} S_i$ in view of the fact that a weak John domain with finitely many points being removed is still a weak John domain by Proposition 2.9.

Theorem 1.4. *Let Ψ_i be as in Example 1.3*(ii) *and η_i be as in (1-22). Let $\bar{\eta}_i(B) = \sup\{\eta_i(x) : x \in B\}$ and*

$$\rho_1(x) = \prod_{i=1}^{l} \Psi_i(\eta_i(x))^{a_i}, \quad \rho_2(x) = \prod_{i=1}^{l} \Psi_i(\eta_i(x))^{b_i}, \quad \rho_0(x) = \prod_{i=1}^{l} \Psi_i(\eta_i(x))^{\gamma_i}$$

with $a_i, b_i, \gamma_i \in \mathbb{R}$, $a_i > 0$ for all i. Under the assumption of Theorem 1.1(I), *except that (1-9) in condition* (ii) *is being replaced by*

$$\text{(1-25)}\quad \textit{for each } j, \quad \mu^*(B)^{1/q} a(Q) \prod_{i=1}^{l} \Psi_i(\bar{\eta}_i(Q))^{a_i/q - b_i/p} \le C_1$$
$$\textit{for all balls } B \textit{ with center in } \Omega_j$$
$$\textit{and balls } Q \subset B,\ Q/\delta \subset \Omega_j \textit{ with } r(Q) \ge c\delta r(B)/(4\tau);$$

and the Vitali-type property holds for $(\rho_1\mu, \mu_a^*)$ *on each* Ω_j $\big($where $\mu_a^*(B) = \mu^*(B)\prod_{i=1}^{l}\Psi_i(\bar{\eta}_i(B))^{a_i}\big)$ *instead of (1-10).*

(I) *Then* (denoting $\rho_1\, d\mu$ by $\rho_1\mu$ and similarly for $\rho_0\, d\sigma$ and $\rho_2\, dw$)

$$\text{(1-26)}\qquad \|f - f_{B'_j,\sigma}\|_{L^q_{\rho_1\mu}(\Omega_j)} \le C c_T C_1 V_\mu^{1/q} \|g\|_{L^p_{\rho_2 w}(\Omega_j)} \quad \textit{for all } j,$$

where the constant C depends also on $\{a_i, b_i, C_{\Psi_i}\}_{i=1}^{l}$ besides those listed in Theorem 1.1 for (1-11).

(II)(a) *If (1-12) is being replaced by* (*again* $1 \le p_0 \le q$)

$$\text{(1-27)}\qquad \mu(\Omega_j)^{1/q}\sigma(\Omega_j)^{-1/p_0} \prod_{i=1}^{l} \Psi_i(\bar{\eta}_i(B'_j))^{a_i/q - \gamma_i/p_0} \le C_2 \quad \textit{for all } j,$$

then

$$\text{(1-28)}\qquad \|f\|_{L^q_{\rho_1\mu}(\Omega)} \le C\big(C_2 M^{1/p_0}\|f\|_{L^{p_0}_{\rho_0\sigma}(\Omega)} + C_1 c_T V_\mu^{1/q} M^{1/p}\|g\|_{L^p_{\rho_2 w}(\Omega)}\big)$$

for all $(f, g) \in \mathfrak{S}$ where C depends on $\{C_{\Psi_i}, a_i, b_i, \gamma_i\}_{i=1}^{l}$ besides those parameters listed in Theorem 1.1.

(b) *Furthermore, if $\rho_1\mu(\Omega) < \infty$, then for every sequence $\{(f_n, g_n)\}$ in $\mathfrak{S}$ such that $\{f_n\}$ and $\{g_n\}$ are bounded in $L^{p_0}_{\rho_0\sigma}(\Omega)$ and $L^p_{\rho_2 w}(\Omega)$ respectively, $\{f_n\}$ has a subsequence that converges in $L^{q_0}_{\rho_1\mu}(\Omega)$ for $1 \le q_0 < q$ to a function in $L^q_{\rho_1\mu}(\Omega)$.*

(c) *If $\rho_1\mu(\Omega_j)^{1/q-1/p_0} \le C_2$ instead of (1-27)* (*and* $1 \le p_0 < q$), *then similar conclusions hold as in part* (*a*) *and* (*b*) *with $L^{p_0}_{\rho_0\sigma}(\Omega)$ being replaced by $L^{p_0}_{\rho_1\mu}(\Omega)$.*

Remark 1.5. Similarly, if we only assume (1-4) holds without the truncation property, then for any $1 \le q_0 < q$, any $L^{p_0}_{\rho_0\sigma}(\Omega) \times L^p_{\rho_2 w}(\Omega)$ bounded sequence $\{(f_n, g_n)\}$ in $\mathfrak{S}$ has a subsequence $\{f_{n_k}\}$ that converges in $L^{q_0}_{\rho_1\mu}(\Omega)$ provided $\rho_1\mu(\Omega) < \infty$; see Remark 1.2(1).

As mentioned earlier, assumptions become simpler and sharp in $\mathbb{R}^n$. In particular, the following is an extension of [Chanillo and Wheeden 1992, Theorem 1; Gatto and Wheeden 1989, Corollary 1.4].

Corollary 1.6. *Let $\Omega \in J'(c)$ $(0 < c < 1)$, $\Omega \subset \mathbb{R}^n$, $1 \le p < q < \infty$, $w \in A_p$ and $v = \rho w$ such that ρ is essentially constant on δ-balls of Ω (1-21). Suppose μ is* *any Borel measure such that there is a doubling ball set function* μ^* (with doubling constant D_μ^*) *with* $\mu(B\cap\Omega)\le\mu^*(B)$ *for all balls* B *with center in* Ω*. If*

$$\mu^*(B)^{1/q}|B|^{\alpha/n}\le C_1^* v(B)^{1/p}\quad \textit{for all } \delta\textit{-balls in } \Omega, \tag{1-29}$$

then for all $f\in\widehat{W}_v^{\alpha,p}(\Omega)$ *when* $0<\alpha<1$ $(f\in E_v^p(\Omega)$ *when* $\alpha=1)$, *we have*

$$\|f-f_{B'}\|_{L_\mu^q(\Omega)}\le C(c,p,q,n,D_\mu^*)e_\rho^{1/p}C_1^*C_w\|\nabla_{\alpha,p}^\Omega f\|_{L_v^p(\Omega)}, \tag{1-30}$$

where B' *is the "central" ball of* Ω (see Remark 1.2(5) for C_w) *and hence*

$$\|f-f_{\Omega,\mu}\|_{L_\mu^q(\Omega)}\le C(c,p,q,n,D_\mu^*)e_\rho^{1/p}C_1^*C_w\|\nabla_{\alpha,p}^\Omega f\|_{L_v^p(\Omega)}. \tag{1-31}$$

Moreover, *if* $\mathcal{D}\in J(c,\infty)$ *is a generalized John domain* [Chua 2009, Definition 1.2] *such that* (1-29) *holds for all* δ*-balls in* $\mathcal{D}$, *and*

$$\lim_{r\to\infty}\inf\{\mu(B_r(x)):x\in\mathcal{D}\}=\infty, \tag{1-32}$$

then for all $1\le p_0<q,\ f\in L^{p_0}(\mathcal{D})\cap E_v^p(\mathcal{D})$ *if* $\alpha=1$, $(L^{p_0}(\mathcal{D})\cap\widehat{W}_v^{\alpha,p}(\mathcal{D})$ if $0<\alpha<1)$,

$$\|f\|_{L_\mu^q(\mathcal{D})}\le C(c,p,q,n)e_\rho^{1/p}C_1^*C_w\|\nabla_{\alpha,p}^{\mathcal{D}} f\|_{L_v^p(\mathcal{D})}. \tag{1-33}$$

Proof. We will use Theorem 1.1 with $d\sigma=dx$, the Lebesgue measure and $\delta=\frac{1}{5}$. It is clear that (μ,μ^*) satisfies the Vitali-type property (1-10). Next, since $w\in A_p$, we have the Poincaré inequality (1-2) with $a(Q)=C_w|Q|^{\alpha/n}w(Q)^{-1/p}$ $(C_w=C(w))$ for all balls Q with $5Q\subset\Omega$; see Remark 1.2(5). Next, since ρ is essentially constant on δ-balls of Ω, we have for all δ-balls Q of Ω,

$$\frac{1}{|Q|}\|f-f_Q\|_{L^1(Q)}\le C(n)e_\rho^{1/p}C_w|Q|^{\alpha/n}v(Q)^{-1/p}\|\nabla_{\alpha,p}^\Omega f\|_{L_v^p(Q)}. \tag{1-34}$$

Let $\mathfrak{S}=\{(f,g): f\in\mathfrak{S}_\alpha(\Omega),\nabla_{\alpha,p}^\Omega f\in L_v^p(\Omega)\}$ (see Remark 1.2(5)). Then $\mathfrak{S}$ satisfies (1-4) (with $d\sigma=dx$, $\tau=1$, $w=v$) with the truncation property by Proposition 2.14. Next, (1-29) implies (1-9) with $C_1=C(D_\mu^*)C_we_\rho^{1/p}C_1^*$ as μ^* is doubling. Indeed,

$$\mu^*(Q)^{1/q}|Q|^{\alpha/n}v(Q)^{-1/p}\le C(D_\mu^*)C_1^*.$$

Moreover, (1-8) holds with $A_1,A_2,\theta_1,\theta_2$ depending on D_μ^* $(r_m^x=\operatorname{diam}(\Omega)/2^{m-1})$. Furthermore, (1-10) holds with $V_\mu=C(D_\mu^*)$. We can then conclude (1-30) for $f\in\mathfrak{S}_\alpha(\Omega)$ by Theorem 1.1(I). For $\alpha<1$, it is then clear that (1-30) holds for $f\in\widehat{W}_v^{\alpha,p}(\Omega)$. For $\alpha=1$, first recall that for any ball B,

$$\|f-f_{B,w}\|_{L_w^p(B)}\le C_w|B|^{1/n}\|\nabla f\|_{L_w^p(B)}\quad\text{for } f\in E_w^p(\Omega) \text{ as } w\in A_p.$$

By Propositions 2.12 and 2.11, we conclude by a density argument that (1-30) holds for all $f\in E_v^p(\Omega)$. Next, (1-30) implies (1-31) by Remark 1.2(10). For the second assertion, note that as $\mathcal{D} \in J(c, \infty)$, for all $K > 0$, there exists $\{\Omega_j^K\} \subset J'(c)$ such that $\operatorname{diam}(\Omega_j^K) \sim K$, "center ball" B_j^K of Ω_j^K with $r(B_j^K) \sim K$, $\bigcup \Omega_j^K = \mathcal{D}$ and $\sum \chi_{\Omega_j^K} \le M = C(n)$. From the first part, we have (1-31) for $\Omega = \Omega_j^K$ for each j. Hence by the triangle inequality and Hölder's inequality, (and $\nabla_{\alpha,p}^{\Omega_j^K} f \le \nabla_{\alpha,p}^{\mathcal{D}} f$)

$$\|f\|_{L^q_\mu(\Omega_j^K)} \le \mu(\Omega_j^K)^{1/q-1/p_0} \|f\|_{L^{p_0}_\mu(\Omega_j^K)} + C(c, n, p, q, D^*_\mu) e_\rho^{1/p} C_w C_1^* \|\nabla_{\alpha,p}^{\mathcal{D}} f\|_{L^p_v(\Omega_j^K)}.$$

Now using the fact that $q \ge p_0$, p and summing up the above with respect to j, we have

$$\|f\|^q_{L^q_\mu(\mathcal{D})} \le 2^{q-1} M \left(\sup_j \mu(\Omega_j^K)^{1-q/p_0} \|f\|^q_{L^{p_0}_\mu(\mathcal{D})} + C \|\nabla_{\alpha,p}^{\mathcal{D}} f\|^q_{L^p_v(\mathcal{D})} \right).$$

Letting $K \to \infty$, we conclude (1-33) by (1-32). □

Remark 1.7. (1) In [Chanillo and Wheeden 1992; Gatto and Wheeden 1989], ρ has been assumed to be a very special case (1-23) while we allow any general weight that is essentially constant on δ-balls and we only assume (1-29) for δ-balls. Moreover, [Chanillo and Wheeden 1992] only consider Ω to be balls, $p > 1$, $\alpha = 1$ and μ is doubling. By using Corollary 1.6, we are able to extend the weight ρ to (1-22) with each S_i consisting of finitely many points. However, we need to observe that $\Omega = B \setminus \left(\bigcup_{i=1}^{l''} S_i\right) \in J'(c)$ for some fixed constant c depending only the total number of distinct points in $\bigcup_{i=1}^{l''} S_i$ (Proposition 2.9) and the fact that ρ is essentially constant on δ-balls of Ω. Hence (1-30) will hold with $\alpha = 1$ for balls B if we assume the following balanced condition (given in [Chanillo and Wheeden 1992]):

$$\left(\frac{|Q|}{|B|}\right)^{1/n} \left(\frac{\mu(Q)}{\mu(B)}\right)^{1/q} \le C \left(\frac{v(Q)}{v(B)}\right)^{1/p} \tag{1-35}$$

for all δ-balls Q in $B \setminus \left(\bigcup_{i=1}^{l''} S_i\right)$ (instead of all balls Q in B given in [Chanillo and Wheeden 1992]). Next, as $\mathbb{R}^n \setminus \left(\bigcup_{i=1}^{l''} S_i\right) \in J(c, \infty)$ [Chua 2009, Proposition 2.24], we obtain [Gatto and Wheeden 1989, Corollary 1.4].

(2) It has been observed that if both μ and v are doubling, $\alpha = 1$ and Ω is a ball, then (1-35) is indeed necessary for (1-31) to hold for all Lipschitz continuous functions [Chanillo and Wheeden 1992]; see also [Chanillo and Wheeden 1985, p. 1192]. Note that (for $\alpha = 1$) it is enough to assume only $\mu = \mu^*$ is doubling without assuming v be doubling so that (1-29) is necessary for (1-31) to hold for all Lipschitz continuous functions. To this end, first observe that when μ is doubling, suppose f is a Lipschitz function that vanishes on a δ-ball $B_0 \subset \Omega$, by (1-19),

taking $\mathcal{D}' = B_0$ and $\mathcal{D} = \Omega$, (1-31) will imply
(1-36)
$$\|f\|_{L^q_\mu(\Omega)} \le C(c, p, q, n, D^*_\mu) e_\rho^{1/p} C_1^* C_w \left(1 + \left(\frac{\mu(\Omega)}{\mu(B_0)}\right)^{1/q}\right) \|\nabla^\Omega_{\alpha,p} f\|_{L^p_v(\Omega)}.$$

We now fix a Lipschitz function $\phi(x)$ on $[0, \infty)$ such that $\chi_{[0,1/2]} \le \phi \le \chi_{[0,1]}$ with $\phi(x) = 2 - 2x$ on $\left[\frac{1}{2}, 1\right]$. Given any δ-ball B in Ω, by translation, we may assume 0 is the center of B. Let $f(x) = \phi(|x|/r)$, where $r = r(B)$. Then f vanishes outside B. In particular, it vanishes on a ball $\widetilde{B}$ such that $\Omega \subset C(c, \delta)\widetilde{B}$. Hence by (1-36) and (1-31), we have

$$\mu(B/2)^{1/p} \le C r^{-1} v(B)^{1/q} \quad (\text{if } \alpha = 1).$$

Since μ is doubling, we have (1-29) with $\mu^* = \mu$. Unfortunately, for $0 < \alpha < 1$, the same method only produces (1-29) for δ-balls with radius comparable to $\rho_\Omega(x_B)$ (x_B is the center of B). This is not really surprising in view of the definition of our fractional Sobolev norm.

(3) For $0 < \alpha < 1$, we can extend a result of Bourgain, Brezis, and Mironescu. In [Bourgain et al. 2002], they discuss what happens in the fractional Poincaré inequality on unit cubes when $\alpha \to 1$. Recall that in [Mazya and Shaposhnikova 2002, Corollary 2 (see also the Erratum)] when $\alpha p < n$, $\frac{1}{p^*} = \frac{1}{p} - \frac{\alpha}{n}$, Q is a unit cube in $\mathbb{R}^n$ and $f \in L^1(Q)$,

$$\text{(1-37)} \quad \|f - f_Q\|^p_{L^{p^*}(Q)} \le C(n, p) \frac{1-\alpha}{(n - \alpha p)^{p-1}} \|f\|^p_{W^{\alpha,p}(Q)} = C(n, p) \frac{1-\alpha}{(n - \alpha p)^{p-1}} \int_Q \int_Q \frac{|f(x) - f(y)|^p}{|x - y|^{n+\alpha p}} \, dy \, dx.$$

Hence by dilation, for any cube Q, we have by Jensen's inequality,

$$\text{(1-38)} \quad \left(\frac{1}{|Q|} \|f - f_Q\|_{L^1(Q)}\right)^p \le \left(\frac{1}{|Q|}\right)^{p/p^*} \|f - f_Q\|^p_{L^{p^*}(Q)} \le C(n, p) |Q|^{\frac{\alpha p}{n} - 1} \frac{1-\alpha}{(n - \alpha p)^{p-1}} \|f\|^p_{W^{\alpha,p}(Q)}.$$

Now let $\Omega \in J'(c)$. and suppose ρ is a weight that is essentially constant on δ-balls of Ω (1-21). As cubes are metric balls under the metric

$$d_\infty(x, y) = \max_{1 \le i \le n} \{|x_i - y_i|\},$$

for easy computation, we will use this metric instead of the Euclidean metric. Then $Q \subset B(x, \rho_\Omega(x)/2)$ for all $x \in Q$ whenever $5Q \subset \Omega$. Using (1-21) for ρ, we have

$$\text{(1-39)} \quad \frac{1}{|Q|} \|f - f_Q\|_{L^1(Q)} \le \left(C(n) |Q|^{\alpha p/n} \rho(Q)^{-1} e_\rho \frac{1-\alpha}{(n-\alpha p)^{p-1}}\right)^{1/p} \|\nabla^\Omega_{\alpha,p} f\|_{L^p_\rho(Q)}.$$

If we assume that $\mu(Q)^{1/q}\rho(Q)^{-1/p}|Q|^{\alpha/n} \le C_*$ (with $q > p$) for all cubes Q with $5Q \subset \Omega$ and μ is doubling with doubling constant D_μ, then we can use Theorem 1.4 (by similar argument as in the proof of Corollary 1.6) to get

$$\begin{aligned}\text{(1-40)}\quad \|f - f_{Q'}\|^p_{L^q_\mu(\Omega)} &\le C(n, c, p, q, D_\mu)e_\rho(C_*C_w)^p \frac{1-\alpha}{(n-\alpha p)^{p-1}}\|f\|^p_{\widehat{W}^{\alpha,p}_\rho(\Omega)} \\ &= C(n, c, p, q, D_\mu)e_\rho(C_w C_*)^p \frac{1-\alpha}{(n-\alpha p)^{p-1}} \\ &\quad \times \int_\Omega \int_{B(x,\rho_\Omega(x)/2)} \frac{|f(x)-f(y)|^p}{|x-y|^{n+\alpha p}}\, dy\, \rho(x)dx,\end{aligned}$$

where Q' is the "central cube" in Ω. Thus, we have extended the results of [Mazya and Shaposhnikova 2002; Bourgain et al. 2002] to weighted fractional Sobolev inequalities on John domains. Again, by Remark 1.2(10) we can replace $f_{Q'}$ in (1-40) by $f_{\Omega,\mu}$.

We now discuss applications on $\mathbb{R}^n$. As mentioned earlier, conditions are now simpler and mostly sharp.

Theorem 1.8. (I) *Let* $\Omega \subset \mathbb{R}^n$, $\Omega \in J'(c)$ (hence a John domain), $0 < c < 1$. *Let* $1 \le p < q < \infty$. *Let* $\Omega_0 \subset \Omega^c$ *and define* $\rho(x) = d(x, \Omega_0) = \inf\{|x - y| : y \in \Omega_0\}$. *Let* $\mathfrak{S}_\alpha(\Omega)$ *be as in Remark 1.2*(5). *Let* w *be a weight on* Ω *and* $0 < \alpha \le 1$ *such that the Poincaré inequality* (1-2) *holds for all balls* Q *with* $2Q \subset \Omega$ *and* $f \in \mathfrak{S}_\alpha(\Omega)$. *Suppose* $C_* > 0$, $\beta \in \mathbb{R}$ *such that*

$$\text{(1-41)}\qquad a(Q) \le C_* r(Q)^\beta \quad \textit{for all balls } Q \textit{ with } 2Q \subset \Omega.$$

Suppose μ *is another weight on* $\mathbb{R}^n$ *such that there exist* $C_\mu, N > 0$ *with*

$$\text{(1-42)}\qquad \mu(B \cap \Omega) \le C_\mu r(B)^N \quad \textit{for all balls } B.$$

Let $a \ge 0$, $b \in \mathbb{R}$. *We define* $\mu_a(E) = \int_E \rho(x)^a\, d\mu$ *and* w_b *similarly. Suppose*

$$\text{(1-43)}\qquad \beta + \frac{N}{q} + \min\Big\{0, \frac{a}{q} - \frac{b}{p}\Big\} \ge 0.$$

Then

$$\text{(1-44)}\qquad \|f - f_{B'}\|_{L^q_{\mu_a}(\Omega)} \le C C_* C_\mu^{1/q} \bar{\rho}(\Omega)^{\beta+(N+a)/q-b/p} \|\nabla^\Omega_{\alpha,p} f\|_{L^p_{w_b}(\Omega)}$$

for all $f \in \mathfrak{S}_\alpha(\Omega)$, *where* $f_{B'} = \int_{B'} f\, dx/|B'|$, $B' = B(x', d(x', \Omega^c)/4)$, x' *is the center of* Ω *where* C *depends only on* c, N, n, p, q, a, b *and* β.

(II) *Suppose* $\mathcal{D}$ *is a countable union of* $\Omega_j \in J'(c)$ $(0 < c < 1$ *is fixed*) *such that* $\sum_j \chi_{\Omega_j} \le M$, $M \in \mathbb{N}$ *and* $M_1 \le |\Omega_j| \le M_2$ *for all* j, $M_1, M_2 > 0$. *Assume* $\Omega_0 \subset \mathcal{D}^c$

and

$$\text{(1-45)} \quad \textit{for all } j, \quad \mu(B \cap \Omega_j) \le C_\mu \min\{r(B)^N, r(B)^{N_1} \bar{\rho}(B)^{N_2}\} \quad \textit{for all balls } B, r(B) \le \operatorname{diam}(\Omega_j),$$

where $\bar{\rho}(B) = \sup\{\rho(x) : x \in B\}$, $N_1, N_2 \in \mathbb{R}$, (usually $N \ge N_1 + N_2$, $N_1 > 0$, $N_2 < 0$) *and*

$$\text{(1-46)} \qquad a(Q) \le C_* r(Q)^{\beta_1} \bar{\rho}(Q)^{\beta_2} \quad \textit{for all balls } Q \textit{ such that } 2Q \subset \Omega_j,$$

where $\beta_1, \beta_2 \in \mathbb{R}$. *Moreover, for any* $\gamma \in \mathbb{R}$, *we use* ρ^γ *to denote the measure defined by* $\rho^\gamma(E) = \int_E \rho(x)^\gamma \, dx$. *Suppose* $1 \le p_0 \le q$ *such that*

(i) $\beta_1 + \frac{N}{q} + \min\bigl\{0, \beta_2 + \frac{a}{q} - \frac{b}{p}\bigr\} \ge 0$; *and*

(ii) *both* $\min\{a, N_2 + a\}/q \le \gamma / p_0$ *and* $\beta_2 + \frac{a}{q} - \frac{b}{p} \le 0$ *in case* ρ *is unbounded on* $\mathcal{D}$.

Then for all $f \in \mathfrak{S}_\alpha(\Omega)$,

$$\text{(1-47)} \qquad \|f\|_{L^q_{\mu_a}(\mathcal{D})} \le C C_\mu^{1/q} \bigl(M^{1/p_0} \|f\|_{L^{p_0}_{\rho^\gamma}(\mathcal{D})} + C_* M^{1/p} \|\nabla^{\mathcal{D}}_{\alpha,p} f\|_{L^p_{w_b}(\mathcal{D})}\bigr),$$

where C *depends also on* $N_1, N_2, p_0, \gamma, M_1$ *and* M_2 *besides those listed above for* (1-44). *Furthermore, if we have strict inequalities in both* (i) *and* (ii) *and* $\mu_a\{x \in \mathcal{D} : \rho(x) < r\} < \infty$ *for any* $r > 0$, *then given any sequence* $\{f_k\} \subset \mathfrak{S}_\alpha(\Omega)$ *such that both* $\|f_k\|_{L^{p_0}_{\rho^\gamma}(\mathcal{D})}$ *and* $\|\nabla^{\mathcal{D}}_{\alpha,p} f_k\|_{L^p_{w_b}(\mathcal{D})}$ *are bounded, it has a subsequence that converges in* $L^q_{\mu_a}(\mathcal{D})$.

Remark 1.9. (1) In view of the fact that a John domain with finitely many points removed is still a John domain (see Proposition 2.9), instead of assuming $\Omega_0 \subset \Omega^c$, it suffices to assume $\Omega_0 \setminus F \subset \Omega^c$ (or $\mathcal{D}^c$), where F is a set of finite points. Note that $\operatorname{Lip}_{\text{loc}}(\Omega) \subset \operatorname{Lip}_{\text{loc}}(\Omega \setminus F)$ and $L^{p_0}_\sigma(\Omega) \cap E^p_w(\Omega) \subset L^{p_0}_\sigma(\Omega \setminus F) \cap E^p_w(\Omega \setminus F)$.

(2) Any finite union of John domains is an example of domain $\mathcal{D}$ for the above theorem. Indeed, $\mathcal{D}$ can be a generalized John domain [Chua 2009, Definition 1.2 and Proposition 2.21].

(3) Strict inequalities in conditions (i) and (ii) will ensure that (1-47) holds with some $\tilde{q} > q$ instead of q. Note that $L^{\tilde{q}}_{\mu_a}(\mathcal{D}) \subset L^q_{\mu_a}(\mathcal{D})$ when $\mu_a(\mathcal{D}) < \infty$ and $\tilde{q} > q$.

(4) Similar to the previous two theorems, we can replace $f_{B'}$ by f_{Ω,μ_a} in (1-44). Equation (1-47) will then also hold with $\|f\|_{L^{p_0}_{\rho^\gamma}(\mathcal{D})}$ being replaced by $\|f\|_{L^{p_0}_{\mu_a}(\mathcal{D})}$ if $1 \le p_0 < q$ and $\sup_j \mu_a(\Omega_j)^{1/q - 1/p_0} < \infty$. Conditions involving γ will then be redundant.

(5) By a standard density argument, one could obtain compact embedding result for the closure of $\operatorname{Lip}_{\text{loc}}(\mathcal{D}) \cap L^{p_0}_{\rho^\gamma}(\mathcal{D}) \cap E^p_{w_b}(\mathcal{D})$ in $L^{p_0}_{\rho^\gamma}(\mathcal{D}) \cap E^p_{w_b}(\mathcal{D})$.

(6) Some discussions of power-type weights (including logarithm) on special union of $C^{0,s}$ domains (bounded and unbounded) can be found in [Gurka and Opic 1988; 1989; 1991]. Note that weights are assumed to be positive and continuous on the domain there.

(7) For the necessity of conditions, see Remark 1.11.

(8) If $d\mu = dw = dx$ is the Lebesgue measure, then $N = N_1 = n,\ \beta = \alpha - \frac{n}{p}$ and $N_2 = 0$. The case $\alpha = 1$ has already been studied in [Chua and Wheeden 2011; Hajłasz and Koskela 1998].

(9) In most cases, $N_1 = n,\ N_2 \le 0$ and $N \le n$ in the above theorem. A typical example (a special case of Example 1.3(iii)) of μ will be

$$\mu(E) = \int_E |x - z_1|^{a_1} |x - z_2|^{a_2}\, dx, \quad \text{where } \ -n < a_1, a_2 < 0,\ z_1 \ne z_2.$$

Note that $\mu(\mathbb{R}^n) < \infty$ (and hence μ cannot be doubling on $\mathbb{R}^n$) if $a_1 + a_2 < -n$. Indeed, if $\bar\rho(B) = \sup\bigl\{\min\{|x - z_1|, |x - z_2|\} : x \in B\bigr\}$, then for any ball B with $r(B) \le C_0$, we have

$$\mu(B) \le C(C_0) \min\{r(B)^N, r(B)^n \bar\rho(B)^{a_1+a_2}\} \quad \text{with } \ N = \min\{n + a_1, n + a_2\}.$$

For more details, see Proposition A.4.

(10) When Ω is a John domain, the case $d\mu = \rho_\Omega^a\, dx,\ a < 0$ such that $\rho_\Omega^a(\Omega) < \infty$ but ρ_Ω^a may not be doubling has been studied in [Chua 2016].

In particular, when $\Omega_0 \setminus F \subset \mathrm{G}$ where G is the graph of a Lipschitz function $\psi : \mathbb{R}^{n-1} \to \mathbb{R}$ with F being a finite set of points and $\mathcal{D} = \mathbb{R}^n \setminus (\mathrm{G} \cup F)$, we have an extension of [Mazya 2011, Theorem 1.4.2.1]. Indeed, we use only the fact that $\mathbb{R}^n \setminus \mathrm{G} \in J(c, \infty)$ (generalized John domain). For example G can be a finite union of hyperplanes that pass through a fixed point.

Corollary 1.10. *Let $1 \le p,\ p_0 < q$ and $0 < \alpha \le 1$. Let F, G, Ω_0 be as above. Let $\rho(x) = \inf\{|x - z| : z \in \Omega_0\},\ N > 0,\ a \ge 0,\ \gamma, b \in \mathbb{R}$ and μ be a weight on $\mathbb{R}^n$ such that*

$$\mu(B) \le C r(B)^N \quad \textit{for all balls } B.$$

Recall that $\mu_a(E) = \int_E \rho(x)^a\, d\mu$ and $\rho^\gamma(E) = \int_E \rho(x)^\gamma\, dx$. If $\frac{N+a}{q} - \frac{n+\gamma}{p_0} < 0$, and

$$\alpha + \frac{N+a}{q} - \frac{n+b}{p} = 0 \quad \textit{and} \quad \frac{a}{q} - \min\left\{\frac{b}{p}, \frac{\gamma}{p_0}\right\} \le 0, \tag{1-48}$$

then for all $f \in L^{p_0}_{\rho^\gamma}(\mathbb{R}^n) \cap E^p_{\rho^b}(\mathcal{D})$ when $\alpha = 1$ and $f \in L^{p_0}_{\rho^\gamma}(\mathbb{R}^n) \cap \widehat{W}^{\alpha,p}_{\rho^b}(\mathcal{D})$ when $\alpha < 1$, where $\mathcal{D} = \mathbb{R}^n \setminus (\mathrm{G} \cup F)$,

$$\|f\|_{L^q_{\mu_a}(\mathbb{R}^n)} \le C \|\nabla^{\mathcal{D}}_{\alpha,p} f\|_{L^p_{\rho^b}(\mathcal{D})}. \tag{1-49}$$

Furthermore, (1-49) *also holds for* $f \in L^{p_0}_{\mu_a}(\mathbb{R}^n) \cap E^p_{\rho^b}(\mathcal{D})$ (*or* $L^{p_0}_{\mu_a}(\mathbb{R}^n) \cap \widehat{W}^{\alpha,p}_{\rho^b}(\mathcal{D})$ *when* $\alpha < 1$) *provided*

$$\alpha + \frac{N+a}{q} - \frac{n+b}{p} = 0 \quad \textit{and} \quad \frac{a}{q} - \frac{b}{p} \le 0 \tag{1-50}$$

$$\textit{and} \quad \lim_{r\to\infty} \inf\{\mu_a(B_r(x)) : x \in \mathbb{R}^n\} = \infty. \tag{1-51}$$

Remark 1.11. (1) Mazya [2011] considered the special case where $\alpha = 1$, $a = b = 0$ and $f \in C_0^\infty(\mathbb{R}^n)$. Of course, $C_0^\infty(\mathbb{R}^n) \subset L^{p_0}_{\rho^\gamma}(\mathbb{R}^n) \cap E^p_{\rho^b}(\mathbb{R}^n) \subset L^{p_0}_{\rho^\gamma}(\mathbb{R}^n) \cap E^p_{\rho^b}(\mathcal{D})$ when ρ^b and ρ^γ are both locally integrable. In general, $C_0^\infty(\mathcal{D}) \subset L^{p_0}_{\rho^\gamma}(\mathbb{R}^n) \cap E^p_{\rho^b}(\mathcal{D})$.

(2) The above result is sharp. For example, when $\mu(B) \ge Cr(B)^N$ for all δ-balls B of Ω, then (1-50) is indeed necessary. It can be done by a standard translation and dilation technique. We will only demonstrate the case where $0 < \alpha < 1$. Fix a C_0^∞ (or Lipschitz) function ϕ as in Remark 1.7(2). For simplicity, let us assume $\Omega_0 = \{(x_1, \dots, x_n) \in \mathbb{R}^n : x_i = 0 \text{ for some } i\}$ and F is a finite set. Suppose (1-49) holds. Then we have if B is any δ-ball in $\mathcal{D} = \mathbb{R}^n \setminus (G \cup F)$, as any appropriate translation and dilation of ϕ is C_0^∞ (or Lipschitz with compact support), we have

$$\mu_a(B/2)^{1/q} \le Cr(B)^{-\alpha}(\rho^b(B))^{1/p}.$$

Hence,

$$\bar{\rho}(B)^{a/q} r(B)^{N/q} \le Cr(B)^{-\alpha+n/p} \bar{\rho}(B)^{b/p}.$$

As we can take δ-balls B with $\bar{\rho}(B)$ comparable to $r(B)$, the first condition of (1-50) must hold. If we fix $r(B)$ but let $\bar{\rho}(B) \to \infty$, we see that $\frac{a}{q} - \frac{b}{p} \le 0$.

Next we have another application that extends a compact embedding result of [Xuan 2005, Theorem 2.1]. For simplicity, we shall only state that for Sobolev space (i.e., $\alpha = 1$).

Corollary 1.12. *Let* $1 \le p < q$, μ *and* ρ *be as in Corollary 1.10. Suppose* $\mathcal{D}$ *is a bounded domain. If*

$$1 + \frac{N}{q} - \frac{n}{p} + \min\left\{\frac{a}{q} - \frac{b}{p}, 0\right\} \ge 0, \tag{1-52}$$

then

$$\|f\|_{L^q_{\mu_a}(\mathcal{D})} \le C\|\nabla f\|_{L^p_{\rho^b}(\mathcal{D})} \tag{1-53}$$

for all $f \in C_0^\infty(\mathcal{D})$. *Furthermore, if in addition we have strict inequality in* (1-52), *then the embedding of the closure of* $C_0^\infty(\mathcal{D})$ *in* $E^p_{\rho^b}(\mathcal{D})$ *to* $L^q_{\mu_a}(\mathcal{D})$ *is compact.*

Remark 1.13. (1) In particular, the above can be applied to compact embedding of $C_0^\infty(\mathcal{D}) \cap E^p_{\rho^\beta}(\mathcal{D})$ to $L^q_{\rho^b}(\mathcal{D})$ when $\Omega_0 = F = \{0\} \subset \mathcal{D}$. Note that $E^p_{\rho^\beta}(\mathcal{D}) \subset E^p_{\rho^\beta}(\mathcal{D} \setminus \{0\})$. To apply Corollary 1.12, we will take $d\mu = dx$ when $\beta \ge 0$ and $\mu(B) = \int_{B\cap\Omega} |x|^\beta \, dx$ when $-n < \beta < 0$. If B is any ball, it is clear that $\rho^\beta(B \cap \Omega) \le$

$Cr(B)^{n+\beta}$ when $-n < \beta < 0$ (and hence $N = n + \beta$ in (1-52)). We obtain the same conclusion as [Xuan 2005, Theorem 2.1] for $\beta > -n$. However, [Xuan 2005] further assumes that $\beta > p - n$, $p > 1$ and $\mathcal{D}$ has C^1 boundary.

(2) From the same construction as in Remark 1.11, (1-53) will imply (1-52) and thus (1-52) is necessary. Note that $\bar{\rho}(B)$ will be bounded when B is a ball inside $\mathcal{D}$.

Finally, we discuss an application related to Caffarelli, Kohn and Nirenberg-type inequalities [Caffarelli et al. 1984]. Instead of considering only powers of $|x|$ (i.e., $\Omega_0 = \{0\}$), we will consider more general power weights and include fractional derivatives. The next theorem allows the case $p = q$ as we will apply results from [Chua 2009] instead of Theorem 2.4. For a more general extension, see Remark 3.2.

Theorem 1.14. *Let $\mathcal{D} \subset \mathbb{R}^n$, $0 < \alpha \le 1$ and $1 \le p, p_0 \le q$. Suppose there exist $M > 0$, $0 < c < 1$ such that $\mathcal{D} = \bigcup_{j=1}^{\infty} \Omega_j$, $\Omega_j \in J'(c)$ with $\varepsilon_0/c_0 \le \operatorname{diam}(\Omega_j) \le c_0\varepsilon_0$, $(c_0, \varepsilon_0 > 0)$ for all j and $\sum \chi_{\Omega_j} \le M$. Let $\{z_i\}_{i=1}^{l} \subset \mathbb{R}^n$, $l \in \mathbb{N}$ ($z_i \ne z_m$ for $i \ne m$) and*

$$\rho_1(x) = \prod_{i=1}^{l} |x - z_i|^{a_i}, \quad \rho_2(x) = \prod_{i=1}^{l} |x - z_i|^{b_i}, \quad \rho_0(x) = \prod_{i=1}^{l} |x - z_i|^{\gamma_i}, \tag{1-54}$$

with $a_i, b_i, \gamma_i \in \mathbb{R}$ and $a_i > -n$ for all i. Let $I^- = \{i : a_i < 0\}$. Suppose further that

(i) $$b = \min\Big\{\alpha - \frac{n+b_i}{p} + \frac{n+a_i}{q} : i = 1, \dots, l\Big\} \ge 0 \quad \textit{and}$$

(ii) $$\sum \frac{a_i}{q} \le \min\Big\{\sum \frac{b_i}{p}, \sum \frac{\gamma_i}{p_0}\Big\} \quad \Big(a = \frac{n + \sum_{i=1}^{l} \gamma_i}{p_0} - \frac{n + \sum_{i=1}^{l} a_i}{q}\Big).$$

Then for all $f \in L^{p_0}_{\rho_0}(\mathcal{D}) \cap E^p_{\rho_2}(\mathcal{D})$ when $\alpha = 1$ $\big(f \in L^{p_0}_{\rho_0}(\mathcal{D}) \cap \widehat{W}^{\alpha,p}_{\rho_2}(\mathcal{D})$ when $\alpha < 1\big)$,

$$\|f\|_{L^q_{\rho_1}(\mathcal{D})} \le C\big(M^{1/p_0}\varepsilon_0^{-a}\|f\|_{L^{p_0}_{\rho_0}(\mathcal{D})} + M^{1/p}\varepsilon_0^{b}\|\nabla^{\mathcal{D}}_{\alpha,p} f\|_{L^p_{\rho_2}(\mathcal{D})}\big), \tag{1-55}$$

where C depends only on

$$c, \{a_i, b_i, \gamma_i\}_{i=1}^{l}, n, p, q, p_0, l \quad \textit{and} \quad \max\{\operatorname{diam}(\Omega_j) : j \in \mathbb{N}\}/\zeta$$

(where $\zeta = \min\{|z_i - z_m| : i \ne m, i, m \in I^-\}$, taking $\zeta = \infty$ when I^- has ≤ 1 element). *Furthermore*, *if we have strict inequalities in both* (i) *and* (ii), *then the natural embedding of $L^{p_0}_{\rho_0}(\mathcal{D}) \cap E^p_{\rho_2}(\mathcal{D})$)* (or $L^{p_0}_{\rho_0}(\mathcal{D}) \cap \widehat{W}^{\alpha,p}_{\rho_2}(\mathcal{D})$ when $\alpha < 1$) *to $L^q_{\rho_1}(\mathcal{D})$ is compact.*

Finally, *if $\mathcal{D} \in J(c, \varepsilon_0)$* (generalized John domains [Chua 2009]), *then*

$$\|f\|_{L^q_{\rho_1}(\mathcal{D})} \le C\varepsilon^{-a}\|f\|_{L^{p_0}_{\rho_0}(\mathcal{D})} + C\varepsilon^{b}\|\nabla^{\mathcal{D}}_{\alpha,p} f\|_{L^p_{\rho_2}(\mathcal{D})} \quad \textit{for all } \varepsilon \in (0, \varepsilon_0), \tag{1-56}$$

with C depending on $c, \{a_i, b_i, \gamma_i\}_{i=1}^{l}, n, p, q, p_0, l$ and ε_0/ζ.

Remark 1.15. (1) If in addition $a, b > 0$, then (1-56) is equivalent to

$$\|f\|_{L^q_{\rho_1}(\mathcal{D})} \le C(\|f\|_{L^{p_0}_{\rho_0}(\mathcal{D})})^{a/(a+b)}\big(\|\nabla^{\mathcal{D}}_{\alpha,p} f\|_{L^p_{\rho_2}(\mathcal{D})} + \varepsilon_0^{-a-b}\|f\|_{L^{p_0}_{\rho_0}(\mathcal{D})}\big)^{b/(a+b)}; \tag{1-57}$$

see [Chua 2009, Remark 1.8(4)] for details.

(2) We may assume I^- in the above has more than one i. In [Chua 2009, Theorem 4.3; Caffarelli et al. 1984], the case with $l = 1$ in (1-54) and $z_1 = 0$ was considered, while we allow $l > 1$. Caffarelli et al. [1984] also showed that the conditions (i) and (ii) are necessary. The main difference (for $l > 1$) is that when $l = 1$ the measure induced is doubling ($|x|^\alpha$ is doubling on $\mathbb{R}^n$ if $\alpha > -n$) while it may not be doubling when $l > 1$ (see Example 1.3(iii)). This creates a problem for necessity of conditions. However, it is still possible to see that some of the conditions remain necessary. Indeed, condition (i) is necessary for the following weighted Poincaré inequality:

$$\|f - f_{\Omega,\rho_1}\|_{L^q_{\rho_1}(\Omega)} \le C\|\nabla^{\Omega}_{\alpha,p} f\|_{L^p_{\rho_2}(\Omega)} \quad \text{for all } f \in \mathrm{Lip}_{\mathrm{loc}}(\Omega) \tag{1-58}$$

for any John domain Ω. To see this, just use the same Lipschitz function ϕ constructed in Remark 1.7(2) to see that

$$\rho_1(Q/2)^{1/q} \le Cr(Q)^{-\alpha}\rho_2(B)^{1/p}$$

for all δ-balls Q in $\Omega \setminus \{z_i\}_{i=1}^l$. For each fixed i, one could choose $r(Q) \sim \bar{d}_i(Q) = \sup_{x\in Q}|x - z_i|$ and let $r(Q) \to 0$. It is now clear that (i) holds. It will be more complicated if we only assume (1-56) holds. Condition (i) is still necessary for (1-55) provided the $L^q_{\rho_1}$ norm is not dominated by the $L^{p_0}_{\rho_0}$ norm. Indeed using ϕ as above again, for any δ-ball Q in $\mathcal{D} \setminus \{z_i\}_{i=1}^l$, (by translation and dilation) we may assume ϕ has support in $Q/2$ and vanishes outside Q, we have by using (1-56),

$$\rho_1(Q/2)^{1/q} \le C\varepsilon_0^{-a}\rho_0(Q)^{1/p_0} + C\varepsilon_0^{b} r(Q)^{-\alpha}\rho_2(Q)^{1/p}.$$

As $d_i(x) = |x - z_i|$ are essentially constant on δ-balls, we have

$$|Q|^{1/q}\prod \bar{d}_i(Q)^{a_i/q} \le C\varepsilon_0^{-a}|Q|^{1/p_0}\prod \bar{d}_i(Q)^{\gamma_i/p_0} + C\varepsilon_0^{b}|Q|^{-\alpha/n+1/p}\prod \bar{d}_i(Q)^{b_i/p}.$$

For each fixed i we could let $r(Q) \to 0$ with $\bar{d}_i(Q) \sim r(Q)$. So if $\frac{n+a_i}{q} < \frac{n+\gamma_i}{p_0}$, we must have $\frac{n+a_i}{q} \ge \frac{n+b_i}{p} - \alpha$.

Next, if we assume (1-56) holds for all $\mathcal{D} \in J(c, \varepsilon_0)$, then for any ball Q with $r(Q) \ge \varepsilon_0$ such that $2Q \subset \mathbb{R}^n \setminus \{z_i\}_{i=1}^l$, we may assume that Q is a connected component of some $\mathcal{D} \in J(c, \varepsilon_0)$. Taking $f = \chi_Q$, since (1-56) holds, we have

$$|Q|^{1/q}\prod \bar{d}_i(Q)^{a_i/q} \le C\varepsilon_0^{-a}|Q|^{1/p_0}\prod \bar{d}_i(Q)^{\gamma_i/p_0}.$$

It is then easy to see that $\sum \frac{a_i}{q} \le \sum \frac{\gamma_i}{p_0}$ as we could let $\bar{d}_i(Q) \to \infty$ (while fixing $r(Q)$).

2. Preliminaries

For easy reference, we collect in this section some definitions and terminology from [Chua 2009; Chua and Wheeden 2008; 2011].

Definition 2.1. A function d is called a (symmetric) quasimetric on a given set H if $d : H \times H \to [0, \infty)$ and there is a constant $\kappa \geq 1$ such that for all $x, y, z \in \Omega$,

$$\begin{aligned} &d(x, y) = d(y, x),\\ &d(x, y) = 0 \Longleftrightarrow x = y, \quad \text{and} \\ &d(x, y) \leq \kappa[d(x, z) + d(z, y)]. \end{aligned} \tag{2-1}$$

If d is a quasimetric on H, we refer to the pair $\langle H, d\rangle$ as a quasimetric space. In this section, unless otherwise mentioned, H will always be a quasimetric space with quasimetric d and quasimetric constant κ. All measures on H will be defined on a fixed σ-algebra Σ that includes all balls. When $\kappa = 1$, H will be a metric space and we will just assume Σ to be the Borel algebra on H.

First, similar to [Chua and Wheeden 2008] for John domains, we see that δ-doubling is equivalent to doubling on weak John domains.

Proposition 2.2. *Let $0 < \delta \leq \frac{1}{2}\kappa^2$. If $\Omega \subset H$, $\Omega \in J'(c)$ with center x', then*

(i) $$d(x', \Omega^c) \geq c \operatorname{diam}(\Omega)/(2\kappa);$$

(ii) *for any $x \in \Omega$, $0 < r_0 < \operatorname{diam}(\Omega)$, $B(x, r_0)$ contains a δ-ball Q with $r(Q) \geq Cr_0$, where C depends only on κ, δ and c, hence, a measure μ is δ-doubling on Ω if and only if it is doubling on Ω.*

Proof. Given any $\varepsilon > 0$, there exist $z_1, z_2 \in \Omega$ with $d(z_1, z_2) > \operatorname{diam}(\Omega) - \varepsilon$. But

$$d(z_1, z_2) \leq \kappa(d(z_1, x') + d(z_2, x')).$$

Hence, without loss of generality, we may assume $d(z_1, x') \geq d(z_1, z_2)/(2\kappa)$. By the weak John condition (1-7), we have

$$d(x') = d(x', \Omega^c) \geq c\, d(z_1, x') \geq \frac{c(\operatorname{diam}(\Omega) - \varepsilon)}{2\kappa},$$

and (i) will then follow as $\varepsilon > 0$ is arbitrary.

For part (ii), recall from (i) that $d(x') \geq \frac{c}{2\kappa}\operatorname{diam}(\Omega)$. It suffices to show that if $x \in \Omega$ and $\delta d(x) \leq r \leq c \operatorname{diam}(\Omega)/(2\kappa)$, then $B_r(x)$ contains a δ-ball with radius comparable to r (with constant independent of r and x). The case when $x = x'$ in the above is easy. Now suppose $x \neq x'$. It is again clear if $x' \in B_r(x)$. So we may assume $d(x, x') \geq r$. Next, we need only a continuous path $\gamma : [0, l] \to \Omega$ connecting x to x' such that $d(\gamma(t), \Omega^c) \geq c\, d(\gamma(t), x)$. Since $d(\gamma(t), x)$ is a continuous function on $[0, l]$, there exists t_0 such that $d(\gamma(t_0), x) = r/(2\kappa)$ and hence $d(\gamma(t_0)) \geq cr/(2\kappa)$. We now observe that the δ-ball $B_{r'}(\gamma(t_0)) \subset B_r(x)$ with $r' = c\delta r/(2\kappa)$. This concludes the proof of part (ii). $\square$

Remark 2.3. Doubling or δ-doubling will imply reverse doubling if Ω is assumed to have the "nonempty annuli property" (on symmetric quasimetric space; see [Chua and Wheeden 2008, Proposition 2.3]). Clearly, any weak John domain satisfies this "nonempty annuli property."

Now, let us state a theorem that is similar to [Chua and Wheeden 2011, Theorem 1.6].

Theorem 2.4. *Let $\Omega \subset H$, $\Omega \in J'(c)$ with central point x', let $0 < \delta \leq 1/(2\kappa^2)$, $1 \leq \tau \leq 1/(2\delta\kappa^2)$. Let $1 \leq p < q < \infty$. Suppose μ, σ and w are measures* (defined on a fixed σ-algebra that includes all balls and Ω) *where σ is δ-doubling on Ω and μ is absolutely continuous with respect to σ. Let $(f, g) \in L^1_{\sigma,\mathrm{loc}}(\Omega) \times L^p_{w,\mathrm{loc}}(\Omega)$ such that (1-4) holds. Suppose there exists a ball set function μ^* satisfying Condition (R) such that $\mu(B \cap \Omega) \leq \mu^*(B)$ for all balls B with center in Ω and (μ, μ^*) satisfies the Vitali-type property on Ω* ((1-10) in Theorem 1.1). *Suppose further that for any ball B with center in Ω and $r(B) \leq$* diam(Ω),

$$\mu^*(B)^{1/q} a(Q) \leq C_1 \tag{2-2}$$

for all δ-balls $Q \subset B$ such that $r(Q) \geq c\delta r(B)/(4\tau\kappa)$. Then

$$\mu\{x \in \Omega : |f(x) - f_{B',\sigma}| > t\} \leq C C_1^q V_\mu \|g\|^q_{L^p_w(\Omega)}/t^q \quad \text{for all } t > 0, \tag{2-3}$$

where $B' = B(x', \delta d(x'))$, and C depends on $c, A_1, A_2, \theta_1, \theta_2, \delta, \tau, \kappa, p, q$ and the doubling constant D_σ of σ but is independent of C_1, V_μ and diam(Ω). *Moreover*, *if $\mathfrak{S}$ satisfies (1-4) with the truncation property*, *then the following strong-type inequality also holds*:

$$\|f - f_{B',\sigma}\|_{L^q_\mu(\Omega)} \leq C c_T C_1 V_\mu^{1/q} \|g\|_{L^p_w(\Omega)}, \tag{2-4}$$

where C depends on the parameters as above.

Remark 2.5. It follows from standard interpolation argument that (2-3) will imply

$$\|f - f_{B',\sigma}\|_{L^{\tilde{q}}_\mu(\Omega)} \leq C C_1 V_\mu^{1/q} \mu(\Omega)^{1/\tilde{q} - 1/q} \|g\|_{L^p_w(\Omega)}$$

for any $1 \leq \tilde{q} < q$, where the constant C now also depends on $\tilde{q}$; see [Chua and Wheeden 2008, Remark 1.3].

In order to prove the above theorem, we will first extend a Whitney-type lemma similar to [Chua and Wheeden 2008, Proposition 2.6]. For simplicity, we will let $\lambda = \kappa + 2\kappa^2$.

Proposition 2.6. *Let $0 < \delta \le 1/(2\kappa^2)$. Suppose $\Omega \subset H$ such that $d(x, \Omega^c) > 0$ for any $x \in \Omega$* (when $\Omega \neq H$) *and there is a δ-doubling measure σ on Ω with doubling constant D_σ. Then there exists a covering $\widetilde{W} = \{\widetilde{B}_i\}$ of Ω by δ-balls $\widetilde{B}_i$ such that:*

(a) *$r(B_i) \le \delta d(x_{B_i}) \le \lambda^2 r(B_i)$, where x_{B_i} is the center of B_i for all $B_i \in W = \{2\kappa \widetilde{B}_i : \widetilde{B}_i \in \widetilde{W}\}$ and given $x \in \Omega$ there exists $\widetilde{B} \in \widetilde{W}$ such that* ($\delta' = \delta/\lambda^3$)

$$B(x, \delta' d(x)) \subset \widetilde{B} \quad \text{and} \quad B(x, \lambda\delta' d(x)) \subset 2\kappa \widetilde{B} \subset B(x, \delta d(x)) \subset 2\kappa\lambda^2 \widetilde{B}. \tag{2-5}$$

(b) *For every $\tau \ge 1$ that satisfies $\tau\delta \le 1/(2\kappa^2)$, there is a constant K depending only on τ, κ and D_σ so that the balls $\{\tau B_i : B_i \in W\}$ have bounded intercepts with bound K (i.e., each τB_i intersects at most $K - 1$ other τB_j in the family); in particular, the balls $\{\tau B_i : B_i \in W\}$ also have pointwise bounded overlaps with overlap constant K. Indeed, the existence of the δ-doubling measure σ guarantees that any collection of $\{\tau B : B \in \mathfrak{F}\}$ has bounded intercepts whenever $\mathfrak{F}$ consists of disjoint δ-balls.*

Now suppose further that $\Omega \in J'(c)$ with center x'. Then:

(c) *For any $x \in \Omega$, $x \neq x'$, there exists a finite chain of δ-balls $\{B_i\}_{i=0}^L \subset W$, depending on x and with $L = L_x$, such that $x \in B_0$, $x' \in B_L$, B_L is independent of x and satisfies $\lambda^{-2} B(x', \delta d(x')) \subset B_L \subset B(x', \delta d(x'))$, $B_i \cap B_{i+1}$ contains a δ-ball B_i' with $B_i \cup B_{i+1} \subset \lambda^4 B_i'$ for all i, and*

$$B_0 \subset \frac{4\lambda^4\kappa}{c\delta} B_i \quad \text{for all } i. \tag{2-6}$$

Furthermore, there is a finite chain of δ-Whitney balls ($B(x, r)$ is said to be a δ-Whitney ball if $r = \delta d(x)$) *$\{Q_i\}_{i=0}^L$ depending on x with bounded intercepts such that $Q_0 = B(x, \delta d(x))$, $Q_L = B(x', \delta d(x'))$, $(1/\lambda^2) Q_i \subset B_i \subset Q_i$, and $Q_i \cap Q_{i+1}$ contains a δ-ball Q_i' with $Q_i \cup Q_{i+1} \subset \lambda^6 Q_i'$.*

(d) *If $Q_i \not\subset B(x, r)$, then $r(Q_i) \ge c\delta r/(2\kappa)$ where x and Q_i are given in* (c).

(e) *For all $\varepsilon > 0$, the number of disjoint Q_i* (in (c)) *having radius between ε and 2ε is at most C* (depending only on δ, κ, D_σ and c).

Proof. The proof of this proposition is just a simple modification of that of [Chua and Wheeden 2008, Proposition 2.6] even though the assumption on Ω is now weaker. For completeness, we provide this proof in Appendix B; see also [Chua and Wheeden 2015]. □

Proof of Theorem 2.4. The proof of this theorem is indeed similar but much simpler than that of [Chua and Wheeden 2011, Theorem 1.6]. However, as weak John domains are weaker than John domains, we will prove it using [Chua and Wheeden 2008, Theorem 1.2]. For easy reference, we have stated it as Theorem A.1 in Appendix A, where we have changed the notation slightly. First as in [Chua and Wheeden 2011, (1-6)], for each $x \in \Omega$, since μ^* satisfies Condition (R), let $B_j^x = B(x, r_j^x)$ as in (1-8), condition (2) of Theorem A.1 will then hold with $\wp = \mu(\Omega)/\mu(B')$. Moreover, Proposition 2.6(c) enable us to construct (see [Chua and Wheeden 2011, (1-6)]) a sequence $\{Q_i^x\}_{i=1}^\infty$ of δ-balls such that $Q_1^x = B(x', \delta d(x'))$ and $\{Q_i^x\}$ has the intersection property

$$Q_i^x \cap Q_{i+1}^x \text{ contains a } \delta\text{-ball } Q_i' \text{ with } Q_i^x \cup Q_{i+1}^x \subset NQ_i'$$

for some positive constant N independent of x and i. Equation (A-1) will then hold as σ is δ-doubling. Moreover, for large i, Q_i^x is centered at x; in fact, for balls $B_j^x = B(x, r_j^x)$, there exist $K_x, K_x' \in \mathbb{N}$ such that $\tau Q_{i+K_x}^x = B_{i+K_x'}^x$ for $i \geq 0$. B_j^x is a $\tau\delta$-ball if $j \geq K_x$, and Q_i^x is not centered at x if $i \leq K_x$ (indeed, such Q_i^x are δ-Whitney balls constructed in Proposition 2.6(c)). We associate with each ball $B_j^x = B(x, r_j^x)$, $j \geq 1$, the following special subcollection of $\{Q_i^x\}$ as in [Chua and Wheeden 2011, (1-6)]:

$$\mathcal{C}(B_j^x) = \{Q_i^x : \tau Q_i^x \subset B_j^x \text{ and } \tau Q_i^x \not\subset B_{j+1}^x\}. \tag{2-7}$$

In case $j \geq K_x$, then $\mathcal{C}(B_j^x)$ consists of just the single ball $\tau^{-1} B_j^x = Q_j^x$. By Proposition 2.6(d)–(e), we know that each $\mathcal{C}(B)$ has a bounded number (denoted by $L = C(\delta, \kappa, D_\sigma, c)$) of δ-balls Q and each δ-ball has radius $\geq c\delta r(B)/(4\tau\kappa)$. Hence if $I = \{B_\alpha\}$ is a countable collection of pairwise disjoint balls B_j^x in the above, then with the notation of condition (3) in Theorem A.1, we have by (2-2), taking $a_*(Q) = a(Q)\|g\|_{L_w^p(\tau Q)}$,

$$\sum_{B_\alpha \in I} (A(B_\alpha)^q \mu^*(B_\alpha))^{p/q} \leq L^{p/q} \sum_{B_\alpha \in I} C_1^p \|g\|_{L_w^p(B_\alpha)}^p \leq L^{p/q} C_1^p \|g\|_{L_w^p(\Omega)}^p.$$

Thus, (A-4) holds with $\theta = p/q$ and $(C_0^q \mu(\Omega))^{p/q} = C(\delta, \kappa, D_\sigma, c) C_1^p \|g\|_{L_w^p(\Omega)}^p$.

Finally, (A-2) holds with

$$p_0 = 1, \quad C(f, Q_j^x) = f_{Q_j^x, \sigma} \quad \text{and} \quad a_*(Q_j^x) = a(Q_j^x)\|g\|_{L_w^p(\tau Q_j^x)}$$

as $f_{Q_i^x, \sigma} \to f(x)$, σ-a.e. (and hence μ-a.e.) by the Lebesgue differentiation theorem as σ is δ-doubling and note that a Vitali-type property (1-10) holds with $\mu = \mu^* = \sigma$ (on metric spaces, see [Heinonen 2001]). Condition (4) holds because we have assumed the Vitali-type property (1-10) holds. (2-3) now follows from Theorem A.1.

Moreover, if the truncation property holds, the proof of the strong-type inequality (2-4) follows exactly the same argument as in [Chua and Wheeden 2008, proof of Theorem 1.10] (and has been used in many other papers listed there) and hence omitted here. We shall only note that our conclusion follows from [Chua and Wheeden 2011, Theorem 1.9]. □

Next, we prove a self improving Poincaré-type property for balls. Note that a metric ball will be a weak John domain if we assume certain geodesic path property. However, we will establish it without such an assumption.

Proposition 2.7. *Let $1 \le p < q$ and $\mathcal{D}$ be a measurable subset in H such that $d(x, \mathcal{D}^c) > 0$ for all $x \in \mathcal{D}$* (when $\mathcal{D} \neq H$). *Let*

$$0 < \delta \le 1/(2\kappa^2) \quad \textit{and} \quad 1 \le \tau \le 1/(2\delta\kappa^2).$$

Let σ, μ, w be measures on $\mathcal{D}$ such that σ is δ-doubling on $\mathcal{D}$ and μ is absolutely continuous with respect to σ. Suppose (1-4) holds for all $(f, g) \in \mathfrak{S} \subset L^1_{\sigma,\mathrm{loc}}(\mathcal{D}) \times L^p_{w,\mathrm{loc}}(\mathcal{D})$ and δ-balls B in $\mathcal{D}$. Suppose there exists a ball set function μ^* such that $\mu(B) \le \mu^*(B)$ for all δ-balls B in $\mathcal{D}$ and such that Condition (R) *holds for any δ-ball $B_r(x_0)$ with $r_1^x = 2\kappa r$. Suppose further that*

$$\mu^*(\widetilde{Q})^{1/q} a(Q) \le C_1 \quad \textit{for all } \delta\textit{-balls } Q, \widetilde{Q}, \quad Q \subset \widetilde{Q} \textit{ and } r(Q) \ge r(\widetilde{Q})/(2\kappa). \tag{2-8}$$

If (μ, μ^*) satisfies the Vitali-type property (1-10) on $\mathcal{D}$, then for any ball B such that $\lambda\tau B$ is a δ-ball, we have

$$\mu\{x \in B : |f(x) - f_{B,\sigma}| > t\} \le \frac{C C_1^q V_\mu}{t^q} \|g\|^q_{L^p_w(\lambda\tau B)} \quad \textit{for all } t > 0,\ (f, g) \in \mathfrak{S}, \tag{2-9}$$

where C depends on $A_1, A_2, \theta_1, \theta_2, \delta, \tau, \kappa, c, p, q$ and the doubling constant D_σ of σ. Furthermore, if $\mathfrak{S}$ satisfies (1-4) *with the truncation property, then we also have the following strong-type inequality*:

$$\|f - f_{B,\sigma}\|_{L^q_\mu(B)} \le C c_T C_1 V_\mu^{1/q} \|g\|_{L^p_w(\lambda\tau B)} \quad \textit{for all } (f, g) \in \mathfrak{S}. \tag{2-10}$$

Proof. This is again a consequence of Theorem A.1 [Chua and Wheeden 2008, Theorem 1.2]. For each ball $B_r(x_0)$ such that $B_{\lambda\tau r}(x_0)$ is a δ-ball, we will apply Theorem A.1 with $\Omega = B_r(x_0)$. For each $x \in B_r(x_0)$, we define $Q_1^x = B_r(x_0)$, $Q_2^x = B(x, 2\kappa r)$ and let $r_1^x = 2\kappa r$. By Condition (R), there exists a sequence $r_j^x \to 0$ such that $r_j^x/2 \le r_{j+1}^x < r_j^x$ and (1-8) holds. We now take $B_j^x = Q_{j+1}^x = B_{r_j}(x)$ for all $j \ge 1$ and define $\mathcal{C}(B_j^x) = \{B_j^x\}$ for $j > 1$ and $\mathcal{C}(B_1^x) = \{B_1^x, B_r(x_0)\}$. Note that B_j^x are δ-balls and (A-3) holds with $\wp = 1$ by Condition (R). Moreover, (A-1) holds since σ is δ-doubling. Also, let

$$a_*(Q_i^x) = a(Q_i^x)\|g\|_{L^p_w(\tau Q_i^x)}.$$

Similar to the proof of Theorem 2.4, (A-2) holds with $p_0 = 1$ by (1-4). Take $\theta = p/q$. We now observe that if I is a subcollection of pairwise disjoint balls B_j^x

defined above, we have

$$\begin{aligned}\sum_{B\in I}(a_*(B)^q\mu^*(B))^{p/q} &= \sum_{B\in I} a(B)^p\|g\|^p_{L^p_w(\tau B)}\mu^*(B)^{p/q}\\ &\le \sum_{B\in I} C_1^p\|g\|^p_{L^p_w(\cup\tau B)}\\ &\le CC_1^p\|g\|^p_{L^p_w(\lambda\tau B_r(x_0))}\end{aligned}$$

since $\{\tau B\}_{B\in I}$ has bounded overlap (see Proposition 2.6(b)) and $\tau B_i^x\subset\lambda\tau B_r(x_0)$ (see [Chua and Wheeden 2008, Observation 2.1(1)]). Equation (A-4) will then hold with

$$C_0^q\mu(\Omega)=2^qCC_1^q\|g\|^q_{L^p_w(\lambda\tau B_r(x_0))}$$

since

$$a(B_r(x_0))^p\|g\|^p_{L^p_w(B_{\tau r}(x_0))}\mu^*(B_{2\kappa r}(x))^{p/q}\le C_1^p\|g\|^p_{L^p_w(B_{\tau r}(x_0))}\quad\text{for any } x\in B_r(x_0).$$

Again, note that $f_{B_r(x),\sigma}\to f(x)$ for σ-a.e. x as $r\to 0$. The first part of the proposition then follows from Theorem A.1 and once again the second part will follow from the standard truncation argument. □

Remark 2.8. (1) $\lambda=3$ when H is a metric space as $\kappa=1$. Moreover, checking through our proof, λ can be replaced by $(1+\varepsilon)$ (for any fixed $\varepsilon>0$) provided for all $x\in B_r(x_0)$ such that $B_{(1+\varepsilon)r}(x_0)$ is a δ ball, we have

(i) $$\sigma(B_{\varepsilon r}(x)\cap B_r(x_0))\ge C_\sigma\sigma(B_{\varepsilon r}(x)\cup B_r(x_0));$$

(ii) $$\mu^*(B_{\varepsilon r}(x))^{1/q}a(B_r(x_0))\le C_1;$$

(iii) $$\mu(B_r(x_0))\le\wp\mu^*(B_{\varepsilon r}(x)).$$

Indeed, we will then choose Q_2^x to be $B(x,\varepsilon r)$ instead of $B(x,2r)$. The rest of the proof is similar with the help of (i)–(iii).

(2) A similar inequality has been obtained in [Hajłasz and Koskela 2000, Theorem 5.1] on metric spaces with λ being replaced by 5 and $\mu=w$ being doubling and $a(Q)=Cr(Q)\mu(Q)^{-1/p}$ [Hajłasz and Koskela 2000, (22)].

(3) It is often true that metric balls are weak John domains; for example, when the ball satisfies the "geodesic path property." In that case, $\|g\|_{L^p_w(\lambda\tau B)}$ in (2-9) and (2-10) can be replaced by just $\|g\|_{L^p_w(B)}$ using Theorem 2.4; see also [Heinonen 2001, Theorem 9.5] when $\mu=w$ is doubling and the main results in [Franchi et al. 2003] for quasimetric balls. Indeed, in particular we obtain the main result of [Franchi et al. 2003] without the assumption of "geodesic path property" or "chain condition."

(4) Equation (2-10) will imply

$$\|f-f_{B,\mu}\|_{L^q_\mu(B)}\le CC_1V_\mu^{1/q}\|g\|_{L^p_w(\lambda\tau B)}\quad\text{for all } (f,g)\in\mathfrak{S}$$

and hence by Hölder's inequality,

(2-11) $$\|f - f_{B,\mu}\|_{L^p_\mu(B)} \le C C_1 V_\mu^{1/q} \mu(B)^{1/q-1/p} \|g\|_{L^p_w(\lambda\tau B)} \quad \text{for all } (f, g) \in \mathfrak{S}.$$

The idea of John domains has been extended to generalized John domains which include bounded and unbounded John domains in [Chua 2009]. It has been shown in [Chua 2009, Proposition 2.24] that a generalized John domain in a metric space that satisfies some "path property" is still a generalized John domain if a point is being removed. Indeed, by a simple modification of that proof, we can also show that a weak John domain in a metric space satisfying a "path property" (which is slightly weaker than that of [Chua 2009]) is still a weak John domain if a point has been removed. In particular, a John domain in $\mathbb{R}^n$ with finite number of points being removed will still be a John domain.

Proposition 2.9. *Let Ω be a subset of a metric space H and $\Omega \in J'(c)$. Suppose Ω satisfies the following path property*:

> *Given any two points $x, y \in B_r(z)$ with $B_{2r}(z) \subset \Omega$, there exists a continuous path $\eta : [0, 1] \to B_{\theta r_2}(z) \setminus B_{r_1/\theta}(z)$ such that $\eta(0) = x$ and $\eta(1) = y$ where $r_1 = \min\{d(x, z), d(y, z)\}$ and $r_2 = \max\{d(x, z), d(y, z)\}$ and θ is a fixed constant > 1.*

Then $\Omega \setminus \{z\} \in J'(C(c, \theta))$ is also a weak John domain.

Proof. As the proof is very similar to the proof of [Chua 2009, Proposition 2.24], we shall only provide it in Appendix B. □

Remark 2.10. (1) The above mentioned path property is weaker than the one used in [Chua 2009, Proposition 2.24]. Indeed, this property is a consequence of the "linearly connected property" defined in [Heinonen 2001, p. 64].

(2) Consequently, if $\Omega \subset \mathbb{R}^n$ is a weak John domain, then $\Omega \setminus \{z_i\}_{i=1}^l$, $l \in \mathbb{N}$ is also a weak John domain. Indeed, if $\Omega \in J'(c)$, then $\Omega \setminus \{z_i\}_{i=1}^l \in J'(\tilde{c})$ with $0 < \tilde{c} < c$ depending only on c, l and n.

Finally, let us discuss a density theorem that is an extension of [Hajłasz and Koskela 1998, Theorem 3] (see also [Hajłasz 1993]). For convenience, we say $C^\infty(\Omega)$ (or $\mathrm{Lip}_{\mathrm{loc}}(\Omega)$) is dense in a norm space W if $C^\infty(\Omega) \cap W$ (or $\mathrm{Lip}_{\mathrm{loc}}(\Omega) \cap W$) is dense in W.

Proposition 2.11. *Let $1 \le p_0, p < \infty$. Let Ω be a domain in $\mathbb{R}^n$, μ, w, ρ, ρ_0 be weights on Ω such that $\rho, \rho^{-1} \in L^\infty_{w,\mathrm{loc}}(\Omega)$* (locally bounded with respect to the measure dw) *and $\rho_0, \rho_0^{-1} \in L^\infty_{\mu,\mathrm{loc}}(\Omega)$. Suppose $C^\infty(\Omega)$* (or $\mathrm{Lip}_{\mathrm{loc}}(\Omega)$) *is dense in $W^{1,p}_{w,\mathrm{loc}}(\Omega) \cap L^{p_0}_{\mu,\mathrm{loc}}(\Omega)$, i.e.,*

(A) *Given any $x \in \Omega$, there exists $B_{r_x}(x) \subset \Omega$ such that for all*

$$f \in W^{1,p}_{w,\mathrm{loc}}(\Omega) \cap L^{p_0}_{\mu,\mathrm{loc}}(\Omega),$$

and $\varepsilon > 0$, *there exists* $\phi \in C^\infty(\Omega)$ (or $\mathrm{Lip}_{\mathrm{loc}}(\Omega)$) *such that*

$$\|f-\phi\|_{W_w^{1,p}(B_{r_x}(x))} < \varepsilon \quad \textit{and} \quad \|f-\phi\|_{L_\mu^{p_0}(B_{r_x}(x))} < \varepsilon. \tag{2-12}$$

Then $C^\infty(\Omega)$ (or $\mathrm{Lip}_{\mathrm{loc}}(\Omega)$) *is dense in* $W^{1,p}_{w\rho}(\Omega) \cap L^{p_0}_{\mu\rho_0}(\Omega)$.

Proof. For each $x \in \Omega$, let $B_{r_x}(x) \subset \Omega$ such that (A) holds and $\overline{B_{r_x}(x)} \subset \Omega$. Since $\Omega = \bigcup_{x\in\Omega} B(x, r_x/2)$, there exists countable subfamily of bounded overlapping balls $\{B_i\}_{i=1}^\infty$ ($B_i = B(x, r_x/2)$ for some x) such that $\Omega \subset \bigcup_i B_i$. We will then choose a partition of unity. Indeed, for each B_i, we find $h_i \in C_0^\infty(\mathcal{D})$ with $\chi_{B_i} \le h_i \le \chi_{2B_i}$ and define $u_i = h_i / \sum_k h_k$ ($u_i = 0$ if $h_i = 0$). Next, for any $f \in W^{1,p}_{w\rho}(\Omega) \cap L^{p_0}_{\mu\rho_0}(\Omega)$, since $\rho^{-1} \in L^\infty_{w,\mathrm{loc}}(\Omega)$, $\rho_0^{-1} \in L^\infty_{\mu,\mathrm{loc}}(\Omega)$, it is clear that $f \in W^{1,p}_{w,\mathrm{loc}}(\Omega) \cap L^{p_0}_{\mu,\mathrm{loc}}(\Omega)$. Since $\rho \in L^\infty_{w,\mathrm{loc}}(\Omega)$ and $\rho_0 \in L^\infty_{\mu,\mathrm{loc}}(\Omega)$, for each B_i, there exists $A_i > 0$ such that $\rho \le A_i$ on $2B_i$ w-a.e. and $\rho_0 \le A_i$ on $2B_i$ μ-a.e. Now, by (A), given any $\varepsilon > 0$, there exists $g_i \in C^\infty(\Omega)$ such that

$$\|f-g_i\|_{L^p_w(2B_i)} + \|\nabla(f-g_i)\|_{L^p_w(2B_i)} \le \varepsilon / \big(2^i (A_i)^{1/p} \max\{\|\nabla u_i\|_{L^\infty(\Omega)}, 1\}\big)$$

and $\|f-g_i\|_{L^{p_0}_\mu(2B_i)} < \varepsilon/(2^i A_i^{1/p_0})$. Thus, by the triangle inequality and estimates on ρ,

$$\begin{aligned}
&\|\nabla(fu_i - g_iu_i)\|_{L^p_{w\rho}(\Omega)} \\
&\qquad = \|\nabla(fu_i - g_iu_i)\|_{L^p_{w\rho}(2B_i)} \\
&\qquad = \|u_i\nabla(f-g_i) + (f-g_i)\nabla u_i\|_{L^p_{w\rho}(2B_i)} \\
&\qquad \le \|\nabla(f-g_i)\|_{L^p_{w\rho}(2B_i)} + \|\nabla u_i\|_{L^\infty(\Omega)}\|f-g_i\|_{L^p_{w\rho}(2B_i)} \\
&\qquad \le A_i^{1/p}\|\nabla(f-g_i)\|_{L^p_w(2B_i)} + A_i^{1/p}\|\nabla u_i\|_{L^\infty(\Omega)}\|f-g_i\|_{L^p_w(2B_i)} \\
&\qquad \le 2\varepsilon/2^i.
\end{aligned}$$

Hence if $g = \sum g_iu_i$, then $g \in C^\infty(\Omega)$ (or $\mathrm{Lip}_{\mathrm{loc}}(\Omega)$ when $g_i \in \mathrm{Lip}_{\mathrm{loc}}(\Omega)$) and

$$\begin{aligned}
\|\nabla(f-g)\|_{L^p_{w\rho}(\Omega)} &= \big\|\nabla\big(f\textstyle\sum u_i - \sum g_iu_i\big)\big\|_{L^p_{w\rho}(\Omega)} \quad \text{since } \textstyle\sum_i u_i = 1 \\
&= \big\|\textstyle\sum_i \nabla(fu_i - g_iu_i)\big\|_{L^p_{w\rho}(\Omega)} \\
&\le \textstyle\sum_i \|\nabla(fu_i - g_iu_i)\|_{L^p_{w\rho}(\Omega)} \le 2\varepsilon.
\end{aligned}$$

Finally, it is easy to see that

$$\|f-g\|_{L^p_{w\rho}(\Omega)},\ \|f-g\|_{L^{p_0}_{\mu\rho_0}(\Omega)} < 2\varepsilon. \qquad \square$$

It is often true that the Poincaré inequality holds. The following observation is useful in applying the density theorem.

Proposition 2.12. *Let* $1 \le p, p_0 < \infty$, $\tau \ge 1$ *and* μ, w *be locally integrable weights on a domain* $\Omega \subset \mathbb{R}^n$. *Suppose for all balls* B *with* $2\tau B \subset \Omega$ *and* $f \in C^\infty(\Omega)$,

$$\|f - f_{B,\mu}\|_{L^{p_0}_\mu(B)} \le a(B)\|\nabla f\|_{L^p_w(\tau B)}, \tag{2-13}$$

where $a(B)$ is a finite ball set function that is independent of f. Suppose also $C^\infty(\Omega)$ is dense in $E^p_{w,\mathrm{loc}}(\Omega)$, i.e., given any $x \in \Omega$, there exists $B_{r_x}(x) \subset \Omega$ such that for any $\varepsilon > 0$, $f \in E^p_{w,\mathrm{loc}}(\Omega)$, there exists $\phi \in C^\infty(\Omega)$ such that

$$\|\nabla(f-\phi)\|_{L^p_w(B_{r_x}(x))} < \varepsilon. \tag{2-14}$$

Then $C^\infty(\Omega)$ is also dense in $E^p_{w,\mathrm{loc}}(\Omega) \cap L^{p_0}_{\mu,\mathrm{loc}}(\Omega)$.

Proof. The conclusion follows from (2-13) and (2-14). □

Remark 2.13. (1) One could generalize the above density theorem to domains in Riemannian manifolds where there are partitions of unity.

(2) Under the assumptions of Proposition 2.11, $C^\infty(\Omega)$ is also dense in

$$L^p_{w\rho_0,\mathrm{loc}}(\Omega) \cap W^{1,p}_{w\rho,\mathrm{loc}}(\Omega), \quad L^p_{w\rho_0}(\Omega) \cap E^p_{w\rho}(\Omega), \quad \ldots, \quad \text{etc.}$$

To see this, just check through the proof.

(3) If (2-13) holds and $w \in A_p$, then it follows from Proposition 2.12 that $C^\infty(\Omega)$ is dense in $L^{p_0}_\mu(\Omega) \cap E^p_w(\Omega)$ as $C^\infty(\Omega)$ is dense in $W^{1,p}_w(\Omega)$ [Turesson 2000].

(4) Condition (2-12) holds for example when $w \in A_p$ and $\mu \in A_{p_0}$. It is then easy to see that $C^\infty(\Omega)$ is dense in $L^{p_0}_{\mu\rho_0}(\Omega) \cap E^p_{w\rho}(\Omega)$. The case where $w = \mu = 1$, $p_0 = p$ and ρ, ρ_0 are positive continuous on Ω has been obtained in [Hajłasz and Koskela 1998, Theorem 3].

(5) The density theorem for weighted Sobolev spaces of different definitions has been studied in [Chiadò Piat and Serra Cassano 1994].

Finally, note that derivatives and the fractional derivatives satisfy the truncation property.

Proposition 2.14. *Let Ω be an open set in $\mathbb{R}^n$ and $1 \le p < \infty$ and $0 < \alpha \le 1$. Let w be any Borel measure on Ω. Then for any $f \in L^1_{\mathrm{loc}}(\Omega)$* (or $\mathrm{Lip}_{\mathrm{loc}}(\Omega)$ if $\alpha = 1$), *we have*

$$\sum_{k=1}^{\infty} \|\nabla^\Omega_{\alpha,p} f_b^{2^k\omega}\|^p_{L^p_w(\Omega)} \le C(p)\|\nabla^\Omega_{\alpha,p} f\|^p_{L^p_w(\Omega)} \quad \textit{for any } \omega > 0 \textit{ and } b \in \mathbb{R}. \tag{2-15}$$

Proof. The case $\alpha = 1$ is well-known and obvious as

$$\sum_{k=1}^{\infty} \|\nabla f_b^{2^k\omega}\|^p_{L^p_w(\Omega)} \le \|\nabla|f-b|\|^p_{L^p_w(\Omega)} \le \|\nabla f\|^p_{L^p_w(\Omega)}.$$

For $0 < \alpha < 1$, a result has been stated in [Dyda et al. 2016, Theorem 4.1]. Unfortunately, the statement is not quite the same as ours. So we will provide the details here. Fix any $\omega > 0$ and $b \in \mathbb{R}$, let

$$A_i = \left\{x \in \Omega : 2^{i-1}\omega < |f(x)-b| \le 2^i\omega\right\}.$$

Then

$$
\begin{aligned}
&\sum_{k=1}^{\infty} \|\nabla_{\alpha,p}^{\Omega} f_b^{2^k\omega}\|_{L_w^p(\Omega)}^p \\
&\quad = \sum_{k=1}^{\infty} \int_{\Omega} \int_{B(x,\rho_\Omega(x))} \frac{|f_b^{2^k\omega}(x) - f_b^{2^k\omega}(y)|^p}{|x-y|^{n+\alpha p}}\, dy\, dw(x) \\
&\quad = \Biggl(\sum_{k=1}^{\infty} \sum_{i \le k \le j} \int_{A_i} \int_{A_j \cap B(x,\rho_\Omega(x))} \\
&\qquad\qquad + \sum_{k=1}^{\infty} \sum_{j \le k \le i} \int_{A_i} \int_{A_j \cap B(x,\rho_\Omega(x))} \Biggr) \frac{|f_b^{2^k\omega}(x) - f_b^{2^k\omega}(y)|^p}{|x-y|^{n+\alpha p}}\, dy\, dw(x).
\end{aligned}
$$

If $x \in A_i,\ y \in A_j,\ i < j-1$, then

$$
\begin{aligned}
&|f(x) - f(y)| \ge |f(y) - b| - |f(x) - b| \ge 2^{j-2}\omega, \\
\text{and}\quad &|f_b^{2^k\omega}(x) - f_b^{2^k\omega}(y)| \le 2^k\omega \le 4 2^{k-j} |f(x) - f(y)|.
\end{aligned}
$$

On the other hand $|f_b^{2^k\omega}(x) - f_b^{2^k\omega}(y)| \le |f(x) - f(y)|$ for all k. Hence,

$$
|f_b^{2^k\omega}(x) - f_b^{2^k\omega}(y)| \le 4 2^{k-j} |f(x) - f(y)| \quad \text{for all } i \le k \le j. \tag{2-16}
$$

Using the above (2-16), we have

$$
\begin{aligned}
&\sum_{k=1}^{\infty} \sum_{i \le k \le j} \int_{A_i} \int_{A_j \cap B(x,\rho_\Omega(x))} \frac{|f_b^{2^k\omega}(x) - f_b^{2^k\omega}(y)|^p}{|x-y|^{n+\alpha p}}\, dy\, dw(x) \\
&\qquad \le 4^p \sum_{k=1}^{\infty} \sum_{i \le k \le j} 2^{(k-j)p} \int_{A_i} \int_{A_j \cap B(x,\rho_\Omega(x))} \frac{|f(x) - f(y)|^p}{|x-y|^{n+\alpha p}}\, dy\, dw(x) \\
&\qquad \le \frac{4^p}{1 - 2^{-p}} \int_{\Omega} \int_{B(x,\rho_\Omega(x))} \frac{|f(x) - f(y)|^p}{|x-y|^{n+\alpha p}}\, dy\, dw(x).
\end{aligned}
$$

A similar estimate can be done for the remaining term. □

3. Proof of the main theorem and related results

Proof of Theorem 1.1. First, on each Ω_j, by Theorem 2.4, for any $(f, g) \in \mathfrak{S}$,

$$
\begin{aligned}
&\|f - f_{B'_j,\sigma}\|_{L_\mu^q(\Omega_j)} \\
&\qquad \le C\bigl(\theta_1, \theta_2, A_1, A_2, D_\sigma, \delta, \tau, c, q, p\bigr) c_T C_1 V_\mu^{1/q} \|g\|_{L_w^p(\Omega_j)}.
\end{aligned} \tag{3-1}
$$

Hence by the triangle inequality and Hölder's inequality,

$$\|f\|_{L^q_\mu(\Omega_j)} \le \|f_{B'_j,\sigma}\|_{L^q_\mu(\Omega_j)} + \|f - f_{B'_j,\sigma}\|_{L^q_\mu(\Omega_j)} \tag{3-2}$$
$$\le \frac{\mu(\Omega_j)^{1/q}}{\sigma(B'_j)^{1/p_0}}\|f\|_{L^{p_0}_\sigma(B'_j)} + Cc_T C_1 V_\mu^{1/q}\|g\|_{L^p_w(\Omega_j)}$$
$$\le C(c, D_\sigma)C_2\|f\|_{L^{p_0}_\sigma(\Omega_j)} + Cc_T C_1 V_\mu^{1/q}\|g\|_{L^p_w(\Omega_j)}$$

by (1-12) since σ is δ-doubling on Ω_j (with doubling constant D_σ) and $\Omega_j \subset C(c,\delta)B'_j$. Hence,

$$\Big(\sum\|f\|^q_{L^q_\mu(\Omega_j)}\Big)^{1/q} \le CC_2\Big(\sum\|f\|^q_{L^{p_0}_\sigma(\Omega_j)}\Big)^{1/q} + Cc_T C_1 V_\mu^{1/q}\Big(\sum\|g\|^q_{L^p_w(\Omega_j)}\Big)^{1/q}$$
$$\le CC_2\Big(\sum\|f\|^{p_0}_{L^{p_0}_\sigma(\Omega_j)}\Big)^{1/p_0} + Cc_T C_1 V_\mu^{1/q}\Big(\sum\|g\|^p_{L^p_w(\Omega_j)}\Big)^{1/p},$$

since $1 \le p, p_0 \le q$. Thus since $\sum \chi_{\Omega_j} \le M$,

$$\|f\|_{L^q_\mu(\Omega)} \le C\big[C_2 M^{1/p_0}\|f\|_{L^{p_0}_\sigma(\Omega)} + c_T C_1 V_\mu^{1/q} M^{1/p}\|g\|_{L^p_w(\Omega)}\big] \tag{3-3}$$

for all $(f,g) \in \mathfrak{S}$. We will now apply Theorem A.2 to prove Theorem 1.1(II)(b) and (II)(c).

First, by Proposition 2.7 and Remark 2.8(4) and Hölder's inequality, we have

$$\|f - f_{B,\mu}\|_{L^p_\mu(B)} \le C\mu(B)^{1/p-1/q}\|g\|_{L^p_w(3\tau B)} \tag{3-4}$$

for all $(f,g) \in \mathfrak{S}$ and any δ-ball B of any Ω_j. Now suppose $\{(f_n, g_n)\} \subset \mathfrak{S}$ such that $\{f_n\}$ and $\{g_n\}$ are bounded in $L^{p_0}_\sigma(\Omega)$ and $L^p_w(\Omega)$ respectively. Then $\{f_n\}$ is also bounded in $L^q_\mu(\Omega)$ by (3-3). Since $\mu(\Omega) < \infty$, given any $\varepsilon > 0$, there exists $L \in \mathbb{N}$ such that $\mu\big(\Omega \setminus \bigcup_{j=1}^L \Omega_j\big) < \varepsilon/2$. Next, for each $1 \le j \le L$, let $\{Q_{i,j}\}_{i=1}^\infty$ be a collection of bounded intersecting δ-balls of Ω_j such that $\Omega_j = \bigcup Q_{i,j}$ guaranteed by Proposition 2.6(a). Then there exists $k_j \in \mathbb{N}$ such that

$$\mu\big(\Omega_j \setminus \textstyle\bigcup_{i=1}^{k_j} Q_{i,j}\big) < \varepsilon/(2L).$$

For each

$$0 < r < \delta \min\big\{d\big(\Omega_j^c, \textstyle\bigcup_{i=1}^{k_j} Q_{i,j}\big) : 1 \le j \le L\big\}\big/(6\tau), \tag{3-5}$$

we choose any maximum family of pairwise disjoint balls $\{B(x_m, r/3)\}_{m=1}^K$ contained in $\bigcup_{1\le j\le L}\bigcup_{i=1}^{k_j} Q_{i,j}$. Then it is easy to see that each $B_r(x_m)$ is a δ-ball in some Ω_j and

$$\textstyle\bigcup_{m=1}^K B_r(x_m) \supset \bigcup_{1\le j\le L}\bigcup_{i=1}^{k_j} Q_{i,j}.$$

Note that the family $\{B(x_m, 3\tau r)\}_{m=1}^K$ has bounded overlaps. It is now clear by (3-4) that

$$\text{(3-6)}\quad \sum_{m=1}^{K} \|f_n - (f_n)_{B_r(x_m),\mu}\|^p_{L^p_\mu(B_r(x_m))} \le \sum_{m=1}^{K} C\mu(B_r(x_m))^{1-p/q}\|g_n\|^p_{L^p_w(B(x_m,3\tau r))} \le C\sup_m \mu(B_r(x_m))^{1-p/q}\|g_n\|^p_{L^p_w(\Omega)}.$$

We now choose r smaller if necessary such that the right hand side of (3-6) is less than ε^p, which is possible by Remark 1.2(8) and the fact that $\{g_n\}$ is bounded in $L^p_w(\Omega)$.

Taking $\{E_\ell\}$ as $\{B_r(x_m)\}_{m=1}^K$, by Theorem A.2, we conclude the proof of (II)(b). Part (c) of (II) is similar but easier; see Remark 1.2(10).

Finally, note that if we only assume (1-4) without the truncation property, then instead of (3-3), we will only have (if $p_0,\ p \le \tilde{q} < q$)

$$\text{(3-7)}\quad \|f\|_{L^{\tilde{q}}_\mu(\Omega)} \le C\sup_j \mu(\Omega_j)^{1/\tilde{q}-1/q}\big[C_2 M^{1/p_0}\|f\|_{L^{p_0}_\sigma(\Omega)} + C_1 V_\mu^{1/q} M^{1/p}\|g\|_{L^p_w(\Omega)}\big]$$

for all $(f, g) \in \mathfrak{S}$ while (3-4) remains valid. Remark 1.2(1) is now clear.

Proof of Theorem 1.4. First, clearly,

$$\rho_1\mu(B\cap\Omega_j) \le \mu^*(B)\prod_{i=1}^{l}\Psi_i(\bar{\eta}_i(B))^{a_i} \quad \text{for any } \Omega_j.$$

We now see that $\mu^*(B)\prod_{i=1}^{l}\Psi_i(\bar{\eta}_i(B))^{a_i}$ satisfies Condition (R). Indeed since Ψ_i's are monotone increasing, $a_i > 0$ and $\Psi_i(2t) \le C_{\Psi_i}\Psi_i(t)$ for all $t > 0$ and all i, we have

$$\Psi_i(\bar{\eta}_i(B))^{a_i} \le \Psi_i(\bar{\eta}_i(2B))^{a_i} \le C_{\rho_1}\Psi_i(\bar{\eta}_i(B))^{a_i} \quad \text{for all balls } B \text{ with center in } \Omega_j,$$

where $C_{\rho_1} = C\big(\{C_{\Psi_i}, a_i\}_{i=1}^l\big)$. Given any $x \in \Omega_j$, suppose $B_i = B(x, r_i^x)$ is the sequence given in Condition (R) for μ^*. The sequence will then work for $\mu^*(B)\prod_{i=1}^{l}\Psi_i(\bar{\eta}_i(B))^{a_i}$. That is, it satisfies Condition (R) (but with smaller constant A_1 and θ_1 on the left). Next, for any δ-ball Q of Ω_j, we have by (1-4),

$$\text{(3-8)}\quad \|f - f_{Q,\sigma}\|_{L^1_\sigma(Q)} \le a(Q)\|g\|_{L^p_w(\tau Q)} \le C(\{C_{\Psi_i}, b_i\}, p, \tau\delta)a(Q)\prod_{i=1}^{l}\Psi_i(\bar{\eta}_i(Q))^{-b_i/p}\|g\|_{L^p_{\rho_2 w}(\tau Q)}$$

as τQ is a $\tau\delta$-ball and ρ_2 is essentially constant on τQ. Moreover, if $Q \subset B$, where Q is a δ-ball, B is a ball with center in Ω_j such that $r(B) \le \operatorname{diam}(\Omega_j)$ and $r(Q) \ge c\delta r(B)/4$, then since $r(Q) \le \bar{\eta}_i(Q) \le \bar{\eta}_i(B) \le C(\delta, c)\bar{\eta}_i(Q)$ and

$\Psi_i(2t) \le C_{\Psi_i}\Psi_i(t),\ a_i > 0$ for all i, we have by (1-25),

$$\begin{aligned}\mu^*(B)^{1/q}a(Q)\prod_{i=1}^{l}\Psi_i(\bar\eta_i(B))^{a_i/q}\prod_{i=1}^{l}\Psi_i(\bar\eta_i(Q))^{-b_i/p}\\ &\le C(\delta,q,c,\{a_i,b_i,C_{\Psi_i}\})\mu^*(B)^{1/q}a(Q)\prod_{i=1}^{l}\Psi_i(\bar\eta_i(Q))^{a_i/q-b_i/p}\\ &\le C(\delta,q,c,\{a_i,b_i,C_{\Psi_i}\})C_1.\end{aligned}$$

Hence, we have by Theorem 2.4 that (1-26) holds. Next, by the triangle inequality and Hölder's inequality,

$$\|f\|_{L^p_{\rho_1\mu}(\Omega_j)} \le \frac{\rho_1\mu(\Omega_j)^{1/q}}{\sigma(B'_j)}\|f\|_{L^{p_0}_\sigma(B'_j)} + \|f - f_{B'_j,\sigma}\|_{L^p_{\rho_1\mu}(\Omega_j)} = I + II.$$

Using (1-27), noting that σ is δ-doubling on Ω_j on each j with doubling constant D_σ and $\Omega_j \subset C(c,\delta)B'_j$, we have

$$\begin{aligned}I &\le C\big(\delta,\tau,c,\{C_{\Psi_i},a_i\},q,p_0\big)\frac{\mu(\Omega_j)^{1/q}\prod_{i=1}^{l}\Psi_i(\bar\eta_i(B'_j))^{a_i/q}}{\sigma(B'_j)^{1/p_0}}\|f\|_{L^{p_0}_\sigma(B'_j)}\\ &\le C\big(c,\delta,\tau,\{C_{\Psi_i},a_i,\gamma_i\},p_0,q\big)\frac{\prod_{i=1}^{l}\Psi_i(\bar\eta_i(B'_j))^{a_i/q-\gamma_i/p_0}\mu(\Omega_j)^{1/q}}{\sigma(B'_j)^{1/p_0}}\|f\|_{L^{p_0}_{\rho_0\sigma}(B'_j)}\\ &\le C\big(c,\delta,\tau,D_\sigma,\{C_{\Psi_i},a_i,\gamma_i\},p_0,q\big)C_2\|f\|_{L^{p_0}_{\rho_0\sigma}(\Omega_j)},\end{aligned}$$

Combining with (1-26), we have

$$\begin{aligned}\|f\|_{L^p_{\rho_1\mu}(\Omega_j)} &\le C\big(c,\delta,\tau,D_\sigma,\{C_{\Psi_i},a_i,b_i,\gamma_i\},p,p_0,q\big)\\ &\qquad\times\big(C_2\|f\|_{L^{p_0}_{\rho_0\sigma}(\Omega_j)} + C_1c_TV_\mu^{1/q}\|g\|_{L^p_{\rho_2 w}(\Omega_j)}\big).\end{aligned}$$

Finally, we can conclude Theorem 1.4 by an argument as in the proof of Theorem 1.1.

Proof of Theorem 1.8. We will only prove the second part where $\mathcal{D} = \bigcup\Omega_j$. We will use Theorem 1.4 with $d\sigma = dx$ the Lebesgue measure, $\Psi = 1,\ \eta = \rho,\ \delta = \frac{1}{2}$ and $\mu^*(B) = C_\mu r(B)^N$. Since $\Omega_j \subset \mathbb{R}^n$, (μ_a,μ_a^*) (where $\mu_a^*(B) = \bar\rho(B)^a\mu^*(B)$) satisfies the Vitali-type property (1-10) with parameter depending only on n. Let $\mathfrak{S}$ be as in the proof of Corollary 1.6. Then the Poincaré inequality (1-4) holds for $\mathfrak{S}$ with $\sigma = 1$ and $g = \nabla^{\Omega_j}_{\alpha,p}f$ by (1-2). Note that $\nabla^{\Omega_j}_{\alpha,p}f \le \nabla^{\mathcal{D}}_{\alpha,p}f$. Again, $\mathfrak{S}$ satisfies (1-4) with the truncation property by Proposition 2.14.

Next, if B is a ball with center in $\Omega_j,\ r(B) \le \operatorname{diam}(\Omega_j)$ and Q is a δ-ball in B such that $r(Q) \ge c\,r(B)/8$, by the fact that $\bar\rho(Q) \ge Cr(Q)$ and (1-46),

$$\begin{aligned}\mu^*(B)^{1/q}a(Q)\bar\rho(B)^{a/q-b/p} &\le CC_*C_\mu^{1/q}r(Q)^{N/q+\beta_1}\bar\rho(Q)^{\beta_2+a/q-b/p}\\ &\le C\big(M_2,a,b,p,q,N,\beta_1,\beta_2\big)C_*C_\mu^{1/q}\end{aligned}$$

since $\beta_1 + \frac{N}{q} + \min\{0, \beta_2 + \frac{a}{q} - \frac{b}{p}\} \geq 0$ (by (i)) and $\beta_2 + \frac{a}{q} - \frac{b}{p} \leq 0$ when ρ is unbounded (by (ii)). Hence (1-25) holds. We now check that (1-27) holds. As $\Omega_j \subset C(c)B'_j$, by (1-45),

$$\begin{aligned}
(3\text{-}9)\quad & \mu(\Omega_j)^{1/q}|\Omega_j|^{-1/p_0}\bar{\rho}(\Omega_j)^{a/q-\gamma/p_0} \\
& \leq CC_\mu^{1/q}\min\{r(B'_j)^N, r(B'_j)^{N_1}\bar{\rho}(B'_j)^{N_2}\}^{1/q} r(B'_j)^{-n/p_0}\bar{\rho}(\Omega_j)^{a/q-\gamma/p_0} \\
& \leq CC_\mu^{1/q}\min\Big\{r(B'_j)^{N/q-n/p_0}\bar{\rho}(B'_j)^{a/q-\gamma/p_0}, \\
& \qquad\qquad r(B'_j)^{N_1/q-n/p_0}\bar{\rho}(B'_j)^{(N_2+a)/q-\gamma/p_0}\Big\},
\end{aligned}$$

which is bounded by $C(M_1, M_2, a, b, p_0, q, N, N_2, N_1, \gamma)C_\mu^{1/q}$ using (i), (ii) and the fact that $r(B'_j) \geq C(c, M_1)$. Equation (1-47) will then hold for all $f \in \mathfrak{S}_\alpha(\mathcal{D})$ by Theorem 1.4.

For the part of compact embedding, as we now allow $\mu_a(\mathcal{D}) = \infty$, we cannot use Theorem 1.4 directly, we will use Theorem A.3 instead of Theorem A.2. Now, suppose we have strict inequalities in conditions (i) and (ii). Then we can find $\tilde{q} > q$ and $\tilde{a} > a$ such that conditions (i) and (ii) hold with a and q being replaced by $\tilde{a}$ and $\tilde{q}$ respectively. We can then apply the first part of the theorem to conclude that (1-47) holds with either a being replaced by $\tilde{a}$ or q being replaced by $\tilde{q}$.

Now suppose $\{u_i\}_{i=1}^\infty \subset \mathfrak{S}_\alpha(\mathcal{D})$ such that both $\|u_i\|_{L^{p_0}_{\rho^\gamma}(\mathcal{D})}$ and $\|\nabla^{\mathcal{D}}_{\alpha,p}u_i\|_{L^p_{w_b}(\mathcal{D})}$ are bounded. Then $\{u_i\}$ is a bounded sequence in both $L^q_{\mu_{\tilde{a}}}(\mathcal{D})$ and $L^{\tilde{q}}_{\mu_a}(\mathcal{D})$. Hence it has a weakly convergent subsequence (in both $L^q_{\mu_{\tilde{a}}}(\mathcal{D})$ and $L^{\tilde{q}}_{\mu_a}(\mathcal{D})$) and for convenience, we will still denote the subsequence by $\{u_i\}$ and we may also assume that $\|u_i\|_{L^q_{\mu_{\tilde{a}}}(\mathcal{D})} \leq A$ for all i. Now, given any $\eta > 0$, let $\mathcal{D}_\eta = \{x \in \mathcal{D} : \rho(x) < \eta^{q/(a-\tilde{a})}\}$ and $\mathcal{D}'_\eta = \mathcal{D} \setminus \mathcal{D}_\eta$. Then,

$$\begin{aligned}
(3\text{-}10)\quad \|u_i - u_j\|^q_{L^q_{\mu_a}(\mathcal{D}'_\eta)} &= \int_{\mathcal{D}'_\eta} |u_i - u_j|^q \rho(x)^{a-\tilde{a}}\,d\mu_{\tilde{a}} \leq \eta^q \int_{\mathcal{D}'_\eta} |u_i - u_j|^q\,d\mu_{\tilde{a}} \\
&\leq (2A)^q\eta^q.
\end{aligned}$$

Again, by Proposition 2.7, for all i, we know inequality (2-11) holds with $f = u_i$, $g = \nabla^{\mathcal{D}}_{\alpha,p}u_i$, $\mu = \mu_a$, $w = w_b$, $\lambda = 3$ and $\tau = 1$. Next, given any $\varepsilon > 0$, as $q > p$, by Remark 1.2(8), we see that there exists $\delta_\varepsilon > 0$ such that (A-7) holds with $f = u_i$ if $r(B) < \delta_\varepsilon$ and $6B \subset \mathcal{D}$. Further, since $\mu_a(\mathcal{D}_\eta) < \infty$ by assumption, as $\{u_i\}$ and $\{\nabla^{\mathcal{D}}_{\alpha,p}u_i\}$ are bounded in $L^{\tilde{q}}_{\mu_a}(\mathcal{D}_\eta)$ and $L^p_{w_b}(\mathcal{D}_\eta)$ respectively, using Theorem A.3, $\{u_i\}$ has a subsequence (still denoted by $\{u_i\}$) converging in $L^{\tilde{q}}_{\mu_a}(\mathcal{D}_\eta)$ and hence Cauchy. Thus, there exists N_ε such that

$$(3\text{-}11)\qquad \|u_i - u_j\|_{L^q_{\mu_a}(\mathcal{D}_\eta)} \leq \varepsilon \quad \text{if } i, j \geq N_\varepsilon.$$

It is now clear that $\{u_i\}$ is a Cauchy sequence in $L^q_{\mu_a}(\mathcal{D})$.

Proof of Corollary 1.10. Let $f \in \operatorname{Lip}_{\mathrm{loc}}(\mathcal{D}) \cap L^{p_0}_{\rho^\gamma}(\mathbb{R}^n)$ if $\alpha = 1$ (or, if $\alpha < 1$, $f \in \widehat{W}^{\alpha,p}_{\rho^b}(\mathcal{D}) \cap L^{p_0}_{\rho^\gamma}(\mathbb{R}^n)$). It is known that $\mathbb{R}^n \setminus \mathrm{G} \in J(c,\infty)$ [Chua 1995, Proposition 2.7; 2009, Proposition 2.21]. Moreover, $\mathcal{D} = \mathbb{R}^n \setminus (\mathrm{G} \cup F) \in J(\tilde{c},\infty)$ [Chua 2009, Proposition 2.24]. Thus, given any $K > 0$, there exists $\{\Omega^K_j\} \subset J'(\tilde{c})$ such that $\operatorname{diam}(\Omega^K_j) \sim K$, center ball B^K_j of Ω^K_j with $r(B^K_j) \sim K$, $\bigcup \Omega^K_j = \mathcal{D}$ and $\sum \chi_{\Omega^K_j} \le C(n)$.

By (1-44), in Theorem 1.8(I), taking $dw = dx$, $\beta = \alpha - n/p$ and we have

$$\begin{aligned}\|f - f_{B^K_j}\|_{L^q_{\mu_a}(\Omega^K_j)} &\le C\bar{\rho}(R)^{\alpha+N+a/q-n+b/p}\|\nabla^{\mathcal{D}}_{\alpha,p} f\|_{L^p_{\rho^b}(\Omega^K_j)}\\ &= C\|\nabla^{\mathcal{D}}_{\alpha,p} f\|_{L^p_{\rho^b}(\Omega^K_j)}.\end{aligned}$$

Hence, by the triangle inequality, Hölder's inequality, the fact that $\bar{\rho}(B^K_j) \ge C\operatorname{diam}(\Omega^K_j)$ and ρ is essentially constant on B^K_j, we have

$$\begin{aligned}\text{(3-12)}\quad &\|f\|_{L^q_{\mu_a}(B^K_j)}\\ &\le C\mu_a(B^K_j)^{1/q}|B^K_j|^{-1/p_0}\bar{\rho}(B^K_j)^{-\gamma/p_0}\|f\|_{L^{p_0}_{\rho^\gamma}(B^K_j)} + C\|\nabla^{\mathcal{D}}_{\alpha,p} f\|_{L^p_{\rho^b}(\Omega^K_j)}\\ &\le C|\Omega^K_j|^{N/nq-1/p_0}\bar{\rho}(B^K_j)^{a/q-\gamma/p_0}\|f\|_{L^{p_0}_{\rho^\gamma}(B^K_j)} + C\|\nabla^{\mathcal{D}}_{\alpha,p} f\|_{L^p_{\rho^b}(\Omega^K_j)}\\ &\le C\operatorname{diam}(\Omega^K_j)^{(N+a)/q-(n+\gamma)/p_0}\|f\|_{L^{p_0}_{\rho^\gamma}(\Omega^K_j)} + C\|\nabla^{\mathcal{D}}_{\alpha,p} f\|_{L^p_{\rho^b}(\Omega^K_j)}\end{aligned}$$

since $a/q \le \gamma/p_0$. Finally, as $q \ge p, p_0$, we have by summing over Ω^K_j,

$$\text{(3-13)}\qquad \|f\|_{L^q_{\mu_a}(\mathbb{R}^n)} \le CK^{(N+a)/q-(n+\gamma)/p_0}\|f\|_{L^{p_0}_{\rho^\gamma}(\mathcal{D})} + C\|\nabla^{\mathcal{D}}_{\alpha,p} f\|_{L^p_{\rho^b}(\mathbb{R}^n)}.$$

Taking $K \to \infty$, as $(N+a)/q < (n+\gamma)/p_0$, we obtain (1-49) for $\alpha < 1$. For $\alpha = 1$, recall that by Remark 2.13(4), we know $\operatorname{Lip}_{\mathrm{loc}}(\mathcal{D})$ is dense in $L^{p_0}_{\rho^\gamma}(\mathcal{D}) \cap E^p_{\rho^b}(\mathcal{D})$ and this concludes the proof of the first part. Finally, the last part of the corollary follows from Remark 1.2(10) and is similar to the proof of the second part of Corollary 1.6. Indeed, instead of (3-12), we will have

$$\|f\|_{L^q_{\mu_a}(\Omega^k_j)} \le C\mu_a(\Omega^k_j)^{1/q-1/p_0}\|f\|_{L^{p_0}_{\mu_a}(\Omega^k_j)} + C\|\nabla^{\mathcal{D}}_{\alpha,p} f\|_{L^p_{\rho^b}(\Omega^k_j)}.$$

Summing up as before, by (1-51), again letting $K \to \infty$, we now see that (1-49) holds if $f \in \operatorname{Lip}_{\mathrm{loc}}(\mathcal{D}) \cap L^{p_0}_{\mu_a}(\mathbb{R}^n)$ or $f \in L^{p_0}_{\mu_a}(\mathbb{R}^n) \cap \widehat{W}^{\alpha,p}_{\rho^b}(\mathcal{D})$. Obviously, the condition involving γ is now redundant. Furthermore for $\alpha = 1$, (1-49) holds for all $f \in L^{p_0}_{\mu_a}(\mathbb{R}^n) \cap E^p_{\rho^b}(\mathcal{D})$ by Propositions 2.11 and 2.12.

Proof of Corollary 1.12. Since $\mathcal{D}$ is bounded, there exists a finite collection of dyadic cubes $\{R_j\}$ of the same size such that $\mathcal{D} \subset \bigcup \overline{R_j}$ and the center ball B'_j of each $R_j \setminus F$ does not intersect $\mathcal{D}$. In particular $f_{B'_j} = 0$ for each j if $f \in C^\infty_0(\mathcal{D})$. Hence, for each $R_j \setminus F$, by Theorem 1.8(I), we have (note that $R_j \setminus F \in J'(c)$ with c independent of j by Proposition 2.9 since F is finite),

$$\|f\|_{L^q_{\mu_a}(R_j)} = \|f\|_{L^q_{\mu_a}(R_j\setminus F)} \le CC^{1/q}_\mu\bar{\rho}(R_j)^{1+(N+a)/q-(n+b)/p}\|\nabla f\|_{L^p_{\rho^b}(R_j)}.$$

And hence

$$\|f\|_{L^q_{\mu_a}(\mathcal{D})} \le C\|\nabla f\|_{L^p_{\rho^b}(\mathcal{D})} \tag{3-14}$$

since $q \ge p$. Now if the inequality in (1-52) is strict, we can find $\tilde{q} > q$ such that the above inequality (3-14) holds with q being replaced by $\tilde{q}$. We can then apply Theorem A.3 to conclude that the embedding of $C_0^\infty(\mathcal{D})$ (and hence also the closure of $C_0^\infty(\mathcal{D})$ in $E^p_{\rho^b}(\mathcal{D})$) to $L^q_{\mu_a}(\mathcal{D})$ is compact. This completes the proof of Corollary 1.12.

Remark 3.1. If $\mathcal{D}$ is unbounded but there exists a collection of countable dyadic cubes $\{R_j\}$ of the same size such that $\mathcal{D} \subset \bigcup R_j$, $|R_j| \ge |\mathcal{D} \cap R_j|/2$ for all j and ρ is bounded on $\bigcup R_j$, then by taking the "parents" of those R_j (for convenience, we will still denote them by $\{R_j\}$), we may assume that the center ball B'_j of $R_j \setminus F$ does not intersect $\mathcal{D}$. We could then derive (3-14). Compact embedding of $C_0^\infty(\mathcal{D})$ (and hence also the closure of $C_0^\infty(\mathcal{D})$ in $E^p_{\rho^b}(\mathcal{D})$) to $L^q_{\mu_a}(\mathcal{D})$ can again be established under similar assumptions if $\mu_a\{x \in \mathcal{D} : \rho(x) < r\} < \infty$ for any $r > 0$.

Proof of Theorem 1.14. Instead of applying Theorem 1.8, we will apply techniques similar to those of [Chua 2009, Theorem 4.1, 4.3]. Moreover, we will also need either [Chua and Wheeden 2008, Theorem 2.9] or [Chua 2009, Theorem 2.11]. Note that a weak John domain is a Boman domain (see Proposition 2.6(c)). Next, by Proposition 2.9, there exists $\tilde{c}$ depending only on l, c and n such that for each j, $\widetilde{\Omega}_j = \Omega_j \backslash F \in J'(\tilde{c})$, where $F = \{z_i\}_{i=1}^l$. For convenience, we will let

$$\bar{d}_i(B) = \sup_{x \in B} |x - z_i| \quad \text{for each } i. \tag{3-15}$$

If Q is a δ-ball $\left(\delta = \frac{1}{5}\right)$ of $\widetilde{\Omega}_j$ for any j, then by Remark 1.2(5), (1-2) will hold with $a(Q) = C(n)|Q|^{\alpha/n-1/p}$ and $w = 1$. Hence for all $f \in \mathfrak{S}_\alpha(\widetilde{\mathcal{D}})$, where $\widetilde{\mathcal{D}} = \mathcal{D} \setminus F$, since ρ_1, ρ_2 are both essentially constant on δ-balls with constant depending only on $\{a_i\}$ and $\{b_i\}$ respectively,

$$\begin{aligned} &\|f - f_Q\|_{L^q_{\rho_1}(Q)} \\ &\qquad \le C\big(n, p, q, \{a_i, b_i\}_{i=1}^l\big)|Q|^{\alpha/n-1/p+1/q}\bar{\rho}_1(Q)^{1/q}\bar{\rho}_2(Q)^{-1/p}\|\nabla^{\widetilde{\mathcal{D}}}_{\alpha,p} f\|_{L^p_{\rho_2}(Q)}, \end{aligned}$$

where $\bar{\rho}_i(Q) = \sup_{x \in Q} \rho_i(x)$. Thus,

$$\begin{aligned} \|f - f_Q\|_{L^q_{\rho_1}(Q)} &\\ \le C\big(n, p, q, \{a_i, b_i\}_{i=1}^l\big)&r(Q)^{\alpha-n/p+n/q}\prod_{i=1}^l \bar{d}_i(Q)^{a_i/q-b_i/p}\|\nabla^{\widetilde{\mathcal{D}}}_{\alpha,p} f\|_{L^p_{\rho_2}(Q)} \\ \le C\big(\tilde{c}, n, p, q, \{a_i, b_i\}_{i=1}^l, c_0\big)&\varepsilon_0^b\|\nabla_{\alpha,p} f\|_{L^p_{\rho_2}(Q)} \end{aligned} \tag{3-16}$$

since

$$r(Q)^{\alpha-n/p+n/q}\prod_{i=1}^{l}\bar d_i(Q)^{a_i/q-b_i/p}\le C\big(\tilde c,n,p,q,\{a_i,b_i\}_{i=1}^{l}\big)r(Q)^b$$

as $\bar d_i(Q)\ge r(Q)$ and assumptions (i) and (ii).

By Proposition A.4, ρ_1 is δ-doubling on $\widetilde\Omega_j$ with doubling constant

$$C\big(\{a_i\}_{i=1}^{l},c_0\varepsilon_0/\zeta,n\big).$$

we can conclude (by either [Chua 2009, Theorem 2.11] or [Chua and Wheeden 2008, Theorem 2.9] as John domains are Boman domains [Buckley et al. 1996]) that

$$\|f-f_{B'_j}\|_{L^q_{\rho_1}(\widetilde\Omega_j)}\le C\big(\tilde c,n,p,q,\{a_i,b_i\}_{i=1}^{l},c_0\varepsilon_0/\zeta,c_0\big)\varepsilon_0^b\|\nabla^{\widetilde{\mathcal D}}_{\alpha,p}f\|_{L^p_{\rho_2}(\widetilde\Omega_j)}. \tag{3-17}$$

Using the triangle inequality and Hölder's inequality, we have

$$\|f\|_{L^q_{\rho_1}(\widetilde\Omega_j)}\le\rho_1(\widetilde\Omega_j)^{1/q}|B'_j|^{-1/p_0}\|f\|_{L^{p_0}(B'_j)}+C\varepsilon_0^b\|\nabla^{\widetilde{\mathcal D}}_{\alpha,p}f\|_{L^p_{\rho_2}(\widetilde\Omega_j)}=I+II.$$

Using the fact that ρ_0 is essentially constant on B'_j, we have

$$\begin{aligned}
I&\le C\big(p_0,\{\gamma_i\}_{i=1}^{l},\tilde c\big)\rho_1(\widetilde\Omega_j)^{1/q}|B'_j|^{-1/p_0}\prod_{i=1}^{l}\bar d_i(B'_j)^{-\gamma_i/p_0}\|f\|_{L^{p_0}(B'_j)}\\
&\le C\big(p_0,q,\tilde c,\{a_i,\gamma_i\}_{i=1}^{l}\big)|B'_j|^{1/q-1/p_0}\prod_{i=1}^{l}\bar d_i(B'_j)^{a_i/q-\gamma_i/p_0}\|f\|_{L^{p_0}_{\rho_0}(B'_j)}\\
&\le C\big(\tilde c,p_0,q,\{a_i,\gamma_i\}_{i=1}^{l},c_0\big)\varepsilon_0^{1/q-1/p_0+\sum(a_i/q-\gamma_i/p_0)}\|f\|_{L^{p_0}_{\rho_0}(B'_j)}\\
&=C\big(\tilde c,p_0,q,\{a_i,\gamma_i\}_{i=1}^{l},c_0\big)\varepsilon_0^{a}\|f\|_{L^{p_0}_{\rho_0}(B'_j)}
\end{aligned}$$

as $\operatorname{diam}(\widetilde\Omega_j)\sim\varepsilon_0$ (with constant c_0) and $\sum a_i/q\le\sum\gamma_i/p_0$. Since $1\le p,p_0\le q$, we have

$$\begin{aligned}
\|f\|_{L^q_{\rho_1}(\mathcal D)}&\le\Big(\sum_j\|f\|^q_{L^q_{\rho_1}(\widetilde\Omega_j)}\Big)^{1/q}\\
&\le C\varepsilon_0^a\Big(\sum_j\|f\|^q_{L^{p_0}_{\rho_0}(B'_j)}\Big)^{1/q}+C\varepsilon_0^b\Big(\sum_j\|\nabla^{\widetilde{\mathcal D}}_{\alpha,p}f\|^q_{L^p_{\rho_2}(\Omega_j)}\Big)^{1/q}\\
&\le C\varepsilon_0^a\Big(\sum_j\|f\|^{p_0}_{L^{p_0}_{\rho_0}(B'_j)}\Big)^{1/p_0}+C\varepsilon_0^b\Big(\sum_j\|\nabla^{\widetilde{\mathcal D}}_{\alpha,p}f\|^p_{L^p_{\rho_2}(\Omega_j)}\Big)^{1/p}\\
&\le C\varepsilon_0^aM^{1/p_0}\|f\|_{L^{p_0}_{\rho_0}(\mathcal D)}+C\varepsilon_0^bM^{1/p}\|\nabla^{\widetilde{\mathcal D}}_{\alpha,p}f\|_{L^p_{\rho_2}(\mathcal D)}.
\end{aligned}$$

Hence we have (1-55) when $0<\alpha<1$. If $\alpha=1$, we use density of $\mathrm{Lip}_{\mathrm{loc}}(\widetilde{\mathcal{D}})$ in $L^{p_0}_{\rho_0}(\widetilde{\mathcal{D}})\cap E^{p}_{\rho_2}(\widetilde{\mathcal{D}})$ which contains $L^{p_0}_{\rho_0}(\mathcal{D})\cap E^{p}_{\rho_2}(\mathcal{D})$; see Remark 2.13(4).

Next, if we have strict inequalities in both conditions (i) and (ii), we can find $\tilde{q}>q$ and $\alpha_1>a_1$ such that both conditions (i) and (ii) hold with q being replaced by $\tilde{q}$ and a_1 being replaced by α_1. We define

$$\rho_1(x)=\prod_{i=1}^{l}|x-z_i|^{\alpha_i},$$

where $\alpha_i=a_i$ for $i=2,\dots,l$ and α_1 is chosen above. Then (1-55) holds with either q being replaced by $\tilde{q}$ or ρ_1 being replaced by ρ_1. In case $\rho_1(\mathcal{D})<\infty$, the fact about compact embedding will follow from Theorem A.3. Next, in case $\rho_1(\mathcal{D})=\infty$, clearly $\mathcal{D}$ is unbounded. Suppose $\{f_i\}$ is a bounded sequence of functions in $L^{p_0}_{\rho_0}(\mathcal{D})$ and $E^{p}_{\rho_2}(\mathcal{D})$ (or $\widehat{W}^{\alpha,p}_{\rho_2}(\mathcal{D})$). We will show that it has a subsequence that is Cauchy in $L^{q}_{\rho_1}(\mathcal{D})$. First, as (1-55) holds with either q being replaced by $\tilde{q}$ or ρ_1 being replaced by ρ_1, we know the sequence is also bounded in $L^{q}_{\rho_1}(\mathcal{D})$ and $L^{\tilde{q}}_{\rho_1}(\mathcal{D})$. Thus it has a weakly convergent subsequence (still denoted by $\{f_i\}$) in $L^{q}_{\rho_1}(\mathcal{D})$ and $\|f_i\|_{L^{q}_{\rho_1}(\mathcal{D})}\le A$. Similar to the proof of Theorem 1.8, given any $\eta>0$, we define

$$\mathcal{D}_\eta=\left\{x\in\mathcal{D}:|x-z_1|<\eta^{\tilde{q}/(a_1-\alpha_1)}\right\}$$

and $\mathcal{D}'_\eta=\mathcal{D}\setminus\mathcal{D}_\eta$. As the rest of the proof is almost identical to that of Theorem 1.8, we will not repeat it here.

Finally, if in particular $\mathcal{D}\in J(c,\varepsilon_0)$ (see [Chua 2009]), we have (1-55) for all $0<\varepsilon<\varepsilon_0$ with ε being replaced by ε.

Remark 3.2. Suppose μ, w are Borel measures such that μ is δ-doubling on $\mathcal{D}$ with $\mathcal{D}$ given in Theorem 1.14. Checking through the proof above, we see that

$$\|f\|_{L^{q}_{\mu\rho_1}(\mathcal{D})}\le C\big(M^{1/p_0}\varepsilon_0^{-a}\|f\|_{L^{p_0}_{\mu\rho_0}(\mathcal{D})}+M^{1/p}\varepsilon_0^{b}\|g\|_{L^{p}_{w\rho_2}(\mathcal{D})}\big) \tag{3-18}$$

provided f and g are measurable functions on $\mathcal{D}$ such that

$$\|f-f_{Q,\mu}\|_{L^{q}_{\mu}(Q)}\le Cr(Q)^{\beta}\|g\|_{L^{p}_{w}(Q)}\quad\text{for all }\delta\text{-balls } Q \text{ of } \mathcal{D} \tag{3-19}$$

and condition (i) in Theorem 1.14 holds with α being replaced by β ($\beta\ge 0$). See also Theorem 1.8.

Appendix A.

For convenience, we state [Chua and Wheeden 2008, Theorem 1.2] here for easy reference.

Theorem A.1. *Let σ and μ be measures on a σ-algebra Σ of subsets of X. Let Ω be a measurable subset of X and f a fixed measurable function which satisfies* *the following assumptions for some constants* $0 < p_0, q < \infty,\ 0 < \theta < 1,\ C_\sigma \geq 1,$ $0 < \theta_1 < \theta_2 < 1,\ 0 < A_1, A_2 < \infty$ *and* $\wp \geq 1$:

(1) *For each* $x \in \Omega$, *there is a sequence of measurable sets* $\{Q_i^x\}_{i=1}^\infty$, *depending on* x, *and a fixed set* $B' \subset X$ *such that* $Q_1^x = B'$,

$$0 < \sigma(Q_i^x \cup Q_{i+1}^x) \leq C_\sigma \sigma(Q_i^x \cap Q_{i+1}^x) < \infty, \quad i = 1, 2, \dots, \tag{A-1}$$

and

$$\left(\frac{1}{\sigma(Q_i^x)} \int_{Q_i^x} |f - C(f, Q_i^x)|^{p_0}\, d\sigma\right)^{1/p_0} \leq a_*(Q_i^x), \tag{A-2}$$

where $\{C(f, Q_i^x)\}$ *is a sequence of constants that converges to* $f(x)$ *and* $\{a_*(Q_i^x)\}$ *is a sequence of nonnegative numbers.*

(2) *For each* $x \in \Omega$, *there is a sequence* $\{B_j^x\}_{j=1}^\infty$ *of measurable sets and a sequence* $\{\mu^*(B_j^x)\}$ *of positive numbers such that*

$$\mu(\Omega) \leq \wp\mu^*(B_1^x) \quad \textit{and} \quad A_1\theta_1^k \leq \frac{\mu^*(B_{j+k}^x)}{\mu^*(B_j^x)} \leq A_2\theta_2^k, \quad j, k \in \mathbb{N}. \tag{A-3}$$

(3) *Let* $\mathfrak{F} = \{B_j^x\}_{x\in\Omega, j\in\mathbb{N}}$. *Assume for any* $B_j^x \in \mathfrak{F}$, *there is* $\mathcal{C}(B_j^x) \subset \{Q_l^x\}_{l\in\mathbb{N}}$ *such that for each* $x \in \Omega$, $\bigcup_{j\in\mathbb{N}} \mathcal{C}(B_j^x) = \{Q_l^x\}_{l\in\mathbb{N}}$ *and* $\mathcal{C}(B_i^x) \cap \mathcal{C}(B_j^x) = \varnothing$ *when* $i \neq j$. *Further, for any countable subcollection* I *of pairwise disjoint sets* $\{B_\alpha\}$ *in* $\mathfrak{F}$, *let*

$$A(B_\alpha) = \sum_{Q\in\mathcal{C}(B_\alpha)} a_*(Q)$$

and assume that

$$\sum_{B_\alpha\in I} \big(A(B_\alpha)^q \mu^*(B_\alpha)\big)^\theta \leq (C_0^q \mu(\Omega))^\theta. \tag{A-4}$$

(4) *Suppose the collection* $\mathfrak{F}$ *is a cover of Vitali-type of subsets of* Ω *with respect to* (μ, μ^*), *i.e., given any measurable set* $E \subset \Omega$ *and a collection* $\mathcal{B}_E = \{B_{i(x)}^x : x \in E\}$, *there is a countable pairwise disjoint collection* $\mathcal{B}_E' \subset \mathcal{B}_E$ *such that*

$$\mu(E) \leq V_\mu \sum_{B_\alpha\in\mathcal{B}_E'} \mu^*(B_\alpha), \quad V_\mu \geq 1.$$

Then

$$\sup_{t>0} t\mu\{x \in \Omega : |f(x) - f_{B'}| > t\}^{1/q} \leq CC_0[\wp V_\mu\, \mu(\Omega)]^{1/q}, \tag{A-5}$$

where C *depends on* $C_\sigma, p_0, q, A_1, A_2, \theta, \theta_1$ *and* θ_2.

We will now state a general theorem that gives a necessary condition for precompact subsets of L^p spaces.

Theorem A.2 [Chua et al. 2013, Theorem 1.2]. *Let w be a finite measure on a σ-algebra Σ of subsets of a set Ω, with $\Omega \in \Sigma$. Let $1 \le p < \infty$, $1 < N \le \infty$ and $\mathcal{P}$ be a bounded subset of $L^N_\mu(\Omega)$. Suppose there is a positive constant C so that for every $\varepsilon > 0$, there are a finite number of sets $E_\ell \in \Sigma$ with*

(i) $$\mu\big(\Omega \setminus \textstyle\bigcup_\ell E_\ell\big) < \varepsilon \quad \text{and} \quad \mu(E_\ell) > 0;$$

(ii) *for every $f \in \mathcal{P}$,*

$$\sum_\ell \|f - f_{E_\ell,\mu}\|^p_{L^p_\mu(E_\ell)} \le C\varepsilon^p \quad \text{where } f_{E_\ell,\mu} = \int_{E_\ell} f\, d\mu/\mu(E_\ell). \tag{A-6}$$

Then for every sequence $\{f_k\} \subset \mathcal{P}$, there is a single subsequence $\{f_{k_i}\}$ and a function $f \in L^N_\mu(\Omega)$ such that $f_{k_i} \to f$ pointwise μ-a.e. in Ω and in $L^{\tilde q}_\mu(\Omega)$ norm for $1 \le \tilde q < N$.

Next, we state a useful special case of the above on Euclidean spaces. It is an extension of [Chua et al. 2013, Theorem 2.1]. Here we include the case of fractional derivatives. As almost the same proof as in [Chua et al. 2013] will give us the theorem, we shall not prove it.

Theorem A.3 [Chua et al. 2013, Theorem 2.1]. *Let $\widetilde\Omega \subset \Omega$ be both open sets in $\mathbb{R}^n$. Let μ, w be Borel measures on Ω with $\mu(\widetilde\Omega) = \mu(\Omega) < \infty$. Let $1 \le p < \infty$, $0 < \alpha \le 1$, $1 < N \le \infty$, $\tau_0 \ge 1$ and $\mathfrak{S} \subset L^N_\mu(\Omega) \cap E^p_w(\Omega)$ or $L^N_\mu(\Omega) \cap \widehat{W}^{\alpha,p}_w(\Omega)$, and suppose that for all $\varepsilon > 0$, there exists $\delta_\varepsilon > 0$ such that*

$$\|f - f_{B,\mu}\|_{L^p_\mu(B)} \le \varepsilon \|\nabla_{\alpha,p} f\|_{L^p_w(\tau_0 B)} \quad \text{for all } f \in \mathfrak{S} \tag{A-7}$$

and all Euclidean balls B with $r(B) < \delta_\varepsilon$ and $2\tau_0 B \subset \widetilde\Omega$. Then for any sequence $\{f_k\} \subset \mathfrak{S}$ that is bounded in $L^N_\mu(\Omega) \cap E^p_w(\Omega)$ or $L^N_\mu(\Omega) \cap \widehat{W}^{\alpha,p}_w(\Omega)$, there is a subsequence $\{f_{k_i}\}$ and a function $f \in L^N_\mu(\Omega)$ such that $f_{k_i} \to f$ pointwise μ-a.e. in Ω and in $L^{\tilde q}_\mu(\Omega)$ norm for $1 \le \tilde q < N$.

Finally, note that ρ_1 in Theorem 1.14 is δ-doubling with doubling constant independent of $\widetilde\Omega_j$. Indeed, we have the following more general result.

Proposition A.4. *Let $\{S_i\}_{i=1}^l$, $l \in \mathbb{N}$ be such that each S_i is a set of finite points in $\mathbb{R}^n$ and $S_i \cap S_j = \varnothing$ if $i \ne j$. Suppose Ω is an open set with* $\operatorname{diam}(\Omega) \le d$, *$a_i > -n$ for all i and $z \in \Omega^c$ for all $z \in \bigcup_{i=1}^l S_i$. Then the weight $\prod_{i=1}^l d(x, S_i)^{a_i}$ is δ-doubling on Ω with doubling constant depends only on n, $\{a_i\}_{i=1}^l$, and d/ζ, where $\zeta = \min\big\{|z-y| : z \ne y, z, y \in \bigcup_{i\in I^-} S_i = S'\big\}$, $I^- = \{i : a_i < 0\}$* (independent of d when S' has ≤ 1 point).

Proof. The result is easy when S' has ≤ 1 point; recall that $|x|^\alpha$ is doubling on $\mathbb{R}^n$ for $\alpha > -n$ and see Example 1.3(ii). Moreover, again by Example 1.3(ii), we only need to show that $\prod_{i\in I^-} d(x, S_i)^{a_i}$ is δ-doubling on Ω. Thus, we will only show that $\rho(x)=\prod_{i\in I^-} d(x,S_i)^{a_i}$ induces a δ-doubling measure on Ω. For convenience, we will let

$$\bar{d}_i(B)=\sup_{x\in B} d(x,S_i).$$

Let $\beta=\sum_{i\in I^-} a_i$. Given any ball B with $2B\subset\Omega$, clearly (as $a_i<0$ for all i)

$$\rho(B)\geq C(n,\{a_i\})\biggl(\prod_{i\in I^-}\bar{d}_i(B)^{a_i}\biggr)r(B)^n\geq C(n,\{a_i\})d^\beta r(B)^n. \tag{A-8}$$

Now, let $\widetilde{B}$ be a ball with the same center as B and $r(\widetilde{B})\geq 2r(B)$. Since

$$\widetilde{B}\subset\biggl(\bigcup_{z\in S'}(B(z,\zeta/2)\cap\widetilde{B})\biggr)\cup\{x\in\widetilde{B}:|x-z|\geq\zeta/2\ \forall z\in S'\}.$$

For the first term note that the number of such balls $B(z,\zeta/2)$ that intersect $\widetilde{B}$ is less than $C(n)\max\{1,(4r(\widetilde{B})/\zeta)^n)\}$. Now suppose $B(z,\zeta/2)$ intersects $\widetilde{B}$, $z\in S_1$. We see that as $-n<a_i<0$,

$$\begin{aligned}\rho(B(z,\zeta/2)\cap\widetilde{B})&\leq C(n,\{a_i\})(\zeta/2)^{\beta-a_1}\int_{B(z,\zeta/2)\cap\widetilde{B}}|x-z|^{a_1}\,dx\\&\leq C(n,\{a_i\})\zeta^{\beta-a_1}\min\{r(\widetilde{B})^{n+a_1},(\zeta/2)^{n+a_1}\}.\end{aligned}$$

Hence if $r(\widetilde{B})\geq\zeta/4$, we have

$$\begin{aligned}\rho(\widetilde{B})&\leq\sum_{z\in S'}\rho(B(z,\zeta/2)\cap\widetilde{B})+\rho\{x\in\widetilde{B}:|x-z|\geq\zeta/2\ \forall z\in S'\}\\&\leq C(n,\{a_i\})\zeta^\beta(4r(\widetilde{B})/\zeta)^n)\zeta^n+C(n,\{a_i\})\zeta^\beta r(\widetilde{B})^n\\&\leq C(n,\{a_i\})\zeta^\beta r(\widetilde{B})^n.\end{aligned}$$

On the other hand, if $r(\widetilde{B})\leq\zeta/4$, then there is at most one $z_1\in S'$ with $d(z_1,\widetilde{B})<\zeta/4$. For simplicity, let us assume $z_1\in S_1$. We have

$$\begin{aligned}\rho(\widetilde{B})&\leq\rho(B(z_1,\zeta/2)\cap\widetilde{B})+\rho\{x\in\widetilde{B}:|x-z|\geq\zeta/2\ \forall z\in S'\}\\&\leq C(n,\{a_i\})\zeta^{\beta-a_1}r(\widetilde{B})^{n+a_1}+C(n,\{a_i\})\zeta^\beta r(\widetilde{B})^n\\&\leq C(n,\{a_i\})\zeta^{\beta-a_1}r(\widetilde{B})^{n+a_1}.\end{aligned}$$

Moreover, if $d(z,\widetilde{B})\geq\zeta/4$ for all $z\in S'$, we have $\rho(\widetilde{B})\leq C(n,\{a_i\})\zeta^\beta r(\widetilde{B})^n$. It is now easy to see that

$$\rho(\widetilde{B})/\rho(B)\leq C(\zeta,n,\{a_i\}_{i\in I'})\max_i\{(r(\widetilde{B})/r(B))^{n+a_i},(\zeta/d)^{\beta-a_i}\}.$$

In the above, we have assumed that the total number of points in $\bigcup S_i$ is more than 1. If there is only one point z, it is well-known that the weight $|x-z|^a$ induces a measure that is doubling on $\mathbb{R}^n$ if $a>-n$. $\square$

Appendix B.

Proof of Proposition 2.6. In this proof, we will only assume the following condition:

There is a fixed "center" $x' \in \Omega$ such that for any $x \neq x'$ in Ω, there exists $\gamma : [0, l] \to \Omega$ such that $\gamma(0) = x,\ \gamma(1) = x'$ and γ is "continuous," i.e.,

(B-1) for all $\varepsilon > 0$ and $t_0 \in [0, l]$, there exists $\delta > 0$ such that

$$d(\gamma(t), \gamma(t_0)) < \varepsilon \quad \text{when } |t - t_0| < \delta,\ t \in [0, l];$$

and γ satisfies the weak John condition

$$d(\gamma(t), \Omega^c) = \inf\{d(\gamma(t), y) : y \notin \Omega\} \geq c\, d(\gamma(t), x) \quad \text{for all } t. \tag{B-2}$$

Note that while (B-2) remains the same, the main paper assumes γ is Lipschitz continuous instead of (B-1).

Even though we have allowed $\tau\delta \leq 1/(2\kappa^2)$ here instead of $\tau\delta < 1/(2\kappa^2)$ in [Chua and Wheeden 2008, Proposition 2.6], the proof of part (a) and (b) are essentially the same. For (2.5), just see [Chua and Wheeden 2008, (2.6)]. However, the assumptions in (c)–(e) are more different from those of [Chua and Wheeden 2008, Proposition 2.6]; we will provide a proof here. We will now prove (c). Fix a point $x \in \Omega$, and let $\gamma(t),\ t \in [0, l]$, be a curve connecting x and x' satisfying conditions guaranteed by the weak John property (B-2). With $\delta' = \delta/\lambda^3$, we begin by constructing a special sequence of δ'-Whitney balls centered along γ. For $t \in [0, l]$, let

$$\mathcal{R}_{\gamma(t)} = B\big(\gamma(t), \delta' d(\gamma(t))\big).$$

Use (2-5) to pick $\widetilde{B}_0 \in \widetilde{W}$ containing $\mathcal{R}_{\gamma(0)}$, and let

$$t_1 = \sup\{t \in [0, 1] : \gamma(t) \in \widetilde{B}_0\}.$$

Note that $t_1 > 0$ by continuity of γ. Moreover, $\mathcal{R}_{\gamma(t_1)}$ intersects $\widetilde{B}_0$ by definition of t_1 and continuity of γ. We then use (2-5) again to choose a ball $\widetilde{B}_1 \in \widetilde{W}$ containing $\mathcal{R}_{\gamma(t_1)}$. Then clearly $\widetilde{B}_0$ intersects $\widetilde{B}_1$. If $t_1 = l$, we stop the construction process. If $t_1 < l$, we define

$$t_2 = \sup\{t \in [t_1, l] : \gamma(t) \in \widetilde{B}_1\}$$

and choose $\widetilde{B}_2 \in \widetilde{W}$ containing $\mathcal{R}_{\gamma(t_2)}$. Again, $t_1 < t_2 \leq l$ and $\widetilde{B}_1 \cap \widetilde{B}_2 \neq \varnothing$. In general, if $0 = t_0 < t_1 < \cdots < t_k$ and $\widetilde{B}_0, \widetilde{B}_1, \ldots, \widetilde{B}_k$ with $\widetilde{B}_i \cap \widetilde{B}_{i+1} \neq \varnothing$ have been constructed and if $t_k < l$, we continue by defining

$$t_{k+1} = \sup\{t \in [t_k, l] : \gamma(t) \in \widetilde{B}_k\} \tag{B-3}$$

and using (2-5) to pick $\widetilde{B}_{k+1} \in \widetilde{W}$ containing $\mathcal{R}_{\gamma(t_{k+1})}$. As before, we have $t_k < t_{k+1} \le l$ and $\widetilde{B}_k \cap \widetilde{B}_{k+1} \ne \varnothing$. We stop the construction if $t_{k+1} = l$.

Let us show that the process must end after a finite number of steps, i.e., that there is a positive integer $L = L_x$ such that $t_L = l$. To see this, note that since γ is continuous, taking $\varepsilon = \min\{c\delta' d(\gamma(t_1), x), \delta' d(x)\}$, we can find $\eta > 0$ such that

$$d(\gamma(s_1), \gamma(s_2)) < \varepsilon \quad \text{if } |s_1 - s_2| < \eta \text{ and } s_1, s_2 \in [0, l]. \tag{B-4}$$

Claim: $$|t_k - t_{k+1}| \ge \eta \quad \text{for all } k \ge 1 \text{ such that } t_{k+1} < l.$$

Note that we are done if $t_{k+1} = l$. Suppose $|t_{k+1} - t_k| < \eta$, then there exists $l \ge t' > t_{k+1}$ and $|t' - t_k| < \eta$. But by (B-4), we have $d(\gamma(t'), \gamma(t_k)) < \varepsilon$. On the other hand by (B-2)

$$\delta' d(\gamma(t_k)) \ge c\delta' d(\gamma(t_k), x) \ge c\delta' d(\gamma(t_1), x) \ge \varepsilon,$$

as $\gamma(t_k) \notin \mathcal{R}_{\gamma(0)}$ if $k > 1$ and hence $\gamma(t') \in \mathcal{R}_{\gamma(t_k)} \subset \widetilde{B}_k$ while $t' > t_{k+1}$ and it is a contradiction to (B-3). This proves the claim. It is now easy to see that $L - 1 \le l/\eta$.

For each $\widetilde{B}_i$ constructed above, let $B_i = 2\kappa \widetilde{B}_i$ just as in the proof of [Chua and Wheeden 2008, Proposition 2.6(c)], we see that except for (2-6), the first part of (c) is proved.

Let us now prove (2-6). The case when $B_0 \cap B_i \ne \varnothing$ is easy since then $B_0 \subset \lambda^4 B_i$ (see [Chua and Wheeden 2008, p. 2996]) and hence (2-6) is obvious.

Next, suppose that $B_0 \cap B_i = \varnothing$. The following is just a simple modification of [Chua and Wheeden 2008, p. 2996]. Due to the construction of B_i, there is a point $\xi \in \widetilde{B}_i \cap \gamma[0, l]$. Since $\xi \notin B_0$ and $x \in \widetilde{B}_0 = B_0/(2\kappa)$, the quasitriangle inequality gives $d(\xi, x) \ge r(B_0)/(2\kappa)$. Similarly, since $x \notin B_i$ and $\xi \in \widetilde{B}_i$, we have $d(\xi, x) \ge r(B_i)/(2\kappa)$. Hence,

$$d(\xi, x) \ge \frac{1}{2\kappa} \max\{r(B_0), r(B_i)\}.$$

We can use this to show that

$$B_0 \subset \frac{\lambda^2 d(\xi, x)}{r(B_i)} B_i.$$

In fact, if $z \in B_0$ then

$$\begin{aligned} d(z, x_{B_i}) &\le \kappa[d(z, x) + d(x, x_{B_i})] \\ &\le \kappa\big[\kappa\{d(z, x_{B_0}) + d(x, x_{B_0})\} + \kappa\{d(x_{B_i}, \xi) + d(\xi, x)\}\big] \\ &< \kappa\big[2\kappa r(B_0) + \kappa r(\widetilde{B}_i) + \kappa d(\xi, x)\big], \end{aligned}$$

and thus by the previous estimate for $d(\xi, x)$, we have

$$d(z, x_{B_i}) < (4\kappa^3 + 2\kappa^2)\, d(\xi, x) < \lambda^2 d(\xi, x)$$

as desired. To complete the proof of (2-6), we now recall from (B-2) that $d(\xi) \geq c\,d(x,\xi)$. But since $\xi \in B_i$ and B_i is a δ-ball ($\delta \leq 1/(2\kappa^2)$), triangle inequality and (a) give

$$d(\xi) \leq 2\kappa d(x_{B_i}) \leq 2\kappa \frac{\lambda^2}{\delta} r(B_i).$$

Combining estimates, we obtain $d(\xi, x) \leq (2\kappa\lambda^2/(c\delta))r(B_i)$, so that

$$B_0 \subset \frac{\lambda^2 d(\xi, x)}{r(B_i)} B_i \subset \frac{2\kappa\lambda^4}{c\delta} B_i,$$

which proves (2-6) in all cases.

To prove the last statement in (c), we return to the δ'-Whitney balls $\{\mathcal{R}_{\gamma(t_i)}\}_{i=0}^{L}$ centered on the weak John curve γ from x to x', and define balls $\mathcal{Q}_i$ by

$$\mathcal{Q}_i = \lambda^3 \mathcal{R}_{\gamma(t_i)}.$$

Then $\mathcal{Q}_i$ has center on γ and is a δ-Whitney ball since $r(\mathcal{Q}_i) = \lambda^3\delta' d(\gamma(t_i)) = \delta d(\gamma(t_i))$. The same argument as in the proof of [Chua and Wheeden 2008, Proposition 2.6(c)] then establishes the second part of (c).

To verify part (d), note that the hypothesis $\mathcal{Q}_i \not\subset B(x,r)$ implies there exists $z \in \mathcal{Q}_i$ such that $d(z,x) \geq r$. Let $x_i = \gamma(t_i)$ be the center of $\mathcal{Q}_i$ and $r_i = r(\mathcal{Q}_i)$. Then by the triangle inequality and the fact that $d(x_i, x) = d(\gamma(t_i), x) \leq d(\gamma(t_i))/c = r_i/(c\delta)$, we have

$$r \leq d(z,x) \leq \kappa(d(z,x_i) + d(x_i,x)) \leq \kappa \frac{c\delta+1}{c\delta} r_i < \frac{2\kappa r_i}{c\delta}.$$

This completes the proof of (d).

To prove part (e), we will again use the estimate

$$r(\mathcal{Q}_i) = \delta d(\gamma(t_i)) \geq c\delta d(\gamma(t_i), x),$$

which follows from the weak John condition (B-2). Thus if $r(\mathcal{Q}_i) \leq 2\varepsilon$, then

$$2\varepsilon \geq c\delta d(\gamma(t_i), x) \quad \text{and hence} \quad \mathcal{Q} \subset B(x, 4\kappa\varepsilon/(c\delta)).$$

However, as there is a δ-doubling measure σ on Ω, the number of disjoint $\mathcal{Q}$ of radius between ε and 2ε is bounded with bound depending only on D_σ, κ, δ and c. This completes the proof of Proposition 2.6.

Proof of Proposition 2.9. For this proof, we will be again assuming only (B-1) instead of Lipschitz continuity.

Let x' be the central point of Ω and let $d(z, \Omega^c) = (\theta+2)\varepsilon$. We will consider two cases:

Case (i): $x' \in B_\varepsilon(z)$. We will assume $B_\varepsilon(z) \neq \Omega$ as the case $B_\varepsilon(z) = \Omega$ follows immediately from the path property. Using the path property, we know that there exists $x'' \notin B_\varepsilon(z)$ such that $d(x'', z) = \varepsilon$. Moreover, note that

$$d(x', \Omega^c) \leq d(x', z) + d(z, \Omega^c) \leq (\theta + 3)\varepsilon.$$

For any $x \in \Omega \backslash \{z\}$, $x \neq x''$, we will now construct a continuous path connecting x to x''. First suppose $x \in B_\varepsilon(z)$. By assumption, there exists continuous

$$\eta : [0, 1] \to B_{\theta\varepsilon}(z) \setminus B_{d(x,z)/\theta}(z).$$

Clearly $d(\eta(t), \Omega^c) > 2\varepsilon > \frac{2}{\theta} d(\eta(t), z)$ and $d(\eta(t), z) > \frac{1}{1+\theta} d(\eta(t), x)$ since

$$d(\eta(t), x) \leq d(\eta(t), z) + d(x, z) \leq (1+\theta) d(\eta(t), z).$$

Next, suppose $x \notin B_\varepsilon(z)$. Since $\Omega \in J'(c)$, there exists continuous $\gamma : [0, l] \to \Omega$ such that $\gamma(0) = x$, $\gamma(l) = x'$ and

$$d(\gamma(t), \Omega^c) \geq c\, d(\gamma(t), x) \quad \text{for all } t \in [0, l]. \tag{B-5}$$

Since $\gamma(l) \in B(z, \varepsilon)$, we now define

$$t' = \inf\{t \in [0, l] : \gamma(t) \in B_\varepsilon(z)\}.$$

Note that by continuity, we know $d(\gamma(t'), z) = \varepsilon$. Since $t' < l$, by the path property, there exists a continuous $\eta : [t', l] \to B_{\theta\varepsilon}(z) \setminus B_{\varepsilon/\theta}(z)$ such that $\eta(t') = \gamma(t')$ and $\eta(l) = x''$. Note that $d(\eta(t), \Omega^c), d(\eta(t), z) \geq \varepsilon/\theta$. Since

$$\begin{aligned} d(\eta(t), x) &\leq d(\eta(t), z) + d(z, x') + d(x, x') < \theta\varepsilon + \varepsilon + \frac{1}{c} d(x', \Omega^c) \\ &< \frac{2\theta+3}{c}\varepsilon, \end{aligned} \tag{B-6}$$

it is now clear that

$$d(\eta(t), \Omega^c \cup z) \geq c_0 d(\eta(t), x) \quad \text{with } c_0 = \frac{c}{(2\theta + 3)\theta}.$$

Combining γ with η, we obtain a continuous curve satisfying (B-2) connecting x to x''.

Case (ii): $x' \notin B_\varepsilon(z)$. Again, there exists a continuous $\gamma : [0, l] \to \Omega$ such that $\gamma(0) = x$ and $\gamma(l) = x'$ satisfies (B-5). We now consider two subcases.

Subcase (a): $\gamma[0, l] \cap B_\varepsilon(z) = \varnothing$. Then $d(\gamma(t), z) \geq \varepsilon$ for all t. Moreover,

$$d(\gamma(t), \Omega^c) \leq d(\gamma(t), z) + d(z, \Omega^c) \leq (\theta + 3)\, d(\gamma(t), z). \tag{B-7}$$

Hence

$$d(\gamma(t), \Omega^c \cup \{z\}) \geq \frac{1}{\theta+3} d(\gamma(t), \Omega^c) \geq \frac{c}{\theta+3} d(\gamma(t), x).$$

Subcase (b): $\gamma[0, l] \cap B_\varepsilon(z) \neq \varnothing$. Similar to case (i), we will let

$$t' = \inf\{t : \gamma(t) \in B_\varepsilon(z)\}.$$

Moreover, we also let

$$t'' = \sup\{t : \gamma(t) \in B_\varepsilon(z)\}.$$

Again, there exists $\eta : [t', t''] \to B_{\theta\varepsilon}(z) \setminus B_{\varepsilon/\theta}(z)$ with $\eta(t') = \gamma(t'),\ \eta(t'') = \gamma(t'')$.

We now define

$$\tilde{\gamma} = \begin{cases} \gamma(t) & \text{for } t \in [0, t'] \cup [t'', l], \\ \eta(t) & \text{for } t \in [t', t'']. \end{cases}$$

The case $t \in [0, t'] \cup [t'', l]$ follows from (B-7) and the case $t \in [t', t'']$ follows from (B-6).

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A PRO-p GROUP WITH INFINITE NORMAL HAUSDORFF SPECTRA

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Using wreath products, we construct a finitely generated pro-p group G with infinite normal Hausdorff spectrum

$$\mathrm{hspec}_{\trianglelefteq}^{\mathcal{P}}(G) = \{\mathrm{hdim}_G^{\mathcal{P}}(H) \mid H \trianglelefteq_{\mathrm{c}} G\};$$

here $\mathrm{hdim}_G^{\mathcal{P}} : \{X \mid X \subseteq G\} \to [0, 1]$ denotes the Hausdorff dimension function associated to the p-power series $\mathcal{P}$: G^{p^i}, $i \in \mathbb{N}_0$. More precisely, we show that $\mathrm{hspec}_{\trianglelefteq}^{\mathcal{P}}(G) = \left[0, \frac{1}{3}\right] \cup \{1\}$ contains an infinite interval; this settles a question of Shalev. Furthermore, we prove that the normal Hausdorff spectra $\mathrm{hspec}_{\trianglelefteq}^{\mathcal{S}}(G)$ with respect to other filtration series $\mathcal{S}$ have a similar shape. In particular, our analysis applies to standard filtration series such as the Frattini series, the lower p-series and the modular dimension subgroup series.

Lastly, we pin down the ordinary Hausdorff spectra

$$\mathrm{hspec}^{\mathcal{S}}(G) = \{\mathrm{hdim}_G^{\mathcal{S}}(H) \mid H \leq_{\mathrm{c}} G\}$$

with respect to the standard filtration series $\mathcal{S}$. The spectrum $\mathrm{hspec}^{\mathcal{L}}(G)$ for the lower p-series $\mathcal{L}$ displays surprising new features.

1. Introduction

The concept of Hausdorff dimension has led to interesting applications in the context of profinite groups; e.g., [Barnea and Shalev 1997; Barnea and Klopsch 2003; Ershov 2004; 2010; Abért and Virág 2005; Jaikin-Zapirain and Klopsch 2007; Fernández-Alcober et al. 2017; Klopsch et al. 2019]. Let G be a countably based infinite profinite group and consider a *filtration series* $\mathcal{S}$ of G, that is, a descending chain $G = G_0 \supseteq G_1 \supseteq \cdots$ of open normal subgroups $G_i \trianglelefteq_{\mathrm{o}} G$ such that $\bigcap_i G_i = 1$.

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These open normal subgroups form a base of neighbourhoods of the identity and induce a translation-invariant metric on G given by

$$d^{\mathcal{S}}(x, y) = \inf\bigl\{|G : G_i|^{-1} \mid x \equiv y \pmod{G_i}\bigr\}, \quad \text{for } x, y \in G.$$

This, in turn, supplies the *Hausdorff dimension* $\operatorname{hdim}^{\mathcal{S}}_G(U) \in [0, 1]$ of any subset $U \subseteq G$, with respect to the filtration series $\mathcal{S}$.

Barnea and Shalev [1997] established the following "group-theoretic" interpretation of the Hausdorff dimension of a closed subgroup H of G as a logarithmic density:

$$\operatorname{hdim}^{\mathcal{S}}_G(H) = \varliminf_{i\to\infty} \frac{\log|HG_i : G_i|}{\log|G : G_i|}.$$

The *Hausdorff spectrum* of G, with respect to $\mathcal{S}$, is

$$\operatorname{hspec}^{\mathcal{S}}(G) = \{\operatorname{hdim}^{\mathcal{S}}_G(H) \mid H \le_{\mathrm{c}} G\} \subseteq [0, 1],$$

where H runs through all closed subgroups of G. As indicated by Shalev [2000, §4.7], it is also natural to consider the *normal Hausdorff spectrum* of G, with respect to $\mathcal{S}$, namely

$$\operatorname{hspec}^{\mathcal{S}}_{\trianglelefteq}(G) = \{\operatorname{hdim}^{\mathcal{S}}_G(H) \mid H \trianglelefteq_{\mathrm{c}} G\}$$

which reflects the range of Hausdorff dimensions of closed normal subgroups. Apart from the observations in [Shalev 2000, §4.7], very little appears to be known about normal Hausdorff spectra of profinite groups.

Throughout we will be concerned with pro-p groups, where p denotes an odd prime; in the Appendix we indicate how our results extend to $p = 2$. We recall that even for well structured groups, such as p-adic analytic pro-p groups G, the Hausdorff dimension function and the Hausdorff spectrum of G are known to be sensitive to the choice of $\mathcal{S}$; compare [Klopsch et al. 2019]. However, for a finitely generated pro-p group G there are natural choices for $\mathcal{S}$, such as the p-power series $\mathcal{P}$, the Frattini series $\mathcal{F}$, the lower p-series $\mathcal{L}$ and the modular dimension subgroup series $\mathcal{D}$; see Section 2.

In this paper, we are interested in a particular group G constructed as follows. The pro-p wreath product $W = C_p \,\hat{\wr}\, \mathbb{Z}_p$ is the inverse limit $\varprojlim_{k\in\mathbb{N}} C_p \wr C_{p^k}$ of the finite standard wreath products of cyclic groups with respect to the natural projections; clearly, W is 2-generated as a topological group. Let F be the free pro-p group on two generators and let $R \trianglelefteq_{\mathrm{c}} F$ be the kernel of a presentation $\pi : F \to W$. We are interested in the pro-p group

$$G = F/N, \quad \text{where } N = [R, F]R^p \trianglelefteq_{\mathrm{c}} F.$$

Up to isomorphism, the group G does not depend on the particular choice of π, as can be verified using Gaschütz' Lemma; see [Lubotzky 2001, Proposition 2.2].

Indeed, G can be described as the universal covering group for 2-generated central extensions of elementary abelian pro-p groups by W, i.e., for 2-generated pro-p groups E admitting a central elementary abelian subgroup A such that $E/A \cong W$.

Theorem 1.1. *For $p > 2$, the normal Hausdorff spectra of the pro-p group G constructed above, with respect to the standard filtration series $\mathcal{P}$, $\mathcal{D}$, $\mathcal{F}$ and $\mathcal{L}$ respectively, satisfy*:

$$\begin{aligned}
&\mathrm{hspec}^{\mathcal{P}}_{\trianglelefteq}(G) = \mathrm{hspec}^{\mathcal{D}}_{\trianglelefteq}(G) = \left[0, \tfrac{1}{3}\right] \cup \{1\},\\
&\mathrm{hspec}^{\mathcal{F}}_{\trianglelefteq}(G) = [0, 1/(1+p)] \cup \{1\},\\
&\mathrm{hspec}^{\mathcal{L}}_{\trianglelefteq}(G) = \left[0, \tfrac{1}{5}\right] \cup \left\{\tfrac{3}{5}\right\} \cup \{1\}.
\end{aligned}$$

In particular, they each contain an infinite real interval.

This solves a problem posed by Shalev [2000, Problem 16]. We observe that the normal Hausdorff spectrum of G is sensitive to changes in filtration and that the normal Hausdorff spectrum of G with respect to the Frattini series varies with p.

In Section 4 we show that finite direct powers $G \times \cdots \times G$ of the group G provide examples of normal Hausdorff spectra consisting of multiple intervals. Furthermore, the sequence $G \times \overset{m}{\cdots} \times G$, $m \in \mathbb{N}$, has normal Hausdorff spectra "converging" to $[0, 1]$; compare Corollary 4.5. We highlight three natural problems.

Problem 1.2. Does there exist a finitely generated pro-p group H

(a) with countably infinite normal Hausdorff spectrum $\mathrm{hspec}^{\mathcal{S}}_{\trianglelefteq}(H)$,

(b) with full normal Hausdorff spectrum $\mathrm{hspec}^{\mathcal{S}}_{\trianglelefteq}(H) = [0, 1]$,

(c) such that 1 is not an isolated point in $\mathrm{hspec}^{\mathcal{S}}_{\trianglelefteq}(H)$,

for one or several of the standard series $\mathcal{S} \in \{\mathcal{P}, \mathcal{D}, \mathcal{F}, \mathcal{L}\}$?[1]

We also compute the entire Hausdorff spectra of G with respect to the four standard filtration series, answering en route a question raised in [Klopsch 1999, VIII.7.2].

Theorem 1.3. *For $p > 2$, the Hausdorff spectra of the pro-p group G constructed above, with respect to the standard filtration series, satisfy*:

$$\begin{aligned}
&\mathrm{hspec}^{\mathcal{P}}(G) = \mathrm{hspec}^{\mathcal{D}}(G) = \mathrm{hspec}^{\mathcal{F}}(G) = [0, 1],\\
&\mathrm{hspec}^{\mathcal{L}}(G) = \left[0, \tfrac{4}{5}\right) \cup \left\{\tfrac{3}{5} + 2m/(5p^n) \mid m, n \in \mathbb{N}_0 \text{ with } p^n/2 < m \le p^n\right\}.
\end{aligned}$$

[1]Note added in article proof: In the meantime, I. de las Heras and B. Klopsch have modified the construction given in the present paper to obtain a positive answer to question (b), and hence to question (c). Their paper is forthcoming.

The qualitative shape of the spectrum $\mathrm{hspec}^{\mathcal{L}}(G)$, i.e., its decomposition into a continuous and a noncontinuous, but dense part, is unprecedented and of considerable interest; in Corollary 2.11 we show that already the wreath product $W = C_p \,\hat{\wr}\, \mathbb{Z}_p$ has a similar Hausdorff spectrum with respect to the lower p-series.

Organisation. Section 2 contains preliminary results. In Section 3 we give an explicit presentation of the pro-p group G and describe a series of finite quotients G_k, $k \in \mathbb{N}$, such that $G = \varprojlim G_k$. In Section 4 we provide a general description of the normal Hausdorff spectrum of G and, with respect to certain induced filtration series, we generalise this to finite direct powers of G. In Section 5 we compute the normal Hausdorff spectrum of G with respect to the p-power series $\mathcal{P}$, and in Section 6 we compute the normal Hausdorff spectra of G with respect to the other three standard filtration series $\mathcal{D}$, $\mathcal{F}$, $\mathcal{L}$. In Section 7 we compute the entire Hausdorff spectra of G. Finally, in the Appendix we indicate how our results extend to the case $p = 2$.

Notation. Throughout, p denotes an *odd* prime, although some results hold also for $p = 2$, possibly with minor modifications; only in the Appendix we discuss the analogous pro-2 groups. We denote by $\varliminf_{i\to\infty} a_i$ the lower limit (limit inferior) of a sequence $(a_i)_{i\in\mathbb{N}}$ in $\mathbb{R} \cup \{\pm\infty\}$. Tacitly, subgroups of profinite groups are generally understood to be closed subgroups. Subscripts are used to emphasise that a subgroup is closed respectively open, as in $H \le_{\mathrm{c}} G$ respectively $H \le_{\mathrm{o}} G$. We use left-normed commutators, e.g., $[x, y, z] = [[x, y], z]$.

2. Preliminaries

2A. Let G be a finitely generated pro-p group. We consider four natural filtration series on G. The *p-power series* of G is given by

$$\mathcal{P}\colon\ G^{p^i} = \langle x^{p^i} \mid x \in G\rangle, \quad i \in \mathbb{N}_0.$$

The *lower p-series* (or lower p-central series) of G is given recursively by

$$\mathcal{L}\colon\ P_1(G) = G, \quad \text{and} \quad P_i(G) = P_{i-1}(G)^p\,[P_{i-1}(G), G] \quad \text{for } i \ge 2,$$

while the *Frattini series* of G is given recursively by

$$\mathcal{F}\colon\ \Phi_0(G) = G, \quad \text{and} \quad \Phi_i(G) = \Phi_{i-1}(G)^p[\Phi_{i-1}(G), \Phi_{i-1}(G)] \quad \text{for } i \ge 1.$$

The (modular) *dimension subgroup series* (or Jennings series or Zassenhaus series) of G can be defined recursively by

$$\mathcal{D}\colon\ D_1(G) = G, \quad \text{and} \quad D_i(G) = D_{\lceil i/p\rceil}(G)^p \prod_{1\le j<i} [D_j(G), D_{i-j}(G)] \quad \text{for } i \ge 2.$$

As a default we set $P_0(G) = D_0(G) = G$.

2B. Next, we collect auxiliary results to detect Hausdorff dimensions of closed subgroups of pro-p groups. For a countably based infinite pro-p group G, equipped with a filtration series $\mathcal{S}\colon G = G_0 \supseteq G_1 \supseteq \cdots$, and a closed subgroup $H \leq_{\mathrm{c}} G$ we say that H has *strong Hausdorff dimension in G with respect to* $\mathcal{S}$ if

$$\mathrm{hdim}_G^{\mathcal{S}}(H) = \lim_{i\to\infty} \frac{\log_p |HG_i : G_i|}{\log_p |G : G_i|}$$

is given by a proper limit.

The first lemma is an easy variation of [Klopsch et al. 2019, Lemma 5.3] and we omit the proof.

Lemma 2.1. *Let G be a countably based infinite pro-p group with closed subgroups $K \leq_{\mathrm{c}} H \leq_{\mathrm{c}} G$. Let $\mathcal{S}\colon G = G_0 \supseteq G_1 \supseteq \cdots$ be a filtration series of G and write*

$$\mathcal{S}|_H\colon H = H_0 \supseteq H_1 \supseteq \cdots, \quad \textit{with } H_i = H \cap G_i \textit{ for } i \in \mathbb{N}_0,$$

for the induced filtration series of H. If K has strong Hausdorff dimension in H with respect to $\mathcal{S}|_H$, then

$$\mathrm{hdim}_G^{\mathcal{S}}(K) = \mathrm{hdim}_G^{\mathcal{S}}(H) \cdot \mathrm{hdim}_H^{\mathcal{S}|_H}(K).$$

Lemma 2.2. *Let G be a countably based infinite pro-p group with closed subgroups $N \trianglelefteq_{\mathrm{c}} G$ and $H \leq_{\mathrm{c}} G$. Let $\mathcal{S}\colon G = G_0 \supseteq G_1 \supseteq \cdots$ be a filtration series of G, and consider the induced filtration series of N and G/N defined by*

$$\mathcal{S}|_N\colon G_i \cap N, \quad i \in \mathbb{N}_0, \qquad \textit{and} \qquad \mathcal{S}|_{G/N}\colon G_iN/N, \quad i \in \mathbb{N}_0.$$

Suppose that N has strong Hausdorff dimension $\xi = \mathrm{hdim}_G^{\mathcal{S}}(N)$ in G, with respect to $\mathcal{S}$. Then we have

$$(*)\quad \mathrm{hdim}_G^{\mathcal{S}}(H) \geq (1-\xi)\,\mathrm{hdim}_{G/N}^{\mathcal{S}|_{G/N}}(HN/N) + \xi \varliminf_{i\to\infty} \frac{\log_p |HG_i \cap N : G_i \cap N|}{\log_p |N : G_i \cap N|}$$

$$(**)\qquad \geq (1-\xi)\,\mathrm{hdim}_{G/N}^{\mathcal{S}|_{G/N}}(HN/N) + \xi\,\mathrm{hdim}_N^{\mathcal{S}|_N}(H \cap N).$$

Moreover, equality holds in $(*)$, if HN/N has strong Hausdorff dimension in G/N with respect to $\mathcal{S}|_{G/N}$ or if the lower limit on the right-hand side is actually a limit. Similarly, equality holds in $(**)$ if

(i) *$H \cap N \leq_{\mathrm{o}} N$ is an open subgroup or*

(ii) *$G_iN = (G_i \cap H)N$, for all sufficiently large $i \in \mathbb{N}$.*

Proof. We observe that

$$\operatorname{hdim}_G^{\mathcal{S}}(H) = \varliminf_{i\to\infty} \Bigg(\underbrace{\frac{\log_p|G:NG_i|}{\log_p|G:G_i|}}_{\to 1-\xi \text{ as } i\to\infty} \frac{\log_p|HG_iN:G_iN|}{\log_p|G:G_iN|} + \underbrace{\frac{\log_p|NG_i:G_i|}{\log_p|G:G_i|}}_{\to \xi \text{ as } i\to\infty} \frac{\log_p|HG_i\cap NG_i:G_i|}{\log_p|NG_i:G_i|} \Bigg)$$

and that, for each $i \in \mathbb{N}_0$,

$$\frac{\log_p|HG_i\cap NG_i:G_i|}{\log_p|NG_i:G_i|} = \frac{\log_p|HG_i\cap N:G_i\cap N|}{\log_p|N:G_i\cap N|}.$$

Finally,

$$\log_p|HG_i\cap N:G_i\cap N| \geq \log_p|(H\cap N)(G_i\cap N):G_i\cap N|$$

and, if condition (i) or (ii) holds, the difference between the two terms is bounded by a constant that is independent of $i \in \mathbb{N}_0$. $\square$

Lemma 2.3. *Let $Z \cong C_p^{\aleph_0}$ be a countably based infinite elementary abelian pro-p group, equipped with a filtration series $\mathcal{S}$. Then, for every $\eta \in [0,1]$, there exists a closed subgroup $K \leq_{\mathrm{c}} Z$ with strong Hausdorff dimension η in Z with respect to $\mathcal{S}$.*

Proof. Write $\mathcal{S}\colon Z = Z_0 \supseteq Z_1 \supseteq Z_2 \supseteq \cdots$ and let $\eta \in [0,1]$. For $i \in \mathbb{N}$, we have $Z_{i-1}/Z_i \cong C_p^{d_i}$ for nonnegative integers d_i.

Claim: There exist nonnegative integers $e_1, e_2, \dots$ such that, for each $i \in \mathbb{N}$, we have $0 \leq e_i \leq d_i$ and

$$e_1 + \cdots + e_i = \lceil \eta(d_1 + \cdots + d_i) \rceil.$$

Indeed, with $e_1 = \lceil \eta d_1 \rceil$ the statement holds true for $i = 1$. Now, let $i \geq 2$ and suppose that $e_1 + \cdots + e_{i-1} = \lceil \eta(d_1 + \cdots + d_{i-1}) \rceil$. Then

$$\lceil \eta(d_1 + \cdots + d_{i-1}) \rceil \leq \lceil \eta(d_1 + \cdots + d_i) \rceil \leq \lceil \eta(d_1 + \cdots + d_{i-1}) \rceil + d_i$$

and thus we may set

$$e_i = \lceil \eta(d_1 + \cdots + d_i) \rceil - (e_1 + \cdots + e_{i-1}),$$

to satisfy the statement for i. The claim is proved.

For all sufficiently large $i \in \mathbb{N}$ we have $d_1 + \cdots + d_i > 0$ and

$$\eta \leq \frac{e_1 + \cdots + e_i}{d_1 + \cdots + d_i} \leq \eta + \frac{1}{d_1 + \cdots + d_i}.$$

With these preparations, it suffices to display a subgroup $K \le_{\mathrm{c}} Z$ such that

$$\log_p |K Z_i : Z_i| = e_1 + \cdots + e_i.$$

For this purpose, we write

$$Z = \langle z_{1,1}, \ldots, z_{1,d_1},\ z_{2,1}, \ldots, z_{2,d_2},\ \ldots,\ z_{i,1}, \ldots, z_{i,d_i},\ \ldots \rangle$$

such that $Z_{i-1} = \langle z_{i,1}, \ldots, z_{i,d_i} \rangle Z_i$ for each $i \in \mathbb{N}$. Then we set

$$K = \langle z_{1,1}, \ldots, z_{1,e_1},\ z_{2,1}, \ldots, z_{2,e_2},\ \ldots,\ z_{i,1}, \ldots, z_{i,e_i},\ \ldots \rangle. \qquad \square$$

Corollary 2.4. *Let G be a countably based pro-p group, equipped with a filtration series $\mathcal{S}$, and let $N \trianglelefteq_{\mathrm{c}} H \le_{\mathrm{c}} G$ such that $H/N \cong C_p^{\aleph_0}$. Set $\xi = \operatorname{hdim}_G^{\mathcal{S}}(N)$ and $\eta = \operatorname{hdim}_G^{\mathcal{S}}(H)$. If N or H has strong Hausdorff dimension in G with respect to $\mathcal{S}$, then $[\xi, \eta] \subseteq \operatorname{hspec}^{\mathcal{S}}(G)$.*

Proof. If N has strong Hausdorff dimension, we apply Lemmata 2.1, 2.2 and 2.3. If H has strong Hausdorff dimension the claim follows from [Klopsch et al. 2019, Theorem 5.4]. $\square$

2C. For convenience we recall two standard commutator collection formulae.

Proposition 2.5. *Let $G = \langle a, b \rangle$ be a finite p-group, and let $r \in \mathbb{N}$. For $u, v \in G$ let $K(u, v)$ denote the normal closure in G of* (i) *all commutators in $\{u, v\}$ of weight at least p^r that have weight at least 2 in v, together with* (ii) *the p^{r-s+1}-th powers of all commutators in $\{u, v\}$ of weight less than p^s and of weight at least 2 in v for $1 \le s \le r$. Then*

$$(ab)^{p^r} \equiv_{K(a,b)} a^{p^r} b^{p^r} [b,a]^{\binom{p^r}{2}} [b,a,a]^{\binom{p^r}{3}} \cdots [b,a,\overset{p^r-2}{\ldots},a]^{\binom{p^r}{p^r-1}} [b,a,\overset{p^r-1}{\ldots},a], \tag{2-1}$$

$$[a^{p^r}, b] \equiv_{K(a,[a,b])} [a,b]^{p^r} [a,b,a]^{\binom{p^r}{2}} \cdots [a,b,a,\overset{p^r-2}{\ldots},a]^{\binom{p^r}{p^r-1}} [a,b,a,\overset{p^r-1}{\ldots},a]. \tag{2-2}$$

Remark. Under the standing assumption $p \ge 3$ and the extra assumptions

$$\gamma_2(G)^p = 1 \quad \text{and} \quad [\gamma_2(G), \gamma_2(G)] \subseteq Z(G),$$

the congruences (2-1) and (2-2) simplify to

$$(ab)^{p^r} \equiv_{L(a,b)} a^{p^r} b^{p^r} [b,a,\overset{p^r-1}{\ldots},a] \quad \text{and} \quad [a^{p^r}, b] \equiv_{M(a,b)} [a,b,a,\overset{p^r-1}{\ldots},a], \tag{2-3}$$

where $L(a, b)$ denotes the normal closure in G of all commutators in $\{a, b\}$ of weight at least p^r that have weight at least 2 in b and $M(a, b)$ denotes the normal closure in G of all commutators $[[b, a, \overset{i}{\ldots}, a], [b, a, \overset{j}{\ldots}, a]]$ with $i + j \ge p^r$.

The general result is recorded (in a slighter stronger form) in [Leedham-Green and McKay 2002, Proposition 1.1.32]; we remark that (2-2) follows directly from (2-1), due to the identity $[a^{p^r}, b] = a^{-p^r}(a[a,b])^{p^r}$. The first congruence in (2-3) follows directly from (2-1); the second congruence in (2-3) is derived from (2-2) by standard commutator manipulations.

2D. Now we describe, for $k \in \mathbb{N}$, the lower central series, the lower p-series and the Frattini series of the finite wreath product

$$W_k = \langle x, y\rangle = \langle x\rangle \ltimes \langle y, y^x, \dots, y^{x^{p^k-1}}\rangle \cong C_p \wr C_{p^k}$$

with top group $\langle x\rangle \cong C_{p^k}$ and base group $\langle y, y^x, \dots, y^{x^{p^k-1}}\rangle \cong C_p^{\,p^k}$.

Proposition 2.6. *For $k \in \mathbb{N}$, the finite wreath product W_k defined above is nilpotent of class p^k and $W_k^{\,p^k} = \langle y y^x y^{x^2} \cdots y^{x^{p^k-1}}\rangle \cong C_p$.*

(1) *The lower central series of W_k satisfies*

$$W_k = \gamma_1(W_k) = \langle x, y\rangle\, \gamma_2(W_k) \quad \textit{with } W_k/\gamma_2(W_k) \cong C_{p^k} \times C_p,$$

$$\gamma_i(W_k) = \langle [y, x, \overset{i-1}{\ldots}, x]\rangle \gamma_{i+1}(W_k) \quad \textit{with } \gamma_i(W_k)/\gamma_{i+1}(W_k) \cong C_p \textit{ for } 2 \le i \le p^k.$$

(2) *The lower p-series of W_k has length p^k; it satisfies, for $1 \le i \le k$,*

$$P_i(W_k) = \langle x^{p^{i-1}}, [y, x, \overset{i-1}{\ldots}, x]\rangle P_{i+1}(W_k) \quad \textit{with } P_i(W_k)/P_{i+1}(W_k) \cong C_p \times C_p,$$

and, for $k < i \le p^k$,

$$P_i(W_k) = \langle [y, x, \overset{i-1}{\ldots}, x]\rangle P_{i+1}(W_k) \quad \textit{with } P_i(W_k)/P_{i+1}(W_k) \cong C_p.$$

(3) *The Frattini series of W_k has length $k+1$; it satisfies, for $0 \le i < k$,*

$$\Phi_i(W_k) = \langle x^{p^i}\rangle \gamma_{(p^i-1)/(p-1)+1}(W_k) \quad \textit{with } \Phi_i(W_k)/\Phi_{i+1}(W_k) \cong C_p \times \overset{p^i+1}{\cdots} \times C_p,$$

$$\Phi_k(W_k) = \gamma_{(p^k-1)/(p-1)+1}(W_k) \quad \textit{with } \Phi_k(W_k)/\Phi_{k+1}(W_k) \cong \underbrace{C_p \times \cdots \times C_p}_{(p^{k+1}-2p^k+1)/p-1}.$$

(4) *The dimension subgroup series of W_k has length p^k; in particular, it satisfies, for $p^{k-1}+1 \le i \le p^k$,*

$$D_i(W_k) = \gamma_i(W_k) = \langle [y, x, \overset{i-1}{\ldots}, x]\rangle D_{i+1}(W_k) \quad \textit{with } D_i(W_k)/D_{i+1}(W_k) \cong C_p.$$

Proof. The assertions are well known and easy to verify from the concrete realisation of W_k as a semidirect product

$$W_k \cong \langle 1+t\rangle / \langle (1+t)^{p^k}\rangle \ltimes \mathbb{F}_p[t]/t^{p^k}\mathbb{F}_p[t] \tag{2-4}$$

in terms of polynomials over the finite field $\mathbb{F}_p$: here y^{x^i} corresponds to $(1+t)^i$ modulo $t^{p^k}\mathbb{F}_p[t]$, and it is easy to describe all normal subgroups. In particular the normal subgroups of W_k contained in the base group form a descending chain, corresponding to the groups $t^{i-1}\mathbb{F}_p[t]/t^{p^k}\mathbb{F}_p[t]$, $1 \le i \le p^k+1$.

For $0 \le m < k$ and $z \in \langle y, y^x, \dots, y^{x^{p^k-1}}\rangle$ the element

$$(x^{p^m}z)^{p^k} = (x^{p^m})^{p^k} z^{x^{(p^k-1)p^m}} \cdots z^{x^{p^m}} z = z^{x^{(p^k-1)p^m}} \cdots z^{x^{p^m}} z$$

corresponds in $\mathbb{F}_p[t]/t^{p^k}\mathbb{F}_p[t]$ to a multiple of

$$\sum_{i=0}^{p^k-1} (1+t)^{ip^m} = \sum_{i=0}^{p^k-1} (1+t^{p^m})^i = \frac{(1+t^{p^m})^{p^k}-1}{(1+t^{p^m})-1} = t^{(p^k-1)p^m};$$

this shows that $W_k^{p^k} = \langle yy^x y^{x^2} \cdots y^{x^{p^k-1}}\rangle \cong C_p$.

Clearly, $\gamma_1(W_k) = W_k$. For $2 \le i \le p^k+1$, the group $\gamma_i(W_k)$ corresponds to the subgroup $t^{i-1}\mathbb{F}_p[t]/t^{p^k}\mathbb{F}_p[t]$ of the base group. In particular, W_k has nilpotency class p^k. For $1 \le i \le k$, we have $P_i(W_k) = \langle x^{p^{i-1}}\rangle\gamma_i(W_k)$, while for $k < i \le p^k$ we get $P_i(W_k) = \gamma_i(W_k)$. For $0 \le i \le k$ a simple induction shows that the group $\Phi_i(W_k)$ is the normal closure in W_k of the two elements

$$x^{p^i} \quad \text{and} \quad [y, x, x^p, x^{p^2}, \dots, x^{p^{i-1}}] = [y, \overbrace{x, \dots, x}^{(p^i-1)/(p-1)}];$$

the intersection of $\Phi_i(W_k)$ with the base group corresponds to

$$t^{(p^i-1)/(p-1)}\mathbb{F}_p[t]/t^{p^k}\mathbb{F}_p[t].$$

Thus $\Phi_i(W_k) = \langle x^{p^i}\rangle\gamma_{(p^i-1)/(p-1)+1}(W_k)$. In particular, $\Phi_k(W_k)$ is elementary abelian and $\Phi_i(W_k) = 1$ for $i > k$. Finally, for $i \ge p^{k-1}+1$, we use [Dixon et al. 1999, Theorem 11.2] to deduce that $D_i(W_k) = \gamma_i(W_k)$. □

The structural results for the finite wreath products W_k transfer naturally to the inverse limit $W \cong \varprojlim_k W_k$, i.e., the pro-$p$ wreath product

(2-5) $$W = \langle x, y\rangle = \langle x\rangle \ltimes B \cong C_p \mathbin{\hat{\wr}} \mathbb{Z}_p$$

with top group $\langle x\rangle \cong \mathbb{Z}_p$ and base group $B = \prod_{i\in\mathbb{Z}}\langle y^{x^i}\rangle \cong C_p^{\aleph_0}$. Compatible with (2-4), the group W has a concrete realisation as a semidirect product

(2-6) $$W \cong \langle 1+t\rangle \ltimes \mathbb{F}_p[\![t]\!], \quad \text{where } \langle 1+t\rangle \le_{\mathrm{c}} \mathbb{F}_p[\![t]\!]^*,$$

in terms of formal power series over the finite field $\mathbb{F}_p$. We record the following lemma on closed normal subgroups of W.

Lemma 2.7. *Let $W = \langle x, y\rangle \cong C_p \mathbin{\hat{\wr}} \mathbb{Z}_p$ with base group B as above, and let $1 \ne K \trianglelefteq_{\mathrm{c}} W$ be a nontrivial closed normal subgroup. Then either K is open in W or K is open in B; in particular, $K \cap B \le_{\mathrm{o}} B$ and $|K \cap B : [K \cap B, W]| = p$.*

Proof. The lower central series of W is well known and easy to compute: $\gamma_1(W)=W$ and $\gamma_i(W) = B_{i-1}$ for $i \geq 2$, where $B = B_0 \geq B_1 \geq B_2 \geq \cdots$ with $B_{i-1} = \langle [y, x, \overset{i-1}{\ldots}, x] \rangle B_i$ and $|B_{i-1} : B_i| = p$; in other words, $\langle x \rangle$ acts uniserially on B; compare Proposition 2.6.

It follows that $1 \neq K \cap B = B_i$ for some nonnegative integer i, hence $K \cap B \leq_{\mathrm{o}} B$ and $|K \cap B : [K \cap B, W]| = |B_i : B_{i+1}| = p$. Suppose now that $K \not\subseteq B$. Then there exists $x^m z \in K$ with $m \in \mathbb{N}$ and $z \in B$. We may assume that $m = p^k$ is a p-power. Then $\langle x^{p^k} z \rangle \ltimes B \cong \langle x \rangle \ltimes (B \times \overset{p^k}{\ldots} \times B)$, where $x^{p^k} z$ maps to x and, on the right-hand side, x acts diagonally and in each coordinate according to the original action in W. Hence we may assume that $x \in K$. Now the description of the lower central series of W yields $\langle x \rangle B_1 \leq_{\mathrm{c}} K$ and thus $K \leq_{\mathrm{o}} W$. $\square$

From Proposition 2.6 and Lemma 2.7 we deduce the following; cf. [Klopsch 1999, Chapter VIII.7].

Corollary 2.8. *The normal Hausdorff spectrum of the pro-p group $W = C_p \mathbin{\hat{\wr}} \mathbb{Z}_p$ with respect to the standard filtration series $\mathcal{P}$, $\mathcal{D}$, $\mathcal{F}$ and $\mathcal{L}$ respectively, satisfies*:

$$\mathrm{hspec}^{\mathcal{P}}_{\trianglelefteq}(W) = \mathrm{hspec}^{\mathcal{D}}_{\trianglelefteq}(W) = \mathrm{hspec}^{\mathcal{F}}_{\trianglelefteq}(W) = \{0, 1\} \quad \textit{and} \quad \mathrm{hspec}^{\mathcal{L}}_{\trianglelefteq}(W) = \left\{0, \tfrac{1}{2}, 1\right\}.$$

The next result is well known (and not difficult to prove directly); compare [Wilson 1998, Corollary 12.5.10]. It gives a first indication that Theorem 1.1 is at least plausible.

Proposition 2.9. *The pro-p group $W = C_p \mathbin{\hat{\wr}} \mathbb{Z}_p$ is not finitely presented.*

The final result in this section concerns the *finitely generated Hausdorff spectrum* of the pro-p group $W = C_p \mathbin{\hat{\wr}} \mathbb{Z}_p$, with respect to a standard filtration series $\mathcal{S}$; it is defined as

$$\mathrm{hspec}^{\mathcal{S}}_{\mathrm{fg}}(W) = \{\mathrm{hdim}^{\mathcal{S}}_{W}(H) \mid H \leq_{\mathrm{c}} W \text{ and } H \text{ finitely generated}\}$$

and reflects the range of Hausdorff dimensions of (topologically) finitely generated subgroups; compare [Shalev 2000, §4.7].

Theorem 2.10. *With respect to the standard filtration series $\mathcal{P}$, $\mathcal{D}$, $\mathcal{F}$ and $\mathcal{L}$ respectively, the pro-p group $W = C_p \mathbin{\hat{\wr}} \mathbb{Z}_p$ satisfies*:

$$\mathrm{hspec}^{\mathcal{P}}_{\mathrm{fg}}(W) = \mathrm{hspec}^{\mathcal{D}}_{\mathrm{fg}}(W) = \mathrm{hspec}^{\mathcal{F}}_{\mathrm{fg}}(W) = \{m/p^n \mid n \in \mathbb{N}_0, 0 \leq m \leq p^n\},$$
$$\mathrm{hspec}^{\mathcal{L}}_{\mathrm{fg}}(W) = \{0\} \cup \left\{\tfrac{1}{2} + m/(2p^n) \mid n \in \mathbb{N}_0, 0 \leq m \leq p^n\right\}.$$

Proof. As above, let B denote the base group of the wreath product $W = \langle x, y \rangle$. Let $\mathcal{S} \in \{\mathcal{P}, \mathcal{D}, \mathcal{F}, \mathcal{L}\}$, and let K be a finitely generated subgroup of W.

If $K \subseteq B$ then K is finite and $\mathrm{hdim}^{\mathcal{S}}_{W}(K) = 0$. Now suppose that $K \not\subseteq B$; in the proof below we will no longer use that K is finitely generated, but it will become clear that this is automatically so. Write $K = \langle x^{p^n} z \rangle \ltimes M$, where $n \in \mathbb{N}_0$,

$z \in B$ and $M = K \cap B$. Let $B = B_0 \geq B_1 \geq \cdots$ be the filtration corresponding to $\mathbb{F}_p[\![t]\!] \geq t\mathbb{F}_p[\![t]\!] \geq \cdots$ under (2-6), as in the proof of Lemma 2.7. We set

$$J = \{j \in \mathbb{N}_0 \mid (M \cap B_j) \not\subseteq B_{j+1}\} \quad \text{and} \quad J_0 = \{j + p^n\mathbb{Z} \mid j \in J\} \subseteq \mathbb{Z}/p^n\mathbb{Z}.$$

Under the isomorphism (2-6), we may regard M as an $\mathbb{F}_p[\![t^{p^n}]\!]$-submodule of $\mathbb{F}_p[\![t]\!]$. Hence $J + p^n\mathbb{N}_0 \subseteq J$ and

$$\lim_{i\to\infty} \frac{\log_p |(K \cap B)B_i : B_i|}{\log_p |B : B_i|} = \frac{|J_0|}{p^n}.$$

From Proposition 2.6 it is easily seen that B has strong Hausdorff dimension

$$\operatorname{hdim}^{\mathcal{P}}_W(B) = \operatorname{hdim}^{\mathcal{D}}_W(B) = \operatorname{hdim}^{\mathcal{F}}_W(B) = 1 \quad \text{and} \quad \operatorname{hdim}^{\mathcal{L}}_W(B) = \tfrac{1}{2};$$

compare Corollary 2.8. Using Lemma 2.2, we deduce that

$$\operatorname{hdim}^{\mathcal{S}}_W(K) = (1 - \operatorname{hdim}^{\mathcal{S}}_W(B)) + \operatorname{hdim}^{\mathcal{S}}_W(B)\frac{|J_0|}{p^n}$$

lies in the desired range; in fact, the argument even shows that K has strong Hausdorff dimension.

Conversely, our analysis above shows that, for $n \in \mathbb{N}_0$ and $0 \leq m \leq p^n$, the subgroup $K_{n,m} = \langle x^{p^n}, [y, x], [y, x, x], \ldots, [y, x, \overset{m}{\ldots}, x]\rangle$ has Hausdorff dimension

$$\operatorname{hdim}^{\mathcal{S}}_W(K_{n,m}) = \begin{cases} \dfrac{m}{p^n} & \text{if } \mathcal{S} \in \{\mathcal{P}, \mathcal{D}, \mathcal{F}\}, \\ \tfrac{1}{2} + \dfrac{m}{2p^n} & \text{if } \mathcal{S} = \mathcal{L}. \end{cases}$$ □

The next corollary answers a question raised in [Klopsch 1999, VIII.7.2]; it was shown there that $\left[0, \tfrac{1}{2}\right] \subseteq \operatorname{hspec}^{\mathcal{L}}(W)$, while $\left(\tfrac{1}{2}, 1\right) \cap \operatorname{hspec}^{\mathcal{L}}(W)$ remained undetermined.

Corollary 2.11. *The Hausdorff spectrum of the pro-p group $W = C_p \,\hat{\wr}\, \mathbb{Z}_p$ with respect to the lower p-series $\mathcal{L}$ is*

$$\operatorname{hspec}^{\mathcal{L}}(W) = \left[0, \tfrac{1}{2}\right] \cup \left\{\tfrac{1}{2} + m/(2p^n) \mid n \in \mathbb{N}_0, 1 \leq m \leq p^n - 1\right\} \cup \{1\}.$$

Furthermore, every subgroup $K \leq_c W$ with $\operatorname{hdim}^{\mathcal{L}}_W(K) > \tfrac{1}{2}$ has strong Hausdorff dimension in W, with respect to $\mathcal{L}$.

Proof. The subgroups contained in the base group B of W yield $\left[0, \tfrac{1}{2}\right]$ as part of the Hausdorff spectrum; see Lemma 2.3. The proof of Theorem 2.10 shows that the subgroups not contained in B yield the remaining part of the claimed spectrum and that each of them has strong Hausdorff dimension in W. □

3. An explicit presentation for the pro-p group G and a description of its finite quotients G_k for $k \in \mathbb{N}$

Recall that p is an odd prime. As indicated in the paragraph before Theorem 1.1, we consider the pro-p group $G = F/N$, where

- $F = \langle x, y \rangle$ is a free pro-p group, and
- $N = [R, F]R^p \trianglelefteq_{\mathrm{c}} F$ for the kernel $R \trianglelefteq_{\mathrm{c}} F$ of the presentation $\pi : F \to W$ sending x, y to the generators of the same name in (2-5).

By producing generators for R and N as closed normal subgroups of F we obtain explicit presentations for the pro-p groups W and G.

It is convenient to write $y_i = y^{x^i}$ for $i \in \mathbb{Z}$. Setting

$$R_k = \left\langle \{x^{p^k}, y^p\} \cup \{[y_0, y_i] \mid 1 \le i \le (p^k - 1)/2\} \right\rangle^F \trianglelefteq_{\mathrm{o}} F \tag{3-1}$$

for $k \in \mathbb{N}$, we obtain a descending chain of open normal subgroups

$$F \supseteq R_1 \supseteq R_2 \supseteq \cdots \tag{3-2}$$

with quotient groups $F/R_k \cong W_k \cong C_p \wr C_{p^k}$. We put

$$R = \langle \{y^p\} \cup \{[y_0, y_i] \mid i \in \mathbb{N}\} \rangle^F \trianglelefteq_{\mathrm{c}} F,$$

and observe that $R_k = \langle x^{p^k} \rangle^F R$ for each $k \in \mathbb{N}$. Since $x^{p^k} \to 1$ as $k \to \infty$, this yields $R = \bigcap_{k \in \mathbb{N}} R_k$ and thus $F/R \cong W \cong C_p \hat{\wr} \mathbb{Z}_p$. With hindsight there is no harm in taking $W_k = F/R_k$ for $k \in \mathbb{N}$ and $W = F/R$.

Setting $N_k = [R_k, F]R_k^p$ for $k \in \mathbb{N}$, we observe that

$$\begin{aligned} N_k = \Big\langle &\{x^{p^{k+1}}, y^{p^2}, [x^{p^k}, y], [y^p, x]\} \cup \{[y_0, y_i]^p \mid 1 \le i \le (p^k - 1)/2\} \\ &\cup \{[y_0, y_i, x] \mid 1 \le i \le (p^k - 1)/2\} \cup \{[y_0, y_i, y] \mid 1 \le i \le (p^k - 1)/2\} \Big\rangle^F \trianglelefteq_{\mathrm{o}} F, \end{aligned}$$

and as in (3-2) we obtain a descending chain $F \supseteq N_1 \supseteq N_2 \supseteq \cdots$ of open normal subgroups. Moreover, it follows that $\bigcap_{k \in \mathbb{N}} N_k \supseteq [R, F]R^p = N$. On the other hand, if $z \notin N$ then there exists an open normal subgroup $K \trianglelefteq_{\mathrm{o}} F$ and $k \in \mathbb{N}$ such that $z \notin NK = [R_k, F]R_k^p K$, hence $z \notin N_k$. Thus we conclude that

$$\bigcap_{k \in \mathbb{N}} N_k = [R, F]R^p = N.$$

Consequently, $G = F/N \cong \varprojlim G_k$, where

$$\begin{aligned} G_k = F/N_k \cong \Big\langle x, y \;\Big|\; &\underline{x^{p^{k+1}}},\ y^{p^2},\ \underline{[x^{p^k}, y]},\ [y^p, x]; \\ &[y_0, y_i]^p,\ [y_0, y_i, x],\ [y_0, y_i, y] \quad \text{for } 1 \le i \le (p^k - 1)/2 \Big\rangle \end{aligned} \tag{3-3}$$

for $k \in \mathbb{N}$, and

$$G \cong \bigl\langle x, y \mid y^{p^2}, [y^p, x];\ [y_0, y_i]^p, [y_0, y_i, x], [y_0, y_i, y] \quad \text{for } i \in \mathbb{N} \bigr\rangle \tag{3-4}$$

is a presentation of G as a pro-p group. Indeed,

$$\widetilde{N} = \bigl\langle \{y^{p^2}, [y^p, x]\} \cup \{[y_0, y_i]^p, [y_0, y_i, x], [y_0, y_i, y] \mid i \in \mathbb{N}\} \bigr\rangle^F \trianglelefteq_{\mathrm{c}} F$$

satisfies, for each $k \in \mathbb{N}$,

$$N_k = \langle x^{p^{k+1}}, [x^{p^k}, y] \rangle^F \, \widetilde{N},$$

where $x^{p^{k+1}}, [x^{p^k}, y] \to 1$ as $k \to \infty$. This yields $\widetilde{N} = \bigcap_{k \in \mathbb{N}} N_k = N$. To facilitate later use, we have underlined the two relations in (3-3) that do not yet occur in (3-4).

To summarise and supplement some of the notation introduced above, we define

$$Y = \langle y_i \mid i \in \mathbb{Z} \rangle R \trianglelefteq_{\mathrm{c}} F, \quad H = Y/N \trianglelefteq_{\mathrm{c}} G, \quad Z = R/N \trianglelefteq_{\mathrm{c}} G.$$

Similarly for $k \in \mathbb{N}$ we set

$$Y_k = \langle y_i \mid i \in \mathbb{Z} \rangle R_k \trianglelefteq_{\mathrm{o}} F, \quad H_k = Y_k/N_k \trianglelefteq G_k, \quad Z_k = R_k/N_k \trianglelefteq G_k.$$

Diagrammatically, we have:

$$\begin{array}{l} \left.\begin{array}{ccc} F & \twoheadrightarrow & G \\ \vert & & \vert \\ Y & \twoheadrightarrow & H \\ \vert & & \vert \\ R & \twoheadrightarrow & Z \end{array}\right\} G/Z \cong W \\ \begin{array}{ccc} \vert & & \vert \\ N & \twoheadrightarrow & 1 \end{array} \end{array} \qquad \begin{array}{r} W_k \cong G_k/Z_k \left\{\begin{array}{ccc} G_k & \twoheadleftarrow & F \\ \vert & & \vert \\ H_k & \twoheadleftarrow & Y_k \\ \vert & & \vert \\ Z_k & \twoheadleftarrow & R_k \end{array}\right. \\ \begin{array}{ccc} \vert & & \vert \\ 1 & \twoheadleftarrow & N_k \end{array} \end{array}$$

Lemma 3.1. *The centre of G is $Z(G) = Z$, and $Z_k \le Z(G_k)$ for $k \in \mathbb{N}$.*

Proof. By construction, $Z \le Z(G)$ and $Z_k \le Z(G_k)$ for $k \in \mathbb{N}$. From (2-6) we see that $G/Z \cong W$ has trivial centre. Therefore $Z = Z(G)$. $\square$

In fact, $Z_k \lneqq Z(G_k)$ for $k \in \mathbb{N}$; see Lemma 5.3 below.

4. General description of the normal Hausdorff spectrum of the pro-p group G and its finite direct powers

We continue to use the notation set up in Section 3 to study the pro-p group G and its finite direct powers.

Proposition 4.1. *Let $K \trianglelefteq_{\mathrm{c}} G$ be a closed normal subgroup such that $K \not\subseteq Z$. Then either K is open in H or K is open in G; in particular, $K \cap H \le_{\mathrm{o}} H$. Furthermore, $[K \cap H, G] \le_{\mathrm{o}} H$.*

Proof. Lemma 2.7 shows: $KZ \cap H \le_{\mathrm{o}} H$; hence it suffices to prove $K \cap Z \le_{\mathrm{o}} Z$. Choose $\hat{y}_1, \hat{y}_2, \ldots \in H$, converging to 1 modulo Z, and $m \in \mathbb{N}$ such that (the images of) $\hat{y}_1, \hat{y}_2, \ldots$ (modulo Z) yield a basis for the elementary abelian pro-p group H/Z and $\hat{y}_{m+1}, \hat{y}_{m+2}, \ldots$ generate $KZ \cap H$ modulo Z.

Recall that Z is central in G and of exponent p. Thus $K \cap Z$ contains $\hat{y}_i^{\,p}$ and $[\hat{y}_i, \hat{y}_j]$ for all $i, j \in \mathbb{N}$ with $i > m$. Hence the finite set

$$\{\hat{y}_i^{\,p} \mid 1 \le i \le m\} \cup \{[\hat{y}_i, \hat{y}_j] \mid 1 \le i \le j \le m\}$$

generates the elementary abelian group Z modulo $K \cap Z$, and $K \cap Z \le_{\mathrm{o}} Z$.

Finally, Lemma 2.7 implies that $[K \cap H, G] \not\subseteq Z$. Hence $[K \cap H, G] \le_{\mathrm{o}} H$. □

From Proposition 4.1, Lemma 3.1 and Lemmata 2.1 and 2.3 we deduce the general shape of the normal Hausdorff spectrum of G.

Corollary 4.2. *Let $\mathcal{S}$ be an arbitrary filtration series of G. Then the normal Hausdorff spectrum of G has the form*

$$\mathrm{hspec}^{\mathcal{S}}_{\trianglelefteq}(G) = [0, \xi] \cup \{\eta\} \cup \{1\},$$

where $\xi = \mathrm{hdim}^{\mathcal{S}}_G(Z)$ and $\eta = \mathrm{hdim}^{\mathcal{S}}_G(H)$.

More generally we obtain a description of the normal Hausdorff spectrum of finite direct powers $G^{(m)} = G \times \overset{m}{\cdots} \times G$ of G, with respect to suitable "product filtration series." For any filtration series $\mathcal{S}\colon G = S_0 \supseteq S_1 \supseteq \cdots$ of G we consider the naturally induced product filtration series on $G^{(m)}$ given by

$$\mathcal{S}^{(m)}\colon G^{(m)} = G \times \overset{m}{\cdots} \times G \supseteq S_1 \times \overset{m}{\cdots} \times S_1 \supseteq S_2 \times \overset{m}{\cdots} \times S_2 \supseteq \cdots.$$

For a standard filtration series $\mathcal{S} \in \{\mathcal{P}, \mathcal{L}, \mathcal{F}, \mathcal{D}\}$ on G the product filtration series $\mathcal{S}^{(m)}$ is actually the corresponding standard filtration series on $G^{(m)}$.

Corollary 4.3. *Let $m \in \mathbb{N}$, and let $K \trianglelefteq_{\mathrm{c}} G^{(m)}$. For $1 \le j \le m$, let $\pi_j\colon G^{(m)} \to G$ be the canonical projection onto the j-th factor and set*

$$\overline{K}(j) = \begin{cases} Z & \text{if } K\pi_j \subseteq Z, \\ G & \text{otherwise}, \end{cases} \quad \text{and} \quad \underline{K}(j) = \begin{cases} 1 & \text{if } K\pi_j \subseteq Z, \\ H & \text{otherwise}. \end{cases}$$

Then $K \le \prod_{j=1}^m \overline{K}(j)$ and K contains an open normal subgroup of $\prod_{j=1}^m \underline{K}(j)$.

Proof. Observe that

$$[K\pi_1, G] \times \cdots \times [K\pi_m, G] = [K, G^{(m)}] \le K \le K\pi_1 \times \cdots \times K\pi_m.$$

Thus K is contained in $\prod_{j=1}^{m} \overline{K}(j)$, and it suffices to show that $[K\pi_j \cap H, G] \leq_{\mathrm{o}} H$ for each j with $K\pi_j \not\subseteq Z$. This follows by Proposition 4.1. $\square$

Corollary 4.4. *Let $m \in \mathbb{N}$, and let $\mathcal{S}$ be a filtration series of G such that*

$$\mathrm{hdim}_G^{\mathcal{S}}(H) = 1.$$

Then the normal Hausdorff spectrum of $G^{(m)}$ has the form

$$\mathrm{hspec}_{\trianglelefteq}^{\mathcal{S}^{(m)}}(G^{(m)}) = [0, \xi] \cup \bigcup_{1 \leq l \leq m-1} \left[\frac{l}{m}, \frac{l+(m-l)\xi}{m}\right] \cup \{1\},$$

where $\xi = \mathrm{hdim}_G^{\mathcal{S}}(Z)$.

Proof. First let $K \trianglelefteq_{\mathrm{c}} G^{(m)}$, and define $\overline{K}(j)$, $\underline{K}(j)$ for $1 \leq j \leq m$ as in Corollary 4.3. From $\mathrm{hdim}_G^{\mathcal{S}}(H) = 1$ we deduce that

$$\begin{aligned} \tfrac{l}{m} = \mathrm{hdim}_{G^{(m)}}^{\mathcal{S}^{(m)}}\big(\textstyle\prod_{j=1}^{m} \underline{K}(j)\big) &\leq \mathrm{hdim}_{G^{(m)}}^{\mathcal{S}^{(m)}}(K) \\ &\leq \mathrm{hdim}_{G^{(m)}}^{\mathcal{S}^{(m)}}\big(\textstyle\prod_{j=1}^{m} \overline{K}(j)\big) = \tfrac{l}{m} + \tfrac{m-l}{m}\xi, \end{aligned}$$

where $l = \#\{j \mid 1 \leq j \leq m \text{ and } \overline{K}(j) = G\}$.

Conversely, for every $l \in \{0, 1, \ldots, m\}$ and $\beta \in \left[\frac{l}{m}, \frac{l+(m-l)\xi}{m}\right]$ there is a normal subgroup

$$K_\beta = G \times \overset{l}{\cdots} \times G \times U \times \overset{m-l}{\cdots} \times U \trianglelefteq_{\mathrm{c}} G^{(m)},$$

where $U \leq_{\mathrm{c}} Z$ for $l < m$ has $\mathrm{hdim}_G^{\mathcal{S}}(U) = \frac{m}{m-l}\big(\beta - \frac{l}{m}\big) \in [0, \xi]$; compare Corollary 4.2. This yields $\beta = \mathrm{hdim}_{G^{(m)}}^{\mathcal{S}^{(m)}}(K_\beta) \in \mathrm{hspec}_{\trianglelefteq}^{\mathcal{S}^{(m)}}(G^{(m)})$. $\square$

Corollary 4.4 shows that, once $\mathrm{hdim}_G^{\mathcal{S}}(H) = 1$, the general shape (e.g., the number of connected components) of the normal Hausdorff spectrum $\mathrm{hspec}_{\trianglelefteq}^{\mathcal{S}^{(m)}}(G^{(m)})$ depends only on the parameters $\xi = \mathrm{hdim}_G^{\mathcal{S}}(Z)$ and $m \in \mathbb{N}$. For instance, if $\xi < \frac{1}{m}$, then $\mathrm{hspec}_{\trianglelefteq}^{\mathcal{S}^{(m)}}(G^{(m)})$ is the union of $m+1$ disjoint intervals, whereas for $\xi \geq \frac{1}{2}$ we obtain $\mathrm{hspec}_{\trianglelefteq}^{\mathcal{S}^{(m)}}(G^{(m)}) = \left[0, 1 - \frac{(1-\xi)}{m}\right] \cup \{1\}$.

The proof of Theorem 1.1 in Sections 5 and 6 will give $\mathrm{hdim}_G^{\mathcal{S}}(H) = 1$ for the standard filtrations $\mathcal{S} \in \{\mathcal{P}, \mathcal{D}, \mathcal{F}\}$ and $\xi = \mathrm{hdim}_G^{\mathcal{P}}(Z) = \mathrm{hdim}_G^{\mathcal{D}}(Z) = \frac{1}{3}$ respectively $\xi = \mathrm{hdim}_G^{\mathcal{F}}(Z) = \frac{1}{p+1}$; the assertion for H is already a consequence of [Klopsch et al. 2019, Proposition 4.2]. We formulate a tailor-made corollary for these situations.

Corollary 4.5. *Let $m, n \in \mathbb{N}$ with $m \geq \max\{2, n-1\}$ and $n \geq 2$. Let $\mathcal{S}$ be a filtration series of G such that $\mathrm{hdim}_G^{\mathcal{S}}(H) = 1$ and $\mathrm{hdim}_G^{\mathcal{S}}(Z) = \frac{1}{n}$. Then*

$$\mathrm{hspec}_{\trianglelefteq}^{\mathcal{S}^{(m)}}(G^{(m)}) = \left[0, \frac{mn-(n-1)^2}{mn}\right] \cup \bigcup_{m-n+2 \leq l \leq m-1} \left[\frac{l}{m}, \frac{m+l(n-1)}{mn}\right] \cup \{1\}$$

consists of n disjoint intervals.

Proof. From Corollary 4.4, we have

$$\operatorname{hspec}_{\trianglelefteq}^{\mathcal{S}^{(m)}}(G^{(m)}) = \left[0, \frac{1}{n}\right] \cup \bigcup_{1 \le l \le m-1} \left[\frac{l}{m}, \frac{m+l(n-1)}{mn}\right] \cup \{1\}.$$

For $m-n+1 \le l \le m-1$ it is easy to verify that

$$\frac{m+l(n-1)}{mn} < \frac{l+1}{m}.$$

Hence it suffices to show that

$$\left[0, \frac{1}{n}\right] \cup \bigcup_{1 \le l \le m-n+1} \left[\frac{l}{m}, \frac{m+l(n-1)}{mn}\right] = \left[0, \frac{mn-(n-1)^2}{mn}\right].$$

For $m = n-1$ this reduces to $\left[0, \frac{1}{n}\right] = [0, (mn-(n-1)^2)/(mn)]$. Now suppose that $m \ge n$. Then the claim follows from

$$\frac{1}{m} \le \frac{1}{n} \quad \text{and} \quad \frac{l+1}{m} \le \frac{m+l(n-1)}{mn} \quad \text{for } 1 \le l \le m-n. \qquad \square$$

5. The normal Hausdorff spectrum of G with respect to the p-power series

We continue to use the notation set up in Section 3 and establish that

$$\xi = \operatorname{hdim}_G^{\mathcal{P}}(Z) = \tfrac{1}{3} \quad \text{and} \quad \eta = \operatorname{hdim}_G^{\mathcal{P}}(H) = 1,$$

with respect to the p-power series $\mathcal{P}$. This proves Theorem 1.1 for the p-power series, in view of Corollary 4.2. Indeed, $\operatorname{hdim}_G^{\mathcal{P}}(H) = 1$ is already a consequence of [Klopsch et al. 2019, Proposition 4.2]. It remains to show that

$$\operatorname{hdim}_G^{\mathcal{P}}(Z) = \varliminf_{i\to\infty} \frac{\log_p |ZG^{p^i} : G^{p^i}|}{\log_p |G : G^{p^i}|} = \frac{1}{3}. \tag{5-1}$$

It is convenient to work with the finite quotients G_k, $k \in \mathbb{N}$, introduced in Section 3. Let $k \in \mathbb{N}$. From (3-3) and (3-4) we observe that

$$|G : G^{p^k}| = |G_k : G_k^{p^k}|.$$

Heuristically, $G_k^{p^k}$ is almost trivial (see Proposition 5.2) and the elementary abelian p-group Z_k requires roughly half the number of generators compared to the elementary abelian p-group H_k/Z_k. This suggests that (3-4) should be true. We now work out the details.

First we compute the order of G_k, using the notation from Section 3.

Lemma 5.1. *The logarithmic order of G_k is*

$$\log_p |G_k| = \tfrac{1}{2}(3p^k + 2k + 3).$$

In particular,

$$Z_k = R_k/N_k = \big\langle \{x^{p^k}, y^p\} \cup \{[y_0, y_i] \mid 1 \le i \le (p^k-1)/2\} \big\rangle N_k/N_k \cong \underbrace{C_p \times \cdots \times C_p}_{(p^k+3)/2}.$$

Proof. Observe from $F/R_k \cong W_k \cong C_p \wr C_{p^k}$ that

$$\log_p|G_k| = \log_p|F : R_k| + \log_p|R_k : N_k| = k + p^k + \log_p|R_k : N_k|.$$

By construction, R_k/N_k is elementary abelian of exponent p. Moreover, (3-1) shows that $\{x^{p^k}, y^p\} \cup \{[y_0, y_i] \mid 1 \le i \le (p^k-1)/2\}$ generates R_k modulo N_k. In order to prove that the generators are independent, we construct a factor group $\widetilde{G}_k$ of G_k that has the maximal possible logarithmic order $\log_p|\widetilde{G}_k| = p^k + k + 2 + (p^k-1)/2$.

Consider the finite p-group

$$M = \langle \tilde{y}_0, \tilde{y}_1, \ldots, \tilde{y}_{p^k-1} \rangle = E/[\Phi(E), E]\Phi(E)^p,$$

where E is a free pro-p group on p^k generators with Frattini subgroup $\Phi(E) = [E, E]E^p$. Then the images of $\tilde{y}_0, \ldots, \tilde{y}_{p^k-1}$ generate independently the elementary abelian quotient $M/\Phi(M)$ and the commutators $[\tilde{y}_i, \tilde{y}_j]$, for $0 \le i < j \le p^k - 1$, together with the p-th powers $\tilde{y}_0^{\,p}, \ldots, \tilde{y}_{p^k-1}^{\,p}$ generate independently the elementary abelian group $\Phi(M)$. The latter can be checked by considering homomorphisms from M onto groups of the form

$$C_p^{\,p^k-1} \times C_{p^2} \quad \text{and} \quad C_p^{\,p^k-2} \times \mathrm{Heis}(\mathbb{F}_p),$$

where $\mathrm{Heis}(\mathbb{F}_p)$ denotes the group of upper unitriangular 3×3 matrices over $\mathbb{F}_p$. Next consider the action of the cyclic group $X = \langle \tilde{x} \rangle \cong C_{p^{k+1}}$, with kernel $\langle \tilde{x}^{p^k} \rangle \cong C_p$, on M that is induced by

$$\tilde{y}_i^{\,\tilde{x}} = \begin{cases} \tilde{y}_{i+1} & \text{if } 0 \le i \le p^k - 2, \\ \tilde{y}_0 & \text{if } i = p^k - 1. \end{cases}$$

This induces a permutation action on our chosen basis for the elementary abelian group $\Phi(M)$; the orbits are given by

$$[\tilde{y}_i, \tilde{y}_j] \equiv_X [\tilde{y}_{i'}, \tilde{y}_{j'}] \leftrightarrow j - i \equiv_{p^k} j' - i' \quad \text{and} \quad \tilde{y}_0^{\,p} \equiv_X \cdots \equiv_X \tilde{y}_{p^k-1}^{\,p}.$$

We define $\widetilde{M} = M/[\Phi(M), X]$ and, for simplicity, continue to write $\tilde{y}_0, \ldots, \tilde{y}_{p^k-1}$ for the images of these elements in $\widetilde{M}$. Then

- the images of $\tilde{y}_0, \ldots, \tilde{y}_{p^k-1}$ generate independently the elementary abelian quotient $\widetilde{M}/\Phi(\widetilde{M})$, and
- the elements $[\tilde{y}_0, \tilde{y}_i]$, for $1 \le i \le (p^k-1)/2$, together with $\tilde{y}_0^{\,p}$ generate independently the elementary abelian group $\Phi(\widetilde{M})$.

In particular, this yields $\log_p|\widetilde{M}| = p^k + (p^k - 1)/2 + 1$.

Finally, we put $\widetilde{y} = \widetilde{y}_0$ and form the semidirect product

$$\widetilde{G}_k = \langle \widetilde{x}, \widetilde{y} \rangle = X \ltimes \widetilde{M}$$

with the induced action. Upon replacing x, y by $\widetilde{x}$, $\widetilde{y}$, we see that all the defining relations of G_k in (3-3) are valid in $\widetilde{G}_k$. Since $\log_p|G_k| \le p^k+k+2+(p^k-1)/2 = \log_p|\widetilde{G}_k|$, we conclude that $G_k \cong \widetilde{G}_k$. □

Our next aim is to prove the following structural result.

Proposition 5.2. *In the set-up from Section 3, for $k \ge 2$, the subgroup $G_k^{p^k} \le G_k$ is elementary abelian and central in G_k; it is generated independently by x^{p^k}, $w = y_{p^k-1} \cdots y_1 y_0$ and $v = w \cdot y_{p^k-1}^{-1} \cdots y_1^{-1} y_0^{-1}$.*

Consequently

$$G_k^{p^k} \cong C_p \times C_p \times C_p, \quad \log_p |G_k : G_k^{p^k}| = \log_p|G_k| - 3$$

and

$$G_k/G_k^{p^k} \cong \Big\langle x, y \;\Big|\; x^{p^k},\ y^{p^2},\ [y^p, x],\ w(x, y),\ v(x, y);\\ [y_0, y_i]^p,\ [y_0, y_i, x],\ [y_0, y_i, y] \quad \textit{for } 1 \le i \le (p^k-1)/2 \Big\rangle.$$

The proof requires a series of lemmata.

Lemma 5.3. *The elements*

$$w = y_{p^k-1} \cdots y_1 y_0 \quad \textit{and} \quad w' = y_{p^k-1}^{-1} \cdots y_1^{-1} y_0^{-1}$$

are of order p in G_k and lie in $G_k^{p^k} \cap Z(G_k)$.

Proof. Recall that $H_k = \langle y_0, y_1, \dots, y_{p^k-1} \rangle Z_k \le G_k$ and observe that $[H_k, H_k]$ is a central subgroup of exponent p in G_k. Furthermore, $[y^p, x] = 1$ implies $y_{p^k-1}^p = \cdots = y_0^p$ in G_k. Thus (2-1) yields

$$w^p = y_{p^k-1}^p \cdots y_1^p y_0^p = y^{p^{k+1}} = 1.$$

As $w \ne 1$ we deduce that w has order p. Likewise one shows that w' has order p.

Clearly, $w = x^{-p^k}(xy)^{p^k}$ and $w' = x^{-p^k}(xy^{-1})^{p^k}$ lie in $G_k^{p^k}$. In order to prove that w is central, it suffices to check that w commutes with the generators x and y of G_k. First we observe that, for $1 \le i \le p^k-1$, the relation $[y_0, y_i, x] = 1$ implies

$$[y_0, y_{p^k-i}]^{-1} = [y_{p^k-i}, y_0] = [y_0, y_i]^{x^{-i}} = [y_0, y_i] \quad \text{in } G_k. \tag{5-2}$$

Since $[H_k, H_k]$ is central in G_k, we deduce inductively that

$$\begin{aligned}
[w, x] &= (y_{p^k-1} \cdots y_1 y_0)^{-1}(y_{p^k-1} \cdots y_1 y_0)^x \\
&= y_0^{-1} y_1^{-1} \cdots y_{p^k-2}^{-1} \cdot y_{p^k-1}^{-1} y_0 y_{p^k-1} \cdot y_{p^k-2} \cdots y_2 y_1 \\
&= y_0^{-1} y_1^{-1} \cdots y_{p^k-2}^{-1} \cdot y_0 [y_0, y_{p^k-1}] \cdot y_{p^k-2} \cdots y_2 y_1 \\
&= y_0^{-1} y_1^{-1} \cdots y_{p^k-3}^{-1} \cdot y_{p^k-2}^{-1} y_0 y_{p^k-2} \cdot y_{p^k-3} \cdots y_2 y_1 \cdot [y_0, y_{p^k-1}] \\
&\;\;\vdots \\
&= [y_0, y_1][y_0, y_2] \cdots [y_0, y_{p^k-2}][y_0, y_{p^k-1}] \\
&= 1 \quad \text{by (5-2)}.
\end{aligned}$$

Likewise, using the relation $[y_0, y_i, y] = 1$ and (5-2), we obtain

$$[w, y] = [y_{p^k-1} \cdots y_1 y_0, y_0] = [y_{p^k-1}, y_0][y_{p^k-2}, y_0] \cdots [y_1, y_0] = 1.$$

A similar computation can be carried out for w'. □

Lemma 5.4. *Putting*

$$v = ww' = y_{p^k-1} \ldots y_1 y_0 \cdot y_{p^k-1}^{-1} \ldots y_1^{-1} y_0^{-1},$$

the subgroup $\langle x^{p^k}, w, v\rangle \le G_k$ *is isomorphic to* $C_p \times C_p \times C_p$ *and lies in* $G_k^{p^k} \cap Z(G_k)$.

Proof. From the presentation (3-3) and from Lemma 5.3 it is clear that the subgroup $\langle x^{p^k}, w, v\rangle \le G_k$ is elementary abelian and lies in $G_k^{p^k} \cap Z(G_k)$. Furthermore, in order to prove that $\langle x^{p^k}, w, v\rangle \cong C_p \times C_p \times C_p$, it suffices to establish that $v \ne 1$.

Upon a similar rearrangement and cancellation as in the proof of Lemma 5.3, we obtain

$$v = \prod_{i=0}^{p^k-2} [y_i, y_{p^k-1}^{-1}][y_i, y_{p^k-2}^{-1}] \cdots [y_i, y_{i+1}^{-1}].$$

Recall that all commutators appearing in the above product are central in G_k. In particular, we have $[y_0, y_{p^k-j}] = [y_0, y_{p^k-j}]^{x^i} = [y_i, y_{p^k-j+i}]$, for $1 \le j \le p^k - 1$ and $1 \le i \le j-1$. This gives

$$\begin{aligned}
v &= [y_0, y_{p^k-1}^{-1}][y_0, y_{p^k-2}^{-1}]^2 \cdots [y_0, y_1^{-1}]^{p^k-1} \\
&= [y_0, y_{p^k-1}]^{-1}[y_0, y_{p^k-2}]^{-2} \cdots [y_0, y_1]^{1-p^k} \\
&= [y_0, y_1][y_0, y_2]^2 \cdots [y_0, y_{(p^k-1)/2}]^{(p^k-1)/2} \\
&\qquad \cdot [y_0, y_{(p^k-1)/2}]^{(p^k-1)/2} \cdots [y_0, y_2]^2 [y_0, y_1] \quad \text{by (5-2)} \\
&= [y_0, y_1]^2 [y_0, y_2]^4 \cdots [y_0, y_{(p^k-1)/2}]^{p^k-1}.
\end{aligned}$$

Taking note of the second statement in Lemma 5.1, it follows that $v \ne 1$. □

Lemma 5.5. *The group $\gamma_2(G_k) \le G_k$ has exponent p.*

Proof. Recall that $H_k = \langle y_0, y_1, \dots, y_{p^k-1}\rangle Z_k \le G_k$ satisfies: $[H_k, H_k]$ is a central subgroup of exponent p in G_k. Since p is odd, (2-1) shows that it suffices to prove that $[y, x]$ has order p. But $[y, x] = y_0^{-1} y_1$; thus (2-1) and $y_0^p = x^{-1} y_0^p x = y_1^p$ imply $[y, x]^p = y_0^{-p} y_1^p = 1$. □

Lemma 5.6. *The group G_k has nilpotency class p^k, and $\gamma_m(G_k)/\gamma_{m+1}(G_k)$ is elementary abelian of rank at most 2 for $2 \le m \le p^k$.*

Proof. Let $2 \le m \le p^k$. Since G_k is a central extension of Z_k by W_k, we deduce from Proposition 2.6 that

$$\gamma_m(G_k) = \big\langle [y, x, \overset{m-1}{\ldots}, x], [y, x, \overset{m-2}{\ldots}, x, y] \big\rangle \gamma_{m+1}(G_k),$$

and Lemma 5.5 shows that $\gamma_m(G_k)/\gamma_{m+1}(G_k)$ is elementary abelian of rank at most 2. Again by Proposition 2.6, the nilpotency class of G_k is at least p^k. Moreover, $\gamma_{p^k}(G_k) Z_k = \langle w \rangle Z_k$, where $w \in Z(G_k)$ by Lemma 5.3. We conclude that G_k has nilpotency class precisely p^k. □

Lemma 5.7. *The group G_k satisfies*

$$G_k^p \subseteq \langle x^p, y^p \rangle \gamma_p(G_k) \quad \textit{and} \quad G_k^{p^j} \subseteq \langle x^{p^j} \rangle \gamma_{p^j}(G_k) \quad \textit{for } j \ge 2.$$

Proof. Recall that $H_k = \langle y_0, y_1, \dots, y_{p^k-1}\rangle Z_k \le G_k$ has exponent p^2, and observe that Proposition 2.5 together with Lemma 5.5 yields $H_k^p = \langle y^p \rangle$. Every element $g \in G$ is of the form $g = x^m h$, with $0 \le m < p^{k+1}$ and $h \in H_k$. Using (2-3), based on Proposition 2.5 and Lemma 5.5, we conclude that

$$g^p = (x^m h)^p \equiv x^{mp} h^p \in \langle x^p, y^p \rangle \mod \gamma_p(G_k),$$

and for $j \ge 2$,

$$g^{p^j} = (x^m h)^{p^j} \equiv x^{mp^j} h^{p^j} = x^{mp^j} \in \langle x^{p^j} \rangle \mod \gamma_{p^j}(G_k). \qquad \square$$

Proof of Proposition 5.2. Apply Lemmata 5.4, 5.6 and 5.7. □

From Lemma 5.1 and Proposition 5.2 we deduce that

$$\log_p |G : G^{p^k}| = \log_p |G_k : G_k^{p^k}| = \tfrac{1}{2}(3p^k + 2k - 3).$$

On the other hand, we observe from Proposition 2.6 that

$$\log_p |G : ZG^{p^k}| = \log_p |W_k : W_k^{p^k}| = p^k + k - 1,$$

hence

$$\log_p |ZG^{p^k} : G^{p^k}| = \tfrac{1}{2}(3p^k + 2k - 3) - (p^k + k - 1) = \tfrac{1}{2}(p^k - 1).$$

Thus (5-1) follows from

$$\lim_{i\to\infty} \frac{\log_p |ZG^{p^i} : G^{p^i}|}{\log_p |G : G^{p^i}|} = \lim_{i\to\infty} \frac{\frac{1}{2}(p^i-1)}{\frac{1}{2}(3p^i+2i-3)} = \frac{1}{3}. \tag{5-3}$$

Remark 5.8. In the literature, one sometimes encounters a variant of the p-power series, the *iterated* p-power series of G which is recursively given by

$$\mathcal{I}\colon I_0(G) = G, \quad \text{and} \quad I_j(G) = I_{j-1}(G)^p \quad \text{for } j \geq 1.$$

By a small modification of the proof of Lemma 5.7 we obtain inductively

$$I_j(G_k) \subseteq \left(\langle x^{p^{j-1}}\rangle \gamma_{p^{j-1}}(G_k)\right)^p \subseteq \langle x^{p^j}\rangle \gamma_{p^j}(G_k) \quad \text{for } j \geq 2,$$

based on the commutator identities (2-3) for $r = 1$. With Proposition 5.2 and Lemma 5.6 this yields $G_k^{p^k} \subseteq I_k(G_k) \subseteq \langle x^{p^k}\rangle \gamma_{p^k}(G_k) = G_k^{p^k}$. We conclude that the p-power series $\mathcal{P}$ and the iterated p-power series $\mathcal{I}$ of G coincide.

One may further note another natural filtration series $\mathcal{N} : \overline{N}_i$, $i \in \mathbb{N}_0$, of G, consisting of the images $\overline{N}_i$ in G of the open normal subgroups N_i defined in Section 3, where we set $\overline{N}_0 = G$. As $\overline{N}_i \leq G^{p^i}$ with $\log_p |G^{p^i} : \overline{N}_i| \leq 4$ for all $i \in \mathbb{N}_0$, we see that the filtration series $\mathcal{P}$ and $\mathcal{N}$ induce the same Hausdorff dimension function on G.

6. The normal Hausdorff spectra of G with respect to the lower p-series, the dimension subgroup series and the Frattini series

We continue to use the notation set up in Section 3 and work with the finite quotients G_k, $k \in \mathbb{N}$, of the pro-p group G. Our aim is to pin down the lower central series, the lower p-series, the dimension subgroup series and the Frattini series of G_k. Subsequently, it will be easy to complete the proof of Theorem 1.1.

Proposition 6.1. *The group G_k is nilpotent of class p^k; its lower central series satisfies*

$$G_k = \gamma_1(G_k) = \langle x, y\rangle \gamma_2(G_k) \quad \textit{with } G_k/\gamma_2(G_k) \cong C_{p^{k+1}} \times C_{p^2}$$

and, for $1 \leq i \leq (p^k-1)/2$,

$$\gamma_{2i}(G_k) = \langle [y, x, \overset{2i-1}{\ldots}, x]\rangle \gamma_{2i+1}(G_k),$$
$$\gamma_{2i+1}(G_k) = \langle [y, x, \overset{2i}{\ldots}, x], [y, x, \overset{2i-1}{\ldots}, x, y]\rangle \gamma_{2i+2}(G_k)$$

with

$$\gamma_{2i}(G_k)/\gamma_{2i+1}(G_k) \cong C_p \quad \textit{and} \quad \gamma_{2i+1}(G_k)/\gamma_{2i+2}(G_k) \cong C_p \times C_p.$$

Proof. By Lemma 5.6 the nilpotency class of G_k is p^k. From $G_k = \langle x, y\rangle$ it is clear that $\gamma_2(G_k) = \langle [x, y]\rangle\gamma_3(G_k)$, and (3-3) gives $G_k/\gamma_2(G_k) \cong C_{p^{k+1}} \times C_{p^2}$. From Lemma 5.1 we know that

$$\log_p|G_k| = (3p^k + 2k + 3)/2 = ((k+1)+2) + \frac{p^k-1}{2}(1+2),$$

and the proof of Lemma 5.6 shows that

$$\gamma_m(G_k) = \big\langle [y, x, \overset{m-1}{\dots}, x], [y, x, \overset{m-2}{\dots}, x, y]\big\rangle\gamma_{m+1}(G_k) \quad \text{for } 2 \le m \le p^k.$$

Consequently, it suffices to prove that $[y, x, \overset{m-2}{\dots}, x, y] \in \gamma_{m+1}(G_k)$ whenever m is even. More generally, we consider the elements

$$b_{j,m} = [[y, x, \overset{m-2}{\dots}, x]^{x^j}, y] \quad \text{for } 2 \le m \le p^k \text{ and } j \in \mathbb{N}_0.$$

Writing $e_i = [y_0, y_i] \in Z_k \subseteq Z(G_k)$ for $i \in \mathbb{Z}$, we recall from Lemma 5.1 that

$$b_{j,m} \in [H_k, H_k] = \langle e_i \mid 1 \le i \le (p^k-1)/2\rangle \cong \underbrace{C_p \times \dots \times C_p}_{(p^k-1)/2}.$$

Induction on m shows that

$$[y, x, \overset{m-2}{\dots}, x] \equiv \prod_{i=0}^{m-2} y_i^{(-1)^{m+i}\binom{m-2}{i}} \quad \text{modulo } Z_k \subseteq Z(G_k),$$

and we deduce that

$$b_{j,m} = \Big[\prod\nolimits_{i=0}^{m-2} y_{j+i}^{(-1)^{m+i}\binom{m-2}{i}}, y\Big] = \prod\nolimits_{i=0}^{m-2} e_{j+i}^{(-1)^{m+i+1}\binom{m-2}{i}}. \tag{6-1}$$

The identities

$$\binom{m-2}{i} - 2\binom{m-1}{i} + \binom{m}{i} = \binom{m-2}{i-2}$$

imply that

$$b_{j,m} \equiv b_{j,m} b_{j,m+1}^2 b_{j,m+2} = b_{j+2,m} \quad \text{modulo } \gamma_{m+1}(G_k). \tag{6-2}$$

Now suppose that m is even, and recall that $p \ne 2$. From (6-2) we obtain inductively $[y, x, \overset{m-2}{\dots}, x, y] = b_{0,m} \equiv b_{j_0,m}$ modulo $\gamma_{m+1}(G_k)$ for

$$j_0 = \begin{cases} \dfrac{p^k+1}{2} - \dfrac{m}{2} & \text{if } p^k + 1 - m \equiv_4 0, \\[2mm] \dfrac{p^k+3}{2} - \dfrac{m}{2} & \text{if } p^k + 1 - m \equiv_4 2. \end{cases}$$

Consequently, it suffices to prove that $b_{j_0,m} \in \gamma_{m+1}(G_k)$. First suppose that $p^k+1 \equiv_4 m$ and hence $j_0 = (p^k+1)/2 - m/2$. From (6-1) and (5-2) we see that

$$\begin{aligned}
b_{j_0,m} &= \prod_{i=0}^{m/2-1} e_{j_0+i}^{(-1)^{i+1}\binom{m-2}{i}} \prod_{i=m/2}^{m-2} e_{p^k-(j_0+i)}^{(-1)^{i}\binom{m-2}{i}}\\
&= \prod_{i=0}^{m/2-1} e_{j_0+i}^{(-1)^{i+1}\binom{m-2}{i}} \prod_{i=m/2}^{m-2} e_{j_0+(m-1-i)}^{(-1)^{m-i}\binom{m-2}{(m-1-i)-1}}\\
&= \prod_{i=0}^{m/2-1} e_{j_0+i}^{(-1)^{i+1}\binom{m-2}{i}} \prod_{i'=1}^{m/2-1} e_{j_0+i'}^{(-1)^{i'+1}\binom{m-2}{i'-1}}\\
&= \prod_{i=0}^{m/2-1} e_{j_0+i}^{(-1)^{i+1}\binom{m-1}{i}}
\end{aligned}$$

and similarly

$$\begin{aligned}
b_{j_0,m+1}^{-1} &= \prod_{i=0}^{m/2-1} e_{j_0+i}^{(-1)^{i+1}\binom{m-1}{i}} \prod_{i=m/2}^{m-1} e_{p^k-(j_0+i)}^{(-1)^{i}\binom{m-1}{i}}\\
&= \prod_{i=0}^{m/2-1} e_{j_0+i}^{(-1)^{i+1}\binom{m-1}{i}} \prod_{i=m/2}^{m-1} e_{j_0+(m-1-i)}^{(-1)^{m-i}\binom{m-1}{m-1-i}}\\
&= \prod_{i=0}^{m/2-1} e_{j_0+i}^{(-1)^{i+1}\binom{m-1}{i}} \prod_{i'=0}^{m/2-1} e_{j_0+i'}^{(-1)^{i'+1}\binom{m-1}{i'}}\\
&= \Big(\prod_{i=0}^{m/2-1} e_{j_0+i}^{(-1)^{i+1}\binom{m-1}{i}}\Big)^2
\end{aligned}$$

Hence $b_{j_0,m}^2 = b_{j_0,m+1}^{-1} \in \gamma_{m+1}(G_k)$, and $p \neq 2$ implies $b_{j_0,m} \in \gamma_{m+1}(G_k)$.

In the remaining case $p^k+1 \equiv_4 m+2$ we have $j_0 = (p^k+3)/2 - m/2$, and a slight variation of the argument above shows that $b_{j_0,m}^2 = b_{j_0-1,m+1}$, hence $b_{j_0,m} \in \gamma_{m+1}(G_k)$. ☐

Corollary 6.2. *For $2 \le m \le p^k$ and $\nu(m) = \lfloor \frac{1}{2}(p^k - m + 2)\rfloor$, we have*

$$\gamma_m(G_k) \cap Z_k = \big\langle [y, x, \overset{2j-1}{\ldots}, x, y] \mid \lfloor \tfrac{m}{2} \rfloor \le j \le (p^k-1)/2 \big\rangle \cong C_p^{\nu(m)}$$

and $\gamma_m(G_k) \cap Z(G_k) = \langle [y, x, \overset{p^k-1}{\ldots}, x] \rangle \times (\gamma_m(G_k) \cap Z_k) \cong C_p^{\nu(m)+1}$. In particular,

$$[y, x, \overset{m-2}{\ldots}, x, y] \in \big\langle [y, x, \overset{2j-1}{\ldots}, x, y] \mid \tfrac{m}{2} \le j \le (p^k-1)/2 \big\rangle \quad \textit{for } m \equiv_2 0.$$

Proof. Clearly, all nontrivial elements of the form $[y, x, \ldots, x, y]$ are central and of order p. By Proposition 6.1 and Lemma 5.5, also $[y, x, \overset{p^k-1}{\ldots}, x]$ is central and of order p. Moreover, Proposition 6.1 shows that every $g \in \gamma_2(G_k)$ can be written as

$$g = \prod_{i=1}^{p^k-1} [y, x, \overset{i}{\ldots}, x]^{\alpha(i)} \prod_{j=1}^{(p^k-1)/2} [y, x, \overset{2j-1}{\ldots}, x, y]^{\beta(j)},$$

where $\alpha(i), \beta(j) \in \{0, 1, \ldots, p-1\}$ are uniquely determined by g. Furthermore, g is central if and only if $\alpha(i) = 0$ for $1 \le i \le p^k - 2$, and $g \in Z_k$ if and only if $\alpha(i) = 0$ for $1 \le i \le p^k - 1$. ☐

Corollary 6.3. *The lower p-series of G_k has length p^k and satisfies*:

$$\begin{aligned} G_k = P_1(G_k) &= \langle x, y\rangle P_2(G_k) \quad \text{with } G_k/P_2(G_k) \cong C_p \times C_p, \\ P_2(G_k) &= \langle x^p, y^p, [y, x]\rangle P_3(G_k) \quad \text{with } P_2(G_k)/P_3(G_k) \cong C_p \times C_p \times C_p, \end{aligned}$$

and, for $3 \le i \le p^k$, the i-th term is $P_i(G_k) = \langle x^{p^{i-1}}\rangle \gamma_i(G_k)$ so that

$$P_i(G_k) = \begin{cases} \langle x^{p^{i-1}}, [y, x, \overset{i-1}{\ldots}, x]\rangle P_{i+1}(G_k) & \text{if } i \equiv_2 0 \text{ and } i \le k+1, \\ \langle x^{p^{i-1}}, [y, x, \overset{i-1}{\ldots}, x], [y, x, \overset{i-2}{\ldots}, x, y]\rangle P_{i+1}(G_k) & \text{if } i \equiv_2 1 \text{ and } i \le k+1, \\ \langle [y, x, \overset{i-1}{\ldots}, x]\rangle P_{i+1}(G_k) & \text{if } i \equiv_2 0 \text{ and } i > k+1, \\ \langle [y, x, \overset{i-1}{\ldots}, x], [y, x, \overset{i-2}{\ldots}, x, y]\rangle P_{i+1}(G_k) & \text{if } i \equiv_2 1 \text{ and } i > k+1 \end{cases}$$

with

$$P_i(G_k)/P_{i+1}(G_k) \cong \begin{cases} C_p \times C_p & \text{if } i \equiv_2 0 \text{ and } i \le k+1, \\ C_p \times C_p \times C_p & \text{if } i \equiv_2 1 \text{ and } i \le k+1, \\ C_p & \text{if } i \equiv_2 0 \text{ and } i > k+1, \\ C_p \times C_p & \text{if } i \equiv_2 1 \text{ and } i > k+1. \end{cases}$$

Proof. The descriptions of $G_k/P_2(G_k)$ and $P_2(G_k)/P_3(G_k)$ are straightforward. Let $i \ge 3$. Clearly, $P_i(G_k) \supseteq \langle x^{p^{i-1}}\rangle \gamma_i(G_k)$. In view of Proposition 6.1, it suffices to prove that $x^{p^{i-1}}$ is central modulo $\gamma_{i+1}(G_k)$. Indeed, from Lemma 5.5 and Proposition 2.5 (recall that $p > 2$) we obtain

$$[x^{p^{i-1}}, y] \equiv [x, y]^{p^{i-1}} = 1 \quad \text{modulo } \gamma_{p^{i-1}+1}(G_k) \subseteq \gamma_{i+1}(G_k). \qquad \square$$

Corollary 6.4. *The dimension subgroup series of G_k has length p^k. For $1 \le i \le p^k$, the i-th term is $D_i(G_k) = G_k^{p^{l(i)}} \gamma_i(G_k)$, where $l(i) = \lceil \log_p i \rceil$.*

Furthermore, if i is not a power of p, equivalently if $l(i+1) = l(i)$, then $D_i(G_k)/D_{i+1}(G_k) \cong \gamma_i(G_k)/\gamma_{i+1}(G_k)$ so that

$$D_i(G_k) = \begin{cases} \langle [y, x, \overset{i-1}{\ldots}, x]\rangle D_{i+1}(G_k) & \text{if } i \equiv_2 0, \\ \langle [y, x, \overset{i-1}{\ldots}, x], [y, x, \overset{i-2}{\ldots}, x, y]\rangle D_{i+1}(G_k) & \text{if } i \equiv_2 1, \end{cases}$$

with

$$D_i(G_k)/D_{i+1}(G_k) \cong \begin{cases} C_p & \text{if } i \equiv_2 0, \\ C_p \times C_p & \text{if } i \equiv_2 1 \end{cases}$$

whereas if $i = p^l$ is a power of p, equivalently if $l(i+1) = l+1$ for $l = l(i)$, then $D_i(G_k)/D_{i+1}(G_k) \cong \langle x^{p^l}\rangle/\langle x^{p^{l+1}}\rangle \times \langle y^{p^l}\rangle/\langle y^{p^{l+1}}\rangle \times \gamma_i(G_k)/\gamma_{i+1}(G_k)$ so that

$$\begin{aligned} D_1(G_k) &= \langle x, y\rangle D_2(G_k), \\ D_p(G_k) &= \langle x^p, y^p, [y, x, \overset{p-1}{\ldots}, x], [y, x, \overset{p-2}{\ldots}, x, y]\rangle D_{p+1}(G_k), \\ D_i(G_k) &= \langle x^{p^l}, [y, x, \overset{i-1}{\ldots}, x], [y, x, \overset{i-2}{\ldots}, x, y]\rangle D_{i+1}(G_k) \end{aligned}$$

with

$$D_i(G_k)/D_{i+1}(G_k) \cong \begin{cases} C_p \times C_p & \text{if } i = 1, \text{ equivalently if } l = 0,\\ C_p \times C_p \times C_p \times C_p & \text{if } i = p, \text{ equivalently if } l = 1,\\ C_p \times C_p \times C_p & \text{if } i = p^l \text{ with } 2 \le l \le k. \end{cases}$$

In particular, for $p^{k-1} + 1 \le i \le p^k$ *and thus* $l(i) = k$,

$$D_i(G_k) = G_k^{p^k} \gamma_i(G_k) = \langle x^{p^k} \rangle \gamma_i(G_k),$$

so that

$$\log_p |D_i(G_k)| = \log_p |\gamma_i(G_k)| + 1.$$

Proof. For $i \in \mathbb{N}$ write $l(i) = \lceil \log_p i \rceil$. From [Dixon et al. 1999, Theorem 11.2] and Lemma 5.5 we obtain $D_i(G_k) = G_k^{p^{l(i)}} \gamma_i(G_k)$. In particular, $D_i(G_k) = 1$ for $i > p^k$, by Proposition 6.1 and Corollary 6.3.

Now suppose that $1 \le i \le p^k$ and put $l = l(i)$. From Lemma 5.7 we observe that $G_k^{p^l} \cap \gamma_i(G_k) \subseteq \gamma_{p^l}(G_k)$. If $l(i+1) = l$ then $\gamma_{p^l}(G_k) \subseteq \gamma_{i+1}(G_k)$, and hence

$$\begin{aligned} D_i(G_k)/D_{i+1}(G_k) &= G_k^{p^l} \gamma_i(G_k)/G_k^{p^l} \gamma_{i+1}(G_k) \\ &\cong \gamma_i(G_k)/(G_k^{p^l} \cap \gamma_i(G_k))\gamma_{i+1}(G_k) \\ &\cong \gamma_i(G_l)/\gamma_{i+1}(G_l). \end{aligned}$$

Now suppose that $l(i+1) = l+1$, equivalently $i = p^l$. We observe that, modulo H_k, the i-th factor of the dimension subgroup series is

$$D_i(G_k)H_k/D_{i+1}(G_k)H_k = \langle x^{p^l} \rangle H_k/\langle x^{p^{l+1}} \rangle H_k \cong C_p.$$

Comparing with the overall order of G_k, conveniently implicit in Corollary 6.3, we deduce that

$$\begin{aligned} D_i(G_k)/D_{i+1}(G_k) &= G_k^{p^l} \gamma_i(G_k)/G_k^{p^{l+1}} \gamma_{i+1}(G_k) \\ &= \langle x^{p^l}, y^{p^l} \rangle \gamma_i(G_l)/\langle x^{p^{l+1}}, y^{p^{l+1}} \rangle \gamma_{i+1}(G_l) \\ &\cong \langle x^{p^l} \rangle/\langle x^{p^{l+1}} \rangle \times \langle y^{p^l} \rangle/\langle y^{p^{l+1}} \rangle \times \gamma_i(G_l)/\gamma_{i+1}(G_l). \end{aligned}$$

All remaining assertions follow readily from Proposition 6.1. $\square$

Proposition 6.5. *The Frattini series of* G_k *has length* $k+2$ *and satisfies*:

$$\begin{aligned} G_k = \Phi_0(G_k) = \langle x, y \rangle \Phi_1(G_k) \quad &\text{with } G_k/\Phi_1(G_k) \cong C_p \times C_p,\\ \Phi_1(G_k) = \big\langle x^p, y^p, [y,x], [y,x,x], \ldots, [y,x, \overset{p}{\ldots}, x], [y,x,y] \big\rangle \Phi_2(G_k) &\\ &\text{with } \Phi_1(G_k)/\Phi_2(G_k) \cong C_p^{p+3}, \end{aligned}$$

and, for $2 \le i \le k$, the i-th term is

$$\Phi_i(G_k) = \Big\langle x^{p^i}, [y, x, \overset{\nu(i)}{\ldots}, x], [y, x, \overset{\nu(i)+1}{\ldots}, x], \ldots, [y, x, \overset{\nu(i+1)-1}{\ldots}, x],$$
$$[y, x, \overset{2\nu(i-1)+1}{\ldots}, x, y], [y, x, \overset{2\nu(i-1)+3}{\ldots}, x, y], \ldots, [y, x, \overset{2\nu(i)-1}{\ldots}, x, y]\Big\rangle \Phi_{i+1}(G_k)$$
$$\text{with } \Phi_i(G_k)/\Phi_{i+1}(G_k) \cong \begin{cases} C_p^{p^i+p^{i-1}+1} & \text{for } i \ne k, \\ C_p^{p^k+1-(p^{k-1}-1)/(p-1)} & \text{for } i = k, \end{cases}$$

where

$$\nu(j) = \min\{(p^j-1)/(p-1), p^k\} = \begin{cases} \dfrac{(p^j-1)}{(p-1)} & \text{for } 1 \le j \le k, \\ p^k & \text{for } j = k+1; \end{cases}$$

lastly,

$$\Phi_{k+1}(G_k) = \big\langle [y, x, \overset{2\nu(k)+1}{\ldots}, x, y], [y, x, \overset{2\nu(k)+3}{\ldots}, x, y], \ldots, [y, x, \overset{p^k-2}{\ldots}, x, y]\big\rangle$$
$$\text{with } \Phi_{k+1}(G_k) \cong C_p^{(p^{k+1}-3p^k-p+3)/(2(p-1))}.$$

Proof. For ease of notation we set $c_1 = y$ and, for $i \ge 2$,

$$c_i = [y, x, \overset{i-1}{\ldots}, x] \quad \text{and} \quad z_i = [c_{i-1}, y] = [y, x, \overset{i-2}{\ldots}, x, y].$$

From Lemma 5.5 we observe that $c_i^p = z_i^p = 1$ for $i \ge 2$; furthermore, the elements $z_i \in [H_k, H_k] \subseteq Z_k$ are central in G_k. We claim that

$$[c_i, c_j] \equiv z_{i+j}^{(-1)^{j-1}} \bmod \gamma_{i+j+1}(G_k) \quad \text{for } i > j \ge 1. \tag{6-3}$$

Indeed, $[c_i, c_1] = [c_i, y] = z_{i+1}$, and, modulo $\gamma_{i+j+1}(G_k)$, the Hall–Witt identity gives

$$1 \equiv [c_i, c_{j-1}, x][c_{j-1}, x, c_i][x, c_i, c_{j-1}] \equiv [c_j, c_i][c_{i+1}, c_{j-1}]^{-1},$$

hence $[c_i, c_j] \equiv [c_{i+1}, c_{j-1}]^{-1}$ from which the result follows by induction.

We use the generators specified in the statement of the proposition to define an ascending chain $1 = L_{k+2} \le L_{k+1} \le \cdots \le L_1 \le L_0 = G_k$ so that each L_i is the desired candidate for $\Phi_i(G_k)$. For $1 \le i \le k+1$ we deduce from Proposition 6.1 and Corollary 6.2 that

$$L_i = \langle x^{p^i} \rangle M_i \quad \text{with } M_i = \langle c_{\nu(i)+1} \rangle \gamma_{\nu(i)+2}(G_k) C_i \trianglelefteq G_k,$$

where $C_i = \langle y^{p^i} \rangle \times \langle z_j \mid 2\nu(i-1)+3 \le j \le p^k \text{ and } j \equiv_2 1 \rangle$ is central in G_k. (Note that the factor $\langle y^{p^i} \rangle$ vanishes if $i \ge 2$.) Applying (2-3), based on Proposition 2.5 and Lemma 5.5, we see that $[x^{p^i}, G_k] = [x^{p^i}, H_k] \subseteq \gamma_{p^i+1}(G_k)$, hence $L_i \trianglelefteq G_k$ for $1 \le i \le k+1$. Using also (6-3), we see that the factor groups L_i/L_{i+1} are elementary abelian for $0 \le i \le k+1$. In particular, this shows that $\Phi_i(G_k) \subseteq L_i$ for $1 \le i \le k+2$.

Clearly, for each $i \in \{0, \dots, k+1\}$, the value of $\log_p|L_i/L_{i+1}| = d(L_i/L_{i+1})$ is bounded by the number of explicit generators used to define L_i modulo L_{i+1}; these numbers are specified in the statement of the proposition and a routine summation shows that they add up to the logarithmic order $\log_p|G_k|$, as given in Lemma 5.1. Therefore each L_i/L_{i+1} has the expected rank and it suffices to show that $\Phi_i(G_k) \supseteq L_i$ for $1 \le i \le k+1$.

Let $i \in \{1, \dots, k+1\}$. It is enough to show that the following elements which generate L_i as a normal subgroup belong to $\Phi_i(G_k)$:

$$x^{p^i}, \quad c_{\nu(i)+1}, \quad \text{and} \quad z_j \quad \text{for } 2\nu(i-1)+3 \le j \le p^k \text{ with } j \equiv_2 1.$$

Clearly, $x^{p^i} \in \Phi_i(G_k)$ and, applying (2-3), based on Proposition 2.5 and Lemma 5.5, we see by induction on i that

$$c_{\nu(i)+1} = [y, x, \overset{\nu(i)}{\ldots}, x] \equiv_{\Phi_i(G_k)} [y, x, x^p, \dots, x^{p^{i-1}}] \equiv_{\Phi_i(G_k)} 1.$$

Now let $2\nu(i-1)+3 \le j \le p^k$ with $j \equiv_2 1$. By Corollary 6.2 and reverse induction on j it suffices to show that z_j is contained in $\Phi_i(G_k)$ modulo $\gamma_{j+1}(G_k)$. This follows from (6-3) and the fact that $c_{\nu(i-1)+1}, c_{j-\nu(i-1)-1} \in \Phi_{i-1}(G_k)$ by induction on i. $\square$

Using Corollary 4.2, we can now complete the proof of Theorem 1.1: it suffices to compute $\operatorname{hdim}_G^{\mathcal{S}}(Z)$ and $\operatorname{hdim}_G^{\mathcal{S}}(H)$ for the standard filtration series $\mathcal{S} \in \{\mathcal{L}, \mathcal{D}, \mathcal{F}\}$.

Corollary 6.3 implies

$$\operatorname{hdim}_G^{\mathcal{L}}(Z) = \varliminf_{i\to\infty} \frac{\log_p|ZP_i(G) : P_i(G)|}{\log_p|G : P_i(G)|} = \lim_{i\to\infty} \frac{i/2}{5i/2} = \frac{1}{5}, \tag{6-4}$$

$$\operatorname{hdim}_G^{\mathcal{L}}(H) = \varliminf_{i\to\infty} \frac{\log_p|HP_i(G) : P_i(G)|}{\log_p|G : P_i(G)|} = \lim_{i\to\infty} \frac{3i/2}{5i/2} = \frac{3}{5}. \tag{6-5}$$

Corollary 6.4 implies

$$\begin{aligned} \operatorname{hdim}_G^{\mathcal{D}}(Z) &= \varliminf_{i\to\infty} \frac{\log_p|ZD_i(G) : D_i(G)|}{\log_p|G : D_i(G)|} = \lim_{i\to\infty} \frac{i/2}{3i/2} = \frac{1}{3}, \\ \operatorname{hdim}_G^{\mathcal{D}}(H) &= \varliminf_{i\to\infty} \frac{\log_p|HD_i(G) : D_i(G)|}{\log_p|G : D_i(G)|} = \lim_{i\to\infty} \frac{3i/2}{3i/2} = 1. \end{aligned} \tag{6-6}$$

Lastly, Proposition 6.5 implies

$$\begin{aligned} \operatorname{hdim}_G^{\mathcal{F}}(Z) &= \varliminf_{i\to\infty} \frac{\log_p|Z\Phi_i(G) : \Phi_i(G)|}{\log_p|G : \Phi_i(G)|} = \lim_{i\to\infty} \frac{\sum_{j=1}^{i-1} p^{j-1}}{\sum_{j=1}^{i-1}(p^j + p^{j-1}+1)} = \frac{1}{p+1}, \\ \operatorname{hdim}_G^{\mathcal{F}}(H) &= \varliminf_{i\to\infty} \frac{\log_p|H\Phi_i(G) : \Phi_i(G)|}{\log_p|G : \Phi_i(G)|} = \lim_{i\to\infty} \frac{\sum_{j=1}^{i-1}(p^j + p^{j-1})}{\sum_{j=1}^{i-1}(p^j + p^{j-1}+1)} = 1. \end{aligned} \tag{6-7}$$

Remark 6.6. From (5-3), (6-4), (6-5), (6-6), (6-7) and the fact that subgroups of Hausdorff dimension 1 automatically have strong Hausdorff dimension we conclude that Z and H have strong Hausdorff dimension in G with respect to all standard filtration series $\mathcal{P}$, $\mathcal{D}$, $\mathcal{F}$ and $\mathcal{L}$.

7. The entire Hausdorff spectra of G with respect to the standard filtration series

We continue to use the notation set up in Section 3 to study and determine the entire Hausdorff spectra of the pro-p group G, with respect to the standard filtration series $\mathcal{P}, \mathcal{D}, \mathcal{F}, \mathcal{L}$.

Proof of Theorem 1.3. As in Sections 2 and 3, we write $W = G/Z \cong C_p \hat{\wr} \mathbb{Z}_p$, and we denote by $\pi : G \to W$ the canonical projection with $\ker \pi = Z$.

First suppose that $\mathcal{S}$ is one of the filtration series $\mathcal{P}$, $\mathcal{D}$, $\mathcal{F}$ on G. By Remark 6.6, the group H has strong Hausdorff dimension 1 in G with respect to $\mathcal{S}$. As every finitely generated subgroup of H is finite, it follows from [Klopsch et al. 2019, Theorem 5.4] that $\operatorname{hspec}^{\mathcal{S}}(G) = [0, 1]$.

It remains to pin down the Hausdorff spectrum of G with respect to the lower p-series $\mathcal{L}$: $P_i(G)$, $i \in \mathbb{N}$, on G. By Remark 6.6, the normal subgroups $Z, H \trianglelefteq_{\mathrm{c}} G$ have strong Hausdorff dimensions $\operatorname{hdim}^{\mathcal{L}}_G(Z) = \frac{1}{5}$ and $\operatorname{hdim}^{\mathcal{L}}_G(H) = \frac{3}{5}$. From Corollary 2.4, Lemma 2.2 and Corollary 2.11 we deduce that $\operatorname{hspec}^{\mathcal{L}}(G)$ contains

$$S = \left[0, \tfrac{3}{5}\right] \cup \left\{\tfrac{3}{5} + \tfrac{2m}{5p^n} \mid m, n \in \mathbb{N}_0 \text{ with } \tfrac{p^n}{2} < m \le p^n\right\}.$$

Thus it suffices to show that

$$\left(\tfrac{3}{5}, \tfrac{4}{5}\right) \subseteq \operatorname{hspec}^{\mathcal{L}}(G) \subseteq \left(\tfrac{3}{5}, \tfrac{4}{5}\right) \cup S. \tag{7-1}$$

First we prove the second inclusion. Let $K \le_{\mathrm{c}} G$ be any closed subgroup with $\operatorname{hdim}^{\mathcal{L}}_G(K) > \frac{3}{5}$. In particular, this implies $K \not\subseteq H$ and hence $KH \le_{\mathrm{o}} G$.

We denote by $\mathcal{L}|_H$ and $\mathcal{L}|_{H\pi}$ the filtration series induced by $\mathcal{L}$ on H, via intersection, and on $H\pi = HZ/Z$, via subsequent reduction modulo Z. We write $\mathcal{L}$ for the filtration series $\mathcal{L}|_W$ induced on $W = G/Z$, as it coincides with the lower p-series of the quotient group. Using Corollary 2.11 and Lemma 2.2, we see that $(K \cap H)\pi$ has strong Hausdorff dimension

$$\alpha = \operatorname{hdim}^{\mathcal{L}|_{H\pi}}_{H\pi}((K \cap H)\pi) = 2 \operatorname{hdim}^{\mathcal{L}}_W(K\pi) - 1 \in [0, 1]$$

in $H\pi$ with respect to $\mathcal{L}|_{H\pi}$. Applying Lemma 2.2 twice, we deduce that

$$\begin{aligned} \operatorname{hdim}^{\mathcal{L}}_G(K) &= \tfrac{2}{5} + \tfrac{3}{5} \operatorname{hdim}^{\mathcal{L}|_H}_H(K \cap H) \\ &\in \tfrac{2}{5} + \tfrac{3}{5}\left(\tfrac{2}{3} \operatorname{hdim}^{\mathcal{L}|_{H\pi}}_{H\pi}((K \cap H)\pi) + \left[0, \tfrac{1}{3}\right]\right) \\ &= \tfrac{2}{5}(1 + \alpha) + \left[0, \tfrac{1}{5}\right]. \end{aligned} \tag{7-2}$$

For $\alpha < \frac{1}{2}$ we obtain $\mathrm{hdim}_G^{\mathcal{L}}(K) < \frac{4}{5}$ and there is nothing further to prove. Now suppose that $\alpha \geq \frac{1}{2}$. It suffices to show that $K \cap Z \leq_{\mathrm{o}} Z$ and hence $\mathrm{hdim}_G^{\mathcal{L}}(K \cap Z) = \frac{1}{5}$: with this extra information we can refine the analysis in (7-2) and use Corollary 2.11 once more to deduce that

$$\mathrm{hdim}_G^{\mathcal{L}}(K) = \tfrac{2}{5}(1+\alpha) + \tfrac{1}{5} = \tfrac{4}{5}\,\mathrm{hdim}_W^{\mathcal{L}}(K\pi) + \tfrac{1}{5} \in S.$$

Let us prove that $K \cap Z \leq_{\mathrm{o}} Z$. As $KH \leq_{\mathrm{o}} G$, we have $KH = \langle x^{p^n} \rangle H$, where $n = \log_p |G : KH| \in \mathbb{N}_0$. Using Lemma 2.2, we deduce from $\alpha \geq \frac{1}{2}$ that

$$\mathrm{hdim}_W^{\mathcal{L}}((K \cap H)\pi) \geq \tfrac{1}{4} = \tfrac{1}{2}\,\mathrm{hdim}_W^{\mathcal{L}}(H\pi). \tag{7-3}$$

At this point it is useful to recall our analysis of $\mathrm{hspec}^{\mathcal{L}}(W)$ in the proof of Theorem 2.10 and also the computations carried out in the proof of Proposition 6.5, involving the elements $c_i = [y, x, \overset{i-1}{\ldots}, x]$ and $z_i = [c_{i-1}, y]$. In particular, for $i \in \mathbb{N}$ with $i \geq 3$ we have

$$(P_i(G) \cap H)\pi = \langle c_j \mid j \geq i \rangle \pi \quad \text{and} \quad P_i(G) \cap Z = \langle z_j \mid j \geq i \text{ and } j \equiv_2 1 \rangle;$$

compare Corollary 6.3. From (7-3) and the proof of Theorem 2.10 we deduce that, subject to replacing K by a suitable open subgroup $\widetilde{K} = K \cap \langle x^{p^{\widetilde{n}}} \rangle H$ with $\widetilde{n} \geq n$ if necessary, we find $m \geq (p^n+1)/2$ and $a_1, \ldots, a_m \in K \cap H$ so that

$$(K \cap H)M/M = \langle a_1, \ldots, a_m \rangle M/M \cong C_p^{\,m}, \quad \text{where } M = (P_{p^n+1}(G) \cap H)Z,$$

and the numbers

$$d(j) = \max\{ i \in \mathbb{N} \mid a_j \in (P_i(G) \cap H)Z \}, \quad 1 \leq j \leq m,$$

form a strictly increasing sequence $1 \leq d(1) < \cdots < d(m) < p^n$. Commuting $a_1, \ldots, a_m$ repeatedly with x^{p^n}, we see as in the proof of Theorem 2.10 that

$$\{d(1), \ldots, d(m)\} + p^n \mathbb{N}_0 \subseteq \big\{ i \in \mathbb{N} \mid \exists g \in K \cap H : g \equiv_{P_{i+1}(G)Z} c_i \big\}.$$

For every $k \in \mathbb{N}$ with $k > p^n$ and $k \equiv_2 1$, the pigeonhole principle (Dirichlet's "Schubfachprinzip") yields $i, j \in \mathbb{N}$ with $i > j \geq 1$ and $i + j = k$, and we find $g_i, g_j \in K \cap H$ with $g_i \equiv_{P_{i+1}(G)Z} c_i$ and $g_j \equiv_{P_{j+1}(G)Z} c_j$ so that (6-3) gives

$$z_k \equiv_{P_{k+1}(G)} [c_i, c_j]^{(-1)^{j-1}} \equiv_{P_{k+1}(G)} [g_i, g_j]^{(-1)^{j-1}} \in K \cap Z.$$

But this implies $K \cap Z \supseteq \langle z_j \mid j > p^n \text{ and } j \equiv_2 1 \rangle = P_{p^n+1}(G) \cap Z$ and thus $K \cap Z \leq_{\mathrm{o}} Z$. This concludes the proof of the second inclusion in (7-1).

Finally we prove the first inclusion in (7-1). Let $\xi \in \left(\frac{2}{5}, \frac{4}{5}\right)$. Choose $m, n \in \mathbb{N}$ such that $1 \leq m < p^n/2$ and

$$\tfrac{1}{5}(2 + (4m-1)/p^n) \leq \xi \leq \tfrac{1}{5}(3 + 2m/p^n).$$

Consider the group $K = \langle x^{p^n}, y_0, y_1, \ldots, y_{m-1} \rangle$. Using the proof of Theorem 2.10 and Lemma 2.2, we show below that K has Hausdorff dimension

$$\begin{aligned}
\text{(7-4)} \qquad \operatorname{hdim}_G^{\mathcal{L}}(K) &= \tfrac{4}{5} \operatorname{hdim}_W^{\mathcal{L}}(K\pi) + \tfrac{1}{5} \operatorname{hdim}_Z^{\mathcal{L}|_Z}(K \cap Z) \\
&= \left(\tfrac{2}{5} + \tfrac{2}{5} m/p^n\right) + \tfrac{1}{5}(2m-1)/p^n \\
&= \tfrac{1}{5}(2 + (4m-1)/p^n).
\end{aligned}$$

In a similar, but much more straightforward way, we see that ZK has strong Hausdorff dimension

$$\operatorname{hdim}_G^{\mathcal{L}}(ZK) = \left(\tfrac{2}{5} + \tfrac{2}{5} m/p^n\right) + \tfrac{1}{5} = \tfrac{1}{5}(3 + (2m)/p^n).$$

An application of [Klopsch et al. 2019, Theorem 5.4] yields $L \le_{\mathrm{c}} G$ with $K \le L \le ZK$ such that $\operatorname{hdim}_G^{\mathcal{L}}(L) = \xi$.

The key to (7-4) consists in showing that

$$\text{(7-5)} \qquad \varliminf_{i \to \infty} \frac{\log_p |K P_i(G) \cap Z : P_i(G) \cap Z|}{\log_p |Z : P_i(G) \cap Z|} = \operatorname{hdim}_Z^{\mathcal{L}|_Z}(K \cap Z) = (2m-1)/p^n.$$

First we examine the lower limit on the left-hand side, restricting to indices of the form $i = p^k + 1$, $k \in \mathbb{N}$. Let $i = p^k + 1$, where $k \ge n$. Recall that $G_k = G/\langle x^{p^{k+1}}, [x^{p^k}, y] \rangle^G$ and consider the canonical projection $\varrho_k \colon G \to G_k$, $g \mapsto \bar{g}$. As before, we write $H_k = H\varrho_k$. Furthermore, we observe that $Z_k = \langle \bar{x}^{p^k} \rangle Z\varrho_k$ with $|Z_k : Z\varrho_k| = p$. By Corollary 6.3, we have

$$|H_k : H_k \cap \underbrace{P_i(G_k)}_{=1}| = |H_k| = |H : H \cap P_i(G)|$$

and hence

$$\frac{\log_p |K P_i(G) \cap Z : P_i(G) \cap Z|}{\log_p |Z : P_i(G) \cap Z|} = \frac{\log_p |K\varrho_k \cap Z\varrho_k|}{\log_p |Z\varrho_k|}.$$

Observe that

$$K\varrho_k \cap H_k = \left\langle \overline{y_j} \mid 0 \le j < p^k \text{ with } j \equiv_{p^n} 0, 1, \ldots, m-1 \right\rangle.$$

From Lemma 5.1 we see that $Z\varrho_k \cong C_p^{(p^k+1)/2}$ and further we deduce that

$$\begin{aligned}
\text{(7-6)} \quad & K\varrho_k \cap Z\varrho_k \\
&= \left\langle \{\bar{y}^p\} \cup \left\{ [\overline{y_0}, \overline{y_j}] \mid 0 \le j < p^k,\ j \equiv_{p^n} 0, \pm 1, \ldots, \pm(m-1),\ j \equiv_2 0 \right\} \right\rangle \\
&\cong C_p^{((2m-1)p^{k-n}+1)/2}.
\end{aligned}$$

This yields

$$\varlimsup_{i\to\infty} \frac{\log_p|K P_i(G)\cap Z : P_i(G)\cap Z|}{\log_p|Z : P_i(G)\cap Z|} \le \varlimsup_{k\to\infty} \frac{\log_p|K\varrho_k \cap Z\varrho_k|}{\log_p|Z\varrho_k|}$$

$$= \lim_{k\to\infty} \frac{(2m-1)p^{k-n}+1}{p^k+1} = \frac{2m-1}{p^n}.$$

In order to establish (7-5) it now suffices to prove that

$$\varliminf_{i\to\infty} \frac{\log_p|(K\cap Z)(P_i(G)\cap Z) : P_i(G)\cap Z|}{\log_p|Z : P_i(G)\cap Z|} \ge \frac{2m-1}{p^n}. \tag{7-7}$$

Our analysis above yields

$$K\cap Z = \big\langle \{y^p\} \cup \big\{[y_0, y_j] \mid j\in\mathbb{N} \text{ with } j \equiv_{p^n} 0, \pm 1, \ldots, \pm(m-1)\big\}\big\rangle.$$

Setting

$$L = \big\langle y_j \mid j\in\mathbb{N}_0 \text{ with } j \equiv_{p^n} 0, \pm 1, \ldots, \pm(m-1)\big\rangle Z,$$

and recalling the notation $c_1 = y = y_0$, we conclude that

$$K\cap Z \supseteq \{[g, c_1] \mid g\in L\}.$$

Next we consider the set

$$D = \{j\in\mathbb{N} \mid \exists g\in L : g \equiv_{P_{j+1}(G)Z} c_j\}.$$

Each element y_j can be written (modulo Z) as a product

$$y_j \equiv_Z \prod_{k=0}^{j} c_{k+1}^{\beta(j,k)} \quad \text{where } \beta(j,k) = \tbinom{j}{k},$$

using the elements $c_i = [y, x, \overset{i-1}{\ldots}, x]$ introduced in the proof of Proposition 6.5. In this product decomposition, the exponents should be read modulo p, and the elementary identity $(1+t)^{j+p^n} = (1+t)^j(1+t^{p^n})$ in $\mathbb{F}_p[\![t]\!]$ translates to

$$y_j^{-1} y_{j+p^n} = y^{-x^j} y^{x^{j+p^n}} \equiv_Z \prod_{k=0}^{j} c_{k+1+p^n}^{\beta(j,k)} \quad \text{for all } j\in\mathbb{N};$$

compare (2-4). Inductively, we obtain

$$D = D_0 + p^n\mathbb{N}_0 \quad \text{for } D_0 = D\cap\{1, \ldots, p^n\}.$$

Observe that $|D_0| = 2m-1$ and that, for each $k\in\mathbb{N}_0$, the set

$$(2kp^n + D_0) \cup ((2k+1)p^n + D_0)$$

consists of $2m-1$ odd and $2m-1$ even numbers.

For each $j \in D$ with $j \equiv_2 0$ there exists $g_j \in L$ with $g_j \equiv_{P_{j+1}(G)Z} c_j$ and we deduce that

$$z_{j+1} = [c_j, c_1] \equiv_{P_{j+2}(G)} [g_j, c_1] \in K \cap Z.$$

For $i = 2p^n q + r \in \mathbb{N}$, where $q, r \in \mathbb{N}_0$ with $0 \le r < 2p^n$, the count

$$\bigl|\{j \in D \mid j \equiv_2 0 \text{ and } j < i-1\}\bigr| \ge q(2m-1) - 1$$

yields

$$\log_p\bigl|(K \cap Z)(P_i(G) \cap Z) : P_i(G) \cap Z\bigr| \ge q(2m-1) - 1.$$

From Corollary 6.3 we observe that, for $i \ge 3$,

$$\log_p|Z : P_i(G) \cap Z| = \left\lfloor \tfrac{i}{2} \right\rfloor \le qp^n + p^n.$$

These estimates show that (7-7) holds. □

Appendix: The case $p = 2$

When p is even, Theorems 1.1 and 1.3, and all the results of Sections 2 and 4, hold with corresponding proofs. The structural results of Sections 5 and 6 however are slightly different and we now sketch these differences below; for complete details, we refer the reader to the supplement [Thillaisundaram 2018].

Firstly, for $p = 2$,

$$\text{(A-1)} \quad G_k = F/N_k \cong \Bigl\langle x, y \;\Big|\; x^{2^{k+1}},\ y^4,\ [x^{2^k}, y],\ [y^2, x]; \\ [y_0, y_i]^2,\ [y_0, y_i, x],\ [y_0, y_i, y] \quad \text{for } 1 \le i \le 2^{k-1} \Bigr\rangle$$

for $k \in \mathbb{N}$, and

$$\text{(A-2)} \qquad G \cong \bigl\langle x, y \mid y^4,\ [y^2, x];\ [y_0, y_i]^2,\ [y_0, y_i, x],\ [y_0, y_i, y] \quad \text{for } i \in \mathbb{N} \bigr\rangle$$

is a presentation of G as a pro-2 group.

Next, we have $\log_2 |G_k| = 2^k + 2^{k-1} + k + 2$ and the exponent of $\gamma_2(G_k)$ is 4. With regards to Lemma 5.3, the elements

$$w = y_{2^k-1} \cdots y_1 y_0 \quad \text{and} \quad [w, x] = [w, y] = [y_0, y_{2^{k-1}}]$$

are of order 2 in G_k and lie in $G_k^{2^k}$. In particular the subgroup $\langle x^{2^k}, w, [w, x]\rangle$ is isomorphic to $C_2 \times C_2 \times C_2$ and lies in $G_k^{2^k}$. Hence, for $k \ge 2$,

$$G_k^{2^k} = \langle x^{2^k}, w, [w, x]\rangle \cong C_2 \times C_2 \times C_2, \quad \log_2 |G_k : G_k^{2^k}| = \log_2|G_k| - 3$$

and

$$G_k/G_k^{2^k} \cong \Bigl\langle x, y \;\Big|\; x^{2^k},\ y^4,\ [y^2, x],\ w(x, y),\ [y_0, y_{2^{k-1}}]; \\ [y_0, y_i]^2,\ [y_0, y_i, x],\ [y_0, y_i, y] \quad \text{for } 1 \le i < 2^{k-1} \Bigr\rangle.$$

Lemma 5.7 is slightly different; here the group G_k satisfies $G_k^2 \subseteq \langle x^2, y^2\rangle \gamma_2(G_k)$ and

$$G_k^{2^j} \subseteq \langle x^{2^j}, [y, x, \overset{2^j-3}{\ldots}, x, y]\rangle \gamma_{2^j}(G_k) \subseteq \langle x^{2^j}\rangle \gamma_{2^j-1}(G_k) \quad \text{for } j \geq 2.$$

The proof is similar, but one needs the fact

$$[y, x, \overset{i}{\ldots}, x]^2 \in [H_k, H_k] \cap \gamma_{2i+1}(G_k), \quad \text{for } i \geq 1,$$

which is proved by induction, using

$$[[y, x, \overset{i-1}{\ldots}, x], x]^2 = [[y, x, \overset{i-1}{\ldots}, x]^x, [y, x, \overset{i-1}{\ldots}, x]^{-1}] \quad \text{for } i \geq 2.$$

Furthermore, $[y, x, \overset{i}{\ldots}, x]^2 \equiv [y, x, \overset{2i-1}{\ldots}, x, y]$ modulo $\gamma_{2i+2}(G_k)$.

The group G_k is nilpotent of class 2^k+1; its lower central series satisfies

$$G_k = \gamma_1(G_k) = \langle x, y\rangle \gamma_2(G_k) \quad \text{with} \quad G_k/\gamma_2(G_k) \cong C_{2^{k+1}} \times C_4$$

and, for $1 \leq i \leq 2^{k-1}$,

$$\begin{aligned} \gamma_{2i}(G_k) &= \langle [y, x, \overset{2i-1}{\ldots}, x]\rangle \gamma_{2i+1}(G_k), \\ \gamma_{2i+1}(G_k) &= \begin{cases} \langle [y, x, \overset{2i}{\ldots}, x], [y, x, \overset{2i-1}{\ldots}, x, y]\rangle \gamma_{2i+2}(G_k) & \text{for } i \neq 2^{k-1}, \\ \langle [y, x, \overset{2i}{\ldots}, x]\rangle \gamma_{2i+2}(G_k) & \text{for } i = 2^{k-1}, \end{cases} \end{aligned}$$

with

$$\begin{aligned} \gamma_{2i}(G_k)/\gamma_{2i+1}(G_k) &\cong C_2, \\ \gamma_{2i+1}(G_k)/\gamma_{2i+2}(G_k) &\cong \begin{cases} C_2 \times C_2 & \text{for } i \neq 2^{k-1}, \\ C_2 & \text{for } i = 2^{k-1}. \end{cases} \end{aligned}$$

The proof of the above is similar to that for the odd prime case, however here one takes

$$j_0 = \begin{cases} 2^{k-1} - \frac{m}{2} & \text{if } m \equiv_4 0, \\ 2^{k-1} + 1 - \frac{m}{2} & \text{if } m \equiv_4 2. \end{cases}$$

For the $m \equiv_4 0$ case, noting that $e_{2^{k-1}} = [w, x] \in \gamma_{2^k+1}(G_k)$, we have $b_{j_0,m} \equiv b_{j_0,m+1}$ modulo $\gamma_{m+1}(G_k)$. The $m \equiv_4 2$ case is similar.

The lower 2-series of G_k has length 2^k+1 and satisfies the corresponding form, based on the lower central series of G_k above.

The dimension subgroup series of G_k has length 2^k+2. For $1 \leq i \leq 2^k+2$, the i-th term is $D_i(G_k) = G_k^{2^{l(i)}} \gamma_{\lceil i/2\rceil}(G_k)^2 \gamma_i(G_k)$, where $l(i) = \lceil \log_2 i\rceil$.

Furthermore, if i is not a power of 2, equivalently if $l(i+1) = l(i)$, then $D_i(G_k)/D_{i+1}(G_k) \cong \gamma_{\lceil i/2\rceil}(G_k)^2 \gamma_i(G_k)/\gamma_{\lceil (i+1)/2\rceil}(G_k)^2 \gamma_{i+1}(G_k)$ so that

$$D_i(G_k) = \begin{cases} \langle [y, x, \overset{i-1}{\ldots}, x]\rangle D_{i+1}(G_k) & \text{if } i \equiv_2 1, \\ \big\langle [y, x, \overset{i-3}{\ldots}, x, y], [y, x, \overset{i-1}{\ldots}, x]\big\rangle D_{i+1}(G_k) & \text{if } i \equiv_2 0, \end{cases}$$

with

$$D_i(G_k)/D_{i+1}(G_k) \cong \begin{cases} C_2 & \text{if } i \equiv_2 1 \text{ and } i < 2^k, \\ C_2 \times C_2 & \text{if } i \equiv_2 0 \text{ and } i < 2^k, \\ 1 & \text{if } i = 2^k+1, \\ C_2 & \text{if } i = 2^k+2. \end{cases}$$

whereas if $i = 2^l$ is a power of 2, equivalently if $l(i+1) = l+1$ for $l = l(i)$, then

$$D_i(G_k)/D_{i+1}(G_k) \cong \langle x^{2^l}\rangle/\langle x^{2^{l+1}}\rangle \times \langle y^{2^l}\rangle/\langle y^{2^{l+1}}\rangle \times \langle [y, x, \overset{i-3}{\ldots}, x, y]\rangle \gamma_i(G_k)/\gamma_{i+1}(G_k)$$

so that

$$\begin{aligned} D_1(G_k) &= \langle x, y\rangle D_2(G_k), \\ D_2(G_k) &= \langle x^2, y^2, [y, x]\rangle D_3(G_k), \\ D_i(G_k) &= \big\langle x^{2^l}, [y, x, \overset{i-3}{\ldots}, x, y], [y, x, \overset{i-1}{\ldots}, x]\big\rangle D_{i+1}(G_k) \end{aligned}$$

with

$$D_i(G_k)/D_{i+1}(G_k) \cong \begin{cases} C_2 \times C_2 & \text{if } i = 1, \text{ equivalently if } l = 0, \\ C_2 \times C_2 \times C_2 & \text{if } i = 2, \text{ equivalently if } l = 1, \\ C_2 \times C_2 \times C_2 & \text{if } i = 2^l \text{ with } 2 \le l \le k. \end{cases}$$

In particular, for $2^{k-1}+1 \le i \le 2^k$ and thus $l(i) = k$,

$$D_i(G_k) = G_k^{2^k} \gamma_i(G_k) = \langle x^{2^k}, [y, x, \overset{2^k-3}{\ldots}, x, y]\rangle \gamma_i(G_k),$$

so that

$$\log_2|D_i(G_k)| = \log_2|\gamma_i(G_k)| + 1.$$

Lastly, the Frattini series of G_k has the corresponding form, though it has length $k+1$.

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INVARIANT CONNECTIONS AND PBW THEOREM FOR LIE GROUPOID PAIRS

CAMILLE LAURENT-GENGOUX AND YANNICK VOGLAIRE

Given a closed wide Lie subgroupoid A of a Lie groupoid L, i.e., a Lie groupoid pair, we interpret the associated Atiyah class as the obstruction to the existence of L-invariant fibrewise affine connections on the homogeneous space L/A. For Lie groupoid pairs with vanishing Atiyah class, we show that the left A-action on the quotient space L/A can be linearized.

In addition to giving an alternative proof of a result of Calaque about the Poincaré–Birkhoff–Witt map for Lie algebroid pairs with vanishing Atiyah class, this result specializes to a necessary and sufficient condition for the linearization of dressing actions, and gives a clear interpretation of the Molino class as an obstruction to simultaneous linearization of all the monodromies.

We also develop a general theory of connections on Lie groupoid equivariant principal bundles.

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1. Introduction

Invariant connections form an important tool for the study of homogeneous spaces, and their study goes back to the work of É. Cartan on Lie groups. Generalizing the

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canonical invariant connection on a symmetric space, Nomizu [1954] studied the existence of invariant connections on reductive homogeneous spaces. Around 1960, Nguyen Van Hai [1964], Vinberg [1960] and Wang [1958] independently characterized the set of G-invariant affine connections on a not necessarily reductive homogeneous space G/H, and computed necessary and sufficient conditions for their existence. In the connected case, the obstruction was given a cohomological meaning in [Hai 1965] as an element in the first Lie algebra cohomology $H^1(\mathfrak{h}, \mathrm{Hom}(\mathfrak{g}/\mathfrak{h} \otimes \mathfrak{g}/\mathfrak{h}, \mathfrak{g}/\mathfrak{h}))$. Recently, this class was rediscovered by Calaque, Căldăraru and Tu [Calaque et al. 2013] and shown to be the obstruction to a Poincaré–Birkhoff–Witt-type theorem for inclusions of Lie algebras. Bordemann [2012] realized and explained the link between the two approaches and gave a geometric interpretation of the PBW theorem using invariant connections.

In this paper, we explore some aspects of the scarcely studied class of homogeneous spaces of Lie groupoids; see [Liu et al. 1998, Section 8] and [Moerdijk and Mrčun 2006, Section 3]. This research was triggered by recent papers of Chen, Stiénon and Xu [Chen et al. 2016], who generalize Atiyah classes [Atiyah 1957] to inclusions of Lie algebroids, and of Calaque [2014], who generalizes the PBW-type theorem to that case as well. One of our intents is to reprove geometrically the latter theorem. We develop along the way the study of invariant connections on homogeneous spaces of Lie groupoids and on equivariant principal groupoid bundles.

A related study, with a somewhat different point of view, was carried out in [Laurent-Gengoux et al. 2014]: while obviously its authors mostly focus on the case of nonvanishing Atiyah class, they also consider the vanishing case, where the corresponding Kapranov dg-manifold is shown to be *linearizable*. This means that it can be represented by an L_∞-algebra structure that only admits a 1-ary bracket while all higher brackets vanish, including the bilinear bracket. As a Kapranov dg-manifold, or as an L_∞-algebra, it is therefore of limited interest, but the fact that it is trivial has interesting consequences. The authors interpret it geometrically as meaning that the natural left A-action on $\boldsymbol{L}/\boldsymbol{A}$ (with $\boldsymbol{L}$ and $\boldsymbol{A}$ local Lie groupoids integrating L and A, respectively) is formally linearizable. They recover as a corollary an interpretation of this vanishing found in [Calaque 2014] in terms of equivariance of the Poincaré–Birkhoff–Witt map. In this paper, we clarify this geometric interpretation, consider the Lie groupoid $\boldsymbol{A}$-action instead of the infinitesimal A-action and replace "formal" by "semilocal". Semilocal meaning here "in a neighborhood of the zero section", i.e., in a neighborhood of the common base manifold M of both $\boldsymbol{L}$ and $\boldsymbol{A}$.

Our main tool in this article will be Lie groupoid pairs, i.e., pairs $(\boldsymbol{L}, \boldsymbol{A})$ with $\boldsymbol{L}$ a Lie groupoid and $\boldsymbol{A} \subset \boldsymbol{L}$ a closed Lie subgroupoid over the same manifold M, or their local counterparts. As mentioned above, their infinitesimal counterparts have been recently studied [Chen et al. 2016; Laurent-Gengoux et al. 2014] under the name of Lie algebroid pairs, which are pairs (L, A) made of a Lie algebroid L together with a Lie subalgebroid A over the same base. In the transitive case, the latter were already studied, although for other reasons, by Kubarski et al. in [Balcerzak et al. 2001; Kubarski 1998]. Lie algebroid pairs provide an efficient manner to unify various branches of differential geometry where (regular) *transverse* structures appear, as can be seen from the following list of examples:

(1) *Lie subalgebras*. Let $\mathfrak{g}$ be a Lie algebra. For any Lie subalgebra $\mathfrak{h}$ of $\mathfrak{g}$, the pair $(\mathfrak{g}, \mathfrak{h})$ is a Lie algebroid pair.

(2) *Foliations*. Let $L = TM$ be the tangent bundle Lie algebroid of a manifold M. For any integrable distribution $A \subset TM$, i.e., any foliation on the manifold M, the pair (L, A) is a Lie algebroid pair.

(3) *Noncommutative integrable systems*. Let $L = T^*M$ be the cotangent algebroid of a Poisson manifold (M, π); see [Crainic and Fernandes 2004]. Consider a coisotropic foliation on M, i.e., a foliation whose leaves are all coisotropic submanifolds. Covectors vanishing on the tangent space of the coisotropic foliation form a Lie subalgebroid A of L, and the pair (L, A) is a Lie algebroid pair. In particular, the coisotropic foliation can be chosen to be a regular integrable system (in the sense of [Laurent-Gengoux et al. 2013, Chapter 12]) or a noncommutative integrable system in the sense of [Fernandes et al. 2018].

(4) *Manifolds with a Lie algebra action*. If M is a manifold with an action of a Lie algebra $\mathfrak{g}$, one can build a matched pair [Mokri 1997] of Lie algebroids $L = TM \times (\mathfrak{g} \ltimes M)$ where $\mathfrak{g} \ltimes M$ is the action Lie algebroid. Taking A to be this action Lie algebroid yields a Lie algebroid pair (L, A).

(5) *Poisson manifolds with a Poisson $\mathfrak{g}$-action*. If P is a Poisson manifold with a Poisson $\mathfrak{g}$-action, Lu [1997] defines a matched pair of Lie algebroids $L = T^*P \times (\mathfrak{g} \ltimes P)$. Taking A to be the action Lie algebroid yields a Lie algebroid pair (L, A).

(6) Enlarging the setting from real Lie algebroids to complex Lie algebroids [Weinstein 2007], one could add *complex manifolds* among the examples, since an almost complex structure J on a smooth manifold X is complex if and only if $(T_{\mathbb{C}}X, T^{0,1}X)$ is a Lie algebroid pair [Laurent-Gengoux et al. 2008].

There is a canonical, Bott-type, A-module structure on L/A which is fundamental for the study of the transverse geometry of L with respect to A. To the best of our knowledge, it was first considered for a general Lie algebroid pair in [Crainic 2003, Example 4], and extensively studied in [Chen et al. 2016]. For foliations, this A-module structure is the Bott connection, while for Lie algebras, it is simply the A-action on L/A induced by the adjoint action. When L is the double of a Lie bialgebra A, then $L/A \simeq A^*$ with the A-module structure defined by the coadjoint action.

As in Wang's original work [1958], we prove our results first in the context of principal bundles. To this end, we introduce a notion of equivariant principal bundle of Lie groupoids (see Definition 3.12). Such bundles include generalized morphisms as particular examples, but we are mostly interested in those which are not of that kind. It turns out that, just like generalized morphisms, equivariant principal bundles may be seen as "morphisms" between Lie groupoids, whose composition is associative up to biequivariant diffeomorphisms (see Proposition 3.13).

For a vector bundle E and an equivariant principal bundle P with structure groupoid the frame groupoid $\boldsymbol{GL}(E)$, we first extend to this context the equivalence between connection 1-forms on P and connections on the associated bundle $P(E)$ (see Theorem 3.30). We then establish, for equivariant principal bundles over a homogeneous space $\boldsymbol{L}/\boldsymbol{A}$, an equivalence between fibered connection 1-forms and some Lie algebroid connections (see Theorem 5.1). Combining these two results, we arrive at a characterization of invariant connections on vector bundles over homogeneous spaces of Lie groupoids (see Theorems 5.2). As a special case, we obtain the following generalization of Wang's theorem (see Theorem 5.3):

Theorem. *Let $(\boldsymbol{L}, \boldsymbol{A})$ be a Lie groupoid pair over M, with Lie algebroid pair (L, A). There is a bijective correspondence between*

(1) *$\boldsymbol{A}$-compatible L-connections on L/A, and*

(2) *$\boldsymbol{L}$-invariant fibrewise affine connections on $\boldsymbol{L}/\boldsymbol{A} \to M$.*

Given a Lie groupoid pair $(\boldsymbol{L}, \boldsymbol{A})$ over M and an $\boldsymbol{A}$-module E, the obstruction to the existence of an invariant connection on the associated vector bundle

$$\frac{\boldsymbol{L} \times_M E}{\boldsymbol{A}}$$

is a class $\alpha_{(\boldsymbol{L},\boldsymbol{A}),E}$ in the degree 1 Lie groupoid cohomology of $\boldsymbol{A}$, that we call the *Atiyah class* of the $\boldsymbol{A}$-module E with respect to the Lie groupoid pair $(\boldsymbol{L}, \boldsymbol{A})$. We relate it to the Atiyah class of E with respect to the Lie algebroid pair (L, A) as introduced in [Chen et al. 2016] (see Proposition 4.14). We also show its invariance with respect to Morita equivalence of pairs of Lie groupoids (see Theorem 4.16). The quotient bundle L/A is naturally an $\boldsymbol{A}$-module, and its Atiyah class is called the Atiyah class of the Lie pair $(\boldsymbol{L}, \boldsymbol{A})$.

It should be noted that, although we characterize the connection forms on $\boldsymbol{L}$-equivariant principal $\boldsymbol{U}$-bundles P over a homogeneous space $\boldsymbol{L}/\boldsymbol{A}$ for all Lie pairs $(\boldsymbol{L}, \boldsymbol{A})$ and all Lie groupoids $\boldsymbol{U}$ (see Definition 3.12 and Theorem 5.1), we only obtain a cohomological obstruction to their existence for *transitive* $\boldsymbol{U}$ (see Proposition 4.9). Indeed, in that case, the obstruction lies in $H^1(\boldsymbol{A}, (L/A)^* \otimes P(U_0))$ where U_0 is the isotropy subalgebroid of the Lie algebroid U of $\boldsymbol{U}$. In order to make sense of this obstruction in the general case, we would need to work in the context of representations up to homotopy, which we reserve for later work.

Provided that the Atiyah class of $(\boldsymbol{L}, \boldsymbol{A})$ is zero, we construct successively:

(1) An $\boldsymbol{L}$-invariant fibrewise affine connection on the fibered manifold $\boldsymbol{L}/\boldsymbol{A} \to M$.

(2) An $\boldsymbol{A}$-equivariant exponential map from L/A to $\boldsymbol{L}/\boldsymbol{A}$, which is well defined in a neighborhood of the zero section $\iota : M \to L/A$ and a diffeomorphism onto its image (see Theorem 6.1).

(3) An $\boldsymbol{A}$-equivariant Poincaré–Birkhoff–Witt isomorphism from $\Gamma(S(L/A))$ to $U(L)/U(L)\cdot\Gamma(A)$ (see Theorem 6.6).

The exponential map above is indeed the exponential of the connection announced in the first item, and its infinitesimal jet is the Poincaré–Birkhoff–Witt isomorphism. The Poincaré–Birkhoff–Witt isomorphism that we eventually obtain gives an alternative proof of Theorem 1.1 in [Calaque 2014], valid under the assumption that the Lie algebroid pair (L, A) integrates to a Lie groupoid pair $(\boldsymbol{L}, \boldsymbol{A})$:[1]

Theorem. *The Atiyah class of a Lie groupoid pair* $(\boldsymbol{L}, \boldsymbol{A})$ *vanishes if and only if there exists a* $\mathrm{Bis}(\boldsymbol{A})$*-equivariant filtered coalgebra isomorphism from* $\Gamma(S(L/A))$ *to* $U(L)/U(L)\cdot\Gamma(A)$.

The latter theorem specializes to give a cohomological interpretation of the linearization of dressing actions (see Corollary 8.4) and an interesting result about monodromies of foliations (see Theorem 8.15) that we quote here.

Theorem. *Let $\mathcal{F}$ be a regular foliation on a manifold M. The Atiyah class of the Lie algebroid pair $(TM, T\mathcal{F})$ vanishes if and only if all the monodromies are simultaneously linearizable.*

The paper is structured as follows. In Section 2, we recall basic facts about Lie groupoids and Lie algebroids. In Section 3, we review generalized morphisms of Lie groupoids, before introducing equivariant principal bundles and associated vector bundles. We describe an action of the tangent groupoid to a Lie groupoid on the anchor map of its Lie algebroid that plays for us the role of an adjoint action. In Section 4, we show that L/A is an $\boldsymbol{A}$-module, introduce the Atiyah classes of generalized morphisms and of $\boldsymbol{A}$-modules, and prove their Morita invariance. In Section 5, we prove our main results about connections on homogeneous spaces of Lie groupoids. In Section 6, we use invariant connections to prove a Poincaré–Birkhoff–Witt theorem. In Section 7, we investigate how our results can be adapted to local Lie groupoid pairs in order to drop some integrability conditions. In Section 8, we work out applications to Lie groups and foliations.

[1] We also have a version with local Lie groupoids which allows us to drop the integrability condition; see Theorem 7.4.

2. Preliminaries

This section recalls classical notions for Lie groupoids, and fixes our notation and conventions: most facts are basic, but are quite dispersed in the literature. We investigate in particular bisections, and introduce the very convenient operation $\star$ that we insist to be a convenient and pedagogical manner to deal with those objects, in particular when one has to see bisections as the group integrating sections of the Lie algebroids. We also introduce the operator κ that shall play a crucial rôle in the proofs, and that we invite the reader to understand as a formalization of the adjoint action of bisections on sections of the Lie algebroid.

Let us state some general conventions about vector bundles. Projections from vector bundles to their base manifold will be denoted by the letter q, with the total space added as a subscript, as in $q_E : E \to M$, if necessary. For E a vector bundle over a manifold M, we shall denote by $\Gamma(E)$ the space of global smooth sections of E and by $\Gamma_{\mathcal{U}}(E)$ the space of smooth sections over an open subset $\mathcal{U} \subset M$. The fiber at a particular point $x \in M$ shall be denoted by E_x. For all $e \in \Gamma(E)$, $e_x \in E_x$ stands for the evaluation at $x \in M$ of the section e. We may also use the notation $e|_x$. For $\epsilon \in E_x$, a section $e \in \Gamma(E)$ is said to be *through* ϵ if $e_x = \epsilon$. For $\phi : N \to M$ a smooth map, we denote by $\phi^* E$ the pullback of E through ϕ, i.e., the fibered product

$$\phi^* E = N \times_M^{\phi, q} E = \{(y, \epsilon) \in N \times E \mid \phi(y) = q(\epsilon)\}.$$

It is a vector bundle over N, with projection $q(y, \epsilon) = y$. For every section $e \in \Gamma(E)$, the pullback of e through ϕ is the section denoted by $\phi^* e$ and defined by $(\phi^* e)_y = (y, e_{\phi(y)})$ for all $y \in N$.

2A. ***Lie groupoids.*** A *groupoid* is a small category in which every morphism is invertible. The morphisms of a groupoid are called the arrows, and the objects are called the units. The *structure maps* of a groupoid are the source and target maps associating to an arrow its source and target objects respectively, the unit map associating to an object the unit arrow from that object to itself, the inversion sending each arrow to its inverse, and the multiplication sending two composable arrows to their composition. A *Lie groupoid* is a groupoid where the set $\boldsymbol{L}$ of arrows and the set M of objects are smooth manifolds, all structure maps are smooth and the source and target maps are surjective submersions; see [Cannas da Silva and Weinstein 1999; Mackenzie 2005]. The manifold M of objects shall be referred to as the *unit manifold*. The unit map can be shown to be a closed embedding, and the unit manifold shall actually be considered as an embedded submanifold of $\boldsymbol{L}$. We will often identify the Lie groupoid with its manifold of arrows and talk about "a Lie groupoid $\boldsymbol{L}$ over a manifold M", written as $\boldsymbol{L} \rightrightarrows M$. For all the groupoids considered, the source map shall be denoted by $\boldsymbol{s}$, the target map by $\boldsymbol{t}$, the unit map by $\mathbf{1}$, the inverse map by $\boldsymbol{i}$, and the multiplication by a dot. The convention in this paper shall be that the product $\gamma_1 \cdot \gamma_2$ of two elements $\gamma_1, \gamma_2 \in \boldsymbol{L}$ is defined if and only if $\boldsymbol{s}(\gamma_1) = \boldsymbol{t}(\gamma_2)$.

A *Lie groupoid morphism* from a Lie groupoid $\boldsymbol{L}$ over M to a Lie groupoid $\boldsymbol{U}$ over N is a pair of smooth maps $\varphi : \boldsymbol{L} \to \boldsymbol{U}$ and $\varphi_0 : M \to N$ such that $\boldsymbol{s} \circ \varphi = \varphi_0 \circ \boldsymbol{s}$, $\boldsymbol{t} \circ \varphi = \varphi_0 \circ \boldsymbol{t}$, and $\varphi(\gamma_1 \cdot \gamma_2) = \varphi(\gamma_1) \cdot \varphi(\gamma_2)$ for all composable $\gamma_1, \gamma_2 \in \boldsymbol{L}$.

Example 2.1. The frame groupoid $\boldsymbol{GL}(E)$ of a vector bundle E over a manifold M is the Lie groupoid whose unit manifold is M and whose set of arrows between two arbitrary points $x, y \in M$ is made of all invertible linear maps from E_x to E_y. The source of such arrows is x and their target is y.

Modules. For a Lie groupoid $\boldsymbol{L}$ over a manifold M, a (left) $\boldsymbol{L}$*-module* is a vector bundle E over M equipped with a Lie groupoid morphism from $\boldsymbol{L}$ to $\boldsymbol{GL}(E)$. It is often convenient to see it as an assignment

$$\boldsymbol{L} \times_M^{\boldsymbol{s},q} E \to E : (\gamma, e) \mapsto \gamma \cdot e \tag{1}$$

satisfying the usual axioms of a left action; see [Mackenzie 2005].

Let us denote by $\boldsymbol{L}_n$ the manifold of all n-tuples $(\gamma_1, \dots, \gamma_n) \in \boldsymbol{L}^n$ such that the product of any two successive elements is defined, i.e., such that $\boldsymbol{s}(\gamma_i) = \boldsymbol{t}(\gamma_{i+1})$ for all $i = 1, \dots, n-1$. The *Lie groupoid cohomology* [Crainic 2003] of an $\boldsymbol{L}$-module E is the cohomology $H^\bullet(\boldsymbol{L}, E)$ of the complex

$$C^0(\boldsymbol{L}, E) \xrightarrow{\partial_0} C^1(\boldsymbol{L}, E) \xrightarrow{\partial_1} C^2(\boldsymbol{L}, E) \xrightarrow{\partial_2} C^3(\boldsymbol{L}, E) \xrightarrow{\partial_3} \cdots, \tag{2}$$

where

(1) $C^0(\boldsymbol{L}, E)$ is the space $\Gamma(E)$ of sections of E;

(2) for all $n \in \mathbb{N}_*$, $C^n(\boldsymbol{L}, E)$ is the space[2] of smooth functions F from $\boldsymbol{L}_n$ to E such that $F(\gamma_1, \dots, \gamma_n) \in E_{\boldsymbol{t}(\gamma_1)}$ for all $(\gamma_1, \dots, \gamma_n) \in \boldsymbol{L}_n$;

(3) for all $e \in \Gamma(E)$, $\partial_0 e$ is the element of $C^1(\boldsymbol{L}, E)$ defined by
$$\partial_0 e(\gamma) = \gamma \cdot e_{\boldsymbol{s}(\gamma)} - e_{\boldsymbol{t}(\gamma)}$$
for all $\gamma \in \boldsymbol{L}_1 = \boldsymbol{L}$;

(4) for all $n \in \mathbb{N}$ and all $F \in C^n(\boldsymbol{L}, E)$, $\partial_n F$ is the element of $C^{n+1}(\boldsymbol{L}, E)$ defined by

$$\partial_n F(\gamma_0, \dots, \gamma_n) = \gamma_0 \cdot F(\gamma_1, \dots, \gamma_{n-1}) - \sum_{i=0}^{n-1} (-1)^i F(\gamma_0, \dots, \gamma_i \cdot \gamma_{i+1}, \dots, \gamma_n) \\ - (-1)^n F(\gamma_0, \dots, \gamma_{n-1})$$

for all $(\gamma_0, \dots, \gamma_n) \in \boldsymbol{L}_{n+1}$.

[2] The space $C^n(\boldsymbol{L}, E)$ can also be described as the space of sections of the vector bundle $\boldsymbol{t}^* E \to \boldsymbol{L}_n$ where $\boldsymbol{t} : \boldsymbol{L}_n \to M$ stands for the map $(\gamma_1, \dots, \gamma_n) \mapsto \boldsymbol{t}(\gamma_1)$.

Since we will mostly be interested in the first cohomology space $H^1(\boldsymbol{L}, E)$, it is worth describing it more explicitly. On the one hand, 1-cocycles are functions F from $\boldsymbol{L}$ to E such that $F(\gamma) \in E_{\boldsymbol{t}(\gamma)}$ for all $\gamma \in \boldsymbol{L}$ and satisfying the *cocycle identity*

$$F(\gamma_1 \cdot \gamma_2) = \gamma_1 \cdot F(\gamma_2) + F(\gamma_1) \tag{3}$$

for all γ_1, γ_2 in $\boldsymbol{L}$. On the other hand, 1-coboundaries are E-valued functions on $\boldsymbol{L}$ of the form

$$F(\gamma) = \gamma \cdot e_{\boldsymbol{s}(\gamma)} - e_{\boldsymbol{t}(\gamma)} \tag{4}$$

for some section $e \in \Gamma(E)$.

Subgroupoids. A *Lie subgroupoid* of a Lie groupoid $\boldsymbol{L} \rightrightarrows M$ is a Lie groupoid $\boldsymbol{A} \rightrightarrows N$ together with a Lie groupoid morphism (φ, φ_0) from $\boldsymbol{A}$ to $\boldsymbol{L}$ such that both φ and φ_0 are injective immersions. A Lie subgroupoid $\boldsymbol{A}$ is said to be *wide* if its unit manifold is M and $\varphi_0 = \mathrm{id}$. A wide Lie subgroupoid is said to be *closed* if the inclusion $\varphi : \boldsymbol{A} \to \boldsymbol{L}$ is a closed embedding.

Definition 2.2. A *Lie groupoid pair* is a pair $(\boldsymbol{L}, \boldsymbol{A})$ with $\boldsymbol{L}$ a Lie groupoid and $\boldsymbol{A}$ a closed wide Lie subgroupoid of $\boldsymbol{L}$.

For $\boldsymbol{A}$ a closed wide subgroupoid of $\boldsymbol{L}$, the quotient space $\boldsymbol{L}/\boldsymbol{A}$ is a (Hausdorff) manifold that fibers over M through a surjective submersion $\underline{\boldsymbol{t}}$ (see [Moerdijk and Mrčun 2006, Section 3]) defined as the unique map making the following diagram commutative:

(5)
$$\begin{tikzcd} & \boldsymbol{L} \arrow[dl, "\boldsymbol{t}"'] \arrow[d, "\pi"] \\ M & \boldsymbol{L}/\boldsymbol{A} \arrow[l, dotted, "\underline{\boldsymbol{t}}"] \end{tikzcd}$$

Projections to quotients by a group(oid) action will generally be denoted by the letter π. The source will be added as a subscript, as in $\pi_P : P \to P/\boldsymbol{U}$, when a risk of confusion exists.

The quotient $\boldsymbol{L}/\boldsymbol{A}$ is a *homogeneous space* of $\boldsymbol{L}$ in the following sense [Liu et al. 1998]: it is a smooth manifold X with a map to M such that there exists a smooth section $\sigma : M \to X$ with $\boldsymbol{L} \cdot \sigma(M) = X$. Given such data, the *stabilizer* of σ is the closed subgroupoid $\boldsymbol{A}$ of $\boldsymbol{L}$ that sends $\sigma(M)$ to itself, and this yields an equivariant diffeomorphism $X \cong \boldsymbol{L}/\boldsymbol{A}$.

Pullbacks. Let $\boldsymbol{L} \rightrightarrows M$ be a groupoid and $\phi : N \to M$ a map. Consider the *anchor* $\rho : \boldsymbol{L} \to M \times M : \gamma \mapsto (\boldsymbol{t}(\gamma), \boldsymbol{s}(\gamma))$ of $\boldsymbol{L}$. The *pullback* $\phi^! \boldsymbol{L}$ of $\boldsymbol{L}$ by ϕ is, as a set, the pullback of the anchor by $\phi \times \phi$:

(6)
$$\begin{tikzcd} \phi^! \boldsymbol{L} \arrow[r] \arrow[d] & \boldsymbol{L} \arrow[d, "\rho"] \\ N \times N \arrow[r, "\phi \times \phi"'] & M \times M \end{tikzcd}$$

Explicitly, we set $\phi^! \boldsymbol{L} = N \times_M^{\phi,\boldsymbol{t}} \boldsymbol{L} \times_M^{\boldsymbol{s},\phi} N$. The structure maps $\boldsymbol{s}(y, \gamma, x) = x$, $\boldsymbol{t}(y, \gamma, x) = y$ and multiplication

$$(z, \gamma, y) \cdot (y, \gamma', x) = (z, \gamma \cdot \gamma', x)$$

on $\phi^! \boldsymbol{L}$ make (6) a commutative diagram of groupoid morphisms, with left arrow the anchor of $\phi^! \boldsymbol{L}$ and top arrow the projection on the second component.

When $\boldsymbol{L}$ is a Lie groupoid, we require ϕ to be a smooth map such that

$$\boldsymbol{t} \circ \mathrm{pr}_1 : \boldsymbol{L} \times_M^{\boldsymbol{s},\phi} N \to M \tag{7}$$

is a surjective submersion. In that case, $\phi^! \boldsymbol{L}$ becomes a Lie groupoid such that (6) is a commutative diagram of Lie groupoid morphisms with the appropriate universal property.

Tangent groupoid. The tangent bundle $T\boldsymbol{L}$ of a Lie groupoid $\boldsymbol{L}$ over M canonically becomes a Lie groupoid over TM by applying the tangent functor to all the structure maps (see [Mackenzie 2005], or [Courant 1994] for its infinitesimal counterpart). In what follows, we will denote the groupoid multiplication in $T\boldsymbol{L}$ by

$$u \bullet u' = T_{(\gamma,\gamma')}\, \mathrm{m}(u, u'), \tag{8}$$

for all $u \in T_\gamma \boldsymbol{L}$, $u' \in T_{\gamma'} \boldsymbol{L}$, where m denotes the multiplication in $\boldsymbol{L}$. We will denote by u^{-1} the inverse $T\boldsymbol{i}(u)$, and by 0_γ the zero vector at γ.

2B. *Lie algebroids.* A *Lie algebroid* is a vector bundle L over a smooth manifold M together with a Lie bracket $[\,\cdot\,,\cdot\,]$ on the space $\Gamma(L)$ of global sections of L and a bundle map $\rho : L \to TM$ called the *anchor map*, related by the Leibniz rule

$$[l_1, f l_2] = f[l_1, l_2] + \rho(l_1)(f) l_2 \tag{9}$$

for all $l_1, l_2 \in \Gamma(L)$ and $f \in C^\infty(M)$. All vector bundles will be real in this paper, and we shall use the letter ρ, with the Lie algebroid as subscript if necessary, for the anchor map and $[\,\cdot\,,\cdot\,]$ for the Lie bracket of all the Lie algebroids that we consider. We refer to [Mackenzie 2005] for the general theory of Lie algebroids.

A *base-preserving Lie algebroid morphism* from $L \to M$ to $U \to M$ is a bundle map $\phi : L \to U$ covering the identity of M, such that $\rho_L = \rho_U \circ \phi$ and $[\phi(l_1), \phi(l_2)] - \phi[l_1, l_2] = 0$ for all $l_1, l_2 \in \Gamma(L)$ (see below for more on the first condition). A (*wide*) *Lie subalgebroid* of a Lie algebroid $L \to M$ is an injective base-preserving morphism $A \to L$.

We recall [Moerdijk and Mrčun 2003; Huebschmann 2004] that the universal enveloping algebra of a Lie algebroid L is constructed by taking the quotient of the augmentation ideal of the universal enveloping algebra of the semidirect product Lie algebra $\Gamma(L) \ltimes_\rho C^\infty(M)$ by the relations $f \cdot l = fl$, and $f \cdot g = fg$ for all $f, g \in C^\infty(M)$ and $l \in \Gamma(L)$. It is a coalgebra, and, for $A \subset L$ a Lie subalgebroid, $U(L)/U(L)\cdot\Gamma(A)$ inherits a coalgebra structure [Calaque 2014].

Every Lie groupoid $\boldsymbol{L}$ with unit manifold M admits a Lie algebroid $L \to M$. In the present article, for all $x \in M$, L_x shall be defined as the kernel of $T_x\boldsymbol{s} : T_x\boldsymbol{L} \to T_xM$ (i.e., the tangent space at x to the $\boldsymbol{s}$-fiber over x), while the anchor map $\rho : L \to TM$ at x is the restriction to L_x of $T_x\boldsymbol{t} : T_x\boldsymbol{L} \to T_xM$. To every section $l \in \Gamma(L)$ there correspond two vector fields on $\boldsymbol{L}$, namely the *left-invariant vector field* $L(l)$, and the *right-invariant vector field* $R(l)$. The values of these vector fields at a generic element $\gamma \in \boldsymbol{L}$ with source x and target y are given by

$$L(l)|_\gamma = 0_\gamma \bullet (-l_x^{-1}) \quad \text{and} \quad R(l)|_\gamma = l_y \bullet 0_\gamma. \tag{10}$$

The sign convention is chosen so that, evaluated at a unit $x \in M$, the left- and right-invariant vector fields $L(l)|_x = -T_x\boldsymbol{i}(l_x)$ and $R(l)|_x = l_x$ project to the same element in the normal bundle $T_x\boldsymbol{L}/T_xM$. The commutator of two right-invariant vector fields is again right-invariant. Hence the sections of L acquire a Lie bracket by transporting the commutator of (right-invariant) vector fields through the isomorphism $l \mapsto R(l)$, completing the description of the Lie algebroid of a Lie groupoid.

Example 2.3. Let us describe the Lie algebroid of the frame groupoid $\boldsymbol{GL}(E)$ of a vector bundle E (Example 2.1). The $\boldsymbol{s}$-fiber at a point $x \in M$ is the manifold of all linear isomorphisms from E_x to E_y for all $y \in M$. Its tangent space at Id_{E_x} is the vector space of linear maps $X : E_x \to TE|_{E_x}$ which are sections of the canonical projection $TE|_{E_x} \to E_x$. In particular, for each such X there exists an element $X_M \in T_xM$ making the diagram

$$\begin{tikzcd} E_x \arrow[r, "X"] \arrow[d, "q"'] & TE|_{E_x} \arrow[d, "Tq"] \\ \{x\} \arrow[r] & \{X_M\} \end{tikzcd}$$

commute. The collection of these tangent spaces forms a vector bundle $T^{\mathrm{lin}}E$ whose sections are the *linear vector fields* $\mathfrak{X}^{\mathrm{lin}}(E)$, i.e., the bundle maps $E \to TE$ that are sections of the canonical projection bundle map $TE \to E$ over $TM \to M$. These vector fields are closed under the Lie bracket of vector fields and, together with the anchor map $X \mapsto X_M$, this gives $T^{\mathrm{lin}}E$ the structure of a Lie algebroid.

A common description of $T^{\mathrm{lin}}E = \mathrm{Lie}(\boldsymbol{GL}(E))$ is as the Lie algebroid $\mathcal{D}(E)$ whose sections are the *derivative endomorphisms* of E, i.e., the $\mathbb{R}$-linear endomorphisms D of $\Gamma(E)$ such that there exists a vector field D_M on M with

$$D(fe) = D_M(f)e + fD(e) \tag{11}$$

for all $e \in \Gamma(E)$ and $f \in C^\infty(M)$. The explicit correspondence between $\mathcal{D}(E)$

and $T^{\mathrm{lin}}E$ is as follows (see [Mackenzie 2005, Section 3.4] for more detail).

Any $D \in \Gamma(\mathcal{D}(E))$ yields a dual $D^* \in \Gamma(\mathcal{D}(E^*))$ such that

$$\langle D^*(\epsilon), e\rangle = D_M(\langle \epsilon, e\rangle) - \langle \epsilon, D(e)\rangle$$

for all $\epsilon \in \Gamma(E^*)$ and $e \in \Gamma(E)$. This D^* in turn induces a linear vector field $X \in \mathfrak{X}^{\mathrm{lin}}(E)$ defined by

$$X(l_\epsilon) = l_{D^*(\epsilon)}, \qquad X(q^* f) = q^*(D_M(f))$$

for all $\epsilon \in \Gamma(E^*)$ and $f \in C^\infty(M)$. Here, l_ϵ is the fibrewise-linear function on E corresponding to the section ϵ. We used the fact that linear vector fields are determined by their action on linear functions and on pullbacks of functions on the base, and that they preserve the latter two subspaces of functions. The association $D \mapsto X$ is $C^\infty(M)$-linear and induces a Lie algebroid isomorphism

$$\mathcal{L} : \mathcal{D}(E) \to T^{\mathrm{lin}}(E). \tag{12}$$

Pullbacks. The pullback $\phi^! U$ of a Lie algebroid $U \to N$ by a smooth map $\phi : M \to N$ is defined in a similar way to the Lie groupoid case; see, e.g., [Higgins and Mackenzie 1990]. As a set, it is the pullback of its anchor by $T\phi$:

$$\begin{tikzcd}
\phi^! U \arrow[r] \arrow[d] & U \arrow[d, "\rho"] \\
TM \arrow[r, "T\phi"'] & TN
\end{tikzcd}$$

To see when it is a vector bundle, it is best to replace the right-hand column in the above diagram by its pullback $\phi^* U \to \phi^* TN$ by ϕ, to get a diagram of vector bundles over M. Then $\phi^! U$ is a vector subbundle of $TM \oplus \phi^* U$ if and only if the bundle map $\psi : TM \oplus \phi^* U \to \phi^* TN : (X, u) \mapsto T\phi(X) - \rho(u)$ has constant rank. For simplicity, we require ψ to have maximal rank, i.e., we require $T\phi$ and ρ to be transverse, in which case the kernel of ψ,

$$\phi^! U = TM \times_{\phi^* TN} \phi^* U,$$

has rank

$$\mathrm{rk}(\phi^! U) = \mathrm{rk}(U) + \dim M - \dim N.$$

The vector bundle $\phi^! U$ then becomes a Lie algebroid with anchor map given by the first projection and Lie bracket defined by

$$\begin{aligned}\Big[(X, \sum_i f_i \phi^* u_i), (X', \sum_j f'_j \phi^* u'_j)\Big] \\ = \Big([X, X'], \sum_{i,j} (f_i f'_j \phi^*[u_i, u'_j] + f X(f')\phi^* u' - f' X'(f)\phi^* u)\Big)\end{aligned} \tag{13}$$

for all $X, X' \in \Gamma(TM)$, $f_i, f'_j \in C^\infty(M)$ and $u_i, u'_j \in \Gamma(U)$ such that $T\phi(X) = \sum_i f_i \phi^*(\rho(u_i))$ and $T\phi(X') = \sum_j f'_j \phi^*(\rho(u'_j))$.

When $\boldsymbol{U} \rightrightarrows N$ is a Lie groupoid and $\phi : M \to N$ a smooth map such that (7) is a surjective submersion, we have that $T\phi$ is transverse to ρ and there is a natural isomorphism $\phi^!(\mathrm{Lie}(\boldsymbol{U})) \cong \mathrm{Lie}(\phi^! \boldsymbol{U})$.

Morphisms not preserving the base. Consider two Lie algebroids $L \to M$ and $U \to N$ and a bundle map $\Phi : L \to U$ over $\phi : M \to N$. The pullback $\phi^! U$ is not a vector bundle for general ϕ, but the Lie bracket (13) on

$$\phi^! \Gamma(U) := \Gamma(TM) \times_{\Gamma(\phi^* TN)} \Gamma(\phi^* U)$$

always makes sense. Moreover, Φ always induces a base-preserving map $\Phi^* : L \to \phi^* U$ and thus a map of sections $\Phi^! = (\rho, \Phi^*) : \Gamma(L) \to \phi^! \Gamma(U)$. Hence, Φ is said to be a *Lie algebroid morphism* if

(1) it is *anchored*, i.e., it commutes with the anchors: $\rho_U \circ \Phi = T\phi \circ \rho_L$,

(2) the induced map $\Gamma(L) \to \phi^! \Gamma(U)$ is a Lie algebra morphism.

Connections. Let $L \to M$ be a Lie algebroid, and $E \to M$ a vector bundle. An *L-connection on E* is an $\mathbb{R}$-bilinear assignment

$$\Gamma(L) \times \Gamma(E) \to \Gamma(E) : (l, e) \mapsto \nabla_l e$$

which satisfies

$$\nabla_{fl} e = f \nabla_l e \quad \text{and} \quad \nabla_l (fe) = f \nabla_l e + \rho(l)(f) e$$

for all $f \in C^\infty(M)$, $l \in \Gamma(L)$, and $e \in \Gamma(E)$. An L-connection ∇ on E is said to be *flat* when

$$\nabla_{l_1} \nabla_{l_2} e - \nabla_{l_1} \nabla_{l_2} e = \nabla_{[l_1, l_2]} e$$

for all $l_1, l_2 \in \Gamma(L)$ and $e \in \Gamma(E)$. A vector bundle $E \to M$ equipped with a flat L-connection is said to be an *L-module*.

For each $l \in \Gamma(L)$, the map $\nabla_l : \Gamma(E) \to \Gamma(E)$ is a derivative endomorphism as in Example 2.3 (with associated vector field $\rho(l)$), and the assignment $l \mapsto \nabla_l$ is $C^\infty(M)$-linear. Hence, a connection ∇ can be recast (see [Kosmann-Schwarzbach and Mackenzie 2002]) as an anchored map $L \to \mathcal{D}(E)$. A connection is flat if and only if the corresponding anchored map is a Lie algebroid morphism.

The above is the "covariant derivative" picture. The corresponding horizontal lift is obtained by composing with the Lie algebroid isomorphism (12), to get an anchored map $L \to T^{\mathrm{lin}}(E)$. This horizontal lift point of view of anchored maps $L \to T^{\mathrm{lin}}(E)$, seen as maps $q_L^* E \to TE$, was extensively studied in [Fernandes 2002].

Replacing $\mathcal{D}(E)$ by any Lie algebroid U, not necessarily over the same base, we may consider anchored maps from L to U as generalized connections. Anchored maps have been used by many authors, and their use in Lie algebroid theory goes back at least to [Balcerzak et al. 2001]. The *curvature* of an anchored map ∇ from L to U is the bundle map $R^\nabla : L \wedge L \to r^*U$ defined on sections by

$$R^\nabla(l, l') = [\nabla^!(l), \nabla^!(l')] - \nabla^!([l, l']).$$

When U is regular, the curvature actually lands in r^*U_0, where U_0 is the isotropy subalgebroid of U, i.e., the kernel of its anchor map.

A *connection on a vector bundle* $E \to M$ is a TM-connection on E, i.e., an anchored map $TM \to \mathcal{D}(E)$. If the manifold M is fibered over another manifold N through a surjective submersion $f : M \to N$, a *fibered connection on* E is by definition a $T^f M$-connection on E, where $T^f M = \ker Tf \subset TM$. It is thus a smooth family of connections on the vector bundles $i_x^* E$, for $x \in N$, where $i_x : f^{-1}(x) \to M$ is the inclusion of the fiber over x.

An *affine connection* on a manifold M is a connection on the vector bundle TM, i.e., an anchored map $TM \to \mathcal{D}(TM)$. If the manifold M is fibered over N through a surjective submersion $f : M \to N$, a *fibrewise affine connection* is a $T^f M$-connection on $T^f M$. It is thus a smooth family of affine connections on the fibers of f.

2C. *Bisections.* An open submanifold Σ of $\boldsymbol{L}$ to which the restrictions of $\boldsymbol{s}$ and of $\boldsymbol{t}$ are both diffeomorphisms onto their respective images is called a *local bisection* of $\boldsymbol{L}$. The open subsets $\boldsymbol{t}(\Sigma)$ and $\boldsymbol{s}(\Sigma)$ are called the *target* and *source* of Σ respectively. When $\boldsymbol{t}(\Sigma) = \boldsymbol{s}(\Sigma) = M$, we speak of a *global bisection*. A local bisection is said to be *through an element* $\gamma \in \boldsymbol{A}$ when $\gamma \in \Sigma$, and to be *through an element* $u \in T_\gamma \boldsymbol{A}$ when $\gamma \in \Sigma$ and $u \in T_\gamma \Sigma$.

It is often convenient to see a local bisection Σ as a section of the target map, that we then denote by $\Sigma_{\boldsymbol{t}} : \boldsymbol{t}(\Sigma) \to \boldsymbol{L}$, or as a section of the source map, that we then denote by $\Sigma_{\boldsymbol{s}} : \boldsymbol{s}(\Sigma) \to \boldsymbol{L}$. A global bisection Σ induces a diffeomorphism of M denoted by $\underline{\Sigma}$ and defined by

$$\underline{\Sigma} := \boldsymbol{t} \circ \Sigma_{\boldsymbol{s}}. \tag{14}$$

For Σ a local bisection, (14) still makes sense as a diffeomorphism from the source to the target of Σ.

The composition of two local bisections $\Sigma', \Sigma \in \boldsymbol{L}$ is defined by

$$\Sigma' \star \Sigma := \{\gamma' \cdot \gamma \mid \gamma' \in \Sigma', \gamma \in \Sigma, \boldsymbol{s}(\gamma') = \boldsymbol{t}(\gamma)\}. \tag{15}$$

Global bisections form a group under $\star$, and the product of two local bisections is a local bisection. In the whole text, we simply write *bisection* when referring to a local bisection, since all constructions considered in this paper are local by nature. Local bisections only form a pseudogroup, that we denote by $\mathrm{Bis}(\boldsymbol{L})$. We shall often speak of inverses and products without mentioning that we only have a pseudogroup.

For E an $\boldsymbol{L}$-module, $e \in \Gamma(E)$ and Σ a local bisection, we again use the notation $\star$ and denote by $\Sigma \star e$ the local section of E of Σ given by

$$\Sigma \star e|_x := \Sigma_{\boldsymbol{t}}(x) \cdot e_{\underline{\Sigma}^{-1}(x)}$$

for all $x \in M$ where the right-hand side is defined. For any pair Σ', Σ of bisections, the relation $(\Sigma' \star \Sigma) \star e = \Sigma' \star (\Sigma \star e)$ holds, allowing us to erase the parentheses and to write simply $\Sigma' \star \Sigma \star e$ for such expressions.

The Lie algebra $\Gamma(L)$ is "the Lie algebra of the group of bisections". For example, for any smooth[3] 1-parameter family $\Sigma(t)$ of bisections, defined for t in a neighborhood of $0 \in \mathbb{R}$, and such that $\Sigma(0)$ is the unit manifold of $\boldsymbol{L}$, the map defined, for all $x \in M$, by

$$x \mapsto \frac{\mathrm{d}}{\mathrm{d}t} \Sigma(t)_{\boldsymbol{s}}(x) \bigg|_{t=0} \tag{16}$$

takes values in the kernel of the source map in $T_x \boldsymbol{L}$, i.e., is a section of the Lie algebroid L.

For any $\boldsymbol{L}$-module E, an L-module structure (i.e., a flat L-connection) on E is induced by

$$\nabla_l e = \frac{\mathrm{d}}{\mathrm{d}t} \Sigma(t)^{-1} \star e \bigg|_{t=0}, \tag{17}$$

for any smooth 1-parameter family $\Sigma(t)$ of local bisections with $l = \frac{\mathrm{d}}{\mathrm{d}t} \Sigma(t)_{\boldsymbol{s}}|_{t=0}$.

The group of bisections of a Lie groupoid $\boldsymbol{L}$ naturally acts by the adjoint action on the Lie algebra of sections of L,

$$\mathrm{Ad}_\Sigma\, l|_x := \frac{\mathrm{d}}{\mathrm{d}t} (\Sigma \star \Sigma(t) \star \Sigma^{-1})_{\boldsymbol{s}}(x) \bigg|_{t=0}, \tag{18}$$

where $\Sigma \in \mathrm{Bis}(\boldsymbol{L})$, $l \in \Gamma(L)$, and $\Sigma(t)$ is as in the previous paragraph.

Example 2.4. The bisections of the frame groupoid of a vector bundle E are the *automorphisms* of E, i.e., the diffeomorphisms $E \to E$ that send fibers to fibers linearly. The Lie algebra $\mathrm{Der}(E)$ of this infinite-dimensional Lie group is composed of the vector fields on E whose flows are by automorphisms of E, i.e., the linear vector fields $\mathfrak{X}^{\mathrm{lin}}(E) = \Gamma(T^{\mathrm{lin}}(E))$ of Example 2.3.

The action of $\mathrm{Bis}(\boldsymbol{GL}(E))$ on $\mathfrak{X}^{\mathrm{lin}}(E)$ is given by

$$\mathrm{Ad}_\phi X = T\phi \circ X \circ \phi^{-1} \tag{19}$$

for all $\phi \in \mathrm{Bis}(\boldsymbol{GL}(E))$ and $X \in \mathfrak{X}^{\mathrm{lin}}(E)$. When the base manifold is a point, this boils down to the action of $GL(V)$ on $\mathfrak{gl}(V)$ by matrix conjugation, $\mathrm{Ad}_g X = gXg^{-1}$, for a vector space V.

[3] A 1-parameter family of bisections is said to be smooth if the map $(x, t) \mapsto \Sigma(t)_{\boldsymbol{s}}(x)$ is smooth.

Since the group of bisections also acts on the smooth functions on M by $\Sigma \cdot f = \underline{\Sigma}^* f$ for all functions f and all bisections Σ, this action extends to $U(L)$ by coalgebra morphisms. Indeed, for all $\Sigma \in \mathrm{Bis}(\boldsymbol{L})$ and $u = l_1 \cdots l_k \in U(L)$, with $l_1, \ldots, l_k$ sections of L, we have an action

$$\Sigma \cdot u = \mathrm{Ad}_\Sigma\, l_1 \cdots \mathrm{Ad}_\Sigma\, l_k.$$

Moreover, for $(\boldsymbol{L}, \boldsymbol{A})$ a Lie groupoid pair, the group of bisections of $\boldsymbol{A}$, seen as a subgroup of the group of bisections of $\boldsymbol{L}$, acts on $U(L)/U(L)\cdot\Gamma(A)$ by coalgebra morphisms. The following proposition is easy to prove.

Proposition 2.5. *Let $(\boldsymbol{L}, \boldsymbol{A})$ be a Lie groupoid pair. Then the (pseudo-)group $\mathrm{Bis}(\boldsymbol{A})$ of bisections of $\boldsymbol{A}$ acts on $U(L)/U(L)\cdot\Gamma(A)$. The infinitesimal action of this action is simply left-multiplication by sections of A,*

$$a \cdot \bar{u} = \overline{a \cdot u}$$

for all $a \in \Gamma(A)$ and all $u \in U(L)$. Here, $u \mapsto \bar{u}$ is the projection from $U(L)$ to $U(L)/U(L)\cdot\Gamma(A)$.

Exponential map. Given a section $l \in \Gamma(L)$, for each $t \in \mathbb{R}$ and $\gamma \in \boldsymbol{L}$ for which is it defined, we denote by $\Phi_t(\gamma)$ the flow of the right-invariant vector field $R(l)$ starting from γ and evaluated at time t. Every point $m \in M$ admits a neighborhood $\mathcal{U}$ such that the submanifold $\Phi_t(\mathbf{1}(\mathcal{U}))$ is a local bisection of $\boldsymbol{L}$ for all t small enough. We denote by $t \to \exp(tl)$ this map, about which we recall three important properties.

Proposition 2.6 [Mackenzie 2005]. *Let $\boldsymbol{L}$ be a Lie groupoid with Lie algebroid L.*

(1) *For all $l \in \Gamma(L)$, and all t_1, t_2 such that $\exp(t_1 l)$, $\exp(t_2 l)$, and $\exp((t_1+t_2)l)$ exist, the identity*

$$\exp(t_1 l) \star \exp(t_2 l) = \exp((t_1+t_2)l)$$

holds.

(2) *For all $l \in \Gamma(L)$ and all local bisections Σ,*

$$\exp(\mathrm{Ad}_\Sigma\, l) = \Sigma \star \exp(l) \star \Sigma^{-1}. \tag{20}$$

(3) *For all $l, l' \in \Gamma(L)$,*

$$[l, l'] = \frac{d}{dt}\, \mathrm{Ad}_{\exp(-tl)}\, l' \Big|_{t=0}. \tag{21}$$

3. Equivariant principal bundles

3A. ***Generalized morphisms.*** In this section, we collect some facts about Lie groupoid generalized morphisms (see [Blohmann 2008] and references 15, 18, 19, 25 and 26 therein for more details). We then go on by introducing a Lie algebroid morphism κ related to the adjoint action that will be useful in the next sections.

We adopt the point of view of bibundles: a generalized morphism from $\boldsymbol{L}$ to $\boldsymbol{U}$ is a manifold with two commuting actions of $\boldsymbol{L}$ and $\boldsymbol{U}$ such that the $\boldsymbol{U}$-action is free and proper (i.e., principal) with orbit space the base of $\boldsymbol{L}$.

Definition 3.1. Let $\boldsymbol{L} \rightrightarrows M$ and $\boldsymbol{U} \rightrightarrows N$ be two Lie groupoids. A *generalized morphism from* $\boldsymbol{L}$ *to* $\boldsymbol{U}$ is a smooth manifold P with a left $\boldsymbol{L}$-action on a map $l : P \to M$ and a right $\boldsymbol{U}$-action on a map $r : P \to N$ such that

(1) the left and right actions commute,

(2) l is a surjective submersion,

(3) the map

$$P \times_N \boldsymbol{U} \to P \times_M P : (p, \upsilon) \mapsto (p, p \cdot \upsilon) \tag{22}$$

is a diffeomorphism.

The manifold P is called the manifold of arrows, and the maps l and r are called the left and right moment maps, respectively.

Note that both sides of the map (22) have a structure of Lie groupoid over P: the action groupoid for the right $\boldsymbol{U}$-action on P on the left-hand side (with source $\boldsymbol{s}(p, \upsilon) = p \cdot \upsilon$ and target $\boldsymbol{t}(p, \upsilon) = p$) and the Lie groupoid induced by the submersion $l : P \to M$ on the right-hand side (with source $\boldsymbol{s}(p, p') = p'$ and target $\boldsymbol{t}(p, p') = p$). With these structures, the map is actually a Lie groupoid morphism.

The second component

$$D_P : P \times_M P \to \boldsymbol{U} \tag{23}$$

of the inverse of (22) is called the *division map* of P. Since (22) and $\mathrm{pr}_2 : P \rtimes \boldsymbol{U} \to \boldsymbol{U}$ are Lie groupoid morphisms, the division map is also a Lie groupoid morphism. Moreover, it is $\boldsymbol{L}$*-invariant* and $\boldsymbol{U}$*-equivariant*, in the sense that

$$D_P(\gamma \cdot p, \gamma \cdot p') = D_P(p, p'), \tag{24}$$

$$D_P(p \cdot \upsilon, p' \cdot \upsilon') = \upsilon^{-1} \cdot D_P(p, p') \cdot \upsilon' \tag{25}$$

for all $p, p' \in P$ in the same l-fiber, $\gamma \in \boldsymbol{L}$ such that $\boldsymbol{s}(\gamma) = l(p)$, and $\upsilon, \upsilon' \in \boldsymbol{U}$ such that $r(p) = \boldsymbol{t}(\upsilon)$ and $r(p') = \boldsymbol{t}(\upsilon')$.

Generalized morphisms can be composed: if P is a generalized morphism from $\boldsymbol{L}$ to $\boldsymbol{U}$, and Q is a generalized morphism from $\boldsymbol{U}$ to $\boldsymbol{V}$, then $P \times_N Q$ is a smooth manifold thanks to condition (2) (here, N is the manifold of units of $\boldsymbol{U}$). Moreover, by condition (3) it has a proper and free (right) $\boldsymbol{U}$-action $((p, q), \upsilon) \mapsto (p \cdot \upsilon, \upsilon^{-1} \cdot q)$, so that the quotient $(P \times_N Q)/\boldsymbol{U}$ is a smooth manifold as well. The latter still has a free and fiber-transitive $\boldsymbol{V}$-action and is in fact a generalized morphism from $\boldsymbol{L}$ to $\boldsymbol{V}$, which we call the *composition* $P \circ Q$ of P and Q.

There is a natural notion of equivalence between generalized morphisms with same source and target Lie groupoids. An equivalence between two generalized morphisms P and P' from $\boldsymbol{L}$ to $\boldsymbol{U}$ is a smooth map $\phi : P \to P'$ which is *biequivariant*: it commutes with the left and right moment maps and with the left and right actions. Since the left moment maps are surjective submersions and the right actions are transitive on the l-fibers, such biequivariant maps are necessarily diffeomorphisms.

Example 3.2 (units). Any Lie groupoid $\boldsymbol{L} \rightrightarrows M$ defines a generalized morphism, the *unit generalized morphism* $\mathrm{Id}_{\boldsymbol{L}}$ from $\boldsymbol{L}$ to $\boldsymbol{L}$. Its manifold of arrows is $\boldsymbol{L}$, with the left and right multiplications as left and right actions, respectively. It is a unit for the composition of generalized morphisms, in the sense that if P is a generalized morphism from $\boldsymbol{L}$ to $\boldsymbol{U}$, then there are natural biequivariant diffeomorphisms $\mathrm{Id}_{\boldsymbol{L}} \circ P \simeq P$ and $P \circ \mathrm{Id}_{\boldsymbol{U}} \simeq P$ induced by the left and right actions, respectively.

Similarly, the composition of generalized morphisms is associative up to coherent biequivariant diffeomorphisms. More precisely, the above structures fit together to form a bicategory (see [Blohmann 2008, Proposition 2.12], for example).

Proposition 3.3. *The Lie groupoids with generalized morphisms as* 1*-morphisms and bi-equivariant maps as* 2*-morphisms form a bicategory.*

Example 3.4 (morphisms). Any Lie groupoid morphism φ from $\boldsymbol{L} \rightrightarrows M$ to $\boldsymbol{U} \rightrightarrows N$ defines a generalized morphism from $\boldsymbol{L}$ to $\boldsymbol{U}$ which, following [Blohmann 2008], will be called its *bundlization*. Its manifold of arrows is $P_\varphi = M \times_N^{\varphi_0, \boldsymbol{t}} \boldsymbol{U}$, the moment maps are $l(x, \upsilon) = x$ and $r(x, \upsilon) = \boldsymbol{s}(\upsilon)$, the left action is $\gamma \cdot (x, \upsilon) = (\gamma \cdot x, \varphi(\gamma) \cdot \upsilon)$, and the right action is $(x, \upsilon) \cdot \upsilon' = (x, \upsilon \cdot \upsilon')$.

Any manifold P with a left $\boldsymbol{L}$-action on a map l and a right $\boldsymbol{U}$-action on a map r, has an *opposite* manifold P^{op} with a left $\boldsymbol{U}$-action and a right $\boldsymbol{L}$-action. It is defined by $P^{\mathrm{op}} = P$, $l^{\mathrm{op}} = r$, $r^{\mathrm{op}} = l$, with left action $\upsilon \cdot_{\mathrm{op}} p = p \cdot \upsilon^{-1}$ and right action $p \cdot_{\mathrm{op}} \gamma = \gamma^{-1} \cdot p$. If P and P^{op} are both generalized morphisms, P is then *weakly invertible* in the sense that

$$P \circ P^{\mathrm{op}} \to \mathrm{Id}_{\boldsymbol{L}} : [(p, p')] \mapsto D_{P^{\mathrm{op}}}(p, p'), \tag{26}$$

$$P^{\mathrm{op}} \circ P \to \mathrm{Id}_{\boldsymbol{U}} : [(p, p')] \mapsto D_P(p, p') \tag{27}$$

are bi-equivariant diffeomorphisms. Such weakly invertible generalized morphisms are called *Morita morphisms*. Two Lie groupoids are called *Morita equivalent* if there exists a Morita morphism between them.

Some Lie groupoid morphisms, although not invertible themselves, have a weakly invertible bundlization, as shows the following basic example.

Example 3.5 (pullbacks). Consider the pullback $\varphi_0^! \boldsymbol{L}$ of a Lie groupoid $\boldsymbol{L} \rightrightarrows M$ by a surjective submersion $\varphi_0 : N \to M$, and consider the corresponding morphism $\varphi : \varphi_0^! \boldsymbol{L} \to \boldsymbol{L} : (x, \gamma, x') \mapsto \gamma$. Its bundlization is $P_\varphi = N \times_M \boldsymbol{L}$ with the actions described in Example 3.4. Now it is easy to see that $(P_\varphi)^{\mathrm{op}}$ is also a generalized morphism, with division map

$$D_{(P_\varphi)^{\mathrm{op}}}((x,\gamma),(x',\gamma')) = (x, \gamma\cdot{\gamma'}^{-1}, x').$$

More generally, it is sufficient that φ_0 be a smooth map such that $\boldsymbol{s}\circ\mathrm{pr}_2 : N\times_M \boldsymbol{L}\to M$ is a surjective submersion for the pullback groupoid to be a Lie groupoid and for the associated generalized morphism to be a Morita morphism from $\varphi_0^!\boldsymbol{L}$ to $\boldsymbol{L}$.

A generalized morphism P from $\boldsymbol{L}$ to $\boldsymbol{U}$ with moment maps l and r induces a morphism Φ_P from the pullback $l^!\boldsymbol{L}$ to $\boldsymbol{U}$ over r. This *induced morphism* is defined by

$$\Phi_P(p,\gamma,p') = D_P(p,\gamma\cdot p'), \tag{28}$$

where D_P is the division map of P, i.e., $\Phi_P(p,\gamma,p')$ is the unique $\upsilon\in\boldsymbol{U}$ such that $\gamma\cdot p' = p\cdot\upsilon$. Hence, a generalized morphism may be pictured as

$$\begin{tikzcd} & l^!\boldsymbol{L} \arrow[dl, "\mathrm{pr}_2"'] \arrow[d, shift left] \arrow[d, shift right] \arrow[dr, "\Phi_P"] & \\ \boldsymbol{L} \arrow[d, shift left] \arrow[d, shift right] & P \arrow[dl, "l"'] \arrow[dr, "r"] & \boldsymbol{U} \arrow[d, shift left] \arrow[d, shift right] \\ M & & N \end{tikzcd} \tag{29}$$

When P is a Morita morphism, r is also a surjective submersion and we may also pull back $\boldsymbol{U}$ to P. The morphism Φ_P then induces a base-preserving morphism

$$\tilde\Phi_P : l^!\boldsymbol{L}\to r^!\boldsymbol{U} \tag{30}$$

which is readily seen to be a diffeomorphism, with inverse $\tilde\Phi_{P^{\mathrm{op}}}$.

Example 3.6. Any global section $\sigma : M\to P$ of the left moment map l yields a Lie groupoid morphism $\varphi_\sigma : \boldsymbol{L}\to\boldsymbol{U}$ defined by

$$\varphi_\sigma(\gamma) = \Phi_P(\sigma(\boldsymbol{t}(\gamma)),\gamma,\sigma(\boldsymbol{s}(\gamma))),$$

and P is then bi-equivariantly diffeomorphic to the bundlization of φ_σ through the map $M\times_N\boldsymbol{U}\to P : (m,\upsilon)\mapsto\sigma(m)\cdot\upsilon$. Conversely, any bundlization has an obvious global section. Hence, l has a global section if and only if P is isomorphic to the bundlization of a Lie groupoid morphism.

Example 3.7 (induced morphism of units). The induced morphism $\Phi_{\mathrm{Id}_L} : \boldsymbol{t}^!\boldsymbol{L}\to\boldsymbol{L}$ (over $\boldsymbol{s}:\boldsymbol{L}\to M$) of a unit generalized morphism Id_L is

$$\Phi_{\mathrm{Id}_L} : \boldsymbol{L}\times_M^{\boldsymbol{t},\boldsymbol{t}}\boldsymbol{L}\times_M^{\boldsymbol{s},\boldsymbol{t}}\boldsymbol{L}\to\boldsymbol{L} : (\gamma_1,\gamma_2,\gamma_3)\mapsto\gamma_1^{-1}\cdot\gamma_2\cdot\gamma_3. \tag{31}$$

Example 3.8 (induced morphism of bundlizations). The induced morphism Φ_{P_φ} : $l^!\boldsymbol{L} \to \boldsymbol{U}$ (over $r : P_\varphi \to N$) of the bundlization $P_\varphi = M \times_N \boldsymbol{U}$ of a morphism $\varphi : \boldsymbol{L} \to \boldsymbol{U}$ as in Example 3.4 is

$$\Phi_{P_\varphi} = \Phi_{\mathrm{Id}_U} \circ \tilde{\varphi}, \tag{32}$$

where $\tilde{\varphi}$ is the Lie groupoid morphism from $l^!\boldsymbol{L} \rightrightarrows P_\varphi$ to $\boldsymbol{t}^!\boldsymbol{U} \rightrightarrows \boldsymbol{U}$ given by $((m, \upsilon), \gamma, (m', \upsilon')) \mapsto (\upsilon, \varphi(\gamma), \upsilon')$.

3B. *An adjoint action.* It is well known that representations of Lie groupoids in the sense of (1) are not general enough to include a natural notion of adjoint representation. Instead, representations up to homotopy [Arias Abad and Crainic 2013] or VB-groupoids [Gracia-Saz and Mehta 2017] are necessary. Here, we do not need a full-blown adjoint representation as, in the end, our Atiyah class lies in the cohomology with values in a usual module. As a computational replacement, the following $T\boldsymbol{L}$-action on the anchor $L \to TM$ will be sufficient. Although very much related, it should not be confused with the representation of the first jet bundle $J^1\boldsymbol{L}$ on the vector bundle $L \to M$ [Crainic and Fernandes 2005].

Consider the Lie algebroid morphism

$$\kappa = \mathrm{Lie}(\Phi_{\mathrm{Id}_L}) : \boldsymbol{t}^! L \to L, \tag{33}$$

over $\boldsymbol{s} : \boldsymbol{L} \to M$ corresponding to the Lie groupoid morphism of Example 3.7.

Lemma 3.9. *The Lie algebroid morphism κ reads*

$$\kappa(u, \lambda) = u^{-1} \bullet \lambda \bullet 0_\gamma \tag{34}$$

for all $(u, \lambda) \in (\boldsymbol{t}^! L)_\gamma$, $\gamma \in \boldsymbol{L}$.

Proof. Let $(\gamma^u(t), \gamma^\lambda(t), \gamma)$ be a path through $1_\gamma = (\gamma, 1_{\boldsymbol{t}(\gamma)}, \gamma)$ in $\boldsymbol{t}^!\boldsymbol{L}$, with $\gamma^u(t)$ (respectively, $\gamma^\lambda(t)$) tangent to u (respectively, λ) at 0. Then

$$\begin{aligned}\kappa(u, \lambda) &= \frac{d}{dt}\gamma^u(t)^{-1} \cdot \gamma^\lambda(t) \cdot \gamma\bigg|_{t=0} \\ &= u^{-1} \bullet \lambda \bullet 0_\gamma.\end{aligned}$$

□

As expected from its definition, κ is closely related to the (right) adjoint action of bisections on sections of the Lie algebroid.

Lemma 3.10. *Let Σ be a local bisection of the groupoid $\boldsymbol{L}$ and $l \in \Gamma(L)$ a section of its Lie algebroid L. For all $\gamma \in \Sigma$ with source x and target y, the value at $x \in M$ of the adjoint action of Σ on l depends only on l_y and on the unique tangent vector in $T_\gamma\Sigma$ that $T_\gamma \boldsymbol{t}$ maps to $\rho(l_y)$. Explicitly*:

$$(\mathrm{Ad}_{\Sigma^{-1}}\, l)_x = \kappa(u, l_y), \tag{35}$$

where $u = T\Sigma_{\boldsymbol{t}}(\rho(l_y))$.

Proof. For all $\gamma \in \Sigma$ with source x and target y, we have

$$\begin{aligned}\mathrm{Ad}_{\Sigma^{-1}} l|_x &= \frac{\mathrm{d}}{\mathrm{d}t}(\Sigma^{-1} \star \exp(tl) \star \Sigma)_{\boldsymbol{s}}(x)\Big|_{t=0} \\ &= \frac{\mathrm{d}}{\mathrm{d}t}(\Sigma_{\boldsymbol{t}}(\boldsymbol{t}(\exp(tl)_{\boldsymbol{s}}(y))))^{-1} \cdot \exp(tl)_{\boldsymbol{s}}(y) \cdot \gamma\Big|_{t=0} \\ &= (T\Sigma_{\boldsymbol{t}}(\rho(l_y)))^{-1} \bullet l_y \bullet 0_\gamma = \kappa(u, l_y),\end{aligned}$$

where $u = T\Sigma_{\boldsymbol{t}}(\rho(l_y))$. □

We list here some properties of κ that follow in a straightforward manner from the definitions. Below, $L(\cdot)$ and $R(\cdot)$ are the left- and right-invariant vector fields defined in (10).

Proposition 3.11. *For every $\gamma \in \boldsymbol{L}$ with source x and target y, we have*

(1) $\kappa(L(\lambda)|_\gamma, \lambda) = 0$ *for all* $\lambda \in L_x$,

(2) $\kappa(R(\lambda)|_\gamma, 0_x) = -\lambda$ *for all* $\lambda \in L_y$,

(3) $\kappa(0_x, \lambda) = \lambda$ *for all* $\lambda \in L_x$.

For every $(u, \lambda) \in (\boldsymbol{t}^! L)|_\gamma$ and every $u' \in T\boldsymbol{L}$, we have

(4) $\kappa(u \bullet u', \lambda) = \kappa(u', \kappa(u, \lambda))$ *whenever $u \bullet u'$ is defined.*

By items (3) and (4) of Proposition 3.11, we may see the map

$$\kappa : T\boldsymbol{L} \times_{TM}^{T\boldsymbol{t},\rho} L \to L$$

as a *right $T\boldsymbol{L}$-action on the anchor map $\rho : L \to TM$.* In that context, we will use the notation

$$\kappa_u = \kappa(u, \cdot) : \rho^{-1}(T\boldsymbol{t}(u)) \to \rho^{-1}(T\boldsymbol{s}(u)) \tag{36}$$

for all $u \in T\boldsymbol{L}$.

3C. ***Equivariant principal bundles.*** In this section, we slightly extend the notion of generalized morphism. Specifically, we consider (right) principal bundles with a compatible left action of a Lie groupoid, without requiring the base manifolds of the principal bundle and of the Lie groupoid acting on the left to agree.

In the case of groups instead of groupoids, these objects are already very natural and were considered in [Wang 1958] and [Bordemann 2012], for example. Apart from the passage to groupoids, what seems to be new here is the fact that these objects, as well as the connection forms on them, can be composed.

Definition We start with the definition of our bundles and their composition.

Definition 3.12. Let $\boldsymbol{L} \rightrightarrows M$ and $\boldsymbol{U} \rightrightarrows N$ be two Lie groupoids. An *$\boldsymbol{L}$-equivariant principal $\boldsymbol{U}$-bundle* over a manifold X is a surjective submersion $\pi : P \to X$ from a manifold P with a left $\boldsymbol{L}$-action on a map $l : P \to M$ and a right $\boldsymbol{U}$-action on a map $r : P \to N$ such that

(1) the left and right actions commute,

(2) l is a surjective submersion,

(3) the map

$$P \times_N \boldsymbol{U} \to P \times_X P : (p, \upsilon) \mapsto (p, p \cdot \upsilon) \tag{37}$$

is a diffeomorphism.

The maps l and r are called the left and right moment maps, respectively.

As before, the diffeomorphism (37) is a Lie groupoid morphism, which yields a *division map* $D_P : P \times_X P \to \boldsymbol{U}$ with the same invariance and equivariance properties as those of generalized morphisms (see (23)–(25)).

The axioms imply that l descends to $\bar{l} : X \to M$, and P will often be represented by the diagram

$$\begin{tikzcd}
\boldsymbol{L} \arrow[d, shift left] \arrow[d, shift right] & P \arrow[dl, "l"'] \arrow[d, two heads, "\pi"] \arrow[dr, "r"] & \boldsymbol{U} \arrow[d, shift left] \arrow[d, shift right] \\
M & X \arrow[l, two heads, "\bar{l}"'] & N
\end{tikzcd}$$

When there can be no confusion about the actions, we will use the notation ${}_{\boldsymbol{L}}P_{\boldsymbol{U}}$ as shorthand for the above diagram.

When $X = M$ and $l = \pi$, we recover the notion of *generalized morphism* between Lie groupoids. Just as with generalized morphisms, equivariant principal bundles may be composed: if P is an $\boldsymbol{L}$-equivariant principal $\boldsymbol{U}$-bundle, and Q is a $\boldsymbol{U}$-equivariant principal $\boldsymbol{V}$-bundle, then $P \times_N Q$ is a smooth manifold thanks to condition (2). Moreover, by condition (3) it has a proper and free $\boldsymbol{U}$-action $(u, (p, q)) \mapsto (pu^{-1}, uq)$, so that the quotient $P \circ Q = (P \times_N Q)/\boldsymbol{U}$ is a smooth manifold as well. The latter still has a free and proper $\boldsymbol{V}$-action and is in fact an $\boldsymbol{L}$-equivariant principal $\boldsymbol{V}$-bundle over the manifold $(P \circ Q)/\boldsymbol{V}$, which we call the *composition* of P and Q.

The equivalences between two $\boldsymbol{L}$-equivariant principal $\boldsymbol{U}$-bundles P and P' (over X and X', respectively) are again the bi-equivariant diffeomorphisms $\phi : P \to P'$. Note that these induce $\boldsymbol{L}$-equivariant maps $\psi : X \to X'$ on the bases such that $\pi' \circ \phi = \psi \circ \pi$.

The proof of the following result is a straightforward adaptation of the corresponding proof for generalized morphisms in, e.g., [Blohmann 2008].

Proposition 3.13. *The Lie groupoids with equivariant principal bundles as* 1*-morphisms and bi-equivariant diffeomorphisms as* 2*-morphisms form a bicategory.*

The equivariant principal bundles form a generalization of the generalized morphisms which only includes more "degenerate" morphisms. Indeed note that, keeping our previous notation, the base $(P \circ Q)/V$ of a composition $P \circ Q$ fibers over X through a surjective submersion whose fibers are those of $\bar{l}_Q : Y \to N$, where Y is the base of Q. As a result, the dimension of the fibers of $\bar{l}_{P\circ Q}$ is the sum of the dimensions of the fibers of $\bar{l}_P$ and of $\bar{l}_Q$. This implies that a weakly invertible equivariant principal bundle is, up to bi-equivariant diffeomorphism, a weakly invertible generalized morphism (i.e., a Morita morphism).

Examples. The main example of "degenerate" morphism that we will consider is induced by a Lie groupoid pair $(\boldsymbol{L}, \boldsymbol{A})$. Given such a pair, $\boldsymbol{L}$ can be considered in two ways as an equivariant principal bundle: either as an $\boldsymbol{A}$-equivariant principal $\boldsymbol{L}$-bundle, or as an $\boldsymbol{L}$-equivariant principal $\boldsymbol{A}$-bundle. Those are denoted, respectively, by ${}_{\boldsymbol{A}}\boldsymbol{L}_{\boldsymbol{L}}$ and ${}_{\boldsymbol{L}}\boldsymbol{L}_{\boldsymbol{A}}$. In both cases, the left and right moment maps are just the target and source maps, respectively, and the actions are by left and right translations. The first version, ${}_{\boldsymbol{A}}\boldsymbol{L}_{\boldsymbol{L}}$, has $X = M$ and is isomorphic to the bundlization P_i of the inclusion morphism $i : \boldsymbol{A} \to \boldsymbol{L}$, since $P_i = M \times_M \boldsymbol{L}$ is bi-equivariantly diffeomorphic to $\boldsymbol{L}$. It is thus a generalized morphism. The second version, ${}_{\boldsymbol{L}}\boldsymbol{L}_{\boldsymbol{A}}$, sits over the homogeneous space $X = \boldsymbol{L}/\boldsymbol{A}$ and is not a generalized morphism as soon as $X \neq M$.

The composition of the $\boldsymbol{L}$-equivariant principal $\boldsymbol{A}$-bundle ${}_{\boldsymbol{L}}\boldsymbol{L}_{\boldsymbol{A}}$ with a generalized morphism P from $\boldsymbol{A}$ to a Lie groupoid $\boldsymbol{U}$ yields an $\boldsymbol{L}$-equivariant principal $\boldsymbol{U}$-bundle $Q = {}_{\boldsymbol{L}}\boldsymbol{L}_{\boldsymbol{A}} \circ P$ over $\boldsymbol{L}/\boldsymbol{A}$. This kind of composition will be studied extensively.

Example 3.14. Let $\varphi : \boldsymbol{A} \to \boldsymbol{U}$ be a Lie groupoid morphism over $\varphi_0 : M \to N$. Then the fibered product $\boldsymbol{L} \times_N \boldsymbol{U} = \boldsymbol{L} \times_N^{\varphi_0\circ \boldsymbol{s}, \boldsymbol{t}} \boldsymbol{U}$ is a smooth manifold which admits a free and proper right $\boldsymbol{A}$-action defined by

$$(\boldsymbol{L} \times_N \boldsymbol{U}) \times_M \boldsymbol{A} \to \boldsymbol{L} \times_N \boldsymbol{U} : ((\gamma, \upsilon), \gamma') \mapsto (\gamma \cdot \gamma', \varphi(\gamma'^{-1}) \cdot \upsilon).$$

The corresponding quotient

$$Q = \frac{\boldsymbol{L} \times_N \boldsymbol{U}}{\boldsymbol{A}} \tag{38}$$

is then an $\boldsymbol{L}$-equivariant principal $\boldsymbol{U}$-bundle over $\boldsymbol{L}/\boldsymbol{A}$ when endowed with the left and right moment maps $l : Q \to M : [(g, u)] \mapsto \boldsymbol{t}(g)$ and $r : Q \to N : (g, u) \mapsto \boldsymbol{s}(u)$, with the projection $\pi : Q \to \boldsymbol{L}/\boldsymbol{A} : [(g, u)] \mapsto [g]$, and with the actions

$$\boldsymbol{L} \times_M Q \to Q : (\gamma, [(\gamma', \upsilon)]) \mapsto [(\gamma \cdot \gamma', \upsilon)],$$
$$Q \times_N \boldsymbol{U} \to Q : ([(\gamma, \upsilon)], \upsilon') \mapsto [(\gamma, \upsilon \cdot \upsilon')].$$

It is canonically isomorphic to the composition ${}_{\boldsymbol{L}}\boldsymbol{L}_{\boldsymbol{A}} \circ P_\varphi$.

The bundles constructed in Example 3.14 exhaust all $\boldsymbol{L}$-equivariant principal $\boldsymbol{U}$-bundles Q over X such that

(1) the $\boldsymbol{L}$-action on X is transitive, and

(2) the left moment map has a smooth global section.

Indeed, let σ be such a section, let $\bar{\sigma} = \pi \circ \sigma$ be the corresponding section of $\bar{l}$, and denote by $\boldsymbol{A}$ the closed subgroupoid of $\boldsymbol{L}$ that sends $\bar{\sigma}(M)$ to itself. Then, X is equivariantly diffeomorphic to $\boldsymbol{L}/\boldsymbol{A}$. Moreover, there is a Lie groupoid morphism $\phi : \boldsymbol{A} \to \boldsymbol{U}$ defined by the relation $\gamma \cdot \sigma(\boldsymbol{s}(\gamma)) = \sigma(\boldsymbol{t}(\gamma)) \cdot \phi(\gamma)$. Now, we have a map $r \circ \sigma : M \to N$ and we may consider $\boldsymbol{L} \times_N \boldsymbol{U} \to Q : (\gamma, \upsilon) \mapsto \gamma \cdot \sigma(\boldsymbol{s}(\gamma)) \cdot \upsilon$, which descends to an isomorphism (i.e., bi-equivariant diffeomorphism) $(\boldsymbol{L} \times_N \boldsymbol{U})/\boldsymbol{A} \to Q$ as promised.

Dropping the existence of a section of the left moment map, we still have that X is a homogeneous space of $\boldsymbol{L}$ and thus has a section $\bar{\sigma} : M \to X$. Defining $\boldsymbol{A}$ as above and $P = \pi^{-1}(\sigma(M))$, we get that P is a generalized morphism from $\boldsymbol{A}$ to $\boldsymbol{U}$ and that there is a map $\boldsymbol{L} \times_M P \to Q : (\gamma, p) \mapsto \gamma \cdot p$, which descends to an isomorphism $(\boldsymbol{L} \times_M P)/\boldsymbol{A} \to Q$.

We have thus proved the following result about principal bundles over homogeneous spaces.

Proposition 3.15. *Any $\boldsymbol{L}$-equivariant principal bundle Q over X for which the $\boldsymbol{L}$-action on X is transitive is isomorphic to a composition ${}_{\boldsymbol{L}}\boldsymbol{L}_{\boldsymbol{A}} \circ P$ where $\boldsymbol{A}$ is the stabilizer of some section $\sigma : M \to X$ and P is a generalized morphism. The latter generalized morphism is isomorphic to (the bundlization of) a morphism if and only if the left moment map of Q admits a section.*

Remark 3.16. If P is an $\boldsymbol{L}$-equivariant principal $\boldsymbol{U}$-bundle over X, there is an induced $\boldsymbol{L}$-action on X. Hence, we may consider the action groupoid $\boldsymbol{L} \ltimes X$ over X. Then P is actually a generalized morphism from $\boldsymbol{L} \ltimes X$ to $\boldsymbol{U}$ with left action defined by $(\gamma, x) \cdot p = \gamma \cdot p$ whenever $\pi(p) = x$.

$$
\begin{tikzcd}
\boldsymbol{L} \arrow[d, shift left] \arrow[d, shift right] & P \arrow[dl, "l"'] \arrow[d, "\pi"] \arrow[dr, "r"] & \boldsymbol{U} \arrow[d, shift left] \arrow[d, shift right] \\
M & X \arrow[l, two heads, "\bar{l}"'] & N
\end{tikzcd}
\quad \rightsquigarrow \quad
\begin{tikzcd}
\boldsymbol{L} \ltimes X \arrow[d, shift left] \arrow[d, shift right] & P \arrow[dl, "\pi"'] \arrow[dr, "r"] & \boldsymbol{U} \arrow[d, shift left] \arrow[d, shift right] \\
X & & N
\end{tikzcd}
$$

So in some sense, equivariant principal bundles are just a special kind of generalized morphisms, but we do not want to see them in this way. We really want to see them as “morphisms” from $\boldsymbol{L}$ to $\boldsymbol{U}$.

Example 3.17. While the association $X \mapsto \underline{X} = (X \rightrightarrows X)$ realizes the category of manifolds as a full subcategory of the bicategory of Lie groupoids defined in Proposition 3.3, the analogous result is not true for the bicategory where generalized morphisms as 1-morphisms are replaced by equivariant principal bundles as in Proposition 3.13. Indeed, the equivariant principal bundles between $\underline{X}$ and $\underline{Y}$ for two smooth manifolds X and Y are the *multivalued functions from X to Y*. Here, a multivalued function from X to Y is a smooth manifold Z together with a surjective submersion to X and a smooth map to Y.

Connections. The connection forms defined below are natural extensions of those on usual principal bundles with structure group, and on principal bundles with structure groupoid. To define them, let us first explain some notation.

If $\boldsymbol{L} \times_M P \to P$ is a left action on a map $P \to M$, there is an induced $T\boldsymbol{L}$-action on TP simply obtained by applying the tangent functor. We will write $\gamma \cdot p$ for the action of $\gamma \in \boldsymbol{L}$ on $p \in P$, and $u \cdot X$ for the action of $u \in T\boldsymbol{L}$ on $X \in TP$, whenever defined. We use the same notation for a right action $P \times_N \boldsymbol{U} \to P$, and write $p \cdot \upsilon$ for the action of $\upsilon \in \boldsymbol{U}$ on $p \in P$, and $X \cdot v$ for the action of $v \in T\boldsymbol{U}$ on $X \in TP$, whenever defined. The zero vector at a point $p \in P$ is denoted by 0_p. Recall that $T^l P$ is the subbundle of TP of vectors tangent to the l-fibers, $T^l P = \ker Tl$, and similarly for $T^\pi P$.

Definition 3.18. The *infinitesimal vector fields* of a right action $R : P \times_N \boldsymbol{U} \to P$ of a Lie groupoid $\boldsymbol{U} \rightrightarrows N$ on a manifold P are the vector fields $\hat{v} \in \mathfrak{X}(P)$ defined by

$$\hat{v}|_p = \frac{d}{dt} R_{\exp(tv)^{-1}}(p)\bigg|_{t=0} = 0_p \cdot (v|_p)^{-1}$$

for all $v \in \Gamma(U)$ and $p \in P$.

Let us consider now an equivariant principal bundle P and momentarily denote by ψ the Lie groupoid diffeomorphism (37). Then the infinitesimal vector fields map coincides with the Lie algebroid isomorphism

$$r^*U \cong \operatorname{Lie}(P \rtimes \boldsymbol{U}) \xrightarrow{\operatorname{Lie}(\psi)} \operatorname{Lie}(P \times_X P) \cong T^\pi P. \tag{39}$$

A connection form is a bundle map from TP to r^*U that extends the inverse of the above map, in an equivariant way.

Definition 3.19. A *connection form* (resp., *fibered connection form*) on an $\boldsymbol{L}$-equivariant principal $\boldsymbol{U}$-bundle P is an r^*U-valued 1-form $\omega \in \Omega^1(P, r^*U)$ (resp., an r^*U-valued 1-form on the l-fibers $\omega \in \Omega^1_l(P, r^*U)$) such that

(F1) $\omega(\hat{v}) = r^*v$, for all $v \in \Gamma(U)$,

(F2) $\operatorname{Ad}_{\Sigma^{-1}} \circ\, \omega = R^*_\Sigma \omega$, for all $\Sigma \in \operatorname{Bis}(\boldsymbol{U})$,

(F3) $L^*_\Sigma \omega = \omega$, for all $\Sigma \in \operatorname{Bis}(\boldsymbol{L})$.

Remark 3.20. Fibered connection forms are specifically designed for equivariant principal bundles which are *not* generalized morphisms. Indeed, if P is a generalized morphism then $l = \pi$, the infinitesimal vector fields of the right $\boldsymbol{U}$-action span the tangent space to the l-fibers at all points, and condition (F1) in Definition 3.19 entirely determines the values of ω at all points. On the other hand, since $R_\Sigma(\hat{v}) = (\mathrm{Ad}_{\Sigma^{-1}}(v))^\wedge$ and since the left and right actions commute, the map defined by (F1) also satisfies (F2) and (F3). Hence, there exists one and only one fibered connection form on a generalized morphism, given by the inverse of (39). We will call it the *Maurer–Cartan form* of a generalized morphism.

Connection forms, on the other hand, reduce to the usual notion of connection form on a principal bundle when $\boldsymbol{U}$ is a Lie group and $\boldsymbol{L}$ is the (trivial) groupoid $M \rightrightarrows M$ of a manifold. Moreover, when $\boldsymbol{U}$ is a Lie group and $\boldsymbol{L}$ is any Lie groupoid, our connection forms coincide with the connection forms on a principal bundle over a groupoid defined in [Laurent-Gengoux et al. 2007].

We stress that both kinds of connections need not exist in general, due to the left-invariance condition, just like G-invariant connections on a homogeneous space G/H need not exist in general. It is the very purpose of this paper to study the obstruction to their existence and some constructions that can be made when such connections exist.

In this paper, we will only use *fibered* connection forms $\omega \in \Omega^1_l(P, r^*U)$ and, more precisely, we will only use the corresponding bundle maps

$$\begin{array}{ccc} T^lP & \xrightarrow{\omega} & U \\ \downarrow & & \downarrow \\ P & \xrightarrow{r} & N \end{array}$$

We will use the same letter ω for fibered connection forms and the corresponding bundle maps, and call both *fibered connection forms*. These bundle maps enjoy similar properties to (F1)–(F3) above, however, in case we want to avoid using bisections, we have two simpler axioms: $T\boldsymbol{U}$-equivariance and $\boldsymbol{L}$-invariance.

Proposition 3.21. *A vector bundle morphism $\omega : T^lP \to U$ over $r : P \to N$ is* (*the bundle map of*) *a fibered connection form if and only if it is an anchored map such that*, *for all $Y \in T^lP$, $v \in T\boldsymbol{U}$ and $\gamma \in \boldsymbol{L}$*,

(B1) $\kappa_v\omega(Y) = \omega(Y \cdot v)$ *whenever* $Tr(Y) = T\boldsymbol{t}(v)$,

(B2) $\omega(0_\gamma \cdot Y) = \omega(Y)$ *whenever* $Y \in T^l_pP$ *with* $l(p) = \boldsymbol{s}(\gamma)$.

Proof. We will show that (B1) is equivalent to (F1) + (F2), and that (B2) is equivalent to (F3).

Assume $\omega : T^lP \to U$ satisfies (B1). Taking $Y = 0_p$ and $v = u^{-1}$ with $u \in U_{r(p)}$, we get

$$u = u \bullet 0_{1_{r(p)}} \bullet 0_{(1_{r(p)})^{-1}} = \kappa(u^{-1}, 0_{1_{r(p)}}) = \omega(0_p \cdot u^{-1}) = \omega(\hat{u}|_p),$$

which is (F1). By Lemma 3.10, (B1) also implies (F2). Conversely, assume that $\omega : T^l P \to U$ is a bundle map satisfying (F1) and (F2). Notice that any pair $(Y, v) \in T^l_{(p,v)}(P \times_N \boldsymbol{U})$ can be written as

$$(Y, v) = (0_p, 0_v \bullet u^{-1}) + (Y, T\Sigma_{\boldsymbol{t}}(Tr(Y)))$$

for some bisection $\Sigma \in \mathrm{Bis}(\boldsymbol{U})$ and some $u \in U_{\boldsymbol{s}(v)}$. The same arguments as for the converse show that (B1) holds for each term in this sum. Hence, it holds in general.

The equivalence between (B2) and (F3) follows from the fact that, for a bisection $\Sigma \in \mathrm{Bis}(\boldsymbol{L})$ and a vector $Y \in T^l_p P$, we have

$$\begin{aligned}\Sigma \star Y &= T\Sigma_{\boldsymbol{s}}(Tl(Y)) \cdot Y \\ &= T\Sigma_{\boldsymbol{s}}(0_{l(p)}) \cdot Y \\ &= 0_{\Sigma_s(l(p))} \cdot Y. \end{aligned} \qquad \square$$

Example 3.22 (units). The Maurer–Cartan form (see Remark 3.20) of a unit generalized morphism $\mathrm{Id}_{\boldsymbol{L}}$ is the bundle map $\tau = \tau_{\boldsymbol{L}} : T^{\boldsymbol{t}}\boldsymbol{L} \to L$ defined by

$$\tau(u) = u^{-1} \bullet 0_\gamma = \kappa(u, 0_{\boldsymbol{t}(\gamma)}) \tag{40}$$

for all $u \in (T^{\boldsymbol{t}}\boldsymbol{L})_\gamma$. Hence, it is the usual Maurer–Cartan form of the Lie groupoid $\boldsymbol{L}$. It is natural in $\boldsymbol{L}$: if $\phi : \boldsymbol{L} \to \boldsymbol{U}$ is a Lie groupoid morphism, then $\tau_{\boldsymbol{U}} \circ T\phi = \mathrm{Lie}(\phi) \circ \tau_{\boldsymbol{L}}$.

Example 3.23 (bundlizations). The Maurer–Cartan form of the bundlization of a morphism $\varphi : \boldsymbol{L} \to \boldsymbol{U}$ is induced from the Maurer–Cartan form of $\boldsymbol{U}$. Indeed, the fibered tangent bundle $T^l P_\varphi$ is the set of tangent vectors (X, v) in $TM \times_{TN} T\boldsymbol{U}$ that project to zero through the projection on the first component, hence the set of vectors $(0, v)$ with $v \in T^{\boldsymbol{t}}\boldsymbol{U}$. The connection form on P_φ is then the bundle map $\omega_\varphi : T^l P_\varphi \to U$ defined by

$$\omega_\varphi(0, v) = \tau_{\boldsymbol{U}}(v)$$

for all $(0, v) \in T^l P_\varphi$.

Just like equivariant principal bundles can be composed, connections on such bundles can be composed as well (see Section 5C for an application of that result).

Proposition 3.24. *Let P be an $\boldsymbol{L}$-equivariant principal $\boldsymbol{A}$-bundle, and Q an $\boldsymbol{A}$-equivariant principal $\boldsymbol{U}$-bundle, for some Lie groupoids $\boldsymbol{L}$, $\boldsymbol{A}$, and $\boldsymbol{U}$. Let ω_P and ω_Q be fibered connection forms on P and Q, respectively. Then there is a fibered connection form ω on $P \circ Q$ defined by*

$$\omega([(X, Y)]) = \omega_Q(Y - \omega_P(X) \cdot 0_q)$$

for all $(X, Y) \in T^l(P \times^{r,l}_M Q)$, where M is the base manifold of $\boldsymbol{A}$, and q is the base point of Y.

Proof. Property (B1) for ω_P and property (B2) for ω_Q imply that $(X, Y) \mapsto \omega_Q(Y - \omega_P(X) \cdot 0_q)$ is $T\boldsymbol{A}$-invariant, so ω is well-defined. Then (B1) follows from (B1) for ω_Q and from the commutativity of the left and right actions on P. And (B2) follows from (B2) for ω_P. □

It is straightforward to check that this composition is compatible with the Maurer–Cartan form of generalized morphisms, and that equivariant principal bundles with fibered connection also form a bicategory, which contains generalized morphisms.

3D. *Associated vector bundles.* In this section, for a Lie groupoid $\boldsymbol{L} \rightrightarrows M$ and a vector bundle $E \to N$, we exhibit an explicit correspondence between fibered connection forms on an $\boldsymbol{L}$-equivariant principal $\boldsymbol{GL}(E)$-bundle P and $\boldsymbol{L}$-invariant fibered connections on the associated vector bundle $P(E)$.

The results in this section are natural analogues of the classical notions.

Definition 3.25. Let $\boldsymbol{L}$ and $\boldsymbol{U}$ be Lie groupoids over M and N, respectively, let $E \to N$ be a $\boldsymbol{U}$-module, and let P be an $\boldsymbol{L}$-equivariant principal $\boldsymbol{U}$-bundle over X. The *associated $\boldsymbol{L}$-module* to P and E is the associated vector bundle

$$P(E) = \frac{P \times_N E}{\boldsymbol{U}} \to X$$

with the $\boldsymbol{L}$-module structure $\boldsymbol{L} \times_M P(E) \to P(E)$ defined by

$$\gamma \cdot [(p, e)] = [(\gamma \cdot p, e)].$$

We will denote by μ the (left) $\boldsymbol{U}$-action on $P \times_N E$ that defines $P(E)$:

$$\mu_\upsilon(p, e) = (p \cdot \upsilon^{-1}, \upsilon \cdot e),$$

where $\upsilon \in \boldsymbol{U}$, $p \in P$ and $e \in E$ satisfy $r(p) = q(e) = \boldsymbol{s}(\upsilon)$. Also, we will denote by $\pi_{P(E)}$ the projection $(p, e) \mapsto [(p, e)]$ from $P \times_N E$ to $P(E)$.

Any vector bundle E is canonically a $\boldsymbol{GL}(E)$-module. *In the rest of this section, we will only consider the case where P is an $\boldsymbol{L}$-equivariant principal $\boldsymbol{GL}(E)$-bundle.*

Example 3.26. Let $(\boldsymbol{L}, \boldsymbol{A})$ be a Lie groupoid pair over M and E be an $\boldsymbol{A}$-module. The Lie groupoid pair defines an $\boldsymbol{L}$-equivariant principal $\boldsymbol{A}$-bundle over $\boldsymbol{L}/\boldsymbol{A}$, and the associated $\boldsymbol{L}$-module to ${}_{\boldsymbol{L}}\boldsymbol{L}_{\boldsymbol{A}}$ and E is $(\boldsymbol{L} \times_M E)/\boldsymbol{A}$.

Considering the $\boldsymbol{A}$-module structure on E as a Lie groupoid morphism from $\boldsymbol{A}$ to the frame groupoid $\boldsymbol{GL}(E)$ we get, as in Example 3.14, an $\boldsymbol{L}$-equivariant principal $\boldsymbol{GL}(E)$-bundle $P = (\boldsymbol{L} \times_M \boldsymbol{GL}(E))/\boldsymbol{A}$ over $X = \boldsymbol{L}/\boldsymbol{A}$. The associated $\boldsymbol{L}$-module $P(E) = (P \times_M E)/\boldsymbol{GL}(E)$ is isomorphic to $(\boldsymbol{L} \times_M E)/\boldsymbol{A}$.

The following result will be needed in the proof of Proposition 3.29.

Lemma 3.27. *There is a canonical isomorphism $\Psi : \pi^* P(E) \to P \times_N E$ of vector bundles over P. It is $\boldsymbol{L}$- and $\boldsymbol{GL}(E)$-equivariant, in the sense that*

$$\Psi(\gamma \cdot p, \gamma \cdot \epsilon) = \gamma \cdot \Psi(p, \epsilon),$$
$$\Psi(p \cdot \phi^{-1}, \epsilon) = \mu_\phi \Psi(p, \epsilon)$$

for all $(p, \epsilon) \in \pi^* P(E)$, $\gamma \in \boldsymbol{L}$ such that $\boldsymbol{s}(\gamma) = l(p)$, and $\phi \in \boldsymbol{GL}(E)$ such that $\boldsymbol{s}(\phi) = r(p)$.

Proof. This follows directly from the isomorphism (37). Explicitly, consider the map

$$P \times_X (P \times_N E) \to P \times_N E : (p', (p, e)) \mapsto (p', D_P(p', p) \cdot e). \tag{41}$$

It is smooth and invariant under the $\boldsymbol{GL}(E)$-action on $P \times_X (P \times_N E)$ given by $(\phi, (p', (p, e))) \mapsto (p', \mu_\phi(p, e))$. Hence it descends to a smooth map

$$\Psi : P \times_X P(E) = \pi^* P(E) \to P \times_N E$$

which is, moreover, an inverse of the map $P \times_N E \to \pi^* P(E) : (p, e) \mapsto (p, [(p, e)])$.

The equivariance is now obvious from (41) and the equivariance of the division map D_P. ∎

We will use the notation

$$\begin{tikzcd}
\boldsymbol{L} \arrow[d, shift left] \arrow[d, shift right] & P \arrow[dl, two heads, "l"'] \arrow[d, two heads, "\pi"] \arrow[dr, "r"] & \boldsymbol{GL}(E) \arrow[d, shift left] \arrow[d, shift right] \\
M & X \arrow[l, two heads, "\bar{l}"] & N
\end{tikzcd}$$

Note that X is still fibered over M, so that we may consider the subbundle $T^{\bar{l}} X = \ker T\bar{l} \subset TX$, and correspondingly consider *fibered* differential k-forms on X. A *$P(E)$-valued fibered k-form on X* is a section of $\Lambda^k (T^{\bar{l}} X)^* \otimes P(E) \to X$.

On the other hand, we can consider the *E-valued fibered k-forms on P*, i.e., the bundle maps $\alpha : \Lambda^k (T^l P) \to E$ over $r : P \to N$. We make the following definition.

Definition 3.28. An E-valued fibered k-form α on P is *horizontal* if it vanishes whenever one of its arguments is in $\ker T\pi \subset T^l P$, where $\pi : P \to X$ is the projection:

$$\alpha_p(Y_1, \ldots, Y_k) = 0 \quad \text{if } Y_i \in \ker T\pi \text{ for some } i \in \{1, \ldots, k\},$$

for all $p \in P$ and $Y_1, \ldots, Y_k \in T^l_p P$. It is *equivariant* if it is equivariant for the $\boldsymbol{GL}(E)$-actions on P and E:

$$R^*_{\phi^{-1}} \alpha = \phi \circ \alpha \quad \text{for all } \phi \in \operatorname{Bis}(\boldsymbol{GL}(E)).$$

On the right-hand side, ϕ is considered as in Example 2.4 as a map $E \to E$.

Proposition 3.29. *There is a* $\mathrm{Bis}(\boldsymbol{L})$*-equivariant isomorphism of* $C^\infty(X)$*-modules*

$$\Omega^k_{\bar{l}}(X, P(E)) \xrightarrow{\sim} \Omega^k_{\mathrm{hor}}(P, E)^{\boldsymbol{GL}(E)}$$

between the space $\Omega^k_{\bar{l}}(X, P(E))$ *of* $P(E)$*-valued fibered* k*-forms on* X *and the space* $\Omega^k_{\mathrm{hor}}(P, E)^{\boldsymbol{GL}(E)}$ *of equivariant horizontal* E*-valued fibered* k*-forms on* P.

Proof. Let α be an equivariant horizontal E-valued fibered k-form on P. Define a $P \times_N E$-valued fibered k-form $\tilde{\eta}$ on P by

$$\tilde{\eta}_p(Y_1, \ldots, Y_k) = (p, \alpha_p(Y_1, \ldots, Y_k))$$

for all $p \in P$ and $Y_i \in T^l_p P$. Since α is horizontal, $\tilde{\eta}$ only depends on $X_i = T\pi(Y_i)$, $i = 1, \ldots, k$. Moreover, since α is equivariant, we have

$$\begin{aligned}(R^*_{\phi^{-1}}\tilde{\eta})_p(Y_1, \ldots, Y_k) &= (p\phi^{-1}, (R^*_{\phi^{-1}}\alpha)_p(Y_1, \ldots, Y_k)) \\ &= (p\phi^{-1}, \phi \circ \alpha_p(Y_1, \ldots, Y_k)) = \mu_\phi(\tilde{\eta}_p(Y_1, \ldots, Y_k))\end{aligned}$$

for all $\phi \in \mathrm{Bis}(\boldsymbol{GL}(E))$, $p \in P$, and $Y_i \in T^l_p P$. Hence the composition $\pi_{P(E)} \circ \tilde{\eta}$ only depends on $x = \pi(p)$ and on $X_i = T\pi(Y_i)$, $i = 1, \ldots, k$, so that it descends to a $P(E)$-valued fibered k-form η on X.

Conversely, let η be a $P(E)$-valued fibered k-form on X. Define an E-valued fibered k-form on P by

$$\alpha_p(Y_1, \ldots, Y_k) = (\mathrm{pr}_2 \circ \Psi)(p, (\pi^*\eta)_p(Y_1, \ldots, Y_k))$$

for all $p \in P$ and $Y_i \in T^l_p P$, where Ψ is defined in Lemma 3.27. By construction, α is horizontal and equivariant.

An easy check now shows that the two assignments $\alpha \mapsto \eta$ and $\eta \mapsto \alpha$

(1) are linear inverses of each other,

(2) are $C^\infty(X)$-linear for the multiplications $(f\alpha)_p = f(\pi(p))\alpha_p$ and $(f\eta)_x = f(x)\eta_x$, where $f \in C^\infty(X)$, and

(3) are $\mathrm{Bis}(\boldsymbol{L})$-equivariant for the actions

$$\begin{aligned}(g \cdot \alpha)_p(Y_1, \ldots, Y_k) &= \alpha_{g^{-1}p}(TL_{g^{-1}}(Y_1), \ldots, TL_{g^{-1}}(Y_k)), \\ (g \cdot \eta)_x(X_1, \ldots, X_k) &= g \cdot (\eta_{g^{-1}x}(TL_{g^{-1}}(X_1), \ldots, TL_{g^{-1}}(X_k))),\end{aligned} \tag{42}$$

where $g \in \mathrm{Bis}(\boldsymbol{L})$. □

A fibered connection on $P(E)$ can be seen as an $\mathbb{R}$-linear map

$$\nabla : \Omega^0_{\bar{l}}(X, P(E)) \to \Omega^1_{\bar{l}}(X, P(E))$$

satisfying the Leibniz rule

$$\nabla(f\epsilon)(Y) = Y(f)\epsilon + f\nabla(\epsilon)(Y)$$

for all $\epsilon \in \Omega^0_{\bar{l}}(X, P(E)) = \Gamma(P(E))$, $f \in C^\infty(X)$ and $Y \in \Gamma(T^{\bar{l}}X)$. Through the correspondence of Proposition 3.29, this becomes an $\mathbb{R}$-linear map

$$\nabla : \Omega^0_{\mathrm{hor}}(P, E)^{\boldsymbol{GL}(E)} \to \Omega^1_{\mathrm{hor}}(P, E)^{\boldsymbol{GL}(E)} \tag{43}$$

satisfying the Leibniz rule

$$\nabla(f\alpha)(Y) = Y(f)\alpha + f\nabla(\alpha)(Y) \tag{44}$$

for all $\alpha \in \Omega^0_{\mathrm{hor}}(P, E)^{\boldsymbol{GL}(E)}$, $f \in C^\infty(P)^{\boldsymbol{GL}(E)}$ and $Y \in \Gamma(T^l P)$.

Theorem 3.30. *Let $\boldsymbol{L}$ be a Lie groupoid, E a vector bundle, and P an $\boldsymbol{L}$-equivariant principal $\boldsymbol{GL}(E)$-bundle. There is a bijective correspondence between*

(1) *fibered connection forms on P, and*

(2) *$\boldsymbol{L}$-equivariant fibered connections on the vector bundle $P(E)$.*

Proof. As explained above, by Proposition 3.29, we can consider $\boldsymbol{L}$-equivariant fibered connections on the vector bundle $P(E)$ as $\boldsymbol{L}$-equivariant maps (43) satisfying the Leibniz rule (44).

Step 1 (from connection forms to connections). Let $\omega : T^l P \to T^{\mathrm{lin}} E$ be a fibered connection form on P. For an equivariant map $\alpha \in \Omega^0_{\mathrm{hor}}(P, E)^{\boldsymbol{GL}(E)}$, we will denote by $T^l\alpha$ its differential $T\alpha : TP \to TE$ restricted to $T^l P$. There is a canonical map $\ker Tq_E \to E$ obtained by considering each vertical vector v at $e \in E_x$ as a vector in E_x. We will denote this map by I.

Define a map $\nabla : \Omega^0_{\mathrm{hor}}(P, E)^{\boldsymbol{GL}(E)} \to \Omega^1_{\mathrm{hor}}(P, E)^{\boldsymbol{GL}(E)}$ by

$$\nabla\alpha = I(T^l\alpha - \omega(\alpha)), \tag{45}$$

for all $\alpha \in \Omega^0_{\mathrm{hor}}(P, E)^{\boldsymbol{GL}(E)}$, where $\omega(\alpha)$ is the map $T^l P \to TE$ defined by $\omega(\alpha)(Y) = \omega(Y)(\alpha(p))$ for all $Y \in T^l_p P$.

Since ω is an anchored map, it follows easily that $Tq_E \circ (\omega(\alpha)) = Tr$. Hence, we have

$$Tq_E \circ (T^l\alpha - \omega(\alpha)) = Tr - Tr = 0.$$

As a result, $\nabla\alpha$ is well defined.

The 1-form $\nabla\alpha$ is horizontal since if $Y \in \ker(T\pi)_p \subset T^l_p P$, then $Y = \hat{D}_p$ for some $D \in (T^{\mathrm{lin}} E)_{r(p)}$, and we have

$$T^l\alpha(\hat{D}) - \omega(\hat{D})(\alpha(p)) = D(\alpha(p)) - D(\alpha(p)) = 0$$

by the equivariance of α and the first property of a fibered connection form.

Let us show that $\nabla\alpha$ is equivariant. Let $\phi \in \mathrm{Bis}(\boldsymbol{GL}(E))$. As in Example 2.4, we consider ϕ as a diffeomorphism $E \to E$ that sends fibers to fibers linearly. Since α satisfies $\alpha \circ R_{\phi^{-1}} = \phi \circ \alpha$, we have

$$T^l\alpha \circ TR_{\phi^{-1}} = T\phi \circ T^l\alpha. \tag{46}$$

The second term satisfies

$$(R^*_{\phi^{-1}}(\omega(\alpha)))(Y) = \omega(\alpha)_{p\cdot\phi^{-1}}(TR_{\phi^{-1}}(Y)) \tag{47}$$
$$= \omega(TR_{\phi^{-1}}(Y))(\alpha(p\cdot\phi^{-1})) = (\mathrm{Ad}_\phi \circ \omega(Y))(\phi\circ\alpha(p))$$
$$= T\phi\circ\omega(Y)(\alpha(p)) = T\phi\circ\omega(\alpha)(Y)$$

for all $p \in P$, $Y \in T^l_p P$, and $\phi \in \mathrm{Bis}(\boldsymbol{GL}(E))$, where we used the equivariance of α and ω, and (19). But ϕ is linear on the fibers so we have $I \circ T\phi|_{\ker Tq_E} = \phi \circ I$. With (46) and (47), this shows that $\nabla\alpha$ is equivariant. Hence, $\nabla\alpha \in \Omega^1_{\mathrm{hor}}(P, E)^{\boldsymbol{GL}(E)}$.

The map ∇ is $\boldsymbol{L}$-equivariant since both parts $\alpha \mapsto T^l\alpha$ and $\alpha \mapsto \omega(\alpha)$ are.

Finally, it satisfies the Leibniz rule since the first term does and the second term is $C^\infty(P)^{\boldsymbol{GL}(E)}$-linear.

Step 2 (from connections to connection forms). Let

$$\nabla : \Omega^0_{\mathrm{hor}}(P, E)^{\boldsymbol{GL}(E)} \to \Omega^1_{\mathrm{hor}}(P, E)^{\boldsymbol{GL}(E)}$$

be an $\boldsymbol{L}$-equivariant map satisfying the Leibniz rule (44). Much as for the map I in Step 1 above, for each $e \in E_x$ there is a canonical map $V_e : E_x \to T^{\mathrm{vert}}_e E = \ker(Tq_E)_e$ such that $I \circ V_e = \mathrm{Id}$. Define a map $\omega : T^l P \to T^{\mathrm{lin}} E$ by

$$\omega(Y)(\alpha(p)) = (T^l\alpha)(Y) - V_{\alpha(p)}(\nabla\alpha)(Y) \tag{48}$$

for all $\alpha \in \Omega^0_{\mathrm{hor}}(P, E)^{\boldsymbol{GL}(E)}$, $Y \in T^l_p P$ and $p \in P$.

By Proposition 3.29, the equivariant maps $P \to E$ correspond to sections of $P(E) \to X$. Since there exist sections through any point, this shows that, given $p \in P$, any $e \in E_{r(p)} \subset E$ can be written as $\alpha(p)$ for some $\alpha \in \Omega^0_{\mathrm{hor}}(P, E)^{\boldsymbol{GL}(E)}$. Hence, (48) defines $\omega(Y) : E_{r(p)} \to TE$ on all of $E_{r(p)}$.

Let us show that for every $Y \in T^l_p P$ and $e \in E$, $\omega(Y)(e)$ is well defined by (48). Let $e \in E$ and let $\alpha, \alpha' \in \Omega^0_{\mathrm{hor}}(P, E)^{\boldsymbol{GL}(E)}$ taking the value e at p. Since $\alpha - \alpha'$ vanishes at p and is equivariant, it vanishes on the whole l-fiber through p. Hence $T^l(\alpha - \alpha')(Y) = 0$. On the other hand, the Leibniz rule (44) shows that $\nabla(\alpha - \alpha')(Y)$ only depends on the derivative of $\alpha - \alpha'$ in the direction of Y, which also vanishes. As a result, $\omega(Y)(e)$ is well defined by (48).

Let us show that $Y \mapsto \omega(Y)$ defines an anchored map $T^l P \to T^{\mathrm{lin}} E$ over $r : P \to N$. We only need to see that $\omega(Y)(e) \in T_e E$ and that $Tq(\omega(Y)(e)) = Tr(Y)$ for all $e \in E$ and $Y \in T^l_p P$ with $r(p) = q(e)$, and these statements are easily checked.

We now proceed to show that ω satisfies the three conditions of Definition 3.19.

Let $D \in \Gamma(T^{\mathrm{lin}} E)$ and $p \in P$. We have

$$T^l\alpha(\hat{D}_p) = \frac{d}{dt}\alpha(p\cdot(\exp tD)^{-1})\bigg|_{t=0} = \frac{d}{dt}\exp tD\cdot\alpha(p)\bigg|_{t=0} = D(\alpha(p)).$$

On the other hand, $V_{\alpha(p)}(\nabla\alpha)(\hat{D}_p) = 0$ since $\hat{D}_p \in \ker T\pi$. Hence, $\omega(\hat{D}) = D$.

Now, let $\phi \in \mathrm{Bis}(\boldsymbol{GL}(E))$. We have

$$\begin{aligned}\omega(TR_\phi Y)(\alpha(p\cdot\phi)) &= T^l\alpha(TR_\phi Y) - V_{\alpha(p\cdot\phi)}(\nabla\alpha)(TR_\phi Y)\\ &= T\phi^{-1}\circ T^l\alpha(Y) - V_{\phi\circ\alpha(p)}(\phi^{-1}\circ(\nabla\alpha)(Y))\\ &= T\phi^{-1}\circ(\omega(Y)(\alpha(p)))\end{aligned}$$

for all $\alpha \in \Omega^0_{\mathrm{hor}}(P,E)^{\boldsymbol{GL}(E)}$, $Y \in T^l_p P$ and $p \in P$. Hence,

$$(R^*_\phi\omega)(Y) = T\phi^{-1}\circ\omega(Y)\circ\phi = (\mathrm{Ad}_{\phi^{-1}}\circ\omega)(Y),$$

i.e., ω is $\boldsymbol{GL}(E)$-equivariant.

Let $g \in \mathrm{Bis}(\boldsymbol{L})$. Recall that ∇ is equivariant for the $\mathrm{Bis}(\boldsymbol{L})$-action (42) on $\Omega^k_{\mathrm{hor}}(P,E)^{\boldsymbol{GL}(E)}$. We have

$$\begin{aligned}\omega(TL_g Y)(\alpha(g\cdot p)) &= T^l\alpha(TL_g Y) - V_{\alpha(g\cdot p)}(\nabla\alpha)(TL_g Y)\\ &= T^l(g^{-1}\cdot\alpha)(Y) - V_{g^{-1}\cdot\alpha(p)}(\nabla(g^{-1}\cdot\alpha))(Y)\\ &= \omega(Y)((g^{-1}\cdot\alpha)(p)) = \omega(Y)(\alpha(g\cdot p))\end{aligned}$$

for all $\alpha \in \Omega^0_{\mathrm{hor}}(P,E)^{\boldsymbol{GL}(E)}$, $Y \in T^l_p P$ and $p \in P$. Hence, $\omega\circ TL_g = \omega$.

So ω is a fibered connection form on P.

Step 3 (bijection). Let us denote the associations (45) and (48) respectively by $\omega \mapsto \nabla^\omega$ and $\nabla \mapsto \omega_\nabla$. Recall that $I\circ V_e = \mathrm{Id}$ and $V_e\circ I|_{T_eE} = \mathrm{Id}$ for all $e \in E$. We have

$$\begin{aligned}(\nabla^{\omega_\nabla}\alpha)(Y) &= I\circ(T^l\alpha - \omega_\nabla(\alpha))(Y)\\ &= I\circ(T^l\alpha - T^l\alpha + V_{\alpha(p)}\circ\nabla(\alpha))(Y) = (\nabla\alpha)(Y)\end{aligned}$$

and

$$\begin{aligned}\omega_{\nabla^\omega}(\alpha)(Y) &= (T^l\alpha(Y) - V_{\alpha(p)}\circ(\nabla^\omega\alpha))(Y)\\ &= (T^l\alpha - T^l\alpha + \omega(\alpha))(Y) = \omega(\alpha)(Y)\end{aligned}$$

for all $\alpha \in \Omega^0_{\mathrm{hor}}(P,E)^{\boldsymbol{GL}(E)}$, $Y \in T^l_p P$ and $p \in P$, which completes the proof. □

4. Global Atiyah class

Throughout this section, we consider a *Lie groupoid pair* $(\boldsymbol{L}, \boldsymbol{A})$ over a manifold M, i.e., a Lie groupoid $\boldsymbol{L}$ over M and a closed wide Lie subgroupoid $\boldsymbol{A}$ of $\boldsymbol{L}$. We define, for any transitive Lie groupoid $\boldsymbol{U}$, the Atiyah class of a generalized morphism from $\boldsymbol{A}$ to $\boldsymbol{U}$ with respect to such a pair. We then specialize to the case where $\boldsymbol{U}$ is the frame groupoid $\boldsymbol{GL}(E)$ of a vector bundle over the same base as $\boldsymbol{A}$ and the generalized morphism is (the bundlization of) an $\boldsymbol{A}$-module structure on E. Finally, we consider the special case of the $\boldsymbol{A}$-module $E = L/A$ (see Section 4A), which defines the Atiyah class of the Lie groupoid pair $(\boldsymbol{L}, \boldsymbol{A})$.

4A. *$\boldsymbol{A}$-action on L/A.* Let L be the algebroid of $\boldsymbol{L}$ and $A \subset L$ the Lie subalgebroid corresponding to the Lie subgroupoid $\boldsymbol{A}$. Although there is no adjoint action of a Lie groupoid on its Lie algebroid, there is a canonical $\boldsymbol{A}$-action on the quotient vector bundle $L/A \to M$, as we proceed to show.

Proposition 4.1. *There is a unique left $\boldsymbol{A}$-module structure*

$$\boldsymbol{A} \times_M L/A \to L/A : (\gamma, \beta) \mapsto \mathrm{Ad}_\gamma \beta$$

on L/A which, when extended to bisections, satisfies

$$\mathrm{Ad}_\Sigma \bar{l} = \overline{\mathrm{Ad}_\Sigma l} \tag{49}$$

for all $\Sigma \in \mathrm{Bis}(\boldsymbol{A})$ and $l \in \Gamma(L)$. It satisfies, for all $\gamma \in \boldsymbol{A}$ and $\beta \in (L/A)_{s(\gamma)}$, the relation

$$\mathrm{Ad}_\gamma \beta = \overline{\kappa_{a^{-1}} \lambda}, \tag{50}$$

where $a \in T_\gamma \boldsymbol{A}$ is any tangent vector and $\lambda \in L$ is any element such that $T\boldsymbol{t}(u) = \rho(\lambda)$ and $\bar{\lambda} = \beta$. Above, $\lambda \mapsto \bar{\lambda}$ stands for the natural projection $L \to L/A$.

Proof. Let (a, λ) and (a', λ') be two pairs satisfying the conditions in the statement. Then $a - a' \in T_\gamma \boldsymbol{A}$ and $\lambda - \lambda' \in A$, and

$$\begin{aligned} \kappa_{a^{-1}} \lambda - \kappa_{(a')^{-1}} \lambda' &= a \bullet \lambda \bullet 0_{\gamma^{-1}} - a' \bullet \lambda' \bullet 0_{\gamma^{-1}} \\ &= (a - a') \bullet (\lambda - \lambda') \bullet 0_{\gamma^{-1}} \end{aligned}$$

is an element in A since all three factors are in $T\boldsymbol{A}$. This proves that $\mathrm{Ad}_\gamma \beta$ is well defined by (50).

The fact that it defines an $\boldsymbol{A}$-module structure is straightforward, and Lemma 3.10 shows that it is a solution of (49). On the other hand, solutions to (49) are obviously unique, which concludes the proof. □

Remark 4.2. As can easily be checked, for Lie groups, the action above is simply induced from the adjoint action of $\boldsymbol{A} \subset \boldsymbol{L}$ on L.

Remark 4.3. Alternatively, using the global structure of the Lie groupoid pair (and not just the $T\boldsymbol{A}$-action on L), there is a geometrical picture describing the above action. Indeed, the Lie groupoid $\boldsymbol{A}$ has a natural left action on the quotient space $\boldsymbol{L}/\boldsymbol{A}$, which is a manifold that fibers over M through $\underline{\boldsymbol{t}}$ as in (5). By construction, this action preserves the unit manifold M seen as a closed embedded submanifold of $\boldsymbol{L}/\boldsymbol{A}$, which automatically implies that the action by an element $\gamma \in \boldsymbol{A}$ with source x and target y maps $T_x\boldsymbol{L}/\boldsymbol{A}$ to $T_y\boldsymbol{L}/\boldsymbol{A}$. Since the latter are isomorphic to $(L/A)_x$ and $(L/A)_y$ respectively, we obtain a linear map that coincides with the map Ad_γ defined in (50).

4B. *Atiyah class.* Let P be a generalized morphism from $\boldsymbol{A}$ to a Lie groupoid $\boldsymbol{U}$ over N with Lie algebroid U. Let us denote by l and r the left and right moment maps of P, respectively.

An *L-U-connection over P* is an anchored map $\nabla : l^! L \to U$ over r, i.e., a bundle map such that

$$\begin{array}{ccc} l^! L & \xrightarrow{\nabla} & U \\ {\scriptstyle \rho = \mathrm{pr}_1}\downarrow & & \downarrow{\scriptstyle \rho} \\ TP & \xrightarrow{Tr} & TN \end{array}$$

commutes. It is said to *extend the generalized morphism* if $\nabla|_{l^! A} = \mathrm{Lie}(\Phi_P)$; see (28)–(29). It is said to be *$T\boldsymbol{U}$-equivariant* if $\nabla \circ R_u = \kappa_u \circ \nabla$ for all $u \in T\boldsymbol{U}$, where $R_u(X, (p, \lambda)) = (X \cdot u, (q, \lambda))$ (here, q is such that $X \cdot u \in T_q P$).

Definition 4.4. An L-U-connection ∇ over P is said to be *P-compatible* if it commutes with the $T(l^! \boldsymbol{A})$-actions, in the sense that the following condition holds:

(C) $\kappa_{T\Phi_P(a)} \circ \nabla = \nabla \circ \kappa_a$ for all $a \in T(l^! \boldsymbol{A})$.

Restricting (C) to zero vectors $(0, (p, 0)) \in l^! L$ and to $a = (0, \alpha^{-1}, X)$ with $\alpha \in A$ shows that P-compatible L-U-connections automatically extend the generalized morphism. Restricting (C) to $a = (X, 0_1, X \cdot u)$ with $(X, u) \in TP \times_{TN} T\boldsymbol{U}$ shows that P-compatible L-U-connections automatically are $T\boldsymbol{U}$-equivariant.

A $T\boldsymbol{U}$-equivariant L-U-connection over P is entirely determined by its restriction to a section of the left moment map, if such a section exists, i.e., if P is the bundlization of a morphism $\phi : \boldsymbol{A} \to \boldsymbol{U}$. So a $T\boldsymbol{U}$-equivariant L-U-connection over the bundlization of a morphism is equivalent to an anchored map $\nabla : L \to U$, and the former exists if and only if the latter does. For that reason, we make the following definition.

Definition 4.5. Given a morphism $\varphi : \boldsymbol{A} \to \boldsymbol{U}$, an anchored map ∇ from L to U is said to be *φ-compatible* if it commutes with the $T\boldsymbol{A}$-actions, in the sense that the following condition holds:

(C′) $\kappa_{T\varphi(a)} \circ \nabla = \nabla \circ \kappa_a$ for all $a \in T\boldsymbol{A}$.

We invite the reader to have the next example in mind.

Example 4.6. For an $\boldsymbol{A}$-module E, take $\boldsymbol{U} = \boldsymbol{GL}(E)$ its frame groupoid, and P the bundlization of the morphism $\boldsymbol{A} \to \boldsymbol{GL}(E)$ defining the $\boldsymbol{A}$-module structure. Then $T\boldsymbol{U}$-equivariant L-U-connections over P are equivalent to anchored maps $L \to T^{\mathrm{lin}} E$ or, after composing with the Lie algebroid isomorphism

$$\mathcal{L}^{-1} : T^{\mathrm{lin}} E \to \mathcal{D}(E)$$

defined in (12), to L-connections on E.

In fact, when the Lie groupoid $\boldsymbol{U}$ is over the same base M as $\boldsymbol{A}$ and $\boldsymbol{L}$ and φ is a morphism covering the identity of M, then φ sends bisections of $\boldsymbol{A}$ to bisections of $\boldsymbol{U}$ and $\mathrm{Lie}(\varphi)$ sends sections of A to sections of U, which makes sense of the following proposition.

Proposition 4.7. *Given a morphism $\varphi : \boldsymbol{A} \to \boldsymbol{U}$ between Lie groupoids over the same base, an anchored map ∇ from L to U is φ-compatible if and only if*

(C1) *it* ***extends the morphism*** $\mathrm{Lie}(\varphi) : A \to U$*, i.e.,*

$$\nabla|_A = \mathrm{Lie}(\varphi),$$

(C2) *it is* ***equivariant****, in the sense that for all bisections $\Sigma \in \mathrm{Bis}(\boldsymbol{A})$,*

$$\begin{array}{ccc} \Gamma(L) & \xrightarrow{\nabla} & \Gamma(U) \\ {\scriptstyle \mathrm{Ad}_\Sigma}\downarrow & & \downarrow{\scriptstyle \mathrm{Ad}_{\varphi(\Sigma)}} \\ \Gamma(L) & \xrightarrow{\nabla} & \Gamma(U) \end{array}$$

Proof. If restricted to the zero vectors in L and with $u = \upsilon^{-1}$ for $\upsilon \in A$, (C′) does indeed imply condition (C1). Also, condition (C2) follows from Lemma 3.10. The other implication follows from arguments similar to those in the proof of Proposition 3.21. □

Assume that $\boldsymbol{U}$ is a *transitive* Lie groupoid, and let $U_0 = \ker \rho_U$ be the isotropy Lie subalgebroid of U. Recall that U_0 is naturally a $\boldsymbol{U}$-module with action defined by

$$\upsilon \cdot u = \kappa_{0_{\upsilon^{-1}}}(u) = 0_\upsilon \bullet u \bullet 0_{\upsilon^{-1}}$$

for all $\upsilon \in \boldsymbol{U}$ and $u \in (U_0)_{\boldsymbol{s}(\upsilon)}$. The generalized morphism P therefore makes the associated vector bundle $P(U_0)$ an $\boldsymbol{A}$-module (see Definition 3.25). There is also an $l^!\boldsymbol{A}$-module r^*U_0 which is isomorphic to $l^*P(U_0)$ as an $l^!\boldsymbol{A}$-module.

Example 4.8. The frame groupoid in Example 4.6 is transitive, and its isotropy Lie algebroid is $U_0 = \mathrm{End}\, E$.

Proposition 4.9. *Let $(\boldsymbol{L}, \boldsymbol{A})$ be a Lie groupoid pair, and let P be a generalized morphism from $\boldsymbol{A}$ to a transitive Lie groupoid $\boldsymbol{U}$.*

(1) *There exist L-U-connections over P extending the generalized morphism.*

(2) *For any such L-U-connection ∇, there is a smooth groupoid 1-cochain $R^\nabla \in C^1(l^!\boldsymbol{A}, l^*(L/A)^* \otimes r^*U_0)$ defined for all $\gamma \in l^*\boldsymbol{A}$ and $\beta \in (l^*(L/A))_{\boldsymbol{t}(\gamma)}$ by*

$$R^\nabla(\gamma)(\beta) = (\kappa_{T\Phi_P(a)^{-1}} \circ \nabla \circ \kappa_a - \nabla)(\lambda), \tag{51}$$

where $a \in T_\gamma(l^!\boldsymbol{A})$ is any tangent vector and $\lambda \in l^!L$ is any element such that $T\boldsymbol{t}(a) = \rho(\lambda)$ and $\bar{\lambda} = \beta$.

(3) *The* 1*-cochain* R^∇ *is closed and its cohomology class* $\tilde{\alpha}_{(\boldsymbol{L},\boldsymbol{A}),P} = [R^\nabla]$ *is independent of the* L*-*U*-connection* ∇ *over* P *extending the generalized morphism.*

(4) *The class* $\tilde{\alpha}_{(\boldsymbol{L},\boldsymbol{A}),P} \in H^1(l^!\boldsymbol{A}, l^*(L/A)^* \otimes r^*U_0)$ *is zero if and only if there exists a* P*-compatible* L*-*U*-connection over* P*.*

Proof. (1) Any transitive Lie algebroid $U \to N$ has Lie algebroid connections [Mackenzie 2005, Corollary 5.2.7], i.e., anchored maps from TN to U over the identity. Let ∇^0 be such a connection. Let $B \subset l^!L$ be a vector subbundle supplementary to $l^!A$, and define a map $\nabla : l^!L \to U$ by $\nabla|_{l^!A} = \mathrm{Lie}(\Phi_P)$ and $\nabla|_B = \nabla^0 \circ Tr \circ \rho_{l^!L}$. By construction, ∇ is an anchored map which extends the morphism $\mathrm{Lie}(\Phi_P)$.

(2) Let (a, λ) and (a', λ') be two pairs satisfying the conditions in the statement. Then $a - a' \in T_\gamma l^!\boldsymbol{A}$ and $\lambda - \lambda' \in l^!A$, and

$$\begin{aligned}
&(\kappa_{T\Phi_P(a)^{-1}} \circ \nabla \circ \kappa_a - \nabla)(\lambda) - (\kappa_{T\Phi_P(a')^{-1}} \circ \nabla \circ \kappa_{a'} - \nabla)(\lambda') \\
&\qquad = T\Phi_P(a) \bullet \nabla(a^{-1} \bullet \lambda \bullet 0_\gamma) \bullet 0_{\Phi_P(\gamma)^{-1}} \\
&\qquad\qquad\qquad - T\Phi_P(a') \bullet \nabla((a')^{-1} \bullet \lambda' \bullet 0_\gamma) \bullet 0_{\Phi_P(\gamma)^{-1}} - \nabla(\lambda - \lambda') \\
&\qquad = T\Phi_P(a-a') \bullet \nabla((a-a')^{-1} \bullet (\lambda - \lambda') \bullet 0_\gamma) \bullet 0_{\Phi_P(\gamma)^{-1}} - \nabla(\lambda - \lambda') \\
&\qquad = T\Phi_P(a-a') \bullet \mathrm{Lie}(\Phi_P)((a-a')^{-1} \bullet (\lambda - \lambda') \bullet 0_\gamma) \bullet 0_{\Phi_P(\gamma)^{-1}} \\
&\qquad\qquad\qquad - \mathrm{Lie}(\Phi_P)(\lambda - \lambda') \\
&\qquad = 0.
\end{aligned}$$

This proves that the right-hand side of (51) only depends on γ and β, and justifies the definition of $R^\nabla(\gamma)(\beta)$.

(3) First note that if $\nu_0 \in U_0$ is written as $\nu_0 = \nu - \nu'$ with $\nu, \nu' \in U$, then for any $u \in T_{\upsilon^{-1}}\boldsymbol{U}$ such that $T\boldsymbol{t}(u) = \rho(\nu)$ we have

$$\upsilon \cdot \nu_0 = \kappa_{0_{\upsilon^{-1}}}(\nu_0) = \kappa_{u-u}(\nu - \nu') = \kappa_u(\nu) - \kappa_u(\nu').$$

Let $\gamma, \gamma' \in l^!\boldsymbol{A}$ be two composable elements and let $\beta \in l^*(L/A)_{\boldsymbol{t}(\gamma)}$. Let $a \in T_\gamma l^!\boldsymbol{A}$, $a' \in T_{\gamma'} l^!\boldsymbol{A}$, and $\lambda \in L_{\boldsymbol{t}(\gamma)}$ be such that $(a \bullet a')^{-1} \bullet \lambda$ is defined and $\overline{\lambda} = \beta$. We have

$$\begin{aligned}
&(\gamma \cdot R^\nabla(\gamma') + R^\nabla(\gamma))(\beta) \\
&\qquad\qquad = \Phi_P(\gamma) \cdot (R^\nabla(\gamma')(\mathrm{Ad}_{\gamma^{-1}} \beta)) + R^\nabla(\gamma)(\beta) \\
&\qquad\qquad = \kappa_{T\Phi_P(a)^{-1}} \circ (\kappa_{T\Phi_P(a')^{-1}} \circ \nabla \circ \kappa_{a'})(\kappa_a \lambda) \\
&\qquad\qquad\qquad - \kappa_{T\Phi_P(a)^{-1}} \circ \nabla(\kappa_a \lambda) + (\kappa_{T\Phi_P(a)^{-1}} \circ \nabla \circ \kappa_a)(\lambda) - \nabla(\lambda) \\
&\qquad\qquad = R^\nabla(\gamma \cdot \gamma')(\beta),
\end{aligned}$$

which shows that the cocycle identity (3) is satisfied.

Let now ∇, ∇' be two L-U-connections over P extending the morphism $\mathrm{Lie}(\Phi_P)$. We have

$$\begin{aligned}(R^{\nabla}(\gamma) - R^{\nabla'}(\gamma))(\beta) &= (\kappa_{T\Phi_P(a)^{-1}} \circ \nabla \circ \kappa_a)(\lambda) - \nabla(\lambda) - (\kappa_{T\Phi_P(a)^{-1}} \circ \nabla' \circ \kappa_a)(\lambda) - \nabla'(\lambda)\\ &= \kappa_{0_{\Phi_P(\gamma)^{-1}}} \circ (\nabla - \nabla') \circ \kappa_a(\lambda) - (\nabla - \nabla')(\lambda) = (\gamma \cdot \mu - \mu)(\lambda),\end{aligned}$$

where μ is $\nabla - \nabla'$ seen as an element of $\Gamma(l^*(L/A)^* \otimes r^*U_0)$. Hence, $\tilde{\alpha}_{(\boldsymbol{L},\boldsymbol{A}),P} = [R^{\nabla}]$ is independent of the chosen connection ∇.

(4) If ∇ is a P-compatible L-U-connection over P, then R^{∇} vanishes and so, too, does $\tilde{\alpha}_{(\boldsymbol{L},\boldsymbol{A}),P}$. Conversely, assume that $\tilde{\alpha}_{(\boldsymbol{L},\boldsymbol{A}),P} = 0$. Then for any L-U-connection over P extending the morphism $\mathrm{Lie}(\Phi_P)$, there exists $\mu \in \Gamma(l^*(L/A)^* \otimes r^*U_0)$ such that $R^{\nabla}(\gamma) = \gamma \cdot \mu - \mu$ for all $\gamma \in l^!\boldsymbol{A}$. Let $\bar{\mu} : l^!L \to U_0$ be the corresponding bundle map vanishing on $l^!A$, and let $\nabla' = \nabla - \bar{\mu}$. We get $0 = R^{\nabla}(\gamma) - (\gamma \cdot \mu - \mu) = R^{\nabla'}$, proving the claim. □

Since the left moment map is a surjective submersion, it induces an isomorphism in cohomology,

$$l^* : H^1(\boldsymbol{A}, (L/A)^* \otimes P(U_0)) \to H^1(l^!\boldsymbol{A}, l^*(L/A)^* \otimes l^*P(U_0)).$$

Using the isomorphism of $l^!\boldsymbol{A}$-modules $r^*U_0 \cong l^*P(U_0)$, we can now define the Atiyah class.

Definition 4.10. The *Atiyah class of the generalized morphism P with respect to the Lie groupoid pair* $(\boldsymbol{L}, \boldsymbol{A})$ is the class

$$\alpha_{(\boldsymbol{L},\boldsymbol{A}),P} \in H^1(\boldsymbol{A}, (L/A)^* \otimes P(U_0))$$

defined by $\alpha_{(\boldsymbol{L},\boldsymbol{A}),P} = (l^*)^{-1}\tilde{\alpha}_{(\boldsymbol{L},\boldsymbol{A}),P}$ where $\tilde{\alpha}_{(\boldsymbol{L},\boldsymbol{A}),P}$ is defined in Proposition 4.9.

When P is the bundlization of a morphism φ, the above Atiyah class may be directly defined using anchored maps from L to U.

The main example is when $\boldsymbol{U} = \boldsymbol{GL}(E)$ is the frame groupoid of a vector bundle $E \to M$, and $\varphi : \boldsymbol{A} \to \boldsymbol{GL}(E)$ is an $\boldsymbol{A}$-module structure on E. The Atiyah class, written $\alpha_{(\boldsymbol{L},\boldsymbol{A}),E}$, is an element of $H^1(\boldsymbol{A}, (L/A)^* \otimes \mathrm{End}\, E)$. Recall the definition of L-connections on a vector bundle from the end of Section 2B.

Corollary 4.11. *Let $(\boldsymbol{L}, \boldsymbol{A})$ be a Lie groupoid pair and E an $\boldsymbol{A}$-module.*

(1) *There exist L-connections on E extending the A-action.*

(2) *For any such L-connection ∇, there is a smooth groupoid 1-cochain $R^{\nabla} \in C^1(\boldsymbol{A}, (L/A)^* \otimes \mathrm{End}\, E)$ defined by*

$$R^{\nabla}(\gamma)(l, e) = \Sigma \star \nabla_{\mathrm{Ad}_{\Sigma^{-1}} l}(\Sigma^{-1} \star e) - \nabla_l e \tag{52}$$

for all bisections $\Sigma \in \mathrm{Bis}(\boldsymbol{A})$ and all sections $l \in \Gamma(L)$ and $e \in \Gamma(E)$.

(3) *The* 1*-cochain* $R^\nabla \in C^1(\boldsymbol{A}, (L/A)^* \otimes \operatorname{End} E)$ *is closed and its cohomology class* $\alpha_{(\boldsymbol{L},\boldsymbol{A}),E} = [R^\nabla]$ *is independent of the choice of* ∇.

(4) *The class* $\alpha_{(\boldsymbol{L},\boldsymbol{A}),E}$ *is zero if and only if there exists an* $\boldsymbol{A}$*-compatible* L*-connection on* E.

Here, we used the following definition.

Definition 4.12. An L-connection extending the A-action is said to be $\boldsymbol{A}$*-compatible* if the 1-cocycle R^∇ defined in (52) vanishes.

In the setting of Corollary 4.11, the class

$$\alpha_{(\boldsymbol{L},\boldsymbol{A}),E} \in H^1(\boldsymbol{A}, (L/A)^* \otimes \operatorname{End} E)$$

is the *Atiyah class of the* $\boldsymbol{A}$*-module* E *with respect to the Lie groupoid pair* $(\boldsymbol{L}, \boldsymbol{A})$.

The case of the $\boldsymbol{A}$ module L/A of Section 4A is of special interest.

Definition 4.13. The *Atiyah class of the Lie groupoid pair* $(\boldsymbol{L}, \boldsymbol{A})$ is the class

$$\alpha_{(\boldsymbol{L},\boldsymbol{A})} \in H^1(\boldsymbol{A}, (L/A)^* \otimes (L/A)^* \otimes L/A)$$

defined by $\alpha_{(\boldsymbol{L},\boldsymbol{A})} = \alpha_{(\boldsymbol{L},\boldsymbol{A}),L/A}$.

We relate our global Atiyah class to the Atiyah class of the A-module E with respect to (L, A), the construction of which we briefly recall, using [Chen et al. 2016] as a guideline. Let (L, A) be a Lie algebroid pair and let E be an A-module. Given an L-connection ∇ on E extending the flat A-connection $\nabla^A : A \to \mathcal{D}(E)$ that defines the module structure, the formula

$$\mathfrak{r}^\nabla(a)(l, e) = \nabla_a \nabla_l e - \nabla_l \nabla_a e - \nabla_{[a,l]} e \tag{53}$$

with $l \in \Gamma(L)$, $a \in \Gamma(A)$ and $e \in \Gamma(E)$ defines a Lie algebroid 1-cochain $\mathfrak{R}^\nabla \in C^1(A, (L/A)^* \otimes \operatorname{End} E)$ as follows. For all $\alpha \in A_x$, $\beta \in (L/A)_x$ and $\epsilon \in E_x$, set

$$\mathfrak{R}^\nabla(\alpha)(\beta, \epsilon) = \mathfrak{r}^\nabla(a)(l, e)|_x$$

with l any section of L such that $\bar{l_x} = \beta$ and a, e any sections through α and ϵ respectively. We say that ∇ is A*-compatible* when $\mathfrak{R}^\nabla = 0$. The 1-cochain $\mathfrak{R}^\nabla$ is closed and its cohomology class $\alpha_{(L,A),E} = [\mathfrak{R}^\nabla]$ is independent of the L-connection ∇ on E extending the natural flat A-connection. The class $\alpha_{(L,A),E}$ is zero if and only if there exists an A-compatible L-connection on E extending the natural A-action, defining therefore a class

$$\alpha_{(L,A),E} \in H^1(A, (L/A)^* \otimes \operatorname{End} E),$$

called the *Atiyah class of the* A*-module* E *with respect to the Lie algebroid pair* (L, A). The next proposition relates both classes; we refer to the work of Marius Crainic [2003] for a definition of the van Est functor.

Proposition 4.14. *Let $(\boldsymbol{L}, \boldsymbol{A})$ be a Lie groupoid pair, and (L, A) be its infinitesimal Lie algebroid pair. Let E be an $\boldsymbol{A}$-module. The van Est functor*

$$H^1(\boldsymbol{A}, (L/A)^* \otimes \operatorname{End} E) \to H^1(A, (L/A)^* \otimes \operatorname{End} E)$$

maps the Atiyah class of the $\boldsymbol{A}$-module E with respect to $(\boldsymbol{L}, \boldsymbol{A})$ to minus the Atiyah class of the A-module E with respect to (L, A).

Proof. Recall that the van Est functor simply assigns to an $\boldsymbol{A}$-cocycle Φ valued in an $\boldsymbol{A}$-module F the F-valued 1-form $\phi : \alpha \mapsto T\Phi(\alpha)$, with the understanding that $\alpha \in A_x$ is seen as an element of $T_x\boldsymbol{A}$. An important feature of this assignment is that for any section a of A, $\phi(a) = \frac{\mathrm{d}}{\mathrm{d}t}\Phi(\exp(ta))|_{t=0}$. Applying this construction to the Atiyah cocycle R^∇, we are left with the task of taking the derivative at $t = 0$ of the quantity

$$\exp(ta) \star \nabla_{\mathrm{Ad}_{\exp(ta)^{-1}} l}(\exp(ta)^{-1} \star e) - \nabla_l e$$

for arbitrary sections $e \in \Gamma(E)$ and $l \in \Gamma(L)$, which yields precisely minus the expression given in (53) in view of (17)–(21) and completes the proof. □

According to Theorem 3 in [Crainic 2003], the van Est map is an isomorphism in degree $\leq n$ and is injective in degree $n+1$ provided that the fibers of the source map of the Lie groupoid are n-connected. As an immediate corollary of the previous proposition, we have the following result:

Corollary 4.15. *Let $(\boldsymbol{L}, \boldsymbol{A})$ be a Lie groupoid pair with $\boldsymbol{A}$ source-connected, let (L, A) be its infinitesimal Lie algebroid pair, and E an $\boldsymbol{A}$-module. Then the Atiyah class of the A-module E with respect to (L, A) vanishes if and only if the Atiyah class of the $\boldsymbol{A}$-module E with respect to $(\boldsymbol{L}, \boldsymbol{A})$ vanishes.*

4C. ***Morita invariance.*** In this section, we prove that our Atiyah classes are invariant under Morita equivalences.

Let us first recall [Crainic 2003] how Morita equivalent Lie groupoids have equivalent categories of representations. Let $\boldsymbol{A}'$ and $\boldsymbol{A}$ be two Lie groupoids, and let Q be a generalized morphism from $\boldsymbol{A}'$ to $\boldsymbol{A}$. Given an $\boldsymbol{A}$-module E, Q and E define the associated $\boldsymbol{A}'$-module $Q(E) = (Q \times_M E)/\boldsymbol{A}$ (see Definition 3.25). Given an $\boldsymbol{A}$-module map $E \to F$, Q naturally induces an $\boldsymbol{A}'$-module map $Q(E) \to Q(F)$, and this defines a functor Q from the category of $\boldsymbol{A}$-modules to that of $\boldsymbol{A}'$-modules. When Q is a Morita morphism, the functor Q becomes an equivalence of categories (see (26)–(27)).

Recall also [Crainic 2003] that a Morita morphism Q induces an isomorphism, denoted by Q^*, from the Lie groupoid cohomology of $\boldsymbol{A}$ valued in E to the Lie groupoid cohomology of $\boldsymbol{A}'$ valued in $Q(E)$.

From now on, let us fix two Lie groupoid pairs, $(\boldsymbol{L}', \boldsymbol{A}')$ over M' and $(\boldsymbol{L}, \boldsymbol{A})$ over M. Recall the following notion from [Laurent-Gengoux 2009]. A *Morita morphism from* $(\boldsymbol{L}', \boldsymbol{A}')$ *to* $(\boldsymbol{L}, \boldsymbol{A})$ is a pair $(\widetilde{Q}, Q)$ with

(1) $\widetilde{Q}$ a Morita morphism from $\boldsymbol{L}'$ to $\boldsymbol{L}$,

(2) Q a Morita morphism from $\boldsymbol{A}'$ to $\boldsymbol{A}$,

(3) $i : Q \hookrightarrow \widetilde{Q}$ an inclusion map that makes Q an immersed submanifold of $\widetilde{Q}$,

such that

(1) the following diagram commutes:

(54)
$$\begin{tikzcd} & \widetilde{Q} \arrow[dl, "\tilde{l}"'] \arrow[dr, "\tilde{r}"] & \\ M' & Q \arrow[l, "l"] \arrow[r, "r"'] \arrow[u, "i"] & M \end{tikzcd}$$

(2) the inclusion map i is equivariant with respect to the left $\boldsymbol{A}'$-action and the right $\boldsymbol{A}$-action.

Note that such a Morita morphism may be expressed with bundlizations of morphisms as

(55)
$$(\widetilde{Q}, Q) \cong ((P_{\tilde{l}})^{-1}, (P_l)^{-1}) \circ (P_{\Phi_{\widetilde{Q}}}, P_{\Phi_Q}).$$

Theorem 4.16. *Let* $(\widetilde{Q}, Q)$ *be a Morita morphism from* $(\boldsymbol{L}', \boldsymbol{A}')$ *to* $(\boldsymbol{L}, \boldsymbol{A})$. *Let* P *be a generalized morphism from* $\boldsymbol{A}$ *to a transitive Lie groupoid* $\boldsymbol{U}$ *and let* $P' = Q \circ P$ *be its composition with* Q. *Then*

(1) *the functor* Q *maps the* $\boldsymbol{A}$*-module* $(L/A)^* \otimes P(U_0)$ *to the* $\boldsymbol{A}'$*-module* $(L'/A')^* \otimes P'(U_0)$,

(2) *the Lie groupoid cohomology isomorphism*

$$Q^* : H^1(\boldsymbol{A}, (L/A)^* \otimes P(U_0)) \to H^1(\boldsymbol{A}', (L'/A')^* \otimes P'(U_0))$$

associated to the Morita morphism Q *maps the Atiyah class of* P *with respect to* $(\boldsymbol{L}, \boldsymbol{A})$ *to the Atiyah class of* P' *with respect to* $(\boldsymbol{L}', \boldsymbol{A}')$.

We start with a lemma.

Lemma 4.17. *Let* $(\widetilde{Q}, Q)$ *be a Morita morphism from* $(\boldsymbol{L}', \boldsymbol{A}')$ *to* $(\boldsymbol{L}, \boldsymbol{A})$. *Then*

$$Q(L/A) \cong L'/A'$$

as $\boldsymbol{A}'$*-modules.*

Proof. Since $\widetilde{Q}$ is a Morita morphism from $\boldsymbol{L}'$ to $\boldsymbol{L}$, there is a natural base-preserving isomorphism (30) of Lie groupoids $\tilde{\Phi}_{\widetilde{Q}} : \tilde{l}^! \boldsymbol{L}' \to \tilde{r}^! \boldsymbol{L}$. Pulling back by the map

$i : Q \to \widetilde{Q}$ and using $\tilde{l} \circ i = l$ and $\tilde{r} \circ i = r$ yields an isomorphism $l^! \boldsymbol{L}' \to r^! \boldsymbol{L}$. Applying the Lie functor, we obtain a base-preserving Lie algebroid isomorphism

$$l^! L' \to r^! L.$$

Since Q is a Morita morphism from $\boldsymbol{A}'$ to $\boldsymbol{A}$, similarly, we obtain a base-preserving Lie algebroid isomorphism

$$l^! A' \to r^! A.$$

The inclusion map i of Q into $\widetilde{Q}$ being compatible with the bibundle structures (see (54)), there is a commutative diagram of Lie algebroids over Q,

$$\begin{tikzcd} l^! A' \arrow[r] \arrow[d, hook] & r^! A \arrow[d, hook] \\ l^! L' \arrow[r] & r^! L \end{tikzcd}$$

where the horizontal arrows are isomorphisms and the vertical arrows are inclusions. As a result, we get an isomorphism

$$l^! L' / l^! A' \to r^! L / r^! A \tag{56}$$

of vector bundles over Q. By construction, this isomorphism intertwines the $l^! \boldsymbol{A}$-module structure and the $r^! \boldsymbol{A}$-module structure.

Since l is a surjective submersion, the projection on the second component $l^! L' \to l^* L'$ induces an isomorphism

$$l^! L' / l^! A' \to l^*(L'/A'). \tag{57}$$

Let us prove that this isomorphism is in fact an $l^! \boldsymbol{A}'$-module isomorphism. Notice that bisections can be pulled-back — for Σ' a local bisection of $\boldsymbol{A}'$, a bisection of $l^! \boldsymbol{A}'$ is defined by

$$l^* \Sigma' = \{(q, \gamma', q') \mid \gamma' \in \Sigma', l(q) = \boldsymbol{t}(\gamma'), l(q') = \boldsymbol{s}(\gamma')\}. \tag{58}$$

Applying (49) to bisections and sections of the previous form, gives immediately that the natural projection from $l^! \boldsymbol{A}'$ to $\boldsymbol{A}'$ intertwines the module structures on $l^! L' / l^! A'$ and L'/A'. This implies the result. The same procedure applies with $\boldsymbol{A}$ and L/A, and yields an isomorphism of modules

$$l^*(L'/A') \to r^*(L/A). \tag{59}$$

Now, in view of Definition 3.25, $r^*(L/A)/\boldsymbol{A} = Q(L/A)$. Since $\boldsymbol{A}$ acts freely on the leaves of $l : Q \to M'$, we of course have $L'/A' \simeq l^*(L'/A')/\boldsymbol{A}$. Taking the quotient by the right action of $\boldsymbol{A}$ on both sides of (59) finally yields

$$L'/A' \simeq \frac{l^*(L'/A')}{\boldsymbol{A}} \simeq \frac{r^*(L/A)}{\boldsymbol{A}} = Q(L/A). \qquad \square$$

Proof of Theorem 4.16. We start with the first item. It is easy to check that the functor Q is compatible with duality and tensor products. Hence, item (1) follows from Lemma 4.17.

We now turn to item (2). Since $Q \mapsto Q^*$ is a functor and sends Morita morphisms to isomorphisms in cohomology, and since we have the decomposition (55), it suffices to prove the result for a Morita morphism of the kind $(P_{\tilde{\varphi}}, P_{\varphi})$ with $\tilde{\varphi}: \boldsymbol{L}' \to \boldsymbol{L}$ and $\varphi : \boldsymbol{A}' \to \boldsymbol{A}$ morphisms such that $\tilde{\varphi}|_{\boldsymbol{A}'} = \varphi$. In that case, we need to show that the top arrow in the diagram

$$\begin{CD} H^1(l^!\boldsymbol{A}, l^*(L/A)^* \otimes l^*P(U_0)) @>{(l^!\varphi)^*}>> H^1(l^!\boldsymbol{A}', l^*(L'/A')^* \otimes l^*P'(U_0)) \\ @VVV @VVV \\ H^1(\boldsymbol{A}, (L/A)^* \otimes P(U_0)) @>{\varphi^*}>> H^1(\boldsymbol{A}', (L'/A')^* \otimes P'(U_0)) \end{CD} \tag{60}$$

sends $\tilde{\alpha}_{(\boldsymbol{L},\boldsymbol{A}),P}$ to $\tilde{\alpha}_{(\boldsymbol{L}',\boldsymbol{A}'),P'}$. Here, $P' = P_\varphi \circ P \cong M' \times_M P$ and we have $\Phi_{P'} = \Phi_P \circ (l^!\varphi)$. Now, if $\nabla : l^!L \to U$ is an L-U-connection over P extending the generalized morphism, a direct computation shows that

$$(l^!\varphi)^* R^\nabla = R^{\nabla \circ \mathrm{Lie}(l^!\tilde{\varphi})},$$

which yields the result. □

5. Connections on homogeneous spaces

Throughout this section, $(\boldsymbol{L}, \boldsymbol{A})$ is a Lie groupoid pair integrating a Lie algebroid pair (L, A) over M, and $\boldsymbol{U}$ is a Lie groupoid over N.

5A. *Equivariant principal bundles.*

Theorem 5.1. *Let Q be an $\boldsymbol{L}$-equivariant principal $\boldsymbol{U}$-bundle over the homogeneous space $X = \boldsymbol{L}/\boldsymbol{A}$. Let P be a generalized morphism, given by Proposition 3.15, such that $Q \cong {}_{\boldsymbol{L}}\boldsymbol{L}_{\boldsymbol{A}} \circ P$. There is a bijection between the following affine spaces*:

(1) *The fibered connection forms on Q (Definition 3.19).*

(2) *The P-compatible L-U-connections (Definition 4.4).*

Proof. Without loss of generality, we may identify Q with ${}_{\boldsymbol{L}}\boldsymbol{L}_{\boldsymbol{A}} \circ P$.

Let $\nabla : l^!L \to U$ be a P-compatible L-U-connection. The elements of Q are equivalence classes $[(\gamma, p)]$ of pairs $(\gamma, p) \in \boldsymbol{L} \times_M^{s,l} P$. We use the same notation for tangent vectors $[(v, X)] \in T_{[(\gamma,p)]}Q$. There is a map

$$\tilde{\tau} : T^t\boldsymbol{L} \times_{TM} TP \to l^!L : (v, X) \mapsto (X, (p, \tau(v))),$$

where X is in T_pP (essentially, $\tilde{\tau} = \tau_{l^!\boldsymbol{L}}$). Define then $\omega : T^l Q \to U$ by

$$\omega([(v, X)]) = \nabla \circ \tilde{\tau}(v, X). \tag{61}$$

The equivariance properties of ∇ and τ and the identity $\Phi_P(p, \gamma^{-1}, \gamma \cdot p) = 1_{r(p)}$ for all compatible $\gamma \in \boldsymbol{A}$ and $p \in P$ imply that $\nabla \circ \tilde{\tau}$ is $\boldsymbol{A}$-basic (i.e., $T\boldsymbol{A}$-invariant), so ω is well defined. Now (B1) directly follows from the equivariance of ∇ and the identity $\Phi_P(p, 1, p \cdot \upsilon) = \upsilon$ for all compatible $p \in P$ and $\upsilon \in \boldsymbol{U}$, and (B2) follows from the fact that τ is left-invariant.

Conversely, let $\omega : T^l Q \to U$ be a fibered connection form on Q. Define, for all $(X, (p, \lambda)) \in l^! L$,

$$\nabla(X, (p, \lambda)) = \omega([(\lambda^{-1}, X)]). \tag{62}$$

For all $(X, (p, \lambda)) \in l^! L$ and $(X, a, X') \in T(l^! \boldsymbol{A})$, using successively (B1), the defining property of Φ_P, and (B2) we get

$$\begin{aligned}\kappa_{T\Phi_P(X,a,X')} \circ \nabla(X, (p, \lambda)) &= \omega([(\lambda^{-1}, X \cdot T\Phi_P(X, a, X'))]) \\ &= \omega([(\lambda^{-1}, a \cdot X')]) = \omega(0_\gamma \cdot [(\lambda^{-1} \bullet u, X')]) \\ &= \omega([((\kappa_a \lambda)^{-1}, X')]) = \nabla \circ \kappa_{(X,a,X')}(X, (p, \lambda)).\end{aligned}$$

This proves (C).

The two associations $\omega \mapsto \nabla$ and $\nabla \mapsto \omega$ are obvious inverses of each other, which concludes the proof. □

5B. ***Associated vector bundles.*** Consider now the case where $\boldsymbol{U} = \boldsymbol{GL}(E)$ for some vector bundle $E \to M$ and where P is the bundlization of a morphism $\varphi : \boldsymbol{A} \to \boldsymbol{GL}(E)$, i.e., of an $\boldsymbol{A}$-module structure on E. We thus have an $\boldsymbol{L}$-equivariant principal $\boldsymbol{GL}(E)$-bundle $Q = (\boldsymbol{L} \times_M \boldsymbol{GL}(E))/\boldsymbol{A}$ (see Examples 3.14 and 3.26 for more details). Composing Theorem 5.1 and Theorem 3.30 yields:

Theorem 5.2. *Let $(\boldsymbol{L}, \boldsymbol{A})$ be a Lie groupoid pair over M, and let E be an $\boldsymbol{A}$-module. There is a bijective correspondence between*

(1) *$\boldsymbol{A}$-compatible L-connections on E, and*

(2) *$\boldsymbol{L}$-invariant fibered connections on the associated vector bundle*
$$\frac{\boldsymbol{L} \times_M E}{\boldsymbol{A}} \to \boldsymbol{L}/\boldsymbol{A} \to M$$
defined in Example 3.26.

We thus arrive at the main theorem of this section.

Theorem 5.3. *Let $(\boldsymbol{L}, \boldsymbol{A})$ be a Lie groupoid pair over M. There is a bijective correspondence between*

(1) *$\boldsymbol{A}$-compatible L-connections on L/A, and*

(2) *$\boldsymbol{L}$-invariant fibrewise affine connections on $\boldsymbol{L}/\boldsymbol{A} \to M$.*

Proof. There is a natural $\boldsymbol{L}$-equivariant isomorphism

$$\theta : \frac{\boldsymbol{L} \times_M L/A}{\boldsymbol{A}} \to T^{\bar{t}}(\boldsymbol{L}/\boldsymbol{A})$$

of vector bundles over $\boldsymbol{L}/\boldsymbol{A}$, defined as follows. The projection $\pi : \boldsymbol{L} \to \boldsymbol{L}/\boldsymbol{A}$ induces an $\boldsymbol{L}$-equivariant map $\pi' : T^{\boldsymbol{t}}\boldsymbol{L} \to T^{\bar{\boldsymbol{t}}}(\boldsymbol{L}/\boldsymbol{A})$. Now the composition of the ($\boldsymbol{L}$-equivariant) map $\boldsymbol{L} \times_M L \to T^{\boldsymbol{t}}\boldsymbol{L} : (\gamma, \lambda) \mapsto 0_\gamma \bullet \lambda^{-1}$ with π' vanishes on $\boldsymbol{L} \times_M A$, hence descends to a map $\boldsymbol{L} \times_M L/A \to T^{\bar{\boldsymbol{t}}}(\boldsymbol{L}/\boldsymbol{A})$. The latter is $\boldsymbol{A}$-invariant, so that it descends to a map θ as above.

Through θ, $\boldsymbol{L}$-invariant fibered connections on the vector bundle

$$\frac{\boldsymbol{L} \times_M L/A}{\boldsymbol{A}} \to \boldsymbol{L}/\boldsymbol{A} \to M$$

become $\boldsymbol{L}$-invariant fibered connections on the vector bundle $T^{\bar{\boldsymbol{t}}}(\boldsymbol{L}/\boldsymbol{A}) \to \boldsymbol{L}/\boldsymbol{A} \to M$, so that the result follows by applying Theorem 5.2 to $E = L/A$. □

Remark 5.4. The correspondence of Theorem 5.2 is by construction obtained by composing the correspondences of Theorems 5.1 and 3.30. We give here a shorter description of it. Let ∇^E be an L-connection on E. There exists a unique fibered connection $\nabla^{\boldsymbol{s}^*E}$ on $\boldsymbol{s}^*E \to \boldsymbol{L} \xrightarrow{\boldsymbol{t}} M$ such that

$$\nabla^{\boldsymbol{s}^*E}_{L(l)} \boldsymbol{s}^* e = \boldsymbol{s}^* \nabla^E_l e,$$

where $L(l)$ is the left-invariant vector field associated to $l \in L$. The vector bundle $\boldsymbol{s}^*E \to \boldsymbol{L}$ is canonically isomorphic to the pullback of $(\boldsymbol{L} \times E)/\boldsymbol{A} \to \boldsymbol{L}/\boldsymbol{A}$ through $\boldsymbol{L} \to \boldsymbol{L}/\boldsymbol{A}$. If ∇^E is φ-compatible, then one can see that the fibered connection $\nabla^{\boldsymbol{s}^*E}$ is in fact the pullback of some (unique) fibered connection $\nabla^{(\boldsymbol{L}\times E)/\boldsymbol{A}}$ on the vector bundle $(\boldsymbol{L} \times E)/\boldsymbol{A} \to \boldsymbol{L}/\boldsymbol{A}$. Spelling out the construction, one can see that

$$\nabla^E \mapsto \nabla^{(\boldsymbol{L}\times E)/\boldsymbol{A}}$$

is the correspondence that we obtained.

We now derive an immediate consequence of Theorem 5.2 and the last item of Corollary 4.11.

Corollary 5.5. *Let $(\boldsymbol{L}, \boldsymbol{A})$ be a Lie groupoid pair over M, and let E be an $\boldsymbol{A}$-module. The Atiyah class of E with respect to $(\boldsymbol{L}, \boldsymbol{A})$ vanishes if and only if there exist $\boldsymbol{L}$-invariant fibered connections on the associated vector bundle $(\boldsymbol{L} \times_M E)/\boldsymbol{A} \to \boldsymbol{L}/\boldsymbol{A} \to M$.*

In the case where $E = L/A$, using Theorem 5.3 instead of Theorem 5.2 yields:

Corollary 5.6. *Let $(\boldsymbol{L}, \boldsymbol{A})$ be a Lie groupoid pair over M. The Atiyah class of the Lie groupoid pair $(\boldsymbol{L}, \boldsymbol{A})$ vanishes if and only if there exist $\boldsymbol{L}$-invariant fibrewise affine connections on $\boldsymbol{L}/\boldsymbol{A} \to M$.*

In view of Corollary 4.15, the following result can be derived:

Corollary 5.7. *Let $(\boldsymbol{L}, \boldsymbol{A})$ be a Lie groupoid pair over M with $\boldsymbol{A}$ source-connected, and let (L, A) be the corresponding infinitesimal Lie algebroid pair.*

(1) *The Atiyah class of an $\boldsymbol{A}$-module E with respect to (L, A) vanishes if and only if there exist $\boldsymbol{L}$-invariant fibered connections on the associated vector bundle*

$$\frac{\boldsymbol{L} \times_M E}{\boldsymbol{A}} \to \boldsymbol{L}/\boldsymbol{A} \to M.$$

(2) *The Atiyah class of the Lie algebroid pair (L, A) vanishes if and only if there exist $\boldsymbol{L}$-invariant fibrewise affine connections on $\boldsymbol{L}/\boldsymbol{A} \to M$.*

5C. *Reductive homogeneous spaces.* Consider a Lie group G viewed as a G-equivariant principal H-bundle over G/H for some closed Lie subgroup H. It is well known (see, e.g., [Kobayashi and Nomizu 1963, II, Theorem 11.1]) that the principal H-bundle G admits a G-invariant connection if and only if G/H is a *reductive homogeneous space*, in the sense that $\mathfrak{h}$ admits an Ad_H-invariant complement in $\mathfrak{g}$. In that case, any G-invariant principal U-bundle over G/H (and any associated vector bundle thereof) also admits a G-invariant connection.

A similar statement holds for Lie groupoid pairs. *For a Lie groupoid pair $(\boldsymbol{L}, \boldsymbol{A})$, the principal $\boldsymbol{A}$-bundle $\boldsymbol{L}$ admits an $\boldsymbol{L}$-invariant fibered connection form if and only if $\boldsymbol{L}/\boldsymbol{A}$ is a reductive homogeneous space, in the sense that there exists a vector subbundle B in L supplementary to A and which is invariant under the* $\mathrm{Bis}(\boldsymbol{A})$*-action on L. In that case, any $\boldsymbol{L}$-equivariant principal bundle over $\boldsymbol{L}/\boldsymbol{A}$ admits fibered connection forms.*

Indeed, by left-invariance, a fibered connection form $\omega : T^{\boldsymbol{t}}\boldsymbol{L} \to \boldsymbol{s}^*A$ is equivalent, through the formula $\omega = \underline{\omega} \circ \tau_{\boldsymbol{L}}$, to a projection $\underline{\omega} : L \to A$ which is anchored and invariant under the $\mathrm{Bis}(\boldsymbol{A})$-actions on L and A. The kernel of $\underline{\omega}$ is then the desired subbundle B. Note that the anchor map restricted to B necessarily vanishes, so $\boldsymbol{L}/\boldsymbol{A}$ is in some sense a "bundle of (Lie group) homogeneous spaces".

By Proposition 3.15, any $\boldsymbol{L}$-equivariant principal bundle Q over $\boldsymbol{L}/\boldsymbol{A}$ is a composition ${}_{\boldsymbol{L}}\boldsymbol{L}_{\boldsymbol{A}} \circ P$ with a generalized morphism P. Such morphisms always have a Maurer–Cartan form (see Remark 3.20), hence by Proposition 3.24 Q always admits fibered connection forms.

5D. *Proper Lie groupoids.* The vanishing theorem for proper Lie groupoids (see Proposition 1 in [Crainic 2003]) states that $H^d(\boldsymbol{A}, E) = 0$ for $d \geq 1$ whenever $\boldsymbol{A}$ is a proper Lie groupoid and E is an $\boldsymbol{A}$-module. Hence the Atiyah class of any generalized morphism from $\boldsymbol{A}$ to a transitive Lie groupoid $\boldsymbol{U}$ vanishes.

In particular, for such an $\boldsymbol{A}$,

(1) any equivariant principal $\boldsymbol{U}$-bundle over a homogeneous space $\boldsymbol{L}/\boldsymbol{A}$ with $\boldsymbol{U}$ transitive admits fibered connection forms,

(2) any equivariant vector bundle over a homogeneous space $\boldsymbol{L}/\boldsymbol{A}$ admits invariant connections,

(3) any homogeneous space $\boldsymbol{L}/\boldsymbol{A}$ admits invariant fibrewise affine connections.

Note that, in contrast to the Lie group case, homogeneous spaces of proper Lie groupoids are in general not reductive homogeneous spaces in the sense of Section 5C. Indeed, there might not even exist an anchored projection $\nabla : L \to A$ since this would imply that the anchor vanishes on the kernel of ∇.

6. Poincaré–Birkhoff–Witt theorem

In this section, for a Lie groupoid pair $(\boldsymbol{L}, \boldsymbol{A})$ we relate the vanishing of the Atiyah class (Definition 4.13) to the existence of an $\boldsymbol{A}$-equivariant Poincaré–Birkhoff–Witt map. The latter map is obtained as the infinite jet of the exponential map of an invariant connection on $\boldsymbol{L}/\boldsymbol{A}$ whose existence was shown in Corollary 5.6 to be equivalent to the vanishing of the Atiyah class.

6A. ***Exponential map of invariant connections.*** Let ∇ be a fibrewise affine connection on $\boldsymbol{L}/\boldsymbol{A} \to M$.

For any $x \in M$ there is, in view of (5), a natural isomorphism of vector spaces

$$T_x^{\underline{\boldsymbol{t}}}(\boldsymbol{L}/\boldsymbol{A}) \cong T_x^{\boldsymbol{t}}\boldsymbol{L}/T_x^{\boldsymbol{t}}\boldsymbol{A}.$$

Since the differentials at x of the inverse maps $\boldsymbol{i}$ of $\boldsymbol{L}$ and $\boldsymbol{A}$ restrict to isomorphisms $L_x \to T_x^{\boldsymbol{t}}\boldsymbol{L}$ and $A_x \to T_x^{\boldsymbol{t}}\boldsymbol{A}$, they further induce an isomorphism

$$T_x\boldsymbol{i} : (L/A)_x \simeq T_x^{\underline{\boldsymbol{t}}}(\boldsymbol{L}/\boldsymbol{A}). \tag{63}$$

Now, the exponential map $\exp_x^\nabla$ at x of the connection ∇ is a diffeomorphism from a neighborhood of $0 \in T_x^{\underline{\boldsymbol{t}}}(\boldsymbol{L}/\boldsymbol{A})$ to a neighborhood of x in the fiber $\underline{\boldsymbol{t}}^{-1}(x)$. Composing $\exp_x^\nabla$ with the isomorphism (63), we get a diffeomorphism from a neighborhood of 0 in L_x/A_x to a neighborhood of x in the fiber $\underline{\boldsymbol{t}}^{-1}(x)$. By a slight abuse of notation, we shall still denote by $\exp_x^\nabla$ this diffeomorphism. This construction can now be done at all points $x \in M$. We may now consider the assignment

$$\beta \mapsto \exp^\nabla_{q(\beta)}(\beta),$$

which is a diffeomorphism from a neighborhood $[M, L/A]$ of M in L/A to a neighborhood $[M, \boldsymbol{L}/\boldsymbol{A}]$ of M in $\boldsymbol{L}/\boldsymbol{A}$. We denote it by $\exp^\nabla : [M, L/A] \to [M, \boldsymbol{L}/\boldsymbol{A}]$.

Let us study the equivariance of $\exp^\nabla$. Notice first that $\exp^\nabla$ is a fibered diffeomorphism that respects M, i.e., the diagrams

$$\begin{tikzcd} & \boldsymbol{L}/\boldsymbol{A} \\ M \arrow[ur, "1"] \arrow[r, "0"'] & L/A \arrow[u, "\exp^\nabla"'] \end{tikzcd} \quad \text{and} \quad \begin{tikzcd} \boldsymbol{L}/\boldsymbol{A} \arrow[dr, "\underline{\boldsymbol{t}}"] & \\ L/A \arrow[u, "\exp^\nabla"] \arrow[r, "q"'] & M \end{tikzcd}$$

are commutative. The commutativity of these diagrams implies that, for all $\gamma \in \boldsymbol{A}$ whose action on a given $\beta \in L/A$ makes sense (i.e., when $\boldsymbol{s}(\gamma) = q(\beta)$), the action of γ on $\exp^\nabla(\beta)$ also makes sense (i.e., $\boldsymbol{s}(\gamma) = \boldsymbol{t} \circ \exp^\nabla(\beta)$), at least when $\exp^\nabla(\beta)$ is defined. Let U be a neighborhood of M in L/A on which exp is defined and let V be its image through the exponential map; we say that the diffeomorphism $\exp^\nabla$ is $\boldsymbol{A}$*-equivariant on* U when the equality

$$\exp^\nabla(\gamma \cdot \beta) = \gamma \cdot \exp^\nabla(\beta)$$

holds for all $\gamma \in \boldsymbol{A}$ and $\beta \in U \subset L/A$ such that $\boldsymbol{s}(\gamma) = q(\beta)$ and $\gamma \cdot \beta \in U$.

Theorem 6.1. *A Lie groupoid pair* $(\boldsymbol{L}, \boldsymbol{A})$ *has vanishing Atiyah class if and only if there exists an* $\boldsymbol{A}$*-equivariant diffeomorphism from a neighborhood of* M *in* L/A *to a neighborhood of* M *in* $\boldsymbol{L}/\boldsymbol{A}$*. In particular, under these equivalent conditions, the* $\boldsymbol{A}$*-action on* $\boldsymbol{L}/\boldsymbol{A}$ *is linearizable. For the "if" part, only the fibered* 2*-jet of such a diffeomorphism is needed.*

Proof. According to the fourth item in Corollary 4.11, the Atiyah class of $(\boldsymbol{L}, \boldsymbol{A})$ vanishes if and only if an $\boldsymbol{A}$-compatible L-connection on L/A exists. By Theorem 5.3, $\boldsymbol{A}$-compatible L-connections on L/A exist if and only if $\boldsymbol{L}$-invariant fibrewise affine connections on $\boldsymbol{L}/\boldsymbol{A} \to M$ exist. We are thus left the task of relating the existence of invariant fibrewise affine connections on $\boldsymbol{L}/\boldsymbol{A}$ to the existence of equivariant diffeomorphisms from a neighborhood of M in L/A to a neighborhood of M in $\boldsymbol{L}/\boldsymbol{A}$. The statement about the linearizability of the action will then follow from the linearity of the $\boldsymbol{A}$-action on L/A.

First, let ∇ be an $\boldsymbol{L}$-invariant fibrewise affine connection on $\boldsymbol{L}/\boldsymbol{A}$. For any diffeomorphism Ψ from $(\boldsymbol{L}/\boldsymbol{A})_x$ to $(\boldsymbol{L}/\boldsymbol{A})_y$ mapping x to y and preserving the connection ∇, the diagram

$$\begin{tikzcd}
T_x(\boldsymbol{L}/\boldsymbol{A})_x \arrow[r, "\exp^\nabla"] \arrow[d, "T_x\Psi"] & (\boldsymbol{L}/\boldsymbol{A})_x \arrow[d, "\Psi"] \\
T_y(\boldsymbol{L}/\boldsymbol{A})_y \arrow[r, "\exp^\nabla"] & (\boldsymbol{L}/\boldsymbol{A})_y
\end{tikzcd}$$

is commutative. Applying this to a left-translation $\Psi = L_\gamma$ for some $\gamma \in \boldsymbol{A}$ with source x and target y yields the desired result, since $TL_\gamma : T_x(\boldsymbol{L}/\boldsymbol{A})_x \to T_y(\boldsymbol{L}/\boldsymbol{A})_y$ coincides with the $\boldsymbol{A}$-action defined in Section 4A, after identifying $T_x(\boldsymbol{L}/\boldsymbol{A})_x$ with $(L/A)_x$ and $T_y(\boldsymbol{L}/\boldsymbol{A})_y$ with $(L/A)_y$.

Conversely, let ϕ be an $\boldsymbol{A}$-equivariant diffeomorphism from a neighborhood of the zero section in L/A to a neighborhood of M in $\boldsymbol{L}/\boldsymbol{A}$. Although it is not the exponential map of a connection, it does define a unique torsion-free fibrewise affine connection ∇ on $\boldsymbol{L}/\boldsymbol{A}$ whose geodesic symmetry agrees with that of ϕ up to order 2. Indeed, transporting ϕ using (63) and the transitive left $\boldsymbol{L}$-action yields a well-defined $\boldsymbol{L}$-equivariant diffeomorphism from a neighborhood of the zero section in $T^{\underline{t}}(\boldsymbol{L}/\boldsymbol{A})$ to a neighborhood of the diagonal in $\boldsymbol{L}/\boldsymbol{A} \times_M \boldsymbol{L}/\boldsymbol{A}$. Let us denote it by $\Phi : X_p \mapsto (p, \Phi_p(X_p))$. For each $p \in \boldsymbol{L}/\boldsymbol{A}$, let s_p be the fibrewise "geodesic symmetry" at p defined by $s_p(\Phi_p(X)) = \Phi_p(-X)$ for sufficiently small $X \in T_p^{\underline{t}}(\boldsymbol{L}/\boldsymbol{A})$. Then, we have $s_p(p) = p$ and $T_p^{\underline{t}} s_p = -\operatorname{Id}$, and the formula

$$(\nabla_X Y)_p = \tfrac{1}{2}[X, Y + (s_p)_* Y]_p$$

defines the announced connection [Bertelson and Bieliavsky 2015, Proposition 1.3]. It only depends on the 2-jet of each s_p at p, and thus of each Φ_p at p. It is $\boldsymbol{L}$-invariant since Φ and hence all s_p are $\boldsymbol{L}$-equivariant. □

6B. *Poincaré–Birkhoff–Witt theorem.* The space $J^\infty([M, L/A])$ of fibered (along the projection $L/A \to M$) jets at M of smooth real-valued functions on L/A is an algebra. It is also a $C^\infty(M)$-module. Let $\mathcal{I}([M, L/A])$ be the ideal of jets of smooth functions on $[M, L/A]$ vanishing identically on M, and consider the decreasing sequence of ideals $(\mathcal{I}^k([M, L/A]))_{k\geq 0}$ of jets along M of functions vanishing on M together with their k first derivatives. Let us denote by $\operatorname{Hom}_{C^\infty(M)}(J^\infty([M, L/A]), C^\infty(M))$ the dual relative to this filtration, that is, the space of $C^\infty(M)$-linear maps from $J^\infty([M, L/A])$ to $C^\infty(M)$ vanishing on $\mathcal{I}^k([M, L/A])$ for some integer k.

Remark 6.2. Let us recall that we do not need to consider the topological dual here. The $C^\infty(M)$-linear maps from $J^\infty([M, L/A])$ to $C^\infty(M)$ vanishing on $\mathcal{I}^k([M, L/A])$ for a given integer k are automatically isomorphic to the space of sections of an ordinary vector bundle over M. When M is a point, for instance, this dual is a vector space of finite dimension.

By construction, $\operatorname{Hom}_{C^\infty(M)}(J^\infty([M, L/A]), C^\infty(M))$ is a filtered coalgebra, with a filtration given by

$$\operatorname{Hom}_{C^\infty(M)}(J^\infty([M, L/A]), C^\infty(M)) = \bigcup_{k\geq 0} J^\infty([M, L/A]))_k^\perp$$

with $J^\infty([M, L/A])_k^\perp$ being, for all $k \geq 0$, the subspace of elements in

$$\operatorname{Hom}_{C^\infty(M)}(J^\infty([M, L/A]), C^\infty(M))$$

vanishing on $\mathcal{I}^k([M, L/A])$. The coalgebra structure is the dual of the algebra structure on $J^\infty([M, L/A])$ and is compatible with the filtration, since

$$\mathcal{I}^k([M, L/A])\mathcal{I}^{k'}([M, L/A]) \subset \mathcal{I}^{k+k'}([M, L/A]).$$

We now intend to describe this coalgebra explicitly. Recall that a section X of L/A can be seen as a vertical vector field $\overline{X}$ on the fibered manifold $L/A \to M$ that is constant on each fiber. The required filtered coalgebra isomorphism is obtained by mapping a section $X_1 \odot \cdots \odot X_k$ in $S^k(L/A)$ (with $X_1, \ldots, X_k \in \Gamma(L/A)$), to the element of $\mathrm{Hom}_{C^\infty(M)}(J^\infty([M, L/A]), C^\infty(M))$ given by

$$F \mapsto \overline{X}_1[\cdots \overline{X}_k[F]]|_M \tag{64}$$

for all $F \in J^\infty([M, L/A])$. The differential operator above vanishes for $F \in \mathcal{I}^k([M, L/A])$, and the correspondence obviously sends $S^k(L/A)$ bijectively to $J^\infty([M, L/A])_k^\perp$.

Lemma 6.3. *The map* (64) *induces a natural filtered coalgebra isomorphism from* $\Gamma(S(L/A))$ *to* $\mathrm{Hom}_{C^\infty(M)}(J^\infty([M, L/A]), C^\infty(M))$.

The same construction can be done considering $J^\infty([M, \boldsymbol{L}/\boldsymbol{A}])$, yielding a filtered coalgebra $\mathrm{Hom}_{C^\infty(M)}(J^\infty([M, \boldsymbol{L}/\boldsymbol{A}]), C^\infty(M))$ of fibered jets at M of smooth functions on $\boldsymbol{L}/\boldsymbol{A}$. Let $\mathcal{I}([M, \boldsymbol{L}/\boldsymbol{A}])$ be the ideal of smooth functions on $[M, \boldsymbol{L}/\boldsymbol{A}]$ vanishing identically on M, and consider the decreasing sequence of ideals $(\mathcal{I}^k([M, \boldsymbol{L}/\boldsymbol{A}]))_{k \geq 0}$ of jets of functions vanishing on M together with their k first derivatives. Let us denote by $\mathrm{Hom}_{C^\infty(M)}(J^\infty([M, \boldsymbol{L}/\boldsymbol{A}]), C^\infty(M))$ the dual relative to this filtration, i.e., the space of $C^\infty(M)$-linear maps from $J^\infty([M, \boldsymbol{L}/\boldsymbol{A}])$ (which is a $C^\infty(M)$-module since $\boldsymbol{L}/\boldsymbol{A}$ fibers over M) to $C^\infty(M)$ vanishing on $\mathcal{I}^k([M, \boldsymbol{L}/\boldsymbol{A}])$ for some integer k.

Since $\boldsymbol{L}$ acts on the left on $\boldsymbol{L}/\boldsymbol{A}$, a section X of L can be seen as a vector field along the fibers of $\boldsymbol{L}/\boldsymbol{A}$ that we denote by $\overline{X}$. Let us map an element $X_1 \cdots X_k$ in $U(L)$ (with $X_1, \ldots, X_k \in \Gamma(L)$), to the element of

$$\mathrm{Hom}_{C^\infty(M)}(J^\infty([M, \boldsymbol{L}/\boldsymbol{A}]), C^\infty(M))$$

given by

$$F \mapsto \overline{X}_k[\cdots \overline{X}_1[F]]|_M \tag{65}$$

for all $F \in J^\infty([M, L/A])$. The map above vanishes on $\mathcal{I}^k([M, \boldsymbol{L}/\boldsymbol{A}])$ and every element in $\mathrm{Hom}_{C^\infty(M)}(J^\infty([M, \boldsymbol{L}/\boldsymbol{A}]), C^\infty(M))$ vanishing on $\mathcal{I}^k([M, \boldsymbol{L}/\boldsymbol{A}])$ is uniquely a linear combination of differential operators of this form. Also, for $X_k \in \Gamma(A)$, the previous differential operator is clearly equal to zero, which eventually leads to the following lemma.

Lemma 6.4. *The map* (65) *induces a filtered coalgebra isomorphism from* $U(L)/U(L) \cdot \Gamma(A)$ *to* $\mathrm{Hom}_{C^\infty(M)}(J^\infty([M, \boldsymbol{L}/\boldsymbol{A}]), C^\infty(M))$.

Assume that we are given a diffeomorphism Φ from a neighborhood $[M, L/A]$ of M in L/A to a neighborhood $[M, \boldsymbol{L}/\boldsymbol{A}]$ of M in $\boldsymbol{L}/\boldsymbol{A}$ which is a *fibered map*, i.e., assume that the diagrams

$$\begin{tikzcd} & \boldsymbol{L}/\boldsymbol{A} \\ M \arrow[ur, "1"] \arrow[r, "0"'] & L/A \arrow[u, "\Phi"'] \end{tikzcd} \quad \text{and} \quad \begin{tikzcd} \boldsymbol{L}/\boldsymbol{A} \arrow[dr, "\underline{t}"] & \\ L/A \arrow[u, "\Phi"] \arrow[r, "q"'] & M \end{tikzcd} \tag{66}$$

are commutative. Since Φ is a diffeomorphism, its pullback

$$\Phi^* : J^\infty([M, \boldsymbol{L}/\boldsymbol{A}]) \to J^\infty([M, L/A]) \tag{67}$$

is an algebra isomorphism. The commutativity of the diagram on the right-hand side of (66) implies that Φ^* is $C^\infty(M)$-linear and the commutativity of the diagram on the left-hand side of (66) implies that the algebra isomorphism Φ^* restricts to an algebra isomorphism, valid for all integer k,

$$\Phi^* : \mathcal{I}^k([M, \boldsymbol{L}/\boldsymbol{A}]) \to \mathcal{I}^k([M, L/A]). \tag{68}$$

Altogether, relations (67) and (68) imply that the algebra isomorphism Φ^* can be dualized again to induce a filtered coalgebra isomorphism

$$\mathrm{Hom}_{C^\infty(M)}(J^\infty([M, L/A]), C^\infty(M)) \to \mathrm{Hom}_{C^\infty(M)}(J^\infty([M, \boldsymbol{L}/\boldsymbol{A}]), C^\infty(M)).$$

By Lemmas 6.3 and 6.4, Φ^* therefore induces a coalgebra isomorphism that we denote by

$$PBW_\Phi : \Gamma(S(L/A)) \to U(L)/U(L) \cdot \Gamma(A)$$

and call the *Poincaré–Birkhoff–Witt map of* Φ. By construction, PBW_Φ makes the diagram

$$\begin{tikzcd} \mathrm{Hom}_{C^\infty(M)}(J^\infty([M, L/A]), C^\infty(M)) \arrow[r] \arrow[d] & \mathrm{Hom}_{C^\infty(M)}(J^\infty([M, \boldsymbol{L}/\boldsymbol{A}]), C^\infty(M)) \arrow[d] \\ \Gamma(S(L/A)) \arrow[r, "PBW_\Phi"] & U(L)/U(L)\cdot\Gamma(A) \end{tikzcd} \tag{69}$$

commutative.

We now intend to explore the consequences of the existence of an $\boldsymbol{A}$-equivariant local diffeomorphism Φ. Every bisection Σ of $\boldsymbol{A}$ induces diffeomorphisms of both $\boldsymbol{L}/\boldsymbol{A}$ and L/A that we denote by $\underline{\Sigma}$. The equivariance of Φ means that the following diagram is commutative:

$$\begin{tikzcd} J^\infty([M, \boldsymbol{L}/\boldsymbol{A}]) \arrow[r, "\Phi^*"] \arrow[d, "\underline{\Sigma}^*"'] & J^\infty([M, L/A]) \arrow[d, "\underline{\Sigma}^*"] \\ J^\infty([M, \boldsymbol{L}/\boldsymbol{A}]) \arrow[r, "\Phi^*"] & J^\infty([M, L/A]) \end{tikzcd} \tag{70}$$

For all integer k, it also restricts to

$$\begin{tikzcd} \mathcal{I}^k([M, \boldsymbol{L}/\boldsymbol{A}]) \arrow[r, "\Phi^*"] \arrow[d, "\underline{\Sigma}^*"] & \mathcal{I}^k([M, L/A]) \arrow[d, "\underline{\Sigma}^*"] \\ \mathcal{I}^k([M, \boldsymbol{L}/\boldsymbol{A}]) \arrow[r, "\Phi^*"] & \mathcal{I}^k([M, L/A]) \end{tikzcd}$$

Altogether, these commutative diagrams allow the dualization of (70), to wit:

$$\begin{tikzcd} \mathrm{Hom}_{C^\infty(M)}(J^\infty([M,\boldsymbol{L}/\boldsymbol{A}]),C^\infty(M)) & \mathrm{Hom}_{C^\infty(M)}(J^\infty([M,L/A]),C^\infty(M)) \arrow[l, "\Phi"'] \\ \mathrm{Hom}_{C^\infty(M)}(J^\infty([M,\boldsymbol{L}/\boldsymbol{A}]),C^\infty(M)) \arrow[u, "\Sigma"] & \mathrm{Hom}_{C^\infty(M)}(J^\infty([M,L/A]),C^\infty(M)) \arrow[l, "\Phi"'] \arrow[u, "\Sigma"'] \end{tikzcd}$$

The isomorphism of filtered coalgebras described in Lemma 6.3 intertwines the action of the pseudogroup of local bisections $\mathrm{Bis}(\boldsymbol{A})$ on

$$\mathrm{Hom}_{C^\infty(M)}(J^\infty([M,\boldsymbol{L}/\boldsymbol{A}]),C^\infty(M))$$

with the action defined in Section 4A. The isomorphism of filtered coalgebras described in Lemma 6.4 intertwines the action of the pseudogroup $\mathrm{Bis}(\boldsymbol{A})$ on $\mathrm{Hom}_{C^\infty(M)}(J^\infty([M,\boldsymbol{L}/\boldsymbol{A}]),C^\infty(M))$ with the action on $U(L)/U(L)\cdot\Gamma(A)$ defined in Proposition 2.5. This proves, in view of (69), the commutativity of

$$\begin{tikzcd} U(L)/U(L)\cdot\Gamma(A) & \Gamma(S(L/A)) \arrow[l, "PBW_\Phi"'] \\ U(L)/U(L)\cdot\Gamma(A) \arrow[u, "\Sigma"] & \Gamma(S(L/A)) \arrow[l, "PBW_\Phi"'] \arrow[u, "\Sigma"'] \end{tikzcd}$$

Tracking the implications in the other direction, we get the following result.

Proposition 6.5. *Let $(\boldsymbol{L},\boldsymbol{A})$ be a Lie groupoid pair. For every $\boldsymbol{A}$-equivariant diffeomorphism Φ from a neighborhood of M in L/A to a neighborhood of M in $\boldsymbol{L}/\boldsymbol{A}$, the map $PBW_\Phi:\Gamma(S(L/A))\to U(L)/U(L)\cdot\Gamma(A)$ defined as above is a* $\mathrm{Bis}(\boldsymbol{A})$*-equivariant isomorphism of filtered coalgebras. Conversely, any such equivariant isomorphism of filtered coalgebras defines an infinite jet of equivariant diffeomorphism from a neighborhood of M in L/A to a neighborhood of M in $\boldsymbol{L}/\boldsymbol{A}$.*

As a direct application of Theorem 6.1 and Proposition 6.5, we get Theorem 6.6, which is an equivalent at the groupoid level of [Calaque 2014, Theorem 1.1], which was also re-proved in [Laurent-Gengoux et al. 2014] using different techniques.

Theorem 6.6. *A Lie groupoid pair $(\boldsymbol{L},\boldsymbol{A})$ has vanishing Atiyah class if and only if there exists a* $\mathrm{Bis}(\boldsymbol{A})$*-equivariant filtered coalgebra isomorphism from $\Gamma(S(L/A))$ to $U(L)/U(L)\cdot\Gamma(A)$.*

7. Local Lie groupoids

We sketch in this section what happens when we work with local Lie groupoids instead of Lie groupoids. Recall that unlike Lie algebras, which are always the tangent space at the unit element of a Lie group, Lie algebroids may not be the infinitesimal object of a Lie groupoid (see [Crainic and Fernandes 2003] for a characterization of integrable Lie algebroids). There is however always a *local*

Lie groupoid (see [Debord 2001, Section 3] for a definition) integrating a Lie algebroid A (as shown in [Crainic and Fernandes 2003, Corollary 5.1]). This local Lie groupoid is not unique: for instance one can always replace it by a neighborhood of the unit submanifold. For any A-module E, there exists moreover such a local Lie groupoid acting on E.

Now, for any Lie algebroid pair (L, A), the Lie algebroid L can be integrated to an $\boldsymbol{s}$-connected local Lie groupoid $\boldsymbol{L}$ and, upon replacing $\boldsymbol{L}$ by a neighborhood of M in $\boldsymbol{L}$ if necessary, we can assume that A is the Lie algebroid of a closed local $\boldsymbol{s}$-connected Lie subgroupoid $\boldsymbol{A} \subset \boldsymbol{L}$. In that case, we shall say that the pair $(\boldsymbol{L}, \boldsymbol{A})$ is a *local Lie groupoid pair* that integrates (L, A). Again, it is not unique. Since $\boldsymbol{A}$ is $\boldsymbol{s}$-connected (hence also $\boldsymbol{t}$-connected), the quotient $\boldsymbol{L}/\boldsymbol{A}$ coincides with the quotient of $\boldsymbol{L}$ by the foliation on $\boldsymbol{L}$ induced by the right Lie algebroid action of A. Since the tangent space of this foliation has, for all $m \in M$, no intersection with $T_m M \subset T_m \boldsymbol{L}$, $\boldsymbol{L}$ can be replaced by a wide, open, local Lie subgroupoid such that the quotient $\boldsymbol{L}/\boldsymbol{A}$ is a smooth manifold. By construction, this submanifold fibers over M and is acted upon on the left by $\boldsymbol{L}$.

Also, for every A-module E, upon shrinking both $\boldsymbol{L}$ and $\boldsymbol{A}$ if necessary, one can assume that E comes equipped with an $\boldsymbol{A}$-module structure, and the induced vector bundle $(\boldsymbol{L} \times_M E)/\boldsymbol{A} \to \boldsymbol{L}/\boldsymbol{A}$ is made sense of through the same construction. Theorems 5.2 and 5.3 extend to local Lie groupoid pairs.

Theorem 7.1. *Let (L, A) be a Lie algebroid pair over M, and let $E \to M$ be an A-module. Then, there exists a local Lie groupoid pair $(\boldsymbol{L}, \boldsymbol{A})$ integrating it such that $\boldsymbol{L}/\boldsymbol{A}$ is a manifold and E is an $\boldsymbol{A}$-module. Moreover, there is a bijective correspondence between*

(1) *A-compatible L-connections on E, and*

(2) *$\boldsymbol{L}$-invariant fibered connections on the associated vector bundle*

$$\frac{\boldsymbol{L} \times_M E}{\boldsymbol{A}} \to \boldsymbol{L}/\boldsymbol{A} \to M.$$

For $E = L/A$, the associated vector bundle $(\boldsymbol{L} \times_M E)/\boldsymbol{A} \to \boldsymbol{L}/\boldsymbol{A} \to M$ is isomorphic to the tangent bundle of the natural projection $\boldsymbol{L}/\boldsymbol{A} \to M$.

The definition of cohomology for a local Lie groupoid $\boldsymbol{A}$ (see Section 2A) must be adapted. Let $\boldsymbol{A}_n$ stand for the manifold of all n-tuples $(\gamma_1, \dots, \gamma_n) \in \boldsymbol{A}^n$ such that the product of any two successive elements is defined. Notice that M is for all $n \in \mathbb{N}$ a submanifold of $\boldsymbol{A}_n$ through the natural assignment $m \mapsto (\mathbf{1}(m), \dots, \mathbf{1}(m))$ (n times). For any $\boldsymbol{A}$-module E, the cohomology $H^\bullet(\boldsymbol{L}, E)$ is defined as being the germification around M of the complex that appears in (2), i.e., the cohomology of

$$C^0_M(\boldsymbol{A}, E) \xrightarrow{\partial_0} C^1_M(\boldsymbol{A}, E) \xrightarrow{\partial_1} C^2_M(\boldsymbol{A}, E) \xrightarrow{\partial_2} C^3_M(\boldsymbol{A}, E) \xrightarrow{\partial_3} \cdots$$

where, for all $n \in \mathbb{N}_*$, $C^n_M(\boldsymbol{A}, E)$ is the space of germs around M of smooth functions from $\boldsymbol{A}_n$ to E such that $F(\gamma_1, \dots, \gamma_n) \in E_{t(\gamma_1)}$ for all $(\gamma_1, \dots, \gamma_n) \in \boldsymbol{A}_n$ while the differential $\partial_n F$ is defined by the same formula, but taken at the level of germs around M. Definition 4.10 of the Atiyah class still makes sense, and Proposition 4.9 is easily adapted, as well as Corollary 4.11 at least for the case of interest for our purpose, namely A-modules.

More precisely, let (L, A) be a Lie algebroid pair and E an A-module. The first item in Corollary 4.11 deals only with algebroids, and therefore holds true again: there exist L-connections on E extending the A-action. To generalize the next items in Corollary 4.11, notice that, for local groupoids, bisections and the assignment κ defined in (33) still make sense and satisfy essentially the same properties, which allows us to extend our proofs to this context without additional difficulties. For any L-connection ∇ on E extending the A-action and for any local Lie groupoid pair $(\boldsymbol{L}, \boldsymbol{A})$ integrating (L, A), a smooth local groupoid 1-cochain $R^\nabla \in C^1(\boldsymbol{A}, (L/A)^* \otimes \operatorname{End} E)$ is still defined by

$$R^\nabla(\gamma)(l, e) = \Sigma \star \nabla_{\mathrm{Ad}_{\Sigma^{-1}} l}(\Sigma^{-1} \star e) - \nabla_l e \tag{71}$$

with $\Sigma \in \operatorname{Bis}(\boldsymbol{A})$ and $l \in \Gamma(L)$, $e \in \Gamma(E)$. It is still true that the 1-cochain $R^\nabla \in C^1(\boldsymbol{A}, (L/A)^* \otimes \operatorname{End} E)$ is closed, that its cohomology class $\alpha_{(\boldsymbol{L},\boldsymbol{A}),\varphi} = [R^\nabla]$ is independent of the choice of ∇ and that the class $\alpha_{(\boldsymbol{L},\boldsymbol{A}),\varphi}$ is zero if and only if there exists an $\boldsymbol{A}$-compatible L-connection on E.

Moreover, Corollary 4.15 holds and yields that the class $\alpha_{(\boldsymbol{L},\boldsymbol{A}),\varphi}$ is zero if the Atiyah class of E with respect to the Lie algebroid (L, A) is zero. Altogether, this last point and Theorem 7.1 imply a variation of Corollary 5.7, which is interesting to state explicitly.

Corollary 7.2. *Let (L, A) be a Lie algebroid pair over M and let E be an A-module. Then there exist a local Lie groupoid pair $(\boldsymbol{L}, \boldsymbol{A})$ integrating (L, A) with $\boldsymbol{A}$ source-connected and such that $\boldsymbol{L}/\boldsymbol{A}$ is a manifold and E is an $\boldsymbol{A}$-module. Moreover, E has vanishing Atiyah class with respect to (L, A) if and only if there exists an $\boldsymbol{L}$-invariant fibered connection on the associated vector bundle $(\boldsymbol{L} \times_M E)/\boldsymbol{A} \to \boldsymbol{L}/\boldsymbol{A} \to M$.*

For $E = L/A$ for instance, we obtain that there exist $\boldsymbol{L}$-invariant fibrewise affine connections on $\boldsymbol{L}/\boldsymbol{A} \to M$ when the Atiyah class of the Lie algebroid pair vanishes.

An $\boldsymbol{L}$-invariant fibrewise affine connection on $\boldsymbol{L}/\boldsymbol{A} \to M$ as in Corollary 7.2 is the only required object for all the arguments in Section 6B. We thus obtain:

Corollary 7.3. *A Lie algebroid pair (L, A) has vanishing Atiyah class if and only if there exists a filtered coalgebra isomorphism from $\Gamma(S(L/A))$ to $U(L)/U(L)\cdot\Gamma(A)$ which intertwines, for all $a \in \Gamma(A)$,*

(1) *the unique derivation of $\Gamma(S(L/A))$ which is given by $\rho(a)$ on smooth functions on M and by the canonical A-action on sections of $\Gamma(L/A)$, and*

(2) *the left multiplication* $L_a : U(L)/U(L) \cdot \Gamma(A) \to U(L)/U(L) \cdot \Gamma(A)$ *by* $a \in \Gamma(A)$.

Corollary 7.3 is the content of Theorem 1.1 in [Calaque 2014] when the Lie algebroids considered are over $\mathbb{R}$. When the Lie algebroid is over $\mathbb{C}$, however, the geometrical interpretation used here is not relevant anymore, and only the methods of [Calaque 2014] or [Laurent-Gengoux et al. 2014] remain valid. Also:

Theorem 7.4. *A Lie algebroid pair* (L, A) *over* M *has vanishing Atiyah class if and only if there exists a local Lie groupoid pair* $(\boldsymbol{L}, \boldsymbol{A})$ *integrating* (L, A) *with* $\boldsymbol{A}$ *source-connected and such that* $\boldsymbol{L}/\boldsymbol{A}$ *is a manifold equipped with an* $\boldsymbol{A}$*-equivariant diffeomorphism from a neighborhood of* M *in* L/A *to a neighborhood of* M *in* $\boldsymbol{L}/\boldsymbol{A}$. *In particular, under these equivalent conditions, the* $\boldsymbol{A}$*-action on* $\boldsymbol{L}/\boldsymbol{A}$ *is linearizable.*

8. Examples and applications

8A. ***Lie group pairs and homogeneous spaces.*** We now explore the case of Lie groups. We shall use the same terminology without the suffix "-oid" and simply speak of Lie group pairs, Lie algebra pairs and so on. Notice that, for $\mathfrak{g}$ a Lie algebra, a $\mathfrak{g}$-connection on a vector space E is simply a bilinear assignment $\mathfrak{g} \times E \to E$. In this case, our results give back well-known results on homogeneous spaces.

Let (G, H) be a Lie group pair, so H is a closed Lie subgroup of G, and let $(\mathfrak{g}, \mathfrak{h})$ be the corresponding Lie algebra pair. Consider the associated homogeneous space G/H. For E an H-module, the associated vector bundle is the vector bundle $(G \times E)/H \to G/H$. Also, the canonical H-module structure on $\mathfrak{g}/\mathfrak{h}$ described in Section 4A is simply induced by the adjoint action under the quotient map. Specializing to this case, Theorem 5.1 yields Wang's characterization [1958, p. 1], Theorem 5.2 yields Proposition 2.7 in [Bordemann 2012] and Theorem 5.3 yields Theorem 1 in [Wang 1958].

Remark 8.1. When H is not closed in G, or when we are only given a Lie algebra pair $(\mathfrak{g}, \mathfrak{h})$, we may consider local Lie groups as in Section 7 and obtain similar results.

Let us turn our attention to the case $E = \mathfrak{g}/\mathfrak{h}$, that is, let us explore the meaning of the vanishing of the Atiyah class of a Lie group pair. First, notice that the Atiyah class of a Lie algebra pair automatically vanishes in the following cases:

(1) When $\mathfrak{h}$ is reductive in $\mathfrak{g}$, i.e., when there exists an $\mathfrak{h}$-invariant subspace $\mathfrak{m}$ in direct sum (as vector spaces) with $\mathfrak{h}$ in $\mathfrak{g}$. In that case, extending the $\mathfrak{h}$-action on $\mathfrak{g}/\mathfrak{h}$ by zero on $\mathfrak{m}$ yields an $\mathfrak{g}$-connection on $\mathfrak{g}/\mathfrak{h}$ with vanishing Atiyah cocycle.

(2) When $\mathfrak{h}$ is semisimple, since then it has no first degree cohomology.

(3) When $\mathfrak{d}$ is the double of a Lie bialgebra $(\mathfrak{g}, \mathfrak{g}^*)$ arising from an r-matrix $r \in \mathfrak{g} \otimes \mathfrak{g}$, the Atiyah class of the Lie pair $(\mathfrak{d}, \mathfrak{g})$ vanishes.

Remark 8.2. Let us explain the third item: we owe this result to Khaoula Abdeljelil, who gave an explicit expression of a connection whose Atiyah cocycle is zero (see also the recent paper of Hong [2019] on this subject). It is, up to a scalar factor, given by $\nabla_\alpha \beta = \mathrm{ad}_{r^\#(\alpha)} \beta$ for all $\alpha, \beta \in \mathfrak{g}^*$. It can be seen conceptually as follows: Drinfeld [1989] showed that a bialgebra $\mathfrak{g}$ is a coboundary if and only if the associated infinitesimal homogeneous space $\mathfrak{d}/\mathfrak{g}$ is reductive, where $\mathfrak{d}$ is the double of $\mathfrak{g}$. Reductive homogeneous spaces are well known to have invariant connections [Nomizu 1954], hence vanishing Atiyah class.

In the case of Lie groups, Theorem 6.1 implies the following result.

Proposition 8.3. *A Lie group pair (G, H) has vanishing Atiyah class if and only if there exists an H-equivariant diffeomorphism from a neighborhood of 0 in $\mathfrak{g}/\mathfrak{h}$ to a neighborhood of eH in G/H. In particular, under these equivalent conditions, the H-action on G/H is linearizable.*

Now, let $D = G \bowtie H$ be a matched pair of Lie groups, i.e., G and H are two Lie subgroups such that the multiplication map m of D restricts to a diffeomorphism $m|_{G\times H} : G \times H \to D$. In this case, there is a D-equivariant diffeomorphism between D/G equipped with the natural left D-action and the Lie group H equipped with the natural left action of H and the dressing action of G. The following is an immediate consequence of Proposition 8.3.

Corollary 8.4. *Let $D = G \bowtie H$ be a matched pair of Lie groups. The Lie group pair (D, G) has vanishing Atiyah class if and only if the dressing action of G on H is linearizable.*

Applying this result to an integrable Lie bialgebra $\mathfrak{g}$ and its double $\mathfrak{d} = \mathfrak{g} \oplus \mathfrak{g}^*$, one sees that the vanishing of the Atiyah class implies that the dressing action of a Poisson–Lie group G on its dual G^* can be linearized in a neighborhood of the identity. Its linearized action is of course the coadjoint action; see [Lu 1990].

Alekseev and Meinrenken [2016] have proved that, for Poisson–Lie groups arising from an r-matrix, the Poisson structure on the dual group G^* is linearizable in a neighborhood of the identity, while our result gives that the dressing action of G on G^* is linearizable. These results are clearly related: the symplectic leaves of the Poisson structure on G^* coincide with the orbits of the dressing action [Lu 1990]. Notice that to linearize the Poisson structure and the dressing action are two different problems. An interesting question is to investigate whether or not the vanishing of the Atiyah class, which gives the linearizability of the dressing action, also implies the linearizability of the Poisson structure on G^*.

Remark 8.5. Since for Poisson–Lie groups, the leaves of the dressing action are precisely the symplectic leaves of the multiplicative Poisson structure while the leaves of the coadjoint action are precisely the symplectic leaves of the linear Poisson structure, it is tempting to believe that a diffeomorphism that intertwines both actions must be a Poisson diffeomorphism. As will be shown in [Abdeljelil and Laurent-Gengoux ≥ 2019], this is *not* the case: there are in general no G-equivariant Poisson diffeomorphisms between the Poisson–Lie group G^* and the linear Poisson structure on $\mathfrak{d}/\mathfrak{g} \simeq \mathfrak{g}^*$.

Given a G-invariant connection on G/H, one can H-equivariantly relate tensors on G/H in a neighborhood of the unit to tensors on $\mathfrak{g}/\mathfrak{h}$ in a neighborhood of zero.

Corollary 8.6. *A Lie group pair (G, H) has vanishing Atiyah class if and only if there exists an H-equivariant one-to-one correspondence between*

(1) *germs at eH of (k, l)-tensors on G/H, and*

(2) *germs at 0 of (k, l)-tensors on $\mathfrak{g}/\mathfrak{h}$ (considered as a manifold).*

This corollary might be more relevant when seen at the level of jets where it immediately implies the following result, which gives back Theorem 1.5 of [Calaque et al. 2013] for Lie algebras over $\mathbb{R}$.

Corollary 8.7. *A Lie group pair (G, H) has vanishing Atiyah class if and only if there exists an H-equivariant one-to-one correspondence between*

(1) *jets at eH of (k, l)-tensors on G/H, and*

(2) *elements in $\widehat{S}((\mathfrak{g}/\mathfrak{h})^*) \bigotimes \otimes^k (\mathfrak{g}/\mathfrak{h})^* \bigotimes \otimes^l (\mathfrak{g}/\mathfrak{h})$.*

8B. ***An interpretation of the Molino class of regular foliations.*** In this section, we give an interpretation of the Molino class of a foliation in terms of linearizability of monodromies. All foliations are assumed to be regular. Throughout, $\mathcal{F}$ is a foliation of rank r on a manifold M of dimension d.

We first fix our vocabulary and notation. We shall denote by $\mathcal{F}_m$ the leaf of $\mathcal{F}$ through $m \in M$, but we shall use the Latin letter F to denote a chosen particular leaf of $\mathcal{F}$. A submanifold T of M is said to be *transverse at $m \in F$ to the leaf F* if it intersects transversally F at m, i.e., if $T_m M = T_m F \oplus T_m T$. A foliation $\mathcal{T}$ on M, defined in a neighborhood $\mathcal{U}$ of the leaf F in $\mathcal{F}$, is said to be *transverse to $\mathcal{F}$* when for all $m \in \mathcal{U}$, the leaf $\mathcal{T}_m$ is transverse to the leaf $\mathcal{F}_m$. Given such a transverse foliation, and given a smooth path $\gamma : I = [0, 1] \to F$ in F, a *parallel lift of γ starting at $n \in \mathcal{T}_{\gamma(0)}$* is a path $\tilde{\gamma} : I \to \mathcal{U} \subset M$ satisfying

(1) $\tilde{\gamma}(0) = n$,

(2) $\tilde{\gamma}(t) \in \mathcal{F}_n$ for all $t \in I$, and

(3) $\tilde{\gamma}(t) \in \mathcal{T}_{\gamma(t)}$ for all $t \in I$.

When γ is given, a parallel lift starting at n exists for all n in a neighborhood of $\gamma(0)$ in $\mathcal{T}_{\gamma(0)}$. Moreover, when it exists, it is unique. This allows us to define the *parallel transport over a smooth path γ in F* as being the germ of local diffeomorphism from $\mathcal{T}_{\gamma(0)}$ to $\mathcal{T}_{\gamma(1)}$ around $\gamma(0)$ mapping a point $n \in \mathcal{T}_{\gamma(0)}$ to the value at $t = 1$ of the parallel lift of γ starting at n. Parallel transport is known to depend on the homotopy class of γ only and, when applied to loops at $m \in F$, it yields a group morphism from $\pi_1(F)$ to the germs of diffeomorphisms of $\mathcal{T}_m$ that we call *the monodromy of $\mathcal{F}$ at m with respect to $\mathcal{T}$*.

Remark 8.8. The monodromy does not depend on the transverse foliation $\mathcal{T}$. More precisely, given two transverse foliations $\mathcal{T}$ and $\mathcal{T}'$, the submanifolds $\mathcal{T}_m$ and $\mathcal{T}'_m$ are always diffeomorphic, in a neighborhood of m, in a canonical manner: the germ of diffeomorphism is obtained by restricting ourselves to a neighborhood $\mathcal{V}$ of m where $\mathcal{F}$ is described by the fibers of a surjective submersion, then by mapping a point in $\mathcal{T}_m \cap \mathcal{V}$ to the point (unique if it exists) in $\mathcal{T}'_m$ which is in the same fiber of this surjective submersion. The monodromies of $\mathcal{F}$ at m with respect to $\mathcal{T}$ and $\mathcal{T}'$ are intertwined by these canonical diffeomorphisms, as is easily seen.

We consider some particular families of submanifolds transversal to the leaves, that we describe as follows.

Definition 8.9. Let $\mathcal{F}$ be a foliation of rank r on a manifold M, and let $N_{\mathcal{F}} = TM/T\mathcal{F}$ be the normal bundle of this foliation. A *system of transversals* is a pair $(\mathcal{U}(N_{\mathcal{F}}), p)$ with $\mathcal{U}(N_{\mathcal{F}})$ a neighborhood of the zero section in the normal bundle $N_{\mathcal{F}}$ and $p : \mathcal{U}(N_{\mathcal{F}}) \to M$ a submersion admitting the zero section $i : M \to \mathcal{U}(N_{\mathcal{F}})$ as right-inverse.

Let us choose a metric on M, and let p be the composition of the identification $N_{\mathcal{F}} \cong T\mathcal{F}^{\perp} \subset TM$ with the exponential map of the Levi-Civita connection. Then there exists a neighborhood $\mathcal{U}(N_{\mathcal{F}})$ of the zero section such that $(\mathcal{U}(N_{\mathcal{F}}), p)$ is a system of transversals. Hence:

Lemma 8.10. *Every foliation admits a system of transversals.*

To see why the previously defined pairs $(\mathcal{U}(N_{\mathcal{F}}), p)$ deserve to be called "system of transversals", denote by $\mathcal{U}(N_{\mathcal{F}})_m$ the intersection of $\mathcal{U}(N_{\mathcal{F}})$ with the fiber over m of the canonical projection $\pi : N_{\mathcal{F}} \to M$. The restriction of π to $\mathcal{U}(N_{\mathcal{F}})$ is still denoted by the same letter. The local inverse theorem implies the following results:

(1) Upon shrinking $\mathcal{U}(N_{\mathcal{F}})$ if necessary, one can assume that for all $m \in \mathcal{U}(N_{\mathcal{F}})$, the image through p of $\mathcal{U}(N_{\mathcal{F}})_m$ is a submanifold of M transverse to $\mathcal{F}_m$ at m that we denote by $\mathcal{T}_m^p$.

(2) Upon shrinking $\mathcal{U}(N_{\mathcal{F}})$ if necessary, one can assume that for all leaves F of $\mathcal{F}$, the map $p : \pi^{-1}(F) \to M$ is a local diffeomorphism onto a neighborhood

$\mathcal{U}(F)$ of F in M. We call that local diffeomorphism a *local neighborhood diffeomorphism at the leaf* F.

(3) Upon shrinking $\mathcal{U}(N_{\mathcal{F}})$ if necessary, one can assume that for each leaf F of $\mathcal{F}$, the disjoint union

$$\bigsqcup_{m\in F} \mathcal{T}_m^p$$

is a foliation $\mathcal{T}^F$ of $\mathcal{U}(F)$ transverse to $\mathcal{F}$ (in a neighborhood of F).

A system of transversals $(\mathcal{U}(N_{\mathcal{F}}), p)$ that satisfies these conditions shall be called a *good system of transversals*.

For $(\mathcal{U}(N_{\mathcal{F}}), p)$ a good system of transversals, we now transport, for each leaf F of $\mathcal{F}$, the foliation $\mathcal{F}$ through the local neighborhood diffeomorphism at the leaf F. This defines a foliation on $\mathcal{U}(N_{\mathcal{F}})$ that we call the *monodromy foliation* and denote by $\mathcal{M}_{\mathcal{F}}$.

Notice that:

(1) When M has dimension d and $\mathcal{F}$ rank r, the monodromy foliation has rank r, but on a manifold of dimension $2d-r$.

(2) By construction, for each leaf F of $\mathcal{F}$, the leaves of $\mathcal{M}_{\mathcal{F}}$ through points above F are contained in $\pi^{-1}(F)$, i.e., the monodromy foliation is tangent to all the $\pi^{-1}(F)$.

Indeed, since the restriction $\mathcal{M}_{\mathcal{F}}|_{\pi^{-1}(F)}$ of $\mathcal{M}_{\mathcal{F}}$ to $\pi^{-1}(F)$ is diffeomorphic, as a foliated manifold, to a neighborhood of F in M, the following holds true by construction:

Proposition 8.11. *Let $\mathcal{F}$ be a foliation on a manifold M, let F be a leaf of $\mathcal{F}$ and let $m\in F$. For every good system of transversals $(\mathcal{U}(N_{\mathcal{F}}), p)$, the local neighborhood diffeomorphism at the leaf F intertwines*

(1) *the monodromy of $\mathcal{F}$ at m with respect to the transverse foliation $\mathcal{T}^F$, and*

(2) *the monodromy of the restriction of $\mathcal{M}_{\mathcal{F}}$ to $\pi^{-1}(F)$ at the point $i(m)$ with respect to the transverse foliation given by the fibers of $\mathcal{U}(N_{\mathcal{F}})|_F \to F$.*

Recall that every flat connection ∇ on a vector bundle $E \to N$ gives rise to a regular foliation $\mathcal{F}^{\nabla}$ on the total space of the vector bundle E: the leaf through $e\in E$ is by definition the subset of all points in E that can be reached from e by parallel transport over paths in M. The leaves of this foliation have the dimension of N and the zero section is a leaf. The same construction applies when $\mathcal{F}$ is a foliation on M and $E\to M$ is a vector bundle equipped with a flat foliated connection. When applied to the Bott connection (the canonical $T\mathcal{F}$-action on $N_{\mathcal{F}}$), this leads to a foliation on the normal bundle $N_{\mathcal{F}}\to M$ that we call the *Bott foliation*. We can now express the following notions.

Definition 8.12. Let $\mathcal{F}$ be a regular foliation on a manifold M.

(1) We say that *the monodromy around a given leaf F is linearizable* when for one (equivalently all) local transverse submanifolds $\mathcal{T}_m$ to F at one (equivalently all) points $m \in M$, the monodromy map $\pi_1(F) \to \mathrm{Diff}_m(\mathcal{T}_m)$ is conjugate to a linear representation of $\pi_1(F)$.

(2) We say that *all the monodromies are simultaneously linearizable* when the Bott foliation and the monodromy foliation (computed with the help of any (equivalently all) good systems of transversal) are diffeomorphic in a neighborhood of the zero section.

The next proposition justifies the assertion "all monodromies are simultaneously linearizable" used in the previous definition:

Proposition 8.13. *Let $\mathcal{F}$ be a regular foliation on a manifold M. If all the monodromies are simultaneously linearizable, then the monodromy around each leaf of $\mathcal{F}$ is linearizable. More precisely, the monodromy of each leaf F of $\mathcal{F}$ linearizes to the* ***holonomy*** *of the Bott connection on the restriction to F of the normal bundle.*

The previous proposition follows immediately from Proposition 8.11 together with the following obvious lemma:

Lemma 8.14. *Let ∇ be a flat connection on a vector bundle $E \to N$. For the associated foliation on E, the monodromy of the zero section $N \subset E$ with respect to the transverse foliation given by the fibers of $E \to N$ is by linear endomorphisms. These linear endomorphisms coincide with the holonomy of ∇.*

We now arrive at the main result of this section:

Theorem 8.15. *Let $\mathcal{F}$ be a regular foliation on a manifold M. The Atiyah class of the Lie algebroid pair $(TM, T\mathcal{F})$ vanishes if and only if all the monodromies are simultaneously linearizable. More precisely, if the monodromy of each leaf F of $\mathcal{F}$ linearizes to the* ***holonomy*** *of the Bott connection on the restriction to F of the normal bundle.*

By construction, the Atiyah class of the Lie algebroid pair $(TM, T\mathcal{F})$ coincides with the *Molino class* defined in [Molino 1973]. The proof of Theorem 8.15 shall of course make use of the Lie algebroid pair $(TM, T\mathcal{F})$. It is not relevant to assume that this Lie algebroid pair integrates to a Lie groupoid pair as there are many natural counter-examples; see [Moerdijk and Mrčun 2006, Examples 12]. For M simply connected, the Lie algebroid TM integrates to the pair Lie groupoid $M \times M \rightrightarrows M$, and $T\mathcal{F}$ integrates to a closed Lie subgroupoid of it if and only if $M/\mathcal{F}$ is a manifold (in which case it integrates to the Lie groupoid $M \times_{\mathcal{F}} M \rightrightarrows M$ of pairs of points in M which are in the same leaf of $\mathcal{F}$, i.e., in the same fiber of the natural projection $M \mapsto M/\mathcal{F}$).

Proof. Let us spell out what the construction, given in Section 7, of the quotient space $\boldsymbol{L}/\boldsymbol{A}$ gives when applied to the particular case of $L = TM$, $A = T\mathcal{F}$. A Lie groupoid $\boldsymbol{L}$ that integrates $L = TM$ is the pair groupoid $\boldsymbol{L} := M \times M \rightrightarrows M$. The Lie algebroid $A = T\mathcal{F}$ acts on $\boldsymbol{L}$ from both sides, i.e.,

(1) it acts on the left by mapping $u \in \Gamma(T\mathcal{F})$ to the vector field on $\boldsymbol{L}$ whose value at $(m, m') \in M \times M$ is $(u_m, 0) \in T_{(m,m')}M \times M \simeq T_m M \times T_{m'} M$,

(2) it acts on the right by mapping $u \in \Gamma(T\mathcal{F})$ to the vector field on $\boldsymbol{L}$ whose value at $(m, m') \in M \times M$ is $(0, -u_{m'}) \in T_{(m,m')}M \times M \simeq T_m M \times T_{m'} M$.

The quotient space $\boldsymbol{L}/\boldsymbol{A}$ can be made sense of as follows: it is the quotient of a neighborhood $\mathcal{U}$ of the diagonal $\Delta(M) \subset M \times M$ by the foliation given by the infinitesimal right action of $A = T\mathcal{F}$. By shrinking $\mathcal{U}$ if necessary, we can assume this quotient to be a manifold, that we denote by $\boldsymbol{L}/\boldsymbol{A}$.

Now, let $(\mathcal{U}(N_{\mathcal{F}}), p)$ be a good system of transversals, with $\mathcal{U}(N_{\mathcal{F}}) \subset N_{\mathcal{F}}$. There is a natural map from $\mathcal{U}(N_{\mathcal{F}})$ to $M \times M$ mapping $x \in N_{\mathcal{F}}|_m \cap \mathcal{U}(N_{\mathcal{F}})$ to $(m, p(m))$. Upon shrinking $\mathcal{U}(N_{\mathcal{F}})$ if necessary, we can assume that this map takes values in the open set $\mathcal{U}$. Upon shrinking $\mathcal{U}(N_{\mathcal{F}})$ once more if necessary, we can then assume that the composition

$$\Phi : \mathcal{U}(N_{\mathcal{F}}) \to \mathcal{U} \to \boldsymbol{L}/\boldsymbol{A} \tag{72}$$

is a local diffeomorphism. By construction, the diffeomorphism Φ defined in (72) intertwines

(1) the monodromy foliation of $\mathcal{U}(N_{\mathcal{F}})$, and

(2) the foliation on $\boldsymbol{L}/\boldsymbol{A}$ given by the left $A = T\mathcal{F}$-action.

By Theorem 7.4, the Atiyah class is zero if and only if there exists an A-equivariant diffeomorphism between $\boldsymbol{L}/\boldsymbol{A}$ and L/A. Since the foliation induced by the A-action on L/A is precisely the Bott foliation, we arrive at the desired condition in view of Lemma 8.14. □

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RANDOM MÖBIUS GROUPS, I: RANDOM SUBGROUPS OF PSL(2, $\mathbb{R}$)

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We introduce a geometrically natural probability measure μ on the group PSL(2, $\mathbb{R}$), identified as the group of all Möbius transformations of the hyperbolic plane, which is mutually absolutely continuous with respect to the Haar measure. Our aim is to study topological generation and random subgroups, in particular random two-generator subgroups where the generators are selected randomly. This probability measure in effect establishes an isomorphism between random n-generator groups and collections of n random pairs of arcs on the circle. Our aim is to estimate the likelihood that such a random group topologically generates (or, conversely, is discrete). We also want to calculate the precise expectation of associated parameters, the geometry and topology, and to establish the effectiveness of tests for discreteness. We achieve an interesting mix of bounds and precise results. For instance, if $f, g \in_* \mathrm{PSL}(2,\mathbb{R})$ (that is, selected via μ), then $0.85 < \Pr\{\overline{\langle f, g\rangle} = \mathrm{PSL}(2,\mathbb{R})\} < 0.9$, thus the probability the group is discrete is at least $\frac{1}{10}$ (Theorem 8.3) and this increases to $\frac{2}{5}$ if we condition the selection to hyperbolic elements (Theorem 11.6). Further, if ζ is a primitive n-th root of unity, $n \geq 2$, and $f(z) = \zeta z$ is the elliptic of order n, and we choose $g \in_* \mathrm{PSL}(2,\mathbb{R})$ conditioned to be hyperbolic, then $\Pr\{\overline{\langle f, g\rangle} = \mathrm{PSL}(2,\mathbb{R})\} = 1 - 2/n^2$ (Theorem 12.5). We establish results such as the p.d.f. for the translation length τ_f of a random hyperbolic to be $H[\tau] = -4/\pi^2 \tanh\frac{\tau}{2} \log\tanh\frac{\tau}{4}$ (Theorem 4.9), along with related geometric invariants.

1. Introduction

This article is motivated in part by generalisations of a couple of specific problems and then explores the more general question of random subgroups of PSL(2, $\mathbb{R}$).

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Here we will mean that generators are selected randomly from a probability distribution on $\mathrm{PSL}(2,\mathbb{R})$ and not the limiting random process as described in [Calegari and Walker 2015] and the references.

First, consider a well known and important result from [Kantor and Lubotzky 1990] (see also [Dixon 1969] and [Liebeck and Shalev 1995]) that shows that the probability that a pair of uniformly and randomly selected elements $u, v \in_u G$ of a classical finite group G generates tends to 1 as the order of the group tends to ∞. Here the notation $\in_u$ means randomly selected from the uniform distribution. So, for instance,

$$\mathbf{Pr}\{\langle u, v\rangle = \mathrm{PSL}(2,q) : u, v \in_u \mathrm{PSL}(2,q)\} \to 1 \quad \text{as } q \to \infty.$$

An earlier result of Auerbach [1934] shows that for a compact Lie group G, a generic pair (u, v) with respect to the product Haar measure on $G \times G$ topologically generates, that is

$$\mathbf{Pr}\{\overline{\langle u, v\rangle} = G : u, v \in_u G\} = 1.$$

There are very recent strengthenings of this result [Noskov 2018]. We ask if we can give meaning to, and answer, a similar question for a noncompact Lie group such as $\mathrm{PSL}(2,\mathbb{R})$ or $\mathrm{PSL}(2,\mathbb{C})$ where there can be no *invariant* probability measure.

For us, there are other questions as well. These are motivated by the increasing number of computer-supported searches of moduli spaces of discrete groups to solve problems in geometry and topology in recent times. These include the smallest volume hyperbolic manifold [Gabai et al. 2011], the noncompact manifold [Cao and Meyerhoff 2001], the orbifold (Siegel's problem) [Gehring and Martin 2009; Marshall and Martin 2012] and perhaps the biggest search of all in [Gabai et al. 2003] establishing topological rigidity. Many of these searches are based on tests for discreteness and related geometric estimates. Thus we ask how effective are elementary discreteness tests such as Jørgensen's inequality? This question can be phrased as follows: Suppose we somehow choose $u, v \in \mathrm{PSL}(2,\mathbb{C})$, what is the probability that $|\operatorname{tr}^2(u) - 4| + |\operatorname{tr}[u, v] - 2| \le 1$?

Another question is, given $\langle u, v\rangle$ discrete in $\mathrm{PSL}(2,\mathbb{R})$ or $\mathrm{PSL}(2,\mathbb{C})$, what is the distribution of the possible topologies of the quotient of the natural action on hyperbolic space. As an example, if we choose two "random" hyperbolic elements which generate a discrete group, then generically the quotient space is either the two-sphere with three holes, or a torus with one hole, with the latter occurring with probability $\frac{1}{3}$ and determined by whether or not the axes cross. We might also ask for the distribution of the dimension of the limit set, or shortest geodesic and so forth. We will answer some of these questions here and leave others to a sequel. For groups generated by two nilpotent elements (parabolic) of $\mathrm{PSL}(2,\mathbb{C})$, we give explicit answers in [Martin et al. 2019].

In each case there are a few problems to address: what generate means, how to measure effectiveness in a probabilistic sense, and what the "correct" probability density is. The first problem is straightforward.

Definition. Let G be a topological group. We say $g_1, g_2, \ldots, g_n$ *topologically generate* if

$$\overline{\langle g_1, g_2, \ldots, g_n \rangle} = G. \tag{1.1}$$

Notice that if G is a Lie group, then the left-hand side is a closed Lie subgroup, and so a Lie group itself. In $\mathrm{PSL}(2, \mathbb{R})$ these closed Lie subgroups can only be finite, discrete, $\mathbb{R}$ or $\mathbb{S}$. While in $\mathrm{PSL}(2, \mathbb{C})$ we have the same description if we add $\mathrm{PSL}(2, \mathbb{R})$. As an example, the n-torus $T^n = \overline{\langle a \rangle}$ for a generic $a \in T^n$ (with respect to the usual volume form). Advancing Auerbach's result, Noskov [2018] proved that for any compact simple Lie group G and any $g \in G \setminus \{I\}$ the subset of $\{h \in G : \overline{\langle g, h \rangle} = G\}$ is nonempty and Zariski open in G.

Now we must discuss probability measures. In the case of locally compact topological groups (which we will not stray from) there is always an invariant Haar measure. However, there can be no invariant probability measure unless the group is compact. Thus for $\mathrm{PSL}(2, \mathbb{R})$ and $\mathrm{PSL}(2, \mathbb{C})$, our first significant problem is to define a geometrically natural probability measure on these spaces. Desirable properties should be that it is mutually absolutely continuous with respect to Haar measure, and invariant under the maximal compact subgroup. This latter property is useful from a computational point of view when using the Iwasawa decomposition. Another desirable property would be that the measure is "geometrically natural" and, finally, that we are able to be compute with it. Unfortunately this will also mean that parabolic elements and elements with a specific finite order occur with probability zero since this is the case for Haar measure. We deal with these cases by conditioning the selection.

In this paper we will focus on the case of $\mathrm{PSL}(2, \mathbb{R})$. This group acts as Möbius transformations (that is, linear fractional transformations or isometries) of hyperbolic 2-space. For us a random group will mean a finitely generated subgroup of $\mathrm{PSL}(2, \mathbb{R})$ where the generators are selected from our probability measure. Our ultimate aim is to study random subgroups of $\mathrm{PSL}(2, \mathbb{C})$ viewed as isometries of hyperbolic 3-space, but the two-dimensional case is quite distinct in many ways — for instance, since the trace is a continuous function to $\mathbb{R}$, the set of precompact cyclic subgroups (the elliptic elements) has nonempty interior, and therefore will have positive measure in any reasonable imposed measure (for our measure, the set of elliptics and the set of hyperbolics are both of measure equal to $\frac{1}{2}$). For $\mathrm{PSL}(2, \mathbb{C})$ this should not be the case.

However, the motivation for the probability measure we chose is similar in both cases. We seek something "geometrically natural" and with which we can compute. We should expect that almost surely (that is, with probability 1) a finitely generated subgroup of the Möbius group is free.

Let us give a couple of examples of the sorts of results we present. We write $f \in_* \mathrm{PSL}(2, \mathbb{R})$ to mean that f is a random variable in $\mathrm{PSL}(2, \mathbb{R})$ selected using the probability density described in Section 2A, although in what follows we chose a Möbius representation for $\mathrm{PSL}(2, \mathbb{R})$.

Theorem 1.2. (1) *Suppose* $f, g \in_* \mathrm{PSL}(2, \mathbb{R})$. *Then*

$$0.85 < \mathbf{Pr}\{\overline{\langle f, g\rangle} = \mathrm{PSL}(2, \mathbb{R})\} < 0.9.$$

(2) *Suppose* $f, g \in_* \mathrm{PSL}(2, \mathbb{R})$ *are hyperbolic. Then*

$$\tfrac{2}{5} < \mathbf{Pr}\{\overline{\langle f, g\rangle} = \mathrm{PSL}(2, \mathbb{R})\} < \tfrac{3}{5}.$$

(3) *For* $f \in_* \mathrm{PSL}(2, \mathbb{R})$ *hyperbolic, the p.d.f. for the translation length* $\tau(f)$ *is*

$$H[\tau] = -\frac{4}{\pi^2}\ \tanh\frac{\tau}{2}\ \log\tanh\ \frac{\tau}{4}.$$

We also consider such things as the probability distribution of the trace of f, the probability that the axes of randomly chosen hyperbolic generators cross and so forth. Finally we look at some specific cases where the calculations simplify a bit. For instance we prove the following theorem.

Theorem 1.3. *Let* $f(z) = \zeta^n z$, n *be an integer at least* 2, *and let* $g \in_* \mathrm{PSL}(2, \mathbb{R})$ *be hyperbolic. Then*

$$\mathbf{Pr}\big\{\overline{\langle f, g\rangle} = \mathrm{PSL}(2, \mathbb{R})\big\} = 1 - \frac{2}{n^2}.$$

To study these questions, our main idea is to set up a topological isomorphism between n pairs of random arcs on the circle and n-generator Möbius groups. We then determine the statistics of a random cyclic group completely and then consider pairs of generators. Unfortunately we are unable to determine the statistics of commutators of pairs of generators. This is an important challenge with topological consequences and which we only partially resolve.

2. Random Möbius groups

We introduce specific definitions in the context of Möbius groups of the hyperbolic plane, identified as the unit disk with the hyperbolic metric. These will naturally motivate more general definitions for the case of Möbius groups of hyperbolic 3-space in later work.

If $A \in \mathrm{PSL}(2, \mathbb{C})$ has the form

$$A = \pm \begin{pmatrix} a & c \\ \bar{c} & \bar{a} \end{pmatrix}, \quad |a|^2 - |c|^2 = 1, \tag{2.1}$$

then the associated linear fractional transformation $f : \hat{\mathbb{C}} \to \hat{\mathbb{C}}$ defined by

$$f(z) = \frac{az + c}{\bar{c}z + \bar{a}} \tag{2.2}$$

preserves the unit circle since

$$\left| \frac{az + c}{\bar{c}z + \bar{a}} \right| = |\bar{z}| \left| \frac{az + c}{\bar{a}\bar{z} + \bar{c}|z|^2} \right|,$$

with the implication that $|z| = 1$ implies $|f(z)| = 1$.

The rotation subgroup $\boldsymbol{K}$ of the disk, $z \mapsto \zeta^2 z$, $|\zeta| = 1$, and the nilpotent or parabolic subgroup $\boldsymbol{P}$ (conjugate to the translations) have the respective representations

$$\begin{pmatrix} \zeta & 0 \\ 0 & \bar{\zeta} \end{pmatrix}, \quad |\zeta| = 1, \quad \begin{pmatrix} 1 + it & t \\ t & 1 - it \end{pmatrix}, \quad t \in \mathbb{R}.$$

The group of all matrices satisfying (2.1) will be denoted $\mathcal{F}$. It is not difficult to construct an algebraic isomorphism $\mathcal{F} \equiv \mathrm{PSL}(2, \mathbb{R}) \equiv \mathrm{Isom}^+(\mathbb{H}^2)$, the isometry group of two-dimensional hyperbolic space (see [Beardon 1983]) and we will often abuse notation and use A from (2.1) and the mapping f from (2.2) interchangeably. Despite some efforts to directly use $\mathrm{PSL}(2, \mathbb{R})$, we feel the approach we take is geometrically more natural by working in $\mathcal{F}$. In particular, our measures are obviously invariant under the action of the compact group $\boldsymbol{K}$. We also seek distributions from which we can make explicit calculations and which are geometrically natural (see, in particular, Lemma 4.2).

2A. ***The probability distribution.*** Our probability space is $(\mathcal{F}, \mu_{\mathcal{F}})$, the space of matrices with the following imposed distributions of the entries of an element of $\mathcal{F}$.

(i) $\zeta = a/|a|$ and $\eta = c/|c|$ are chosen uniformly in the circle $\mathbb{S}$, with arclength measure.

(ii) $t = |a| \geq 1$ is chosen so that

$$2 \arcsin(1/t) \in [0, \pi]$$

is uniformly distributed.

Notice that the product $\zeta\eta$ is uniformly distributed on the circle as a simple consequence of the rotational invariance of arclength measure. Further, this measure is equivalent to the uniform probability measure $\arg(a) \in [0, 2\pi]$. It is thus clear that this selection process is invariant under the rotation subgroup of the circle.

Next, if θ is uniformly distributed in $[0, \pi]$, then the probability distribution function for $\sin\theta$ is $\frac{1}{\pi}(1/\sqrt{1-y^2})$ for $y \in [-1, 1]$. Since $t \mapsto 1/t$, for $t > 0$, is strictly decreasing, we can use the change of variables formula for distribution functions to deduce the p.d.f. for $|a|$.

Lemma 2.3. *The random variable* $|a| \in [1, \infty)$ *has the p.d.f.*

$$F_{|a|}(x) = \frac{2}{\pi}\,\frac{1}{x\sqrt{x^2-1}}.$$

Next notice that the equation $1 + |c|^2 = |a|^2$ tells us that $\arctan(1/|c|)$ is also uniformly distributed in $[0, \pi]$.

Thus we require that the matrix entries a and c have arguments $\arg(a)$ and $\arg(c)$ uniformly distributed on $\mathbb{R}$ mod 2π. We write this as $\arg(a) \in_u [0, 2\pi]_{\mathbb{R}}$ and $\arg(c) \in_u [0, 2\pi]_{\mathbb{R}}$. We illustrate with a lemma.

Lemma 2.4. *If* $\arg(a), \arg(b) \in_u [0, 2\pi]_{\mathbb{R}}$, *then* $\arg(ab), \arg(a/b) \in_u [0, 2\pi]_{\mathbb{R}}$. *Hence* $\arg(a^k) = k\arg(a) \in_u [0, 2\pi]_{\mathbb{R}}$ *for* $k \in \mathbb{Z}$.

Proof. The usual method of calculating probability distributions for combinations of random variables via characteristic functions shows that if θ, η are selected from a uniformly distributed probability measure on $[0, 2\pi]$, then the p.d.f. for $\theta + \eta \in [0, 4\pi]$ is given by

$$g(\zeta) = \begin{cases} \zeta/(8\pi^2), & 0 \le \zeta < 2\pi, \\ (4\pi - \zeta)/(8\pi^2), & 2\pi \le \zeta \le 4\pi. \end{cases} \tag{2.5}$$

We reduce mod 2π and observe

$$\frac{\zeta}{8\pi^2} + \frac{4\pi - \zeta}{8\pi^2} = \frac{1}{2\pi}$$

and this gives us once again the uniform probability density on $[0, 2\pi]$. The remaining results are easy consequences. □

In what follows we will also need to consider variables supported in $[0, \pi]$ or smaller subintervals and as above we will write this as $a \in_u [0, \pi]_{\mathbb{R}}$ and so forth. Most often we will also drop the subscript $\mathbb{R}$.

In a moment we will calculate some distributions naturally associated with Möbius transformations such as traces and translation lengths. Every Möbius transformation of the unit disk $\mathbb{D}$ can be written in the form

$$z \mapsto \zeta^2\,\frac{z - w}{1 - \bar{w}z}, \qquad |\zeta| = 1, \quad w \in \mathbb{D}. \tag{2.6}$$

Thus one could consider another approach by choosing distributions for $\zeta \in \mathbb{S}$ and $w \in \mathbb{D}$. It seems clear one would want ζ uniformly distributed in $\mathbb{S}$. The real question is by what probability measure should w be chosen on $\mathbb{D}$? If w is chosen rotationally invariant, then the choice boils down to probability measures on radii. The choices we have made turn out as follows. The matrix representation of (2.6) in the form (2.1) is

$$\zeta^2\,\frac{z-w}{1-\bar{w}z} \leftrightarrow \begin{pmatrix} \frac{\zeta}{\sqrt{1-|w|^2}} & -\frac{\zeta w}{\sqrt{1-|w|^2}} \\ -\frac{\bar{\zeta}\bar{w}}{\sqrt{1-|w|^2}} & \frac{\bar{\zeta}}{\sqrt{1-|w|^2}} \end{pmatrix}.$$

Hence ζ and $w/|w|$ will be uniformly distributed in $\mathbb{S}$. Then, $|w|<1$ necessarily and

$$\arccos(|w|) = \arcsin(\sqrt{1-|w|^2}) \in [0, \pi/2]$$

is uniformly distributed and we find $|w| = |f(0)|$ has the p.d.f. $2/(\pi\sqrt{1-y^2})$, $y \in [0, 1]$).

Corollary 2.7. *Let $f \in \mathcal{F}$ be a random Möbius transformation. Then the p.d.f. for $y = |f(0)|$ is $2/(\pi\sqrt{1-y^2})$. The expected value of $|f(0)|$ is*

$$E[\|f(0)|] = \frac{2}{\pi}\int_0^1 \frac{y}{\sqrt{1-y^2}}\,dy = \frac{2}{\pi} = 0.63662\ldots$$

The hyperbolic distance here between 0 and $E[|f(0)|]$ is

$$\log\frac{1+|f(0)|}{1-|f(0)|} = \log\frac{\pi+2}{\pi-2} = 1.50494\ldots.$$

3. Fixed points

The fixed points of a random $f \in \mathcal{F}$ are solutions to the same quadratic equation and one should therefore expect some correlation. From (2.2) we see the fixed points are the solutions to $az + c = z(\bar{c}z + \bar{a})$. That is

$$z_\pm = \frac{1}{\bar{c}}(i\Im m(a) \pm \sqrt{\Re e(a)^2 - 1}), \quad |a|^2 = 1 + |c|^2. \tag{3.1}$$

We consider two cases. Further we will soon establish that $\Pr\{|\Re e(a)| \le 1\} = \frac{1}{2}$, so each case occurs with equal probability.

Case 1: (f elliptic or parabolic). $|\Re e(a)| \le 1$ and so $\arg(z_\pm) = \frac{\pi}{2} + \arg(c)$. Thus the argument of both fixed points is the same and that angle is uniformly distributed in $[0, \pi]$.

Case 2: (f hyperbolic). $\Re e(a) > 1$ and $|z_\pm| = 1$. We calculate the derivative

$$|f'(z_\pm)| = \frac{1}{|\bar{c}z_\pm + \bar{a}|^2} = \frac{1}{|\Re e(a) \pm \sqrt{\Re e(a)^2 - 1}|^2}.$$

Hence $|f'(z_+)| < 1$ and z_+ is an *attracting* fixed point, with z_- being *repelling*.

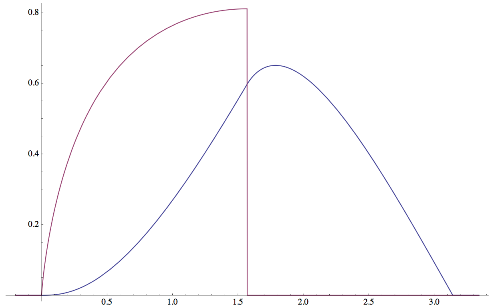

Figure 1. The p.d.f. H_Y for the angle $\phi/2$ between fixed points of a random hyperbolic $f \in \mathcal{F}$ and the convolution $H_Y * H_Y$.

We have chosen $\arg(c)$ to be uniformly distributed and so the argument of either fixed point, say z_+, is uniformly distributed. The interesting question is the distribution of the angle (at 0) between the fixed points. That is the argument of $z_+\bar{z}_-$. This will reflect the correlation we are looking for. This angle is easily seen to be the angle $\phi \in [0, \pi]$ where $\cos(\phi/2) = \Im m(a)/|c|$. Then

$$\cos(\phi/2) = \Im m(a)/|c| = \frac{|a| \sin\theta}{\sqrt{|a|^2 - 1}} = \frac{\sin\theta}{\cos\alpha},$$

where we are able to assume that both θ and α are uniformly distributed in $[0, \pi/2]$ and we are conditioned by $\sin\theta \le \cos\alpha$.

We will calculate the distribution of $\sin\theta/\cos\alpha$ carefully when we come to the calculation of the parameters determining a Möbius group. We report the p.d.f. here as follows.

Theorem 3.2. *The distribution of the random variable* $X = \sin(\theta)/\cos(\alpha)$, *for* θ *and* α *uniformly distributed in* $[0, \pi/2]$ *is given by the formula*

$$h_X(x) = \frac{4}{\pi^2 x} \log\frac{1+x}{1-x}, \qquad 0 \le x < 1. \tag{3.3}$$

We can now use the change of variables formula to compute the p.d.f. for $\phi/2$. That is, we want the distribution for $Y = \cos^{-1}(h_X(x))$, given $h_X(x) \le 1$. We can compute this distribution to be

$$h_Y(y) = \frac{4}{\pi^2} \tan(y) \log\frac{1+\cos(y)}{1-\cos(y)}.$$

Theorem 3.4. *Let* $\phi \in [0, \pi]$ *be the angle subtended at* 0 *by the fixed points of a random hyperbolic element in* $\mathcal{F}$. *Then the p.d.f. for* $\eta = \phi/2$, *as seen in Figure 1, is given by*

$$H_Y(\eta) = \frac{4}{\pi^2} \tan(\eta) \log\frac{1+\cos(\eta)}{1-\cos(\eta)}. \tag{3.5}$$

Some hyperbolic trigonometry reveals the hyperbolic line between a pair of points $z_\pm \in \mathbb{S}$ meets the closed disk of hyperbolic radius r (denoted $\mathbb{D}_\rho(r)$) when the angle ϕ formed at 0 satisfies $\cosh(r) \geq 1/\sin(\phi/2)$. If $z_\pm$ are the fixed points of a hyperbolic element f, then this hyperbolic line joining them is called the axis of f, denoted $\operatorname{axis}(f)$. We can therefore compute the probability that the axis of a random hyperbolic element meets $\mathbb{D}_\rho(r)$ by setting $\delta = \sin^{-1}(1/\cosh(r))$ and computing

$$\begin{aligned}\mathcal{P}(\operatorname{axis}(f) \cap \mathbb{D}_\rho(r) \neq \varnothing) &= \frac{4}{\pi^2} \int_0^\delta \tan(\eta)\ \log \frac{1+\cos(\eta)}{1-\cos(\eta)}\, d\eta \\ &= \frac{4}{\pi^2} \int_0^{\tanh(r)} \frac{1}{x}\ \log \frac{1+x}{1-x}\, dx \\ &= \frac{4}{\pi^2}[\mathrm{Li}_2(\tanh(r)) - \mathrm{Li}_2(-\tanh(r))].\end{aligned}$$

Here $\mathrm{Li}_2(s) = \sum_1^\infty n^{-2}s^n$ is a polylog function. Thus, for instance, this probability exceeds $\frac{1}{2}$ as soon as $r > 0.678\ldots$ and exceeds 0.95 as soon as $r > 2.24419$.

Now, the bisector ζ_f of the smaller circular arc between the fixed points of a random hyperbolic element of f is uniformly distributed on the circle. Then, given f and g random hyperbolic elements of $\mathcal{F}$ and angles ϕ_f and ϕ_g between their fixed points, the p.d.f. for $\phi_f/2 + \phi_g/2$ is the convolution $H_Y * H_Y$. We note that $e^{i\theta} = \xi = \zeta_f \overline{\zeta}_g$ is uniformly distributed as well. Given ξ, the fixed points of f and of g intertwine (so that the axes cross) if both $\phi_f + \phi_g \geq 2\theta$ and $|\phi_f - \phi_g| < 2\theta$. We can use the distributions above to calculate these probabilities, but it is quite complicated and we will find another route to this probability a bit later.

4. Isometric circles and traces

The isometric circles of the Möbius transformation f defined at (2.2) are defined to be the two circles

$$C_+ = \left\{|z + \frac{\bar{a}}{\bar{c}}| = \frac{1}{|c|}\right\}, \quad C_- = \left\{z : |z - \frac{a}{\bar{c}}| = \frac{1}{|c|}\right\},$$

which are paired by the action of f and f^{-1}, with $f^{\pm 1}(C_\pm) = C_\mp$. The *isometric disks* are the finite regions bounded by these two circles. Since $|a|^2 = 1 + |c|^2 \geq 1$, both these circles meet the unit circle in an arc of angle $\theta \in [0, \pi]$. Some elementary trigonometry reveals that

$$\sin(\theta/2) = 1/|a|. \tag{4.1}$$

Thus by our choice of distribution for $|a|$ we obtain the following key result.

Lemma 4.2. *The arcs determined by the intersections of the finite disks bounded by the isometric circles of f, where f is chosen according to the distributions (i) and (ii),* *are centred on uniformly distributed points of* $\mathbb{S}$ *and have arc length uniformly distributed in* $[0, \pi]$.

It is this lemma which supports our claim that the p.d.f. on $\mathcal{F}$ is natural and suggests the way forward for an analysis of random subgroups of $\mathrm{PSL}(2, \mathbb{C})$.

The isometric circles of f are disjoint if

$$\left|\frac{a}{\bar{c}} + \frac{\bar{a}}{\bar{c}}\right| \geq \frac{2}{|c|}.$$

This occurs if $|\mathrm{tr}(f)| = |a + \bar{a}| = 2|\Re e(a)| \geq 2$. Since the disjointness of isometric circles has important geometric consequences we will need to find the p.d.f. for the random variable $t = |\mathrm{tr}(f)|$. As $|\Re e(a)| = |a|\,|\cos(\theta)|$, for a fixed $\theta \in [0, \pi/2]$, the probability

$$\mathrm{Pr}[\{|a| \geq 1/\cos\theta\}] = 1 - \frac{2}{\pi}\int_1^{1/\cos\theta} \frac{dx}{x\sqrt{x^2-1}} = 1 - \frac{2}{\pi}\theta. \tag{4.3}$$

As $a/|a|$ is uniformly distributed on the circle, we have $\theta\,|\,[0, \pi/2]$ uniformly distributed in $[0, \pi/2]$. Therefore using the obvious symmetries we may calculate

$$\mathrm{Pr}[\{|a + \bar{a}| \geq 2\}] = \frac{2}{\pi}\int_0^{\pi/2} 1 - \frac{2}{\pi}\theta \, d\theta = \frac{1}{2}.$$

Corollary 4.4. *Let* $f \in \mathcal{F}$ *be a Möbius transformation chosen randomly from the distribution described in* (i) *and* (ii). *Then the probability that the isometric circles of* f *are disjoint is equal to* $\frac{1}{2}$.

Therefore we have the following simple consequence concerning random cyclic groups.

Corollary 4.5. *Let* $f \in \mathcal{F}$ *be a Möbius transformation chosen randomly from the distribution described in* (i) *and* (ii). *Then the probability that the cyclic group* $\langle f \rangle$ *is discrete is equal to* $\frac{1}{2}$.

Proof. The matrix $A \in \mathrm{SL}(2, \mathbb{C})$ represents an elliptic or parabolic Möbius transformation f if and only if $-2 \leq \mathrm{tr}\, A \leq 2$. This occurs with probability $\frac{1}{2}$. The matrix A represents an elliptic transformation of finite order, or a parabolic transformation if and only if $\mathrm{tr}(A) = \pm 2\cos(p\pi/q),\ \ p, q \in \mathbb{Z}$, and this set is countable and therefore has measure zero. The result follows. □

We now note the following trivial consequence.

Corollary 4.6. *Let* $f, g \in \mathcal{F}$ *be Möbius transformations chosen randomly from the distribution described in* (i) *and* (ii). *Then the probability that the group* $\langle f, g\rangle$ *is discrete is no more than* $\frac{1}{4}$.

Actually we can use (4.3) to determine the p.d.f. for $|\mathrm{tr}(A)|$. We will do this two ways. First, for $s \geq 2$,

$$\begin{aligned}\Pr[\{|\,\mathrm{tr}(A)| \geq s\}] = \Pr[\{2|a|\cos\theta \geq s\}] = \Pr[\{|a| \geq s/(2\cos\theta)\}]\\ = 1 - \frac{4}{\pi^2}\int_0^{\pi/2}\int_1^{s/2\cos\theta}\frac{dx}{x\sqrt{x^2-1}}\,d\theta\\ = 1 - \frac{4}{\pi^2}\int_0^{\pi/2}\cos^{-1}\left(\frac{2\cos\theta}{s}\right)d\theta.\end{aligned}$$

We can now differentiate this function of s under the integral, integrate with respect to θ (using the symmetry to reduce it to being over $[0, \pi/2]$) to obtain the probability density function for $|\mathrm{tr}(A)|$ (for $|\mathrm{tr}(A)| \geq 2$),

$$F[s] = \frac{4}{\pi^2 s}\cosh^{-1}\left[\frac{s}{\sqrt{s^2-4}}\right],$$

with $s \geq 2$. This gives the distribution for $\mathrm{tr}^2 A$ as

$$G[t] = \frac{2}{\pi^2 t}\cosh^{-1}\left(\frac{\sqrt{t}}{\sqrt{t-4}}\right) = \frac{2}{\pi^2 t}\log\frac{\sqrt{t}+2}{\sqrt{t-4}}, \quad t \geq 4.$$

Then the random variable $\beta = \mathrm{tr}^2 A - 4 \geq 0$ has distribution

$$G[\beta] = \frac{1}{\pi^2(\beta+4)}\log\left(1 + \frac{8+4\sqrt{\beta+4}}{\beta}\right), \quad \beta \geq 0. \tag{4.7}$$

We could now follow through a similar, but more difficult, calculation to determine the distribution for β in the interval $-4 \leq \beta \leq 0$. It turns out to be

$$G[\beta] = \frac{1}{\pi^2(\beta+4)}\log\left(\frac{2+\sqrt{\beta+4}}{2-\sqrt{\beta+4}}\right), \quad \beta \in [-4, 0]. \tag{4.8}$$

We will return to this in a moment through a different approach as we can immediately use (4.7) to find the distribution of the translation length of hyperbolic elements.

As we have seen, every element $f \in \mathcal{F}$ which is not elliptic (conjugate to a rotation, equivalently $\beta(f) \in [-4, 0)$) or parabolic (conjugate to a translation, equivalently $\beta(f) = 0$) fixes two points on the circle and the hyperbolic line axis(f) with those points as endpoints. The transformation acts as a translation by constant hyperbolic distance $\tau(f)$ along its axis. This number $\tau(f)$ is called the *translation length* and is related to the trace via the formula $\beta(f) = 4\sinh^2\tau/2$ [Gehring and Martin 1994]. We obtain the distribution for $\tau = \tau(f)$ from the change of variables

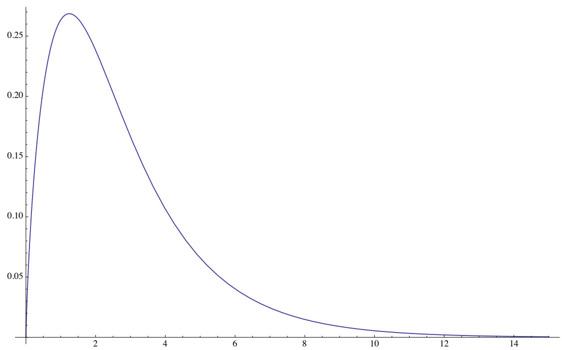

Figure 2. The p.d.f. for the translation length τ of a random hyperbolic element of $\mathcal{F}$.

formula for p.d.f. using (4.7)

$$H[\tau] = \frac{2}{\pi^2}\tanh\frac{\tau}{2}\log\left(\frac{\cosh\frac{\tau}{2}+1}{\cosh\frac{\tau}{2}-1}\right) = -\frac{4}{\pi^2}\tanh\frac{\tau}{2}\log\tanh\frac{\tau}{4}.$$

Unlike our earlier distribution G, the p.d.f. for τ has all moments. In particular once we observe

$$\int_0^\infty t\tanh\frac{t}{2}\log\left[\tanh\frac{t}{4}\right]dt = -\pi^2\log 2,$$

we have the following theorem.

Theorem 4.9. *For randomly selected hyperbolic $f \in_* \mathcal{F}$ the p.d.f. for the translation length $\tau = \tau(f)$, as seen in Figure 2, is*

$$H[\tau] = -\frac{4}{\pi^2}\tanh\frac{\tau}{2}\log\tanh\frac{\tau}{4} \tag{4.10}$$

and the expected value of the translation length is $E[\tau] = 4\log 2 \approx 2.77259\ldots$

However there is another way to see these results and which is more useful in what is to follow in that it more clearly relates to the geometry.

5. The parameter $\beta = \mathrm{tr}^2(A) - 4$

Theorem 5.1. *If a Möbius transformation f is randomly chosen in $\mathcal{F}$, then*

$$\beta(f) = 4\left(\frac{\cos^2(\theta)}{\sin^2(\alpha)} - 1\right), \quad \theta \in_u [0, 2\pi], \quad \alpha \in_u \left[0, \frac{\pi}{2}\right], \tag{5.2}$$

where 2α is the arc length intersection of the isometric circles of f with $\mathbb{S}$ and θ is the argument of the leading entry of A, the matrix representative for f.

Proof. Let $A = \left(\begin{smallmatrix} a & c \\ \bar{c} & \bar{a} \end{smallmatrix}\right)$. Then $\beta = \mathrm{tr}^2 A - 4 = [2\Re e(a)]^2 - 4 = 4|a|^2 \cos^2(\theta) - 4$ and the result follows by (4.1) and Lemma 4.2. □

Theorem 5.3. *The distribution of the random variable*

$$w = \frac{\cos^2(\theta)}{\sin^2(\alpha)} \quad \text{for } \theta \in_u [0, 2\pi] \text{ and } \alpha \in_u \left[0, \frac{\pi}{2}\right]$$

is given by the formula

$$h(w) = \frac{1}{\pi^2 w} \log\left|\frac{\sqrt{w}+1}{\sqrt{w}-1}\right|, \quad w \geq 0. \tag{5.4}$$

Proof. The probability distribution functions of $x = \cos^2(\theta)$ and $y = \sin^2(\alpha)$ are independent and identically distributed $F(x)$ and $F(y)$,

$$F(x) = \frac{1}{\pi\sqrt{x(1-x)}}. \tag{5.5}$$

F is monotonic for $x, y \in \left[0, \frac{1}{2}\right)$ and also for $x, y \in \left(\frac{1}{2}, 1\right]$ and antisymmetric about $\frac{1}{2}$. Therefore we can use the change of variables formula and the Mellin convolution to compute the p.d.f. Write $x = \cos^2(\theta)$, $y = \sin^2(\alpha)$ and $w = \cos^2(\theta)/\sin^2(\alpha)$. We use the Mellin convolution for quotients as in [Springer 1979]. For $x, y \in (0, 1)$ the upper integration limits for the convolution integral are $y < 1 \times \frac{1}{w}$ whenever $w > 1$ and $y < 1$ otherwise; accordingly the Mellin convolution for the quotient of the probability distribution functions over $(0, \infty)$ is calculated as follows, where we have ensured the piecewise differentiability of the integrand.

$$h(w) = \int_0^1 y\, f(x) f(y) dy \ \text{ for } w < 1 \quad \text{and} \quad \int_0^{\frac{1}{w}} y\, f(x) f(y) dy \ \text{ for } w \geq 1 \tag{5.6}$$

and the indefinite integral embedded in both components of (5.6) is given as

$$\begin{aligned} \int y\, f(yw) f(y)\, dy &= \int y\, \frac{1}{\pi\sqrt{yw(1-yw))}} \frac{1}{\pi\sqrt{y(1-y)}}\, dy \\ &= \frac{2}{\pi^2 w} \log\left(w\sqrt{(y-1)} + \sqrt{w(yw-1)}\right). \end{aligned} \tag{5.7}$$

Simplification of the log term in (5.7) yields

$$\log\left(w(w(2y-1) - 1 + 2\sqrt{w(y-1)(yw-1)})\right)$$
$$= \begin{cases} e_0 = \log(-w(w+1-2\sqrt{w})) & \text{at } y = 0, \\ e_1 = \log(w(w-1)) & \text{at } y = 1, \\ e_{\frac{1}{w}} = \log(-w(w-1)) & \text{at } y = \frac{1}{w}, \end{cases}$$

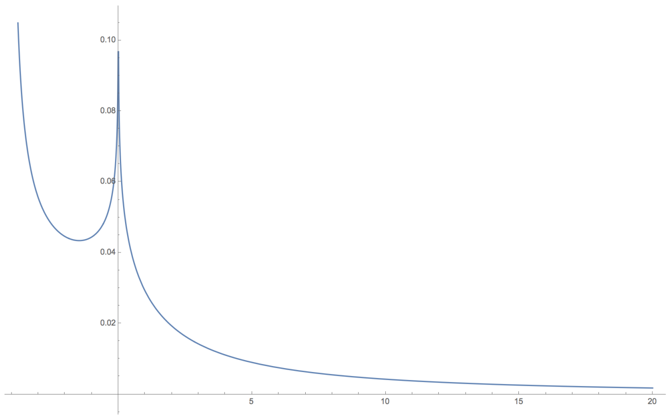

Figure 3. The p.d.f. for the parameter $\beta(f)$ for a random element $f \in \mathcal{F}$.

and accordingly the definite integrals in (5.6) evaluate to

$$\int_0^1 y\, f(yw) f(y) dy = \frac{1}{\pi^2 w}(e_1 - e_0)$$

and

$$\int_0^{\frac{1}{w}} y\, f(yw) f(y) dy = \frac{1}{\pi^2 w}(e_{1/w} - e_0).$$

If we now let $v = \sqrt{w}$, then

$$e_1 - e_0 = \log(w(w-1)) - \log(-w(w+1-2\sqrt{w})) = \log\left(\frac{1+\sqrt{w}}{1-\sqrt{w}}\right)$$

and

$$e_{1/w} - e_0 = \log(-w(w-1)) - \log(-w(w+1-2\sqrt{w})) = \log\left(\frac{\sqrt{w}+1}{\sqrt{w}-1}\right)$$

We deduce that the distribution of $w = \cos^2(\theta)/\sin^2(\alpha)$ is given by (5.4). $\square$

From this, and a little obvious manipulation to see these formulas actually agree with those obtained earlier, we obtain the result we were looking for.

Theorem 5.8. *The distribution of $\beta(f)$ for f randomly chosen from $\mathcal{F}$, as in Figure 3, is given by*

(5.9)
$$G[\beta] = \frac{1}{2\pi^2(\beta+4)} \log\left|\frac{\sqrt{\beta+4}+2}{\sqrt{\beta+4}-2}\right|, \quad \beta \geq -4.$$

This is quite a slowly converging integral, $G[x] \approx 2/(\pi^2 x^{3/2})$ for $x \gg 1$. In order to discuss the effectiveness of Jørgensen's inequality [1976] we will want the

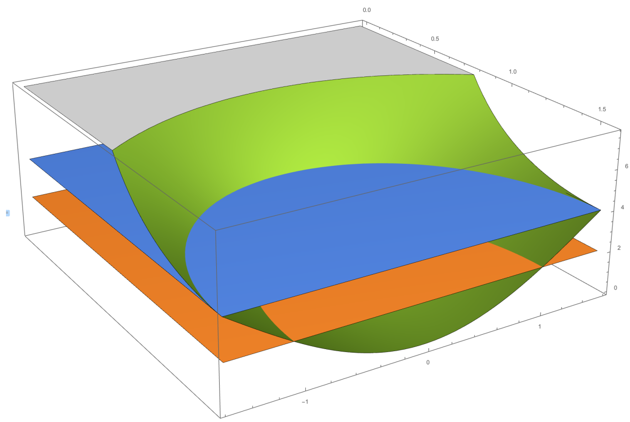

Figure 4. The graph of $\|A-I\|^2$ together with the planes $t^2=2$ and $t^2=4$.

cumulative distribution for $|\beta|$. We put down what we need in the following. The proof simply consists of calculating the integral.

Theorem 5.10. *For f randomly chosen from $\mathcal{F}$, $s \geq 0$, and $\beta = \beta(f)$,*

$$\mathbf{Pr}\{-s \leq \beta \leq 0\} = \frac{1}{2} + \frac{1}{\pi^2}\big(\mathrm{Li}_2(1-s/4) - 4\,\mathrm{Li}_2\big(\sqrt{1-s/4}\big)\big)$$

$$\mathbf{Pr}\{0 \leq \beta \leq s\} = \frac{2}{3} + \frac{2}{\pi^2}\left[\mathrm{Li}_2\left(-\frac{\sqrt{s+4}+2}{\sqrt{s+4}-2}\right) + \mathrm{Li}_2\left(\frac{-4}{\sqrt{s+4}-2}\right) + \log\left(\frac{\sqrt{s+4}+2}{\sqrt{s+4}-2}\right)\log\left(\frac{2\sqrt{s+4}}{\sqrt{s+4}-2}\right)\right].$$

This result gives us an indication of how likely it is that Jørgensen's inequality will have useful content since if we choose a random hyperbolic element in $\mathcal{F}$, then $\mathbf{Pr}\{0 < \beta < 1\} \approx 0.175745$.

5A. ***The metric in* PSL(2, ℝ).** Here we would like to identify the p.d.f. for the distance between an element of PSL(2, ℝ) and the identity when that element $A \in_* \mathrm{PSL}(2,\mathbb{R})$. Again we will see an elliptic/hyperbolic dichotomy in the singularities of the metric. We choose a representative A with positive trace,

$$\begin{pmatrix} e^{i\phi}\csc(\theta) & e^{i\alpha}\cot(\theta) \\ e^{-i\alpha}\cot(\theta) & e^{-i\phi}\csc(\theta) \end{pmatrix}, \quad \theta \in_u \left[0, \frac{\pi}{2}\right], \quad \phi \in_u \left[-\frac{\pi}{2}, \frac{\pi}{2}\right],$$

and calculate

$$\|A-I\|^2 = 2|e^{i\phi}\csc(\theta) - 1|^2 + 2\cot^2(\theta) = 4\csc^2(\theta) - 4\csc(\theta)\cos(\phi),$$

as illustrated in Figure 4.

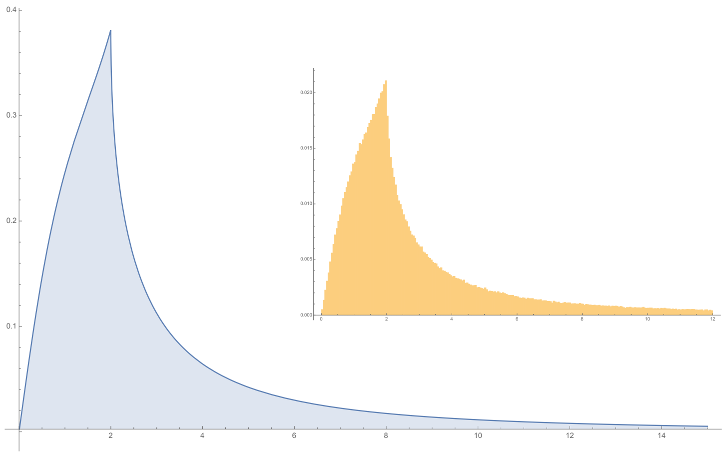

Figure 5. The p.d.f. of $\|A-I\|$. Inset a run on 10^7 random trials.

Then $\|A-I\|^2 \geq t^2$ implies $t^2\sin^2(\theta)+4\sin(\theta)\cos(\phi)-4\leq 0$ and hence, since $\sin\theta \geq 0$,

$$\sin\theta \leq \frac{2}{t^2}\left(\sqrt{\cos^2\phi+t^2}-\cos\phi\right). \tag{5.11}$$

Notice that the right-hand side of (5.11) is ≤ 1. We want to find the measure of the subset of $\left[0,\frac{\pi}{2}\right]\times\left[-\frac{\pi}{2},\frac{\pi}{2}\right]$ where (5.11) holds to find the p.d.f. Fix ϕ, then the length of the θ-interval where (5.11) holds is $\frac{\pi}{2}-\arcsin(2/(t^2)(\sqrt{\cos^2\phi+t^2}-\cos\phi))$, until $2/(t^2)(\sqrt{\cos^2\phi+t^2}-\cos\phi)=1$ whereafter the length stays 0. This latter condition is $1=t^2/4+\cos\phi$ which places no restriction on $\phi\in\left[-\frac{\pi}{2},\frac{\pi}{2}\right]$ as soon as $t^2\geq 4$. Otherwise we only add up the lengths while $|\phi|\leq \arccos\left(1-\frac{t^2}{4}\right)$. We now have the following theorem after making the change of variables $x=\cos(\phi)$ for $t\geq 4$, and related changes for $0\leq t\leq 4$ to simplify their form so as to be able to differentiate under the integral sign to obtain the p.d.f.

Theorem 5.12. *The cumulative distribution for $\|A-I\|$, as shown in Figure 5, is*

$$\frac{4}{\pi^2}\int_{1-\frac{t^2}{4}}^{1}\frac{\pi}{2}-\sin^{-1}\left(\frac{2}{t^2}\left(\sqrt{x^2+t^2}-x\right)\right)\frac{dx}{\sqrt{1-x^2}}$$
$$=\frac{2}{\pi}\cos^{-1}\left(1-\frac{t^2}{4}\right)+\frac{4}{\pi^2}\int_0^1 t\sin^{-1}\left[2z+\frac{2\sqrt{t^4z^2+8t^2(2-z)+16}-8}{t^2}\right]\frac{dz}{\sqrt{z(8-t^2z)}}$$

for $0\leq t\leq 4$, and

$$1-\frac{4}{\pi^2}\int_0^1\sin^{-1}\left(\frac{2}{t^2}\left(\sqrt{x^2+t^2}-x\right)\right)\frac{dx}{\sqrt{1-x^2}}$$

for $4\leq t$.

6. The topology of the quotient space

Topologically there are two surfaces whose fundamental group is isomorphic to F_2, the free group on two generators. These are the 2-sphere with three holes $\mathbb{S}^2_3$, and the torus with one hole T^2_1. Thus a group $\Gamma = \langle f, g\rangle$ generated by two random hyperbolic elements of $\mathcal{F}$ if discrete, has quotient space $\mathbb{D}^2/\Gamma \in \{\mathbb{S}^2_3, T^2_1\}$. We would like to understand the likelihood of one of these topologies over the other. The topology is determined by whether the axes of f and g cross (giving T^2_1) or not (giving $\mathbb{S}^2_3$). This is the same thing as asking if the hyperbolic lines between the fixed points of f and the fixed points of g cross or not, and this in turn is determined by a suitable cross ratio of the fixed points. In fact, the geometry of the commutator $\gamma(f, g) = \operatorname{tr}[f, g] - 2$ determines not only the topology of the quotient, but also the hyperbolic length of the shortest geodesic — it is represented by either f, g, or $[f, g] = fgf^{-1}g^{-1}$ and their Nielsen equivalents. In fact the three numbers $\beta(f)$, $\beta(g)$ and $\gamma(f, g)$ determine the group $\langle f, g\rangle$ uniquely up to conjugacy. Since we have already determined the natural probability densities for $\beta(f)$ and $\beta(g)$ we need only identify the p.d.f. for $\gamma = \gamma(f, g)$ to find a conjugacy invariant way to identify random discrete groups. Unfortunately this is not so straightforward and we do not know this distribution. However important aspects of this distribution can be determined.

6A. ***Commutators and cross ratios.*** We follow [Beardon 1983] and define the cross ratio of four points $z_1, z_2, z_3, z_4 \in \mathbb{C}$ to be

$$[z_1, z_2, z_3, z_4] = \frac{(z_1 - z_3)(z_2 - z_4)}{(z_1 - z_2)(z_3 - z_4)}. \tag{6.1}$$

In order to address the distribution of $\gamma(f, g) = \operatorname{tr}[f, g] - 2$, we need to understand the cross ratio distribution. This is because of the following result from [Beardon 1983, §7.23 and §7.24] together with a little manipulation.

Theorem 6.2. *Let ℓ_1, with endpoints z_1 and z_2, and ℓ_2, with endpoints w_1 and w_2, be hyperbolic lines in the unit disk model of hyperbolic space. So z_1, z_2, w_1, w_2 are in $\mathbb{S}$, the circle at infinity. Let δ be the hyperbolic distance between ℓ_1 and ℓ_2, and should they cross, let $\theta \in [0, \pi/2]$ be the angle at the intersection. Then*

$$\sinh^2\left[\tfrac{1}{2}(\delta + i\theta)\right] \times [z_1, w_1, z_2, w_2] = -1. \tag{6.3}$$

The number $\delta + i\theta$ is called the *complex distance* between the lines ℓ_1 and ℓ_2 where we put $\theta = 0$ if the lines do not meet. The proof of this theorem is simply to use Möbius invariance of the cross ratio and the two different models of the hyperbolic plane. If the two lines do not intersect, we choose the Möbius transformation which sends the disk to the upper half-plane and $\{z_1, z_2\}$ to $\{-1, +1\}$ and $\{w_1, w_2\}$

to $\{-s, s\}$ for some $s > 1$. Then $\delta = \log s$ and

$$[-1, -s, 1, s] = \frac{-4s}{(1-s)^2} = \frac{-4}{(e^{\delta/2} - e^{-\delta/2})^2} = -\frac{1}{\sinh^2(\delta/2)},$$

while if the axes meet at a finite point, we choose a Möbius transformation of the disk so the line endpoints are ± 1 and $e^{\pm i\theta}$ and the result follows similarly.

Next, Lemma 4.2 of [Gehring and Martin 1994] relates the parameters and cross ratios.

Theorem 6.4. *Let f and g be Möbius transformations and let $\delta + i\theta$ be the complex distance between their axes. Then*

$$4\gamma(f, g) = \beta(f)\,\beta(g)\,\sinh^2(\delta + i\theta). \tag{6.5}$$

We note from (6.3) that $\sinh^2(\delta + i\theta) = (1 - 2/[z_1, w_1, z_2, w_2])^2 - 1$. For a pair of hyperbolics f and g we have $\beta(f), \beta(g) \geq 0$ with $\delta = 0$ if the axes meet. Thus the axes cross if and only if $\gamma < 0$, or equivalently,

$$[z_1, w_1, z_2, w_2] > 1. \tag{6.6}$$

Actually to see the latter point, we choose the Möbius transformation which sends $z_1 \mapsto 0$, $z_2 \mapsto \infty$, $w_1 \mapsto 1$. Then $z_2 \mapsto z$, say, and

$$[z_1, w_1, z_2, w_2] = \frac{(0-1)(\infty - z)}{(0-\infty)(1-z)} = \frac{1}{1-z}.$$

The image of the axes (and therefore the axes themselves) cross when $z < 0$, equivalently when (6.6) holds.

6B. ***Cross ratio of fixed points.*** Supposing that f and g are randomly chosen hyperbolic elements, we want to discuss the probability of their axes crossing, if f has fixed points z_1, z_2 and g has fixed points w_1, w_2. We identified the formula for the fixed points above at (3.1) and if we notate the random variables (matrix entries) a, c for f and α, β for g we have

$$z_1, z_2 = \frac{1}{\bar{c}}\big(i\Im m(a) \pm \sqrt{\Re e(a)^2 - 1}\big), \qquad |a|^2 = 1 + |c|^2,$$

$$w_1, w_2 = \frac{1}{\bar{\beta}}\big(i\Im m(\alpha) \pm \sqrt{\Re e(\alpha)^2 - 1}\big), \quad |\alpha|^2 = 1 + |\beta|^2,$$

and as both elements are hyperbolic we have $\Re e(a) \geq 1$ and $\Re e(\alpha) \geq 1$. We put $U = i\Im m(a) + \sqrt{\Re e(a)^2 - 1}$ and $V = i\Im m(\alpha) + \sqrt{\Re e(\alpha)^2 - 1}$. Then

$$[z_1, w_1, z_2, w_2] = \frac{4\sqrt{\Re e(a)^2 - 1}\sqrt{\Re e(\alpha)^2 - 1}}{\bar{c}\,\bar{\beta}\,\left(\frac{U}{\bar{c}} - \frac{V}{\bar{\beta}}\right)\left(\frac{-\bar{U}}{\bar{c}} - \frac{-\bar{V}}{\bar{\beta}}\right)} = \frac{2\sqrt{\Re e(a)^2 - 1}\sqrt{\Re e(\alpha)^2 - 1}}{\Re e[U\bar{V}] - \Re e[c\bar{\beta}]}$$

since, as we recall, $1 = |z_i| = |U|/|c|$, and similarly $|V|/|\beta| = 1$. Thus we want to understand the statistics of the cross ratio, and in particular to determine when

$$[z_1, w_1, z_2, w_2] = \frac{2\sqrt{\Re e(a)^2 - 1}\sqrt{\Re e(\alpha)^2 - 1}}{\Re e[U\bar{V}] - \Re e[c\bar{\beta}]} \geq 1. \tag{6.7}$$

We have

$$a = \frac{1}{\sin\theta}e^{i\phi}, \quad \theta \in_u [0, \pi/2], \quad \phi \in_u [0, 2\pi], \quad c = \cot\theta e^{i\delta}, \quad \delta \in_u [0, 2\pi],$$
$$\alpha = \frac{1}{\sin\eta}e^{i\psi}, \quad \eta \in_u [0, \pi/2], \quad \psi \in_u [0, 2\pi] \quad \beta = \cot\eta e^{i\zeta}, \quad \zeta \in_u [0, 2\pi].$$

Then $\sqrt{\Re e(a)^2 - 1} = \sqrt{\cos^2\phi/\sin^2\theta} - 1$, $\sqrt{\Re e(\alpha)^2 - 1} = \sqrt{\cos^2\psi/\sin^2\eta - 1}$, $\Phi = \arg c\bar{\beta}$ is uniformly distributed in $[0, 2\pi]$ and

$$\Re e[U\bar{V}] - \Re e[c\bar{\beta}] = \frac{\sin\phi}{\sin\theta}\,\frac{\sin\psi}{\sin\eta} + \sqrt{\frac{\cos^2\phi}{\sin^2\theta} - 1}\,\sqrt{\frac{\cos^2\psi}{\sin^2\eta} - 1} - \cot\eta\cot\theta\cos\Phi.$$

This gives

$$\begin{aligned}
&\frac{2\sqrt{\Re e(a)^2 - 1}\,\sqrt{\Re e(\alpha)^2 - 1}}{\Re e[U\bar{V}] - \Re e[c\bar{\beta}]} \\
&\qquad = \frac{2\sqrt{\cos^2\phi - \sin^2\theta}\,\sqrt{\cos^2\psi - \sin^2\eta}}{\sin\phi\,\sin\psi + \sqrt{\cos^2\phi - \sin^2\theta}\,\sqrt{\cos^2\psi - \sin^2\eta} - \cos\eta\cos\theta\cos\Phi} \\
&\qquad = \frac{2\sqrt{1 - X^2}\,\sqrt{1 - Y^2}}{XY + \sqrt{1 - X^2}\,\sqrt{1 - Y^2} - \cos\Phi} = Z,
\end{aligned}$$

where we define the random variables $X = \sin\phi/\cos\theta$, and $Y = \sin\psi/\cos\eta$. To have $Z \geq 1$, we need $|X| \leq 1$, $|Y| \leq 1$ and

$$\sqrt{1 - X^2}\,\sqrt{1 - Y^2} \geq \cos\Phi - XY. \tag{6.8}$$

If this last condition holds, then $[z_1, w_1, z_2, w_2] \geq 1$ requires

$$\sqrt{1 - X^2}\sqrt{1 - Y^2} \geq XY - \cos\Phi. \tag{6.9}$$

Notice that X, Y and $\Phi \in_u [0, 2\pi]$ are independent, with X and Y identically distributed. Unfortunately $\sqrt{1 - X^2}\sqrt{1 - Y^2} \pm XY$ is difficult to find directly as $\sqrt{1 - X^2}\sqrt{1 - Y^2}$ and XY are not independent. We therefore write

$$X = \sin S, \quad S \in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right], \quad Y = \sin T, \quad T \in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right]$$

so that $\sqrt{1-X^2}\sqrt{1-Y^2} \pm XY = \cos(S \mp T)$ and we have the two requirements

$$\cos(S \mp T) \geq \pm\cos(\Phi). \tag{6.10}$$

Following the arguments of Section 5, we have the probability distribution functions X and S, with probability distribution functions, respectively,

$$F_X(x) = \frac{2}{\pi^2 x}\log\left|\frac{1+x}{1-x}\right|, \qquad -1 \leq x \leq 1,$$

$$F_S(\theta) = \frac{2}{\pi^2}\cot(\theta)\log\left|\frac{1+\sin(\theta)}{1-\sin(\theta)}\right|, \qquad -\frac{\pi}{2} \leq \theta \leq \frac{\pi}{2}.$$

We can remove various symmetries and redundancies for the situation to simplify. For instance we may assume $S \geq 0$ and reduce to ranges where cos is either increasing or decreasing so we can remove it. We quickly come to the following conditions equivalent to (6.10) with S and T identically distributed as above and $\Phi \in_u [0, \pi/2]$:

$$0 \leq S, \quad -\Phi \leq S-T \leq \Phi, \quad \text{and} \quad S+T+\Phi \leq \pi. \tag{6.11}$$

This now sets up an integral which we implemented on Mathematica numerically and which returned the value $0.429\ldots$. In the next section we correlate this with independent experiments to determine when $\gamma \leq 0$. This agrees with the results of integration as above at (6.11). We record this in the following.

Theorem 6.12. *Let f, g be randomly chosen hyperbolic elements of $\mathcal{F}$. Then the probability that the axes of f and g cross is ≈ 0.429.*

We should point out here the following well-known observation.

Lemma 6.13. *Let $f, g \in \mathcal{F}$. If $\gamma(f,g) < 0$, then both f and g are hyperbolic.*

Proof. As the result is conjugacy invariant we may first suppose f is hyperbolic and represented by $f = \left(\begin{smallmatrix}\lambda & 0\\ 0 & 1/\lambda\end{smallmatrix}\right)$, and $g = \left(\begin{smallmatrix}a & b\\ c & d\end{smallmatrix}\right)$, with $ad-bc=1$. We calculate $\gamma = -(\lambda - 1/\lambda)^2 bc < 0$. Thus f hyperbolic gives $bc > 0$, $ad = 1+bc > 1$ and $(a+d)^2 > 4$ showing g is hyperbolic. If f is parabolic we put $f = \left(\begin{smallmatrix}1 & 1\\ 0 & 1\end{smallmatrix}\right)$, and calculate $\gamma(f,g) = c^2 \geq 0$. Finally, we write $f = \left(\begin{smallmatrix}\cos\alpha & \sin\alpha\\ -\sin\alpha & \cos\alpha\end{smallmatrix}\right)$ if f is elliptic, and compute that

$$\gamma(f,g) = (a^2+b^2+c^2+d^2-2)\sin^2\alpha \geq 0. \qquad \square$$

In contrast to Theorem 6.12, we have the following result.

Theorem 6.14. *Let ζ_1, ζ_1 and η_1, η_2 be two pairs of points, each randomly and uniformly chosen on the circle. Let α be the hyperbolic line between ζ_1 and ζ_2 and let β be the hyperbolic line between η_1 and η_2. Then the probability that α and β cross is $\frac{1}{3}$.*

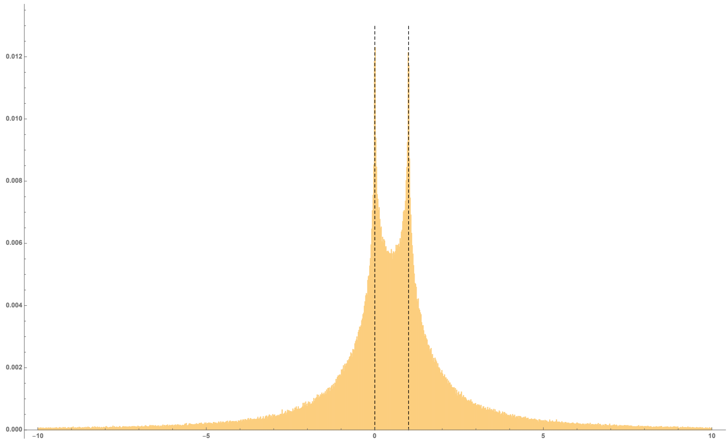

Figure 6. Histogram of the cross ratio of the fixed points of a randomly chosen pair of hyperbolic elements.

Proof. We can forget the points come in pairs and label them z_i, $i = 1, 2, 3, 4$, in order around the circle. There are three different cases, all with the same probability.

- z_1 connects to z_2, hence z_3 to z_4 and the lines are disjoint.
- z_1 connects to z_3, hence z_2 to z_4 and the lines intersect.
- z_1 connects to z_4, hence z_2 to z_3 and the lines are disjoint. □

Together these theorems quantify the degree to which the fixed points are correlated on the circle. We also include the following example.

In the histogram in Figure 6, the singularities are at 0 and 1. We make the observation that it seems quite likely that $\mathbf{Pr}\{[z1, w1, z2, w2] > 1\} = \frac{1}{5}$. It is somewhat of a chore to calculate the cross ratio distribution X_{cr} of four randomly selected points on the circle. This is done in [Martin 2019] and the distribution is very similar to that above, with singularities at 0 and 1. However for that distribution the probabilities are $\mathbf{Pr}\{X_{cr} < 0\} = \mathbf{Pr}\{0 < X_{cr} < 1\} = \mathbf{Pr}\{X_{cr} > 1\} = \frac{1}{3}$ (as can be seen from the action of the group $S4$ on the cross ratio [Beardon 1983]). This shows the distributions are definitely different.

7. The effectiveness of Jørgensen's inequality

In order to computationally explore the moduli spaces of discrete groups we need effective tests for discreteness in groups of Möbius transformations. In practice, it is very difficult to discern if a group is discrete, especially if we know a priori that the group is free on its generators. Discreteness is typically established by constructing a fundamental domain using the Poincaré polyhedral theorem, or using arithmetic information [Gehring et al. 1997], or algorithmically [Gilman 1995]. We would like to discern, with high confidence, that a group is discrete. The most common test is the following from [Jørgensen 1976] (see also [Gehring and Martin 1991a]).

Theorem 7.1 (Jørgensen's inequality). *Let $A, B \in \mathrm{SL}(2, \mathbb{C})$. Suppose that $\langle A, B\rangle$ is discrete and not virtually abelian. Set $\beta = \mathrm{tr}^2(A) - 4$ and $\gamma = \mathrm{tr}[A, B] - 2$. Then $|\gamma| + |\beta| \geq 1$, and if $\gamma \neq \beta$, then $|\beta - \gamma| + |\beta| \geq 1$ also.*

Another common test used can be found in [Gehring and Martin 1991b; Cao 1995].

Theorem 7.2. *Let $A, B \in \mathrm{SL}(2, \mathbb{C})$. Suppose that $\langle A, B\rangle$ is discrete and not virtually abelian. Then*

$$|\gamma(\gamma - \beta)| \geq 2 - 2\cos(\pi/7) = 0.198\ldots$$

All these tests are sharp: there are nonelementary discrete examples where equality holds (for example, lattices). We have already seen that a randomly selected hyperbolic element in $\mathcal{F}$ has $|\beta| < 1$ with probability about 0.175745. Thus for a group generated by random hyperbolics $f_1, f_2, \ldots, f_n$, the probability that one has $|\beta_i| < 1$, so we can even consider the inequality, is quite high:

$$\mathbf{Pr}\{\beta_i < 1 \text{ for some } i = 1, 2\ldots, n\} \geq 1 - \left(\tfrac{33}{40}\right)^n.$$

Further, we are at liberty to consider other generators. For instance in the case of two generators, as in Figure 7, we note that $\langle f, g\rangle = \langle f, gf\rangle = \langle f, gf^{-1}\rangle$ (but do note that if f and g are randomly selected, then fg etc. are not). The unfortunate thing here is that all these pairs of generators have the same commutator,

$$\gamma(f, g) = \gamma(f, gf^{\pm 1}) = \gamma(g, fg^{\pm 1}).$$

In fact the commutator value γ is an invariant of the Nielsen class of generators, and since a random group is free with probability 1, all generating pairs are equivalent. That is, any generating pair has the same value for γ. Thus the principal obstruction to the effectiveness of a discreteness test such as those at Theorems 7.1 and 7.2 is the value of the trace of the commutator. We now explore this.

If we select two random Möbius transformations, say,

$$f = \begin{pmatrix} e^{i\phi_1}\csc(\theta_1) & e^{i(\alpha_1)}\cot(\theta_1) \\ e^{-i\alpha_1}\cot(\theta_1) & e^{-i\phi_1}\csc(\theta_1)\end{pmatrix}, \quad g = \begin{pmatrix} e^{i\phi_2}\csc(\theta_2) & e^{i\alpha_2}\cot(\theta_2) \\ e^{-i\alpha_2}\cot(\theta_2) & e^{-i\phi_2}\csc(\theta_2)\end{pmatrix},$$

and then compute and simplify (making some variable substitutions etc.) $\gamma = \gamma(f, g) = \mathrm{tr}[f, g] - 2$, we find

$$\gamma = 4\csc^2\theta_1\csc^2\theta_2\big[2\cos^2\theta_1(\sin^2\phi_2 - \sin^2\alpha\cos^2\theta_2) + \cos^2\theta_2\sin^2\phi_1 - 2\cos\alpha\cos\theta_1\cos\theta_2\sin\phi_1\sin\phi_2\big]. \tag{7.3}$$

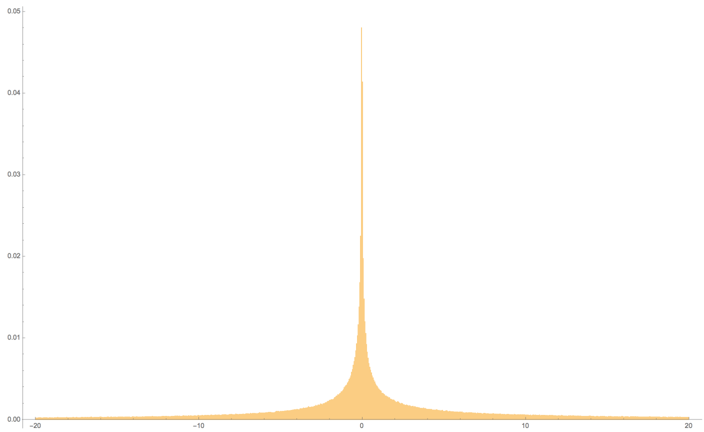

Figure 7. Histogram of γ values conditioned by f and g in $\mathrm{PSL}(2,\mathbb{R})$ hyperbolic.

Here $\theta_1, \theta_2 \in_u [0, \pi/2]$, $\alpha, \phi_1, \phi_2 \in_u [0, \pi]$. There seems to be no easy way to compute this p.d.f.

We made several independent runs through about 10^7 random matrix pairs of hyperbolic elements to generate the histogram in Figure 7. We found the probability that $\gamma < 0$ to be about 0.429601, in alignment with Theorem 6.12. Notice that if $\mathrm{tr}[f, g] \in [-2, 2]$, then almost surely $\langle f, g\rangle$ is not discrete since $[f, g]$ would be elliptic.

We also found

$$\mathbf{Pr}\{-4 \le \gamma \le 0\} \approx 0.162\dots \tag{7.4}$$

$$\mathbf{Pr}\{|\gamma| + |\beta(f)| \le 1 \ \text{ or } \ |\gamma| + |\beta(g)| \le 1\} \approx 0.113\dots \tag{7.5}$$

$$\mathbf{Pr}\{|\gamma(\gamma - \beta(f))| \le 0.198 \ \text{ or } \ |\gamma(\gamma - \beta(g))| \le 0.198\} \approx 0.119\dots \tag{7.6}$$

$$\mathbf{Pr}\{\ fg \text{ or } fg^{-1} \text{ is elliptic }\} \approx 0.203\dots \tag{7.7}$$

Of course these tests for nondiscreteness are not independent. If we put them all together and use additional inequalities found by replacing f by fg or fg^{-1} we found the following.

Conjecture 7.8. *Let $\langle f, g\rangle \in \mathcal{F}$ be randomly chosen hyperbolic elements. Then*

$$\mathbf{Pr}\left\{\overline{\langle f, g\rangle} = \mathcal{F}\right\} > 0.414986\dots$$

That is to say we found that with probability 0.414986... one of the discreteness tests is violated. This probability was not supported by rigorous calculations. However, it is not difficult to establish the lower bound 0.4 rigorously. We discuss this in the next section in a different setting but the ideas are the same.

8. Discreteness

An easy lower bound for the probability a group generated by two random elements of $\mathcal{F}$ is discrete based on the following Klein combination theorem (or "ping pong" lemma).

Lemma 8.1. *Let f_i, $i = 1, 2, \ldots, n$, be hyperbolic transformations of the disk whose isometric disks are all disjoint. Then the group generated by these hyperbolic transformations $\langle f_1, f_2, \ldots, f_n\rangle$ is discrete and isomorphic to the free group F_n.*

We have already seen that the probability that the isometric disks of a randomly chosen $f \in \mathcal{F}$ are disjoint is $\frac{1}{2}$.

Lemma 8.2. *Let α and β be arcs on $\mathbb{S}^1$ with uniformly randomly chosen midpoints ζ_α and ζ_β and subtending angles θ_α and θ_β uniformly chosen from $[0, \pi]$. The probability that α and β meet is $\frac{1}{2}$.*

Proof. The smaller arc subtended between ζ_α and ζ_β has length $\Theta = \arg(\zeta_\alpha \overline{\zeta}_\beta)$ and is uniformly distributed in $[0, \pi]$. Then α and β are disjoint if $\Theta - \theta_\alpha/2 - \theta_\beta/2 \geq 0$. Since $2\Theta - \theta_\alpha - \theta_\beta$ is uniformly distributed in $[-2\pi, 2\pi]$, the probability this number is positive is $\frac{1}{2}$. □

Using Lemma 8.1 this quickly gives us the obvious bound that if $f, g \in \mathcal{F}$ are randomly chosen, then the probability that $\langle f, g\rangle$ is discrete is at least $\frac{1}{64}$. For n generator groups this number is at least $2^{-(2n-1)!}$. However we are going to have to build a bit more theory to prove the following substantial improvements of these estimates.

Theorem 8.3. *The probability that randomly chosen $f, g \in_* \mathcal{F}$ generate a discrete group $\langle f, g\rangle$ is at least $\frac{1}{10}$.*

Theorem 8.4. *The probability that two randomly chosen hyperbolic transformation $f, g \in_* \mathcal{F}$ have disjoint isometric circles, and hence generate a discrete group $\langle f, g\rangle$, is at least $\frac{1}{5}$.*

Theorem 8.3 follows from Theorem 8.4 and Theorem 11.1 (another discreteness test) and the fact that the probability we choose two hyperbolic elements is independent and of probability equal to $\frac{1}{4}$. We now give a proof for Theorem 8.4. It is an immediate consequence of Lemmas 8.1 and 9.4 below.

9. Random arcs on a circle

Let α be an arc on the circle $\mathbb{S}$. We denote its midpoint by $m_\alpha \in \mathbb{S}$ and its arclength by $\ell_\alpha \in [0, 2\pi]$. Conversely, given $m_\alpha \in \mathbb{S}$ and $\ell_\alpha \in [0, 2\pi]$ we determine a unique arc $\alpha = \alpha(m_\alpha, \ell_\alpha)$ with this data.

A random arc α is the arc uniquely determined when we choose $m_\alpha \in \mathbb{S}$ uniformly (equivalently, $\arg(m_\alpha) \in_u [0, 2\pi]$) and $\ell_\alpha \in_u [0, 2\pi]$. We will abuse notation and also refer to random arcs when we restrict to $\ell_\alpha \in_u [0, \pi]$ as for the case of isometric disk intersections. We will make the distinction clear in context.

A simple consequence of our earlier result is the following corollary.

Corollary 9.1. *If $m_\alpha, m_\beta \in_u \mathbb{S}$ and $\ell_\alpha, \ell_\beta \in_u [0, \pi]$, then* $\Pr\{\alpha \cap \beta = \varnothing\} = \frac{1}{2}$.

We need to observe the following lemma.

Lemma 9.2. *If $m_\alpha, m_\beta \in_u \mathbb{S}$ and $\ell_\alpha, \ell_\beta \in_u [0, 2\pi]$, then* $\Pr\{\alpha \cap \beta = \varnothing\} = \frac{1}{6}$.

Proof. We need to calculate the probability that the argument of $\zeta = m_\alpha \overline{m}_\beta$ is greater than $(\ell_\alpha + \ell_\beta)/2$. Now $\theta = \arg(\zeta)$ is uniformly distributed in $[0, \pi]$. The joint distribution is uniform, and so we calculate

$$\Pr\{\theta \geq \ell_\alpha + \ell_\beta\} = \frac{1}{\pi^3} \iiint_{\{\theta \geq \alpha + \beta\}} d\theta\, d\alpha\, d\beta = \frac{1}{\pi^3} \int_0^\pi \int_0^\theta \int_0^{\theta - \alpha} d\beta\, d\alpha\, d\theta = \tfrac{1}{6}. \quad \square$$

Next we consider the probability of disjoint pairs of arcs.

Lemma 9.3. *Let $m_{\alpha_1}, m_{\alpha_2}, m_{\beta_1}, m_{\beta_2} \in_u \mathbb{S}$ and $\ell_\alpha, \ell_\beta \in_u [0, \pi]$. Set*

$$\alpha_i = \alpha(m_{\alpha_i}, \ell_{\alpha_i}), \quad \beta_i = \alpha(m_{\beta_i}, \ell_{\beta_i}).$$

Then the probability that all the arcs α_i, β_i, $i = 1, 2$, are disjoint is $\frac{1}{20}$,

$$\Pr\{(\alpha_1 \cap \alpha_2) \cup (\beta_1 \cap \beta_2) \cup (\alpha_1 \cap \beta_1) \cup (\alpha_1 \cap \beta_2) \cup (\alpha_2 \cap \beta_1) \cup (\alpha_2 \cap \beta_2) = \varnothing\} = \tfrac{1}{20}.$$

Proof. We first observe that the events

$$(\alpha_1 \cap \beta_1) = \varnothing, \quad (\alpha_1 \cap \beta_2) = \varnothing, \quad (\alpha_2 \cap \beta_1) = \varnothing, \quad (\alpha_2 \cap \beta_2) = \varnothing$$

are not independent since (among other reasons) α_1 and α_2, and similarly β_1 and β_2, may overlap. The probability that $(\alpha_1 \cap \beta_1) = \varnothing$ and $(\alpha_2 \cap \beta_2) = \varnothing$ we have already determined to be equal to $\frac{1}{4} = \frac{1}{2} \times \frac{1}{2}$. The result now follows from Lemma 9.4. $\square$

Lemma 9.4. *Let $m_{\alpha_1}, m_{\alpha_2}, m_{\beta_1}, m_{\beta_2} \in_u \mathbb{S}$ and $\ell_\alpha, \ell_\beta \in_u [0, \pi]$. Set*

$$\alpha_i = \alpha(m_{\alpha_i}, \ell_{\alpha_i}), \quad \beta_i = \alpha(m_{\beta_i}, \ell_{\beta_i}),$$

and suppose we are given that $(\alpha_1 \cap \alpha_2) = (\beta_1 \cap \beta_2) = \varnothing$. Then the probability that all the arcs α_i are disjoint from the arcs β_j, $i, j = 1, 2$, is $\frac{1}{5}$,

$$\Pr\{(\alpha_1 \cap \beta_1) \cup (\alpha_1 \cap \beta_2) \cup (\alpha_2 \cap \beta_1) \cup (\alpha_2 \cap \beta_2) = \varnothing\} = \tfrac{1}{5}.$$

Proof. Conditioned by the assumption that α_1 and α_2 are disjoint, and that β_1 and β_2 are disjoint, we note the events

$$(\alpha_1 \cap \beta_1) = \varnothing, \quad (\alpha_1 \cap \beta_2) = \varnothing, \quad (\alpha_2 \cap \beta_1) = \varnothing, \quad (\alpha_2 \cap \beta_2) = \varnothing$$

are independent. A little trigonometry reveals that

$$\alpha_i \cap \beta_j = \varnothing \leftrightarrow \frac{\ell_\alpha + \ell_\beta}{2} \leq 2 \arcsin \frac{|m_{\alpha_i} - m_{\beta_j}|}{2} = \arg(m_{\alpha_i} \overline{m}_{\beta_j}).$$

Now the four variables $\theta_{i,j} = \arg(m_{\alpha_i} \overline{m}_{\beta_j}),\ i, j = 1, 2$, are uniformly distributed in $[0, \pi]$ and independent. We require $\min_{i,j} \theta_{i,j} \geq (\ell_\alpha + \ell_\beta)/2$. Now $\frac{1}{2}(\ell_\alpha + \ell_\beta) = \psi$ is uniformly distributed in $[0, \pi]$ and

$$\Pr\{\min_{i,j} \theta_{i,j} \geq \psi\} = \left(1 - \frac{\psi}{\pi}\right)^4. \tag{9.5}$$

Since $\frac{1}{\pi} \int_0^\pi \left(1 - \frac{\psi}{\pi}\right)^4 = \frac{1}{5}$, the result claimed follows. □

In passing we further note that (9.5) gives us a density function $\rho(\psi) = 4\left(1 - \frac{\psi}{\pi}\right)^3$ and hence an expected value of

$$\frac{4}{\pi^2} \int_0^\pi \psi \left(1 - \frac{\psi}{\pi}\right)^3 d\psi = 4 \int_0^1 (1 - t) t^3 \, dt = \frac{1}{5}.$$

Generalising this result for a greater number of disjoint pairs of arcs quickly gets quite complicated. We state without proof the following, which we will not use.

Lemma 9.6. *Let $m_{\alpha_1}, m_{\alpha_2}, m_{\beta_1}, m_{\beta_2}, m_{\gamma_1}, m_{\gamma_2} \in_u \mathbb{S}$ and $\ell_\alpha, \ell_\beta, \ell_\gamma \in_u [0, \pi]$. Set*

$$\alpha_i = \alpha(m_{\alpha_i}, \ell_{\alpha_i}), \quad \beta_i = \alpha(m_{\beta_i}, \ell_{\beta_i}), \quad \gamma_i = \alpha(m_{\gamma_i}, \ell_{\gamma_i}).$$

Then the probability that all the arcs $\alpha_i, \beta_i, \gamma_i,\ i = 1, 2$, are all disjoint is $\frac{3}{1000}$.

One can get results if there is additional symmetry; for instance, if the lengths of all the arcs are the same.

Theorem 9.7. *Let $m_{i_1}, m_{i_2} \in_u \mathbb{S}^1,\ i = 2, \dots, n$, and $\ell_\alpha \in_u [0, \pi]$. Then the probability that the arcs $\alpha_{ij} = \alpha(m_{i_j}, \ell_\alpha)$ are disjoint is*

$$\frac{1}{(2n)n!} \int_0^1 \sum_{k=0}^{[2-x]} (-1)^k \binom{n}{k} (2 - x - k)^n \, dx. \tag{9.8}$$

Proof. We cyclically order the set $\{m_{i_i} : i = 2, \dots, n,\ j = 1, 2\}$ and let θ_k be the angle between the k-th and $(k+1)$-st point (mod k). Then $\sum_{k=1}^{2n} \theta_k = 2\pi$. The arcs are disjoint if $\theta_k \geq \ell_\alpha$. We have $2n - 1$ independent random variables $\{\theta_k\}_{k=1}^{2n-1}$ which, firstly, must have a minimum which exceeds α, and secondly, must satisfy $2\pi - \sum_{k=1}^{2n-1} \theta_k \geq \ell_\alpha$. The first of these requirements gives us a factor $\frac{1}{2n}$, and from the second we note that the sum of m uniformly distributed random variables in $[0, 1]$ has the Irwin–Hall distribution

$$F_n(x) = \frac{1}{(m-1)!} \sum_{k=0}^{[x]} (-1)^k \binom{m}{k} (x - k)^{m-1}. \tag{9.9}$$

Thus

$$\Pr\left\{2-\frac{\ell_\alpha}{\pi} \geq \sum_{k=1}^{2n-1} \frac{\theta_k}{\pi}\right\} = \int_0^{2-t} F_{2n-1}(t)\, dt.$$

The result follows. □

As an example, for two pairs of equilength arcs we have

$$F_3(x) = \begin{cases} x^2/2, & 0 \leq x \leq 1, \\ (-2x^2+6x-3)/2, & 1 \leq x \leq 2, \\ (x^2-6x+9)/2, & 2 \leq x \leq 3. \end{cases}$$

We see that

$$\int_0^{2-t} F_3(x)\, dx = \int_0^1 F_3(x)\, dx + \int_1^{2-t} F_3(x)\, dx = \frac{1}{6}+\frac{2}{3}-\frac{t}{2}-\frac{t^2}{2}+\frac{t^3}{3}$$

$$\int_0^1 \int_0^{2-t} F_3(x)\, dxdt = \frac{1}{6}+\int_0^1 \frac{2}{3}-\frac{t}{2}-\frac{t^2}{2}+\frac{t^3}{3}\, dt = \frac{1}{6}+\frac{1}{3}=\frac{1}{2}$$

and the probability that two pairs of random equiarclength arcs with arclength uniformly distributed in $[0,\pi]$ are disjoint is $\frac{1}{8}$. Similarly for three pairs the probability is $\frac{9}{200}$.

10. Random arcs to Möbius groups

Given data $m_{\alpha_1}, m_{\alpha_2} \in \mathbb{S}$ with arclength $\ell_\alpha \in [0,\pi]$ we see, just as above, that the arcs centred on the m_{α_i} and of length ℓ_α determine a matrix which can be calculated by examination of the isometric circles. We have

$$(10.1) \qquad A = \begin{pmatrix} a & c \\ \bar{c} & \bar{a} \end{pmatrix}, \quad c = i\sqrt{m_{\alpha_1} m_{\alpha_2}}\, \cot\frac{\ell_\alpha}{2}, \quad a = i\sqrt{\overline{m}_{\alpha_1} m_{\alpha_2}}\, \operatorname{cosec}\frac{\ell_\alpha}{2},$$

where we make a consistent choice of sign by ensuring $c/a = m_{\alpha_1}\cos(\ell_\alpha/2)$. Of course, interchanging m_{α_1} and m_{α_2} sends a to $-\bar{a}$, and so the data actually uniquely determines the cyclic group $\langle f \rangle$ generated by the associated Möbius transformation

$$f(z) = -m_{\alpha_2} \frac{z + m_{\alpha_1}\cos\frac{\ell_\alpha}{2}}{z\,\cos\frac{\ell_\alpha}{2} + m_{\alpha_1}}$$

and not necessarily f itself.

As a consequence we have the following theorem.

Theorem 10.2. *There is a one-to-one correspondence between collections of n pairs of random arcs and n-generator Fuchsian groups preserving the associated probability distributions.*

A randomly chosen $\langle f \rangle \subset \mathcal{F}$ *according to the distribution defined in Section 2A, corresponds uniquely to* $m_{\alpha_1}, m_{\alpha_2} \in_u \mathbb{S}^1$ *and* $\ell_\alpha \in_u [0, \pi]$ *with the distribution defined in Section 9.*

Notice also that if we recognise the association of cyclic groups with the data and say two cyclic groups are close if they have close generators, then this association is continuous.

We have already seen that, for a pair of hyperbolic elements, if all the isometric disks are disjoint then the "ping pong" lemma implies discreteness of the groups in question. Then the association between Fuchsian groups and random arcs quickly establishes Theorems 8.3 and 8.4 via Lemma 9.4.

If f is a parabolic element of $\mathcal{F}$, then the isometric circles are adjacent and meet at the fixed point. Conversely, if two random arcs of arclength ℓ_α are adjacent we have $\arg(m_{\alpha_1}\overline{m}_{\alpha_2}) = \ell_\alpha$, and from (10.1)

$$a = i\left(\cos\frac{\ell_\alpha}{2} + i\sin\frac{\ell_\alpha}{2}\right)\operatorname{cosec}\frac{\ell_\alpha}{2} = -1 + i\cot\frac{\ell_\alpha}{2}$$

and $\operatorname{tr}^2(A) - 4 = 0$ so that A represents a parabolic transformation. Similarly, if the arcs overlap, then $\operatorname{tr}^2(A) \le 2$ and A represents an elliptic transformation.

Theorem 10.3. *Let f, g be randomly chosen parabolic elements in $\mathcal{F}$, by which we mean the isometric circles have diameter chosen as in Section 2A but are conditioned to be tangent. Then the probability $\langle f, g\rangle$ is discrete is at least $\frac{1}{6}$.*

Proof. It is not difficult to see that in fact the point of tangency is uniformly distributed in the circle and from our discussion above we see that this is the same as considering pairs of adjacent arcs. So as f and g are parabolic, their isometric disks are tangent and the point of intersection lies in a random arc of arclength uniformly distributed in $[0, 2\pi]$. Discreteness follows from the "ping pong" lemma and Lemma 9.2. □

11. Another discreteness criterion

Theorem 8.4 gives a discreteness criterion based on the disjointness of isomeric circles. Another criterion can be found as the first condition in [Rosenberger 1986, Theorem 3].

Theorem 11.1. *Let f and g be hyperbolic. If $\gamma(f, g) \le -4$, then $\langle f, g\rangle$ is discrete.*

With f and g selected randomly we recall from (7.3) that the condition $\gamma \le -4$ reads as

$$(11.2)\quad -\sin^2\theta_1 \sin^2\theta_2 \ge 2\cos^2\theta_1(\sin^2\phi_2 - \sin^2\alpha\cos^2\theta_2) + \cos^2\theta_2\sin^2\phi_1 - 2\cos\alpha\cos\theta_1\cos\theta_2\sin\phi_1\sin\phi_2.$$

In our computational investigations we were drawn to the following remarkable observation.

Conjecture 11.3. *Let $f, g \in_* \mathcal{F}$ be hyperbolic and suppose the pairs of isometric circles are not disjoint. Then*

$$\mathbf{Pr}\{\gamma(f, g) \le -4\} = \tfrac{1}{5}. \tag{11.4}$$

The expression in (11.2) provides good gradient bounds for a test and we were able to search this space to verify the conjecture to two decimal places. To gain just a little bit more accuracy without a great deal more care (and time) in our searches, we added in the additional result adapted from [Rosenberger 1986, Theorem 2].

Theorem 11.5. *Let f and g be hyperbolic and $\gamma(f, g) > 0$. Then $\langle f, g\rangle$ is discrete if there are representatives A and B in* $\mathrm{PSL}(2, \mathbb{R})$, *for f and g, respectively, such that*

(1) $0 \le \operatorname{tr}(A) \le \operatorname{tr}(B) \le |\operatorname{tr}(AB)|$,

(2) $\operatorname{tr}(AB) \le -2$.

Of course the theorem applies to Nielsen equivalent pairs of generators. If $f, g \in_* \mathcal{F}$, we can compute

$$\begin{aligned}
\operatorname{tr}(f) &= 2\csc\theta_1\cos\phi_1,\\
\operatorname{tr}(g) &= 2\csc\theta_2\cos\phi_2,\\
\operatorname{tr}(fg) &= 2\csc\theta_1\csc\theta_2(\cos\theta_1\cos\theta_2\cos\alpha + \cos\phi_1+\phi_2),\\
\operatorname{tr}(fg^{-1}) &= 2\csc\theta_1\csc\theta_2(\cos(\phi_1-\phi_2) - 2\cos\theta_1\cos\theta_2\cos\alpha).
\end{aligned}$$

Rearranging to avoid singularities for our gradient estimates (because of our normalisations we use f and g^{-1}), the tests we therefore derive from Theorem 11.5 are

(1) $\sin(\theta_2)\cos(\phi_1) \le \sin(\theta_1)\cos(\phi_2)$,

(2) $\sin(\theta_1)\cos(\phi_2) \le |\cos(\phi_1-\phi_2) - 2\cos(\theta_1)\cos(\theta_2)\cos(\alpha)|$,

(3) $\cos(\phi_1-\phi_2) + \sin(\theta_1)\sin(\theta_2) \le \cos(\theta_1)\cos(\theta_2)\cos(\alpha)$.

A few simple experiments show that if f and g are hyperbolic with intersection isometric circles, then the test above as well as that obtained by the interchange of θ_1 and θ_2 (and the immaterial interchanging of ϕ_1 and ϕ_2) occurs about 5% of the time. It is easy to prove that it happens at least 2% of the time, giving us an easy error bound for our computational verification of Conjecture 11.3. Putting these together, with the bound from isometric circle disjointness yields the following theorem.

Theorem 11.6. *Let $f, g \in_* \mathcal{F}$ be hyperbolic. Then*

$$\mathbf{Pr}\{\langle f, g\rangle \textit{is discrete}\} \ge \tfrac{2}{5}. \tag{11.7}$$

12. Representations of $\mathbb{Z}_n * \mathbb{Z}$ in PSL(2, $\mathbb{R}$)

The discreteness criteria we have used above are not particularly sophisticated, but only minor improvements are known in the generality in which we use them. These amount to looking at deeper level configurations of isometric circles and quickly become extremely complicated. However there is one case where rather more precise results are known in general and that is the case where one generator has order 2. For Fuchsian groups we know more when a generator has finite order. In [Gehring et al. 2001], precise results are given to determine when $G = \langle f, g\rangle$ is discrete, where $\beta(g) = -4$, $\beta(f) \in \mathbb{R}$ and $\gamma(f, g) \in \mathbb{R}$.

It is important to note that this case is not so special, as evidenced by Theorem 12.1.

Theorem 12.1 [Gehring and Martin 1994]. *Let $\langle f, g\rangle$ be a discrete subgroup of* PSL(2, $\mathbb{C}$). *Then there is an elliptic Φ of order* 2 *such that $\langle f, \Phi\rangle$ is discrete, and*

$$\gamma(f, g) = \operatorname{tr}[f, g] - 2 = \operatorname{tr}[f, \Phi] - 2 = \gamma(f, \Phi)$$

This theorem explains in part why we would like to identify the p.d.f. for $\gamma(f, g)$. Care must be taken in using this result in our setting since although f, g might be randomly selected, it is not the case that Φ is.

If we choose a random matrix B conditioned by the assumptions $\operatorname{tr}(B) = 0$, and another random matrix A, then we have the forms

$$A = \begin{pmatrix} e^{i\phi}\csc(\eta) & e^{i\alpha}\cot(\eta) \\ e^{-i\alpha}\cot(\eta) & e^{-i\phi}\csc(\eta)\end{pmatrix}, \quad B = \begin{pmatrix} i\csc(\theta) & e^{i\psi}\cot(\theta) \\ e^{-i\psi}\cot(\theta) & -i\csc(\theta)\end{pmatrix},$$

where all the angles are chosen uniformly in $[0, \pi]$ and we have simplified the variables, replacing η and θ with $\eta/2$ and $\theta/2$ as above:

$$\beta = 4\csc^2(\eta)\cos^2(\phi) - 4,$$

$$\gamma = 4\cot^2(\eta)(\csc^2(\theta) - \cot^2(\theta)\sin^2(\alpha)) + 4\csc^2(\eta)\cot^2(\theta)\sin^2(\phi) \\ -8\cot(\eta)\csc(\eta)\cot(\theta)\csc(\theta)\sin(\phi)\cos(\alpha),$$

where we have assumed $\beta \geq 0$ to simplify the last equation and written α for $\alpha - \psi$ since both are uniformly distributed.

Now by [Gehring et al. 2001, Theorem 3.1], the group $\langle A, B | A^2 = 1\rangle$ projects to a faithful discrete nonelementary subgroup of PSL(2, $\mathbb{R}$) if and only if $4 \leq \beta + 4 \leq \gamma$. After some manipulation, we need to decide when

$$\sin^2(\alpha)\sin^2(\eta)\sin^2(\theta) \leq (\cos(\alpha)\cos(\eta) - \cos(\theta)\cos(\phi))^2.$$

Some parity and symmetry considerations reduce the problem to finding $8/\pi^4$ times the measure of the set

$$\{(\eta, \theta, \alpha, \phi) \in [0, \pi/2]^2 \times [0, \pi]^2 : \sin\alpha\sin\eta\sin\theta \leq \cos\alpha\cos\eta - \cos\theta\cos\phi\}.$$

We could not find a closed form for this number, but used numerical techniques to obtain the following theorem.

Theorem 12.2. *Let $f, g \in_* \mathcal{F}$ be conditioned by $f^2 = 1$. Then*

$$\mathbf{Pr}\{\overline{\langle f, g\rangle}\} = \mathcal{F}\} = 0.706 \pm 0.001.$$

However there is one family of special cases to which we can give a precise theorem. A slight generalisation of [Gehring et al. 2001] yields the following:

Lemma 12.3. *Let $\Gamma = \langle f, g\rangle$ be a Möbius group with $f^n = 1$ and g hyperbolic. Then Γ is discrete and free on its generators if and only if*

$$\gamma \geq \left(\sqrt{\beta+4} + 2\cos\frac{\pi}{n}\right)^2,$$

where $\beta = \operatorname{tr}^2(g) - 4$.

The "boundary groups" are the groups with presentation $\langle a, b | a^n = b^\infty = 1\rangle$.

Thus if $A \sim f : z \to \zeta z$ with $\zeta^n = 1$ and $B \sim g \in_* \mathcal{F}$ is hyperbolic and randomly chosen, then we compute

$$\beta = \operatorname{tr}^2(B) - 4 = 4\csc^2\eta\cos^2\phi - 4, \gamma = \operatorname{tr}[A, B] - 2 = 4\sin^2\frac{\pi}{n}\cot^2\eta,$$

and our test for discreteness is $\gamma \geq \left(\sqrt{\beta+4} + 2\cos\frac{\pi}{n}\right)^2$. That is,

$$4\sin^2\frac{\pi}{n}\cot^2\eta \geq \left(2\csc\eta\cos(\phi) + 2\cos\frac{\pi}{n}\right)^2.$$

We want to take the square roots here. Since $\eta \in_u \left[0, \frac{\pi}{2}\right]$, the left-hand side is positive. Similarly, since $\phi \in_u [0, \pi]$ it makes no difference to assume $\phi \in_u \left[0, \frac{\pi}{2}\right]$. We therefore should determine when

$$\sin\left(\frac{\pi}{n} - \eta\right) \geq \cos(\phi), \quad \eta, \phi \in_u \left[0, \frac{\pi}{2}\right]. \tag{12.4}$$

It is immediate that this probability is no more than $\frac{1}{n}$ as the right-hand side is positive. In fact, this shows that for the angles distributed as above,

$$\Pr\left\{\sin\left(\frac{\pi}{n} - \eta\right) \geq \cos(\phi)\right\} = \frac{1}{n}\Pr\{\sin(\theta) \geq \cos(\phi)\}.$$

This probability is then

$$\frac{4}{\pi^2}\int_0^{\pi/n}\int_0^{\sin(\theta)} \frac{dx\,d\theta}{\sqrt{1-x^2}} = \frac{2}{n^2}.$$

In terms of our original question about topological generation this reads as:

Theorem 12.5. *Let $f(z) = \zeta z$ and $\zeta^n = 1$. Let $g \in_* \mathcal{F}$ be a randomly chosen hyperbolic. Then*

$$\mathbf{Pr}\left\{\overline{\langle f, g\rangle} = \mathcal{F}\right\} = 1 - \frac{2}{n^2}.$$

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PUZZLES IN *K*-HOMOLOGY OF GRASSMANNIANS

PAVLO PYLYAVSKYY AND JED YANG

Knutson, Tao, and Woodward (2004) formulated a Littlewood–Richardson rule for the cohomology ring of Grassmannians in terms of puzzles. Vakil (2006) and Wheeler and Zinn-Justin (2017) have found additional triangular puzzle pieces that allow one to express structure constants for *K*-theory of Grassmannians. Here we introduce two other puzzle pieces of hexagonal shape, each of which gives a Littlewood–Richardson rule for *K*-homology of Grassmannians. We also explore the corresponding eight versions of *K*-theoretic Littlewood–Richardson tableaux.

1. Introduction

Cohomology rings of flag varieties are a major object of interest in algebraic geometry, see [Fulton 1984; Manivel 2001] for an exposition. Perhaps the most well-studied and well-understood examples are the cohomology rings of Grassmannians, with a distinguished basis of Schubert classes. A *Littlewood–Richardson rule* is a combinatorial way to compute the structure constants for this basis. Equivalently, those are the same structure constants $c^{\nu}_{\lambda\mu}$ with which certain symmetric functions — *Schur functions* s_λ — multiply: $s_\lambda s_\mu = \sum_\nu c^{\nu}_{\lambda\mu} s_\nu$. In their groundbreaking work Knutson, Tao, and Woodward [Knutson and Tao 1999; Knutson et al. 2004] introduced *puzzles*, which allow for a powerful formulation of the Littlewood–Richardson rule. Puzzles are tilings of triangular boards with specified boundary conditions by a set of tiles shown in Figure 1. Using puzzles Knutson, Tao, and Woodward studied the faces of the Klyachko cone.

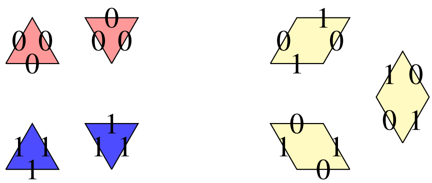


Figure 1. The Knutson–Tao–Woodward tiles.

MSC2010: primary 05E15; secondary 14M15, 52C20.
Keywords: puzzles, hexagon, tiling, K-theory, Grassmannian, Littlewood–Richardson coefficient.

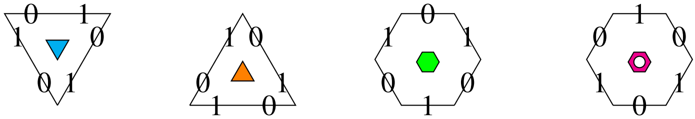


Figure 2. The four K-theoretic tiles.

There is a cohomology theory for each one-dimensional group law [Hazewinkel 1978; Lenart and Zainoulline 2017]. For the additive group law $x \oplus y = x + y$ one has the usual cohomology, while the multiplicative group law $x \oplus y = x + y + xy$ gives the *K-theory*. K-theory of Grassmannians was extensively studied, starting with the works of Lascoux and Schützenberger. In [Lascoux and Schützenberger 1982] they introduced the *Grothendieck polynomials* as representatives of K-theory classes of structure sheaves of Schubert varieties. Fomin and Kirillov [1995] studied those from combinatorial point of view, introducing the *stable Grothendieck polynomials* G_λ. Stable Grothendieck polynomials are symmetric power series that form a rather precise K-theoretic analogue of Schur functions: their multiplicative structure constants are the same as those for classes of the structure sheaves of Schubert varieties in the corresponding K-theory ring.

The first K-theoretic Littlewood–Richardson rule was obtained by Buch [2002]. Vakil [2006] has extended puzzles to K-theory, giving a puzzle version of the rule. His extension works by adding a single additional tile to the set of tiles from the work of Knutson, Tao and Woodward [Knutson et al. 2004]. Later, Wheeler and Zinn-Justin [2017] found an alternative K-theoretic tile, that gives the structure constants of dual K-theory in an appropriate sense. Both Vakil and Wheeler–Zinn-Justin tiles have triangular shape and can be seen in Figure 2.

In this work we present *two new tiles*, adding either one of which to the standard collection allows one to recover structure constants of the Schubert basis in the *K-homology* ring of the Grassmannians, as studied by Lam and Pylyavskyy [2007]. Equivalently, the corresponding puzzles produce a combinatorial rule for the *coproduct* structure constants of the stable Grothendieck polynomials. The first such rule was obtained by Buch [2002]. The tiles have *hexagonal shape* and can be seen in Figure 2.

The paper proceeds as follows. In Section 2 we recall the known results on the cohomology ring of Grassmannians, including tableaux and puzzles formulations of the Littlewood–Richardson rule. In Section 3 we recall the K-theoretic version of the story, and state our main results regarding the two new hexagonal tiles. We also systematize the eight different tableaux formulations of the K-theoretic Littlewood–Richardson rule, some of which are new. The proofs are postponed to Section 4. In Section 5 we conclude with remarks, including the relation of our work to that of Pechenik and Yong [2017] on genomic tableaux.

2. Puzzles and tableaux

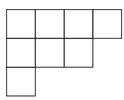
2A. ***Cohomology of Grassmannians.*** Let $\mathrm{Gr}(k, n)$ be the variety of k-dimensional subspaces of $\mathbb{C}^n$. Recall that a *partition* $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_k)$ is a weakly decreasing sequence $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_k \geq 0$ of finitely many nonnegative integers. Restrict to the set of partitions with k parts and with $\lambda_1 \leq n - k$. Fix a complete flag $0 = V_0 \subset V_1 \subset \cdots \subset V_n = \mathbb{C}^n$, with $\dim(V_i) = i$. The *Schubert variety* in $\mathrm{Gr}(k, n)$ associated to λ is the set

$$X_\lambda = \left\{ W \in \mathrm{Gr}(k, n) \mid \dim(W \cap V_{n+k+i-\lambda_i}) \geq i, \ \forall i \in [k] \right\}.$$

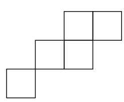
The associated classes $[X_\lambda]$ in the cohomology ring $H_*(\mathrm{Gr}(k, n), \mathbb{Z})$ are known to form a basis, with the structure constants $c_{\lambda\mu}^{\nu}$ called *Littlewood–Richardson coefficients*:

$$[X_\lambda] \cdot [X_\mu] = \sum_\nu c_{\lambda\mu}^{\nu} [X_\nu].$$

Littlewood–Richardson coefficients can also be described in the following elementary way. The Young diagram, or simply, *diagram*, of a partition λ is a collection of boxes, top and left justified, with λ_i boxes in row i. For example, this is the diagram of the partition $\lambda = (4, 3, 1)$:



If λ is a partition whose diagram fits inside that of partition ν, the *skew* diagram of *shape* ν/λ is the diagram consisting of the boxes of the diagram of ν outside that of λ. For example, the following is the diagram of $(4, 3, 1)/(2, 1)$:



Given a (possibly skew) diagram and a set V, a *V-tableau* T is a filling of the boxes with values in V. If V is omitted, it is understood that V is the positive integers. The *shape* of T, denoted $\mathrm{shape}(T)$, is the shape of the diagram. We say that T is *semistandard* if the values are weakly increasing from left to right in rows and strictly increasing from top to bottom in columns. The *reverse row word* of T, denoted $\mathrm{row}(T)$, is the sequence of values of T, read row by row, top to bottom, right to left. For example,

$$T = \begin{array}{|c|c|c|c|} \hline & & 1 & 1 \\ \hline & 2 & 2 & \\ \hline 1 & & & \\ \hline \end{array}$$

is a semistandard tableau with $\mathrm{shape}(T) = (4, 3, 1)/(2, 1)$ and $\mathrm{row}(T) = 11221$.

Let $x_1, x_2, \ldots$ be commutative variables, and let x^T denote the monomial $x_{w_1} x_{w_2} \cdots x_{w_r}$ where $\mathrm{row}(T) = w_1 w_2 \cdots w_r$. The *Schur polynomial* s_λ is given by

$$s_\lambda(x) = \sum_T x^T,$$

where the sum runs over all semistandard tableaux T of shape λ. It is well known that s_λ is symmetric and $\{s_\lambda\}_\lambda$ is a linear basis for the space of all symmetric polynomials (see, e.g., [Stanley 1999]). We may therefore expand the product $s_\lambda s_\mu$ uniquely as a sum of Schur polynomials s_ν as

$$s_\lambda s_\mu = \sum_\nu c^\nu_{\lambda\mu} s_\nu.$$

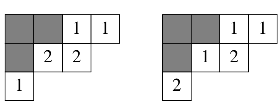
It turns out that the $c^\nu_{\lambda\mu}$ are exactly the Littlewood–Richardson coefficients we described above. They are nonnegative integers, and are zero whenever $|\nu| \neq |\lambda| + |\mu|$, where $|\lambda|$ is the number of boxes of λ. In other words, we can let the sum above run over only ν such that $|\nu| = |\lambda| + |\mu|$. This implies that the sum has finitely many terms.

The Littlewood–Richardson coefficients are ubiquitous, appearing naturally in a variety of contexts. In addition to the Schubert calculus context explained above, they also appear in the representation theory of symmetric groups and of general linear groups, in the theory of orthogonal polynomials, etc. There are also many combinatorial rules for computing $c^\nu_{\lambda\mu}$. In what follows we recall three rules, two involving counting tableaux and one involving counting puzzles.

2B. ***Tableau versions of the Littlewood–Richardson rule.*** Let $w = w_1 w_2 \cdots w_r$ be a sequence of positive integers. The *content* of w, denoted $\mathrm{content}(w)$, is $(m_1, m_2, \ldots, m_k)$ such that m_i is the number of occurrences of i in the sequence w.[1] We say w is *ballot* if $\mathrm{content}(w_1 \cdots w_i)$ is a partition for every i. In other words, in every initial segment of w, the number j occurs at least as many times as the number $j+1$. The *content* of T, denoted $\mathrm{content}(T)$, is simply $\mathrm{content}(\mathrm{row}(T))$. We say that T is *ballot* if $\mathrm{row}(T)$ is.

Theorem 2.1 (Littlewood–Richardson rule, skew version). *For partitions λ, μ, ν such that $|\nu| = |\lambda| + |\mu|$, the coefficient $c^\nu_{\lambda\mu}$ is the number of semistandard ballot tableaux of shape ν/λ and content μ.*

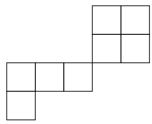
Example 2.2. Let $\lambda = (2, 1)$, $\mu = (3, 2)$, and $\nu = (4, 3, 1)$ in the following examples. The following are the (only) two ways to fill according to the Littlewood–Richardson rule.



[1]For example, if $w = \mathrm{row}(T)$, then in the monomial x^T, the exponent of x_i is m_i.

This shows that $c^{\nu}_{\lambda\mu} = 2$. For visual purposes, we gray out the boxes corresponding to λ instead of removing them. (This will be useful later when we temporarily write numbers in removed boxes.)

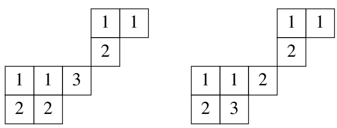
Given two partitions λ and μ, let the $\oplus$ diagram of shape $\mu \oplus \lambda$ be obtained by putting the diagrams of μ and λ corner to corner, with μ to the lower left and λ to the upper right. For example,



is a diagram of shape $(3, 1) \oplus (2, 2)$.

Theorem 2.3 (Littlewood–Richardson rule, $\oplus$ version). *For partitions λ, μ, ν such that $|\nu| = |\lambda| + |\mu|$, the coefficient $c^{\nu}_{\lambda\mu}$ is the number of semistandard ballot tableaux of shape $\mu \oplus \lambda$ and content ν.*

Example 2.4. We continue with λ, μ, ν from the example above. The following are the two corresponding fillings using the $\oplus$ version of the Littlewood–Richardson rule.



These are displayed in the same order under the bijection that is described in later sections.

Of course, any $\oplus$ diagram $\mu \oplus \lambda$ is also a skew diagram of shape

$$(\lambda_1 + \mu_1, \ldots, \lambda_k + \mu_1, \mu_1, \ldots, \mu_k).$$

Nevertheless, we think of these classes of shapes separately, since we will have pairs of tableaux rules, one involving shape ν/λ and one involving shape $\mu \oplus \lambda$. We refer to ν/λ as skew shape (and use grayed out boxes) and refer to $\mu \oplus \lambda$ as $\oplus$ shape (without using grayed out boxes).

2C. *Puzzle version of the Littlewood–Richardson rule.* Let $n \geq k$ be positive integers. Refer to the partition of k rows of length $n - k$ as the *ambient rectangle*. From now on, we consider only partitions whose diagrams fit inside this ambient rectangle. (To consider bigger partitions, simply specify a larger ambient rectangle.) On the lower right boundary of a partition inside the ambient rectangle, write a 0 on each horizontal edge and a 1 on each vertical edge (see Figure 3). A binary string of length n with k ones and $n - k$ zeros is obtained by reading these numbers from top right to bottom left.

Here we consider tilings on the triangular lattice. Knutson, Tao, and Woodward [Knutson et al. 2004] introduced the following *puzzle pieces* (see Figure 4).

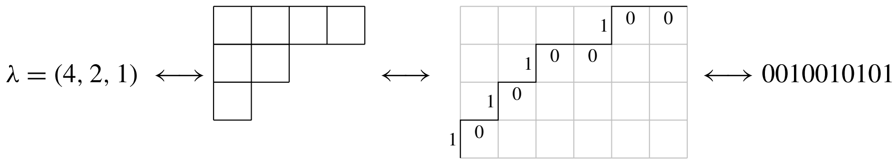


Figure 3. Bijection between partitions, Young diagrams, and binary strings; $n = 10$, $k = 4$.

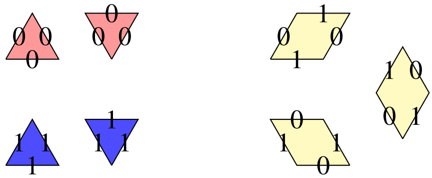


Figure 4. Puzzle pieces.

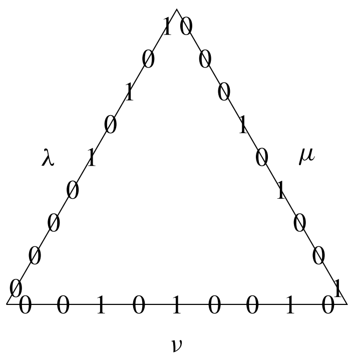


Figure 5. Boundary $\Delta^{\nu}_{\lambda\mu}$ with $\lambda = (2, 1, 0)$, $\mu = (3, 2, 0)$, and $\nu = (4, 3, 1)$.

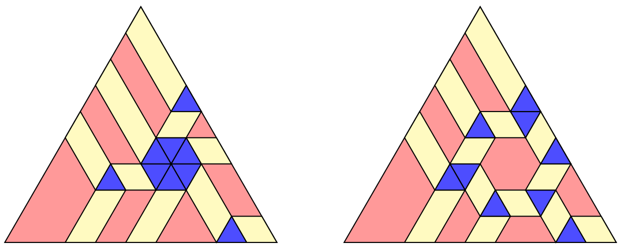
- 0-triangle: unit triangle with edges labeled by 0, two rotations;
- 1-triangle: unit triangle with edges labeled by 1, two rotations; and
- rhombus: formed by gluing two adjacent unit triangles together, with edges labeled by 0 if clockwise of an acute angle and 1 if clockwise of an obtuse angle, three rotations.

A *tiling* is an assembly of (lattice) translated copies of tiles, where edge labels of adjacent tiles must match. We are interested in tiling an upright triangular region $\Delta^{\nu}_{\lambda\mu}$ whose boundary labels of the left, right, and bottom sides, read left-to-right, are the binary strings corresponding to λ, μ, and ν (see Figure 5).

Littlewood–Richardson coefficients can be calculated by counting puzzle tilings:

Theorem 2.5 [Knutson et al. 2004]. *Suppose λ, μ, ν are partitions fitting inside an $(n-k)\times k$ ambient rectangle, with $|\nu| = |\lambda| + |\mu|$. The number of puzzle tilings with boundary $\Delta^{\nu}_{\lambda\mu}$ is $c^{\nu}_{\lambda\mu}$.*

Example 2.6. Continuing with the running example from the previous section, since $c^{\nu}_{\lambda\mu} = 2$, there are two tilings of $\Delta^{\nu}_{\lambda\mu}$:



Here and subsequently, some edges (namely, the edges within a region of 0-triangles and the 1-edges of a sequence of rhombi) are omitted to suggest the structure of puzzle tilings.

The bijection between the tableau rule and the puzzle rule can be seen with Tao's "proof without words" (see [Vakil 2006]). More details of this bijection is given when we generalize it in Section 4B. The reader is encouraged to use Zinn-Justin's puzzle viewer [2016] to aid in visualizing these puzzles.

3. K-theoretic puzzles and tableaux

In this section, we discuss four K-theoretic analogues of the Littlewood–Richardson coefficients. These coefficients can be calculated using four puzzle rules and eight tableaux rules.

3A. ***K-theory and K-homology of Grassmannians.*** Just as in the case of ordinary cohomology, the classes of the structure sheaves $\mathcal{O}_{X_\lambda}$ form a basis for the Grothendieck ring $K^\circ(\mathrm{Gr}(k, n))$. The associated structure constants $c^{\nu}_{\lambda\mu}$ are given by

$$[\mathcal{O}_{X_\lambda}]\cdot[\mathcal{O}_{X_\mu}] = \sum_{\nu} c^{\nu}_{\lambda\mu}[\mathcal{O}_{X_\nu}],$$

and generalize the usual Littlewood–Richardson coefficients in the sense that one recovers the latter for triples λ, μ, ν such that $|\lambda| + |\mu| = |\nu|$. An elementary construction of those structure constants also exists, with the K-theoretic analogue of a Schur function s_λ being the *single stable Grothendieck polynomial* G_λ given by the formula

$$G_\lambda = \sum_{T}(-1)^{|T|-|\lambda|}x^T,$$

where the sum runs over all semistandard set-valued tableaux T of shape λ, and $|T|$ is the length of $\mathrm{row}(T)$. The equivalence of this definition to other definitions is established by Buch [2002].

In addition to the K-theory ring $K^\circ(\mathrm{Gr}(k,n))$ one can also consider a K-homology ring $K_\circ(\mathrm{Gr}(k,n))$. The classes of the ideal sheaves $\mathcal{I}_{X_\lambda}$ of the boundary of the Schubert varieties X_λ form a basis in this ring. It turns out that this basis and the basis of classes of structure sheaves $\mathcal{O}_{X_\lambda}$ in $K^\circ(\mathrm{Gr}(k,n))$ are dual in a precise sense. The structure constants $d^\nu_{\lambda\mu}$ of the classes $[\mathcal{I}_{X_\lambda}]$ are given by

$$[\mathcal{I}_{X_\lambda}]\cdot[\mathcal{I}_{X_\mu}]=\sum_\nu d^\nu_{\lambda\mu}[\mathcal{I}_{X_\nu}],$$

and also constitute a generalization of the classical Littlewood–Richardson coefficients, recovering the latter in the case $|\lambda|+|\mu|=|\nu|$. We refer the reader to [Lam and Pylyavskyy 2007] for details. The same reference also gives a definition of *dual stable Grothendieck polynomials* g_λ, which generalize Schur functions in the sense of their structure constants being exactly the $d^\nu_{\lambda\mu}$.

One can recover the $d^\nu_{\lambda\mu}$ directly from the stable Grothendieck polynomials G_λ however, as follows. Buch has showed that the linear span of $\{G_\lambda\}_\lambda$ inherits from symmetric functions the structure of a bialgebra, with product given by

$$G_\lambda G_\mu=\sum_\nu(-1)^{|\nu|-|\lambda|-|\mu|}c^\nu_{\lambda\mu}G_\nu$$

and coproduct Δ given by

$$\Delta(G_\nu)=\sum_{\lambda,\mu}(-1)^{|\nu|-|\lambda|-|\mu|}d^\nu_{\lambda\mu}G_\lambda\otimes G_\mu.$$

In other words, the product structure constants $c^\nu_{\lambda\mu}$ for the G_λ are the coproduct structure constants for the g_λ, and vice versa.

It turns out that

$$c^\nu_{\lambda\mu}=0\quad\text{when }|\nu|<|\lambda|+|\mu|\qquad\text{and}\qquad d^\nu_{\lambda\mu}=0\quad\text{when }|\nu|>|\lambda|+|\mu|.$$

So we might as well restrict the first and second sums to the cases where $|\nu|\ge|\lambda|+|\mu|$ and $|\nu|\le|\lambda|+|\mu|$, respectively. Unlike the classical case, this does not immediately show that the sums are finite, but indeed they are (Corollaries 5.5 and 6.7 of [Buch 2002]).

As we mentioned above, when $|\nu|=|\lambda|+|\mu|$, the number $c^\nu_{\lambda\mu}$ is indeed the classical Littlewood–Richardson coefficient described in previous sections. Since this is the only case where the classical $c^\nu_{\lambda\mu}$ is possibly nonzero, by an abuse of notation, we use the same symbol to denote both. It is therefore paramount to require $|\nu|=|\lambda|+|\mu|$ when discussing $c^\nu_{\lambda\mu}$ in the classical case.

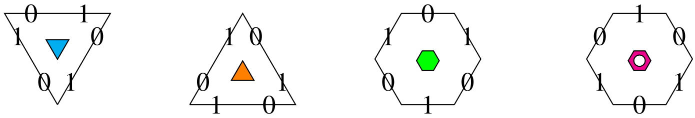


Figure 6. Four additional puzzle pieces.

The following slight variants of $c^{\nu}_{\lambda\mu}$ and $d^{\nu}_{\lambda\mu}$ arise naturally in the study of puzzles. Let $\widetilde{G}_{\lambda} = G_{\lambda} \cdot (1 - G_1)$. Define $\tilde{c}^{\nu}_{\lambda\mu}$ as the unique numbers such that

$$\widetilde{G}_{\lambda} \cdot \widetilde{G}_{\mu} = \sum_{\nu} (-1)^{|\nu|-|\lambda|-|\mu|} \tilde{c}^{\nu}_{\lambda\mu} \widetilde{G}_{\nu}.$$

We again restrict to $|\nu| \geq |\lambda| + |\mu|$, the only time when $\tilde{c}^{\nu}_{\lambda\mu}$ is possibly nonzero. The meaning of the $\widetilde{G}_{\lambda}$ in that they also represent ideal sheaves of Schubert varieties in certain rings is explained in [Wheeler and Zinn-Justin 2017].

Finally, let $\tilde{d}^{\nu}_{\lambda\mu}$ be given by $d^{\nu'}_{\lambda'\mu'}$, where λ' is the transpose of λ, i.e., mirror the diagram of λ across the line $x + y = 0$. Since the number of boxes is preserved, the only time $\tilde{d}^{\nu}_{\lambda\mu}$ is possibly nonzero is when $|\nu| \leq |\lambda| + |\mu|$. The $\tilde{d}^{\nu}_{\lambda\mu}$ form the same collection of structure constants as the $d^{\nu}_{\lambda\mu}$, just indexed differently.

3B. ***The four K-theoretic puzzles.*** Consider the puzzle pieces shown in Figure 6.

We refer to these puzzle pieces using the corresponding pictograms shown in the figure. If X is (the pictogram of) an additional puzzle piece, an X-puzzle is a puzzle tiling where, in additional to the usual puzzle pieces, translated copies of X can be used. There are known interpretations of $\triangledown$-puzzles and $\triangle$-puzzles.

Theorem 3.1 [Vakil 2006]. *Suppose λ, μ, ν are partitions fitting inside an $(n-k)\times k$ ambient rectangle, with $|\nu| \geq |\lambda| + |\mu|$. The number of $\triangledown$-puzzle tilings with boundary $\Delta^{\nu}_{\lambda\mu}$ is $c^{\nu}_{\lambda\mu}$.*

Theorem 3.2 [Wheeler and Zinn-Justin 2017]. *Suppose λ, μ, ν are partitions fitting inside an $(n-k)\times k$ ambient rectangle, with $|\nu| \geq |\lambda| + |\mu|$. The number of $\triangle$-puzzle tilings with boundary $\Delta^{\nu}_{\lambda\mu}$ is $\tilde{c}^{\nu}_{\lambda\mu}$.*

We establish interpretations of ⬢-puzzles and ⬡-puzzles.

Theorem 3.3. *Suppose λ, μ, ν are partitions fitting inside an $(n-k-1)\times k$ ambient rectangle,[2] with $|\nu| \leq |\lambda| + |\mu|$. The number of ⬢-puzzle tilings with boundary $\Delta^{\nu}_{\lambda\mu}$ is $d^{\nu}_{\lambda\mu}$.*

Theorem 3.4. *Suppose λ, μ, ν are partitions fitting inside an $(n-k)\times(k-1)$ ambient rectangle, with $|\nu| \leq |\lambda| + |\mu|$. The number of ⬡-puzzle tilings with boundary $\Delta^{\nu}_{\lambda\mu}$ is $\tilde{d}^{\nu}_{\lambda\mu}$.*

[2]For technical reasons, we require partitions to be slightly smaller. See Section 5A.

3C. ***The eightfold way.*** Like the classical case, where the puzzle rule corresponds to a pair of tableau rules (involving diagrams of shapes ν/λ and $\mu \oplus \lambda$, respectively), we describe four pairs of K-tableau rules corresponding to the four K-puzzle rules.

A *set-valued tableau* is a V-tableau where V consists of nonempty subsets of $\{1, \ldots, k\}$. To understand the semistandard condition in this context, we agree that for $A, B \in V$, A is (strictly) less than B if $\max A$ is (strictly) less than $\min B$. When forming the reverse row word, a value $A \in V$ is expanded as the numbers in the set A, written from largest to smallest.

Buch [2002] gives a combinatorial rule for calculating the K-theory Littlewood–Richardson coefficient $c^{\nu}_{\lambda\mu}$ by counting certain set-valued tableaux of $\oplus$ shape.

Theorem 3.5 ($\blacktriangledown$ rule, $\oplus$ version). *The coefficient $c^{\nu}_{\lambda\mu}$ is the number of semistandard ballot set-valued tableaux of shape $\mu \oplus \lambda$ and content ν.*

To describe the skew version of the K-theory rule, we consider a new kind of tableaux. A *circle tableau* T is a V-tableau where V consists of $\{1, \ldots, k\}$ and the *circled* numbers $\{\textcircled{1}, \ldots, \textcircled{k}\}$.

We say T is a *right* (resp. *left*) circle tableau if each $\textcircled{i}$ is the rightmost (resp. leftmost) i or $\textcircled{i}$ in its row. (In other words, for each i, only the rightmost (resp. leftmost) i in a row is optionally circled.) Moreover, circled values may only occur in the bottom k rows (that is, anywhere in shape ν/λ, bottom half in shape $\mu \oplus \lambda$).

We say T is *semistandard* if it is semistandard when the circled values are treated as if they are not circled. Its *content* is $\text{content}(w)$ where w is $\text{row}(T)$ with the circled values omitted.

Let w be an initial segment of $\text{row}(T)$. If w ends with $\textcircled{i}$, replace it with an uncircled $i+1$. Remove all other circled entries. Call the result the *incremented erasure* of w. Analogously, call the result the *unincremented erasure* of w if the final $\textcircled{i}$ is replaced with an uncircled i instead. We say that a right (left) circle tableau is *ballot* if all its incremented (unincremented) erasures are ballot.

Pechenik and Yong [2017] give a combinatorial rule for calculating the K-theory Littlewood–Richardson coefficient $c^{\nu}_{\lambda\mu}$ by counting certain *genomic* tableaux of skew shape. We give an equivalent formulation (see Section 5C) here in terms of circle tableaux.

Theorem 3.6 ($\blacktriangledown$ rule, skew version). *The coefficient $c^{\nu}_{\lambda\mu}$ is the number of semistandard ballot right circle tableaux of shape ν/λ and content μ.*

An *outer corner* of (the diagram of) a partition μ is a box whose addition results in a diagram of a partition.

Theorem 3.7 ($\blacktriangle$ rule, $\oplus$ version). *The coefficient $\tilde{c}^{\nu}_{\lambda\mu}$ is the number of semistandard ballot set-valued tableaux of shape $\mu^{+} \oplus \lambda$ and content ν, where μ^{+} is μ with some number* (*possibly zero*) *of its outer corners added.*

Theorem 3.8 (△ rule, skew version). *The coefficient $\tilde{c}_{\lambda\mu}^{\nu}$ is the number of semistandard ballot left circle tableaux of shape ν/λ and content μ.*

Recall that a circle tableau of shape $\mu \oplus \lambda$ does not have circles in the rows corresponding to λ.

Theorem 3.9 (⬢ rule, $\oplus$ version). *The coefficient $d_{\lambda\mu}^{\nu}$ is the number of semistandard ballot right circle tableaux of shape $\mu \oplus \lambda$ and content ν.*

An *inner corner* of (the diagram of) a partition λ is a box whose removal results in a diagram of a partition.

Theorem 3.10 (⬢ rule, skew version). *The coefficient $d_{\lambda\mu}^{\nu}$ is the number of semistandard ballot set-valued tableaux of shape ν/λ^- and content μ, where λ^- is λ with some number (possibly zero) of its inner corners removed.*

A circle tableau of shape $\mu \oplus \lambda$ is *limited* if it has no ⓘ in row i of the bottom half for any i.

Theorem 3.11 (⬡ rule, $\oplus$ version). *The coefficient $\tilde{d}_{\lambda\mu}^{\nu}$ is the number of limited semistandard ballot left circle tableaux of shape $\mu \oplus \lambda$ and content ν.*

Theorem 3.12 (⬡ rule, skew version). *The coefficient $\tilde{d}_{\lambda\mu}^{\nu}$ is the number of semistandard ballot set-valued tableaux of shape ν/λ and content μ.*

Note that the limited condition present in the $\oplus$ version of the ⬡ rule does not appear in the skew version. Instead, the limited condition arises implicitly in the skew version of the ▽ rule (Theorem 3.6). In that case, the ballot condition implies the limited condition. See Section 4D for details.

4. Proofs

4A. ***Proof of Theorem 3.10.*** Given a sequence $w = (w_1, \dots, w_r)$ and an interval $[a, b]$, let $w|_{[a,b]}$ be the sequence obtained by shifting the numbers down to the interval $[1, b-a+1]$ by subtracting $a-1$ from each number w_i in the range $[a, b]$ (and omitting numbers that are out of the range).

Theorem 4.1 [Buch 2002]. *The coefficient $d_{\lambda\mu}^{\nu}$ is the number of semistandard set-valued tableaux T of shape ν with content $(\lambda, \mu) = (\lambda_1, \lambda_2, \dots, \lambda_k, \mu_1, \dots, \mu_k)$, such that* $\operatorname{row}(T)|_{[1,k]}$ *and* $\operatorname{row}(T)|_{[k+1,2k]}$ *are both ballot.*

For notational convenience, local to this proof only, a *Buch tableau* is one described in Theorem 4.1. and a ⬢ *tableau* is one described in Theorem 3.10. There is a simple bijection between Buch tableaux and ⬢ tableaux.

Indeed, let T be a ⬢ tableau. Increase each number in T by k. Extend the shape of T to ν by filling in the first λ_i boxes of T with i in row i. The result is clearly a Buch tableau.

Figure 7. Left: a beam of length 3. Right: three beams of length 1.

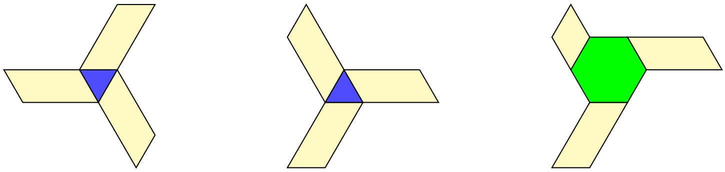


Figure 8. All the ways beams can meet.

Conversely, let T be a Buch tableau. It is easy to see that, as T is semistandard and $\mathrm{row}(T)|_{[1,k]}$ is ballot, the λ_i occurrences of i are exactly in the first λ_i boxes of row i. Remove these "*small*" numbers. A remaining "*big*" number in row i cannot be in the first $\lambda_i - 1$ boxes, since the λ_i-th box contained a small number. It can be in the λ_i-th box only if the λ_i-th box in the next row did not contain a small number. In other words, only if this box is an inner corner of λ. We therefore conclude that the shape of the remaining tableau is ν/λ with some (possibly zero) inner corners of λ added. Decrease k from all the remaining numbers to obtain a ⬢ tableau.

This concludes the proof of Theorem 3.10.

4B. ***Proof of Theorem 3.3.*** We prove Theorem 3.3 by establishing a bijection between ⬢-puzzles and the tableaux described in Theorem 3.10. For notational convenience, we do so by considering an example when $k = 4$. The general case is similar.

First, we consider the structure of a generic ⬢-puzzle. In a tiling, the rhombi form *beams*, a sequence of rhombi adjacent by their 1-edges. The number of rhombi in the beam is its *length*. If beams are adjacent to each other because some rhombi are adjacent by their 0-edges, we consider the beams as separate beams of width one (see Figure 7). Otherwise, three beams can meet at a 1-triangle or a ⬢, as in Figure 8.

If no ⬢ piece is used, the structure is simple, and can be seen in Tao's "proof without words" (see [Vakil 2006]). From the bottom boundary, each 1-edge is adjacent to an *upward* beam (possibly of zero length). The top of each upward beam must be an upright 1-triangle. The left and right side of the 1-triangle are each adjacent to a *leftward* and a *rightward* beam, respectively. A leftward beam terminates either at the left boundary or the right side of an upside-down 1-triangle. Similarly, a rightward beam terminates at the right boundary or the left side of an

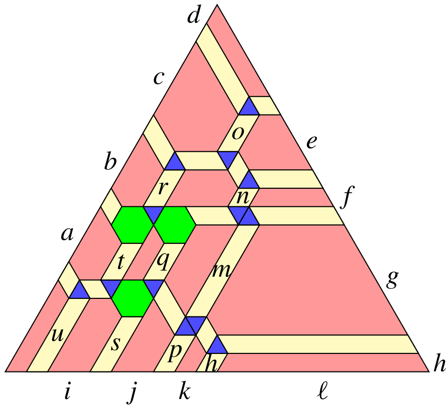


Figure 9. An example tiling.

upside-down 1-triangle. These upside-down 1-triangles have upward beams on their top edges. The rest of the puzzle is filled with 0-triangles.

Now we consider adding in the piece (see Figure 9). Since the piece has 1-edges in the same orientation as the upright 1-triangle, it can be placed on top of an upright beam to replace an upright 1-triangle. It also must have a leftward and a rightward beam adjacent to its two other 1-edges. As compared to using a 1-triangle instead of the piece, the length of the leftward beam is decreased by one, and the rightward beam is shifted up by one.

In Figure 9, the upright beams have labels. We refer to the beam with label x as the x-*beam*. By abuse of notation, we also let x denote the length (that is, the number of rhombi) of the x-beam. For each x-beam, set x' to x. Increment x' by one if the x-beam is capped with a on top (as opposed to a triangle). In the example in the figure, t', q', and s' are the ones that are incremented. The boundary also has some length labels. We use the same labels as those in Tao's "proof without words."

Note that these numbers completely determine the tiling. Indeed, let us describe a process to assemble such a tiling based on the numbers. Place (the rhombi of) the bottom beams according to their lengths (e.g., u, s, p, and h). Place 1-triangles or hexagons on top of them based on whether $x' = x$ or not. Extend the leftmost leftward beam and the rightmost rightward beam to the boundary. In the middle, extend each pair of leftward and rightward beams until they meet each other. That is the unique position to place an upside-down 1-triangle. If we had k beams at the bottom, there are now $k-1$ upside-down 1-triangles. Repeat the process according to the lengths of the second level of upward beams (e.g., t, q, and m). The puzzle can be built level by level, each time with one fewer upward beam. Finally, fill the rest of the puzzle with 0-triangles.

We now describe a bijection from the ⬣-puzzles to skew tableaux. In the boxes of a diagram of shape ν/λ, fill out according to the following schematic plan

				$1u$
			$1t$	$2s$
		$1r$	$2q$	$3p$
	$1o$	$2n$	$3m$	$4h$

where, a number x followed by a letter y in the schematic plan means to fill the number x in y consecutive boxes. If $y' > y$, write an additional x in the *previous* box, without using space. Circle such a number for easy reference. The grayed out boxes correspond to λ and may contain circled numbers; the white boxes correspond to ν/λ and each has exactly one uncircled number. Call this tableau T.

Example 4.2. Applying the bijection described to the puzzle results in the following tableau.

											1	1	1	1
							①	1	1②	2	2	2		
					1	1②	2	2	3	3				
	1	1	2	3	3	3	3	3	4					

From the tiling, one could read off certain equalities and inequalities (see Figure 10).

<u>Shape</u>. The top left picture shows that

$$\nu_2 + 3 = 1 + j + 1 + k + 1 + \ell = s + t + 1 + b + 1 + c + 1 + d = s + t + \lambda_2 + 3,$$

or $\nu_2 - \lambda_2 = s + t$. This means that the $s + t$ uncircled numbers we fill in row 2 of ν/λ precisely takes up the $\nu_2 - \lambda_2$ boxes. In other words, the shape is unaffected by the ⬣ tiles, except for the possibility of writing ① in the shaded boxes, discussed below.

<u>Content</u>. The top right picture shows that $s' + 1 + q' + 1 + n' = h + 1 + g + 1 + h = \mu_2 + 2$, or $\mu_2 = s' + q' + n'$, leading to content$(T) = \mu$ where ⓘ is treated as i.

<u>Ballot</u>. The lower left picture shows that $u' + t' \geq s' + q' \geq p' + m'$. This directly translates to the ballot condition of T, again by treating ⓘ as i.

<u>Semistandard</u>. The lower right picture shows a final type of inequalities, which are slightly more complicated. Let $x \geq_z y$ be a shorthand for $x \geq y + z' - z$. In other words, $x \geq_z y$ means $x \geq y$ if $z' = z$, and means $x > y$ if $z' = z + 1$. If there are no ⬣ tiles, the two thick lines in the picture must not cross, yielding inequalities $b \geq r$ and $b + t \geq r + q$. Because of the ⬣ tiles, these inequalities must be strict. Therefore we get $b \geq_t r$ and $b + t \geq_s r + q$ instead. These inequalities translate to the semistandard condition of T by considering all pairs of numbers in adjacent boxes. Also note that if $b = 0$, then $b \geq_t r$ says that $t = t'$ (and $r = 0$), so there cannot be a ① in row 2 if $\lambda_2 = \lambda_3$. Similarly, there cannot be a ① in row 4 if $\lambda_4 = 0$.

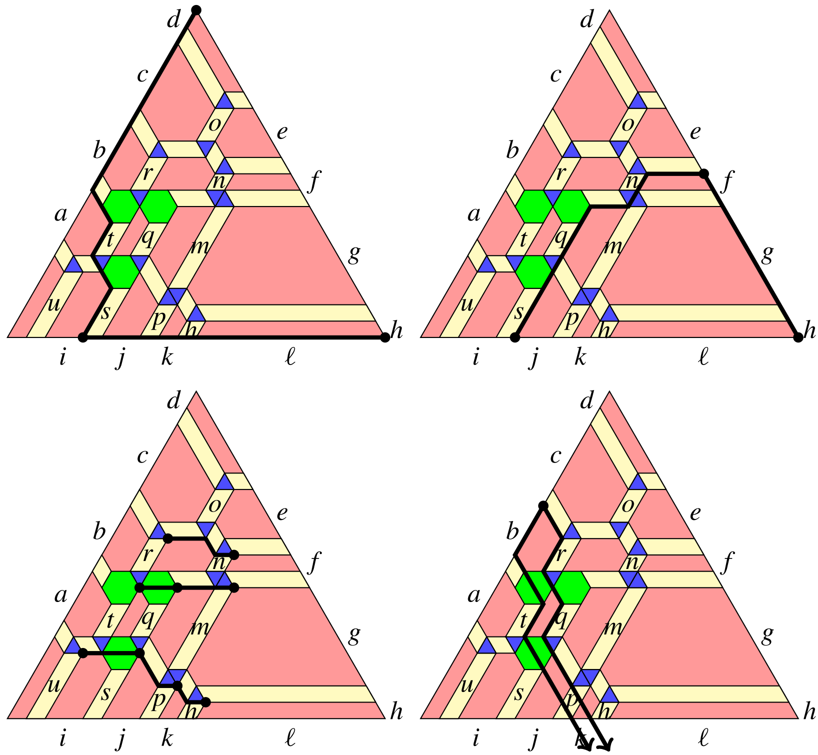


Figure 10. Inequalities from puzzles.

In general, ① can only be written in the boxes corresponding to the *inner corners* of λ.

Finally, uncircle the circled numbers in T. Since circled numbers either share boxes with uncircled numbers or occur in the inner corners of λ, what we get is a set-valued tableau of shape ν/λ^-, where λ^- is λ with some inner corners removed. This concludes one direction of the bijection.

Reversing the bijection is straightforward. First, we reverse the last step. Let T' be a set-valued tableau of shape ν/λ^- and content μ, where λ^- is λ with some of its inner corners removed. Circle all the numbers in boxes corresponding to inner corners of λ and all but the smallest number in each of the boxes corresponding to ν/λ. This tableau with circles is in fact T as described in the middle of the bijection above. Indeed, as T' is ballot, the numbers appearing in row i are all at most i. Also, if we were to get two ⓘ in some row, the right ⓘ is sharing its box with a smaller number, so this row is not weakly increasing from left to right, a contradiction to the fact that T' is semistandard.

It remains to assemble the puzzle from the tableau T by reversing the first half of the bijection. From bottom to top, add in beams of rhombi of the correct height based on the multiplicities of numbers in the tableau, place an upright 1-triangle or hexagon on top of each beam depending on the existence of a corresponding circled number, and join these together using rhombi and upside-down 1-triangles in the only way possible. Repeat with the next set of beams and such. Fill the remaining region with 0-triangles. This construction works, and no tiles need to overlap or extend beyond the boundary, exactly because the inequalities we derived above are satisfied if they came from such a tableau. Checking the details is routine and therefore omitted.

4C. *Proof of Theorem 3.9.* We prove Theorem 3.9 by establishing a bijection between these tableaux and ⬢-puzzles. This bijection is extremely similar to the bijection in the previous proof. We follow the same outline and use the same running examples.

Given a ⬢-puzzle, in the boxes of a diagram of shape $\mu \oplus \lambda$, fill out according to the following schematic plan

$$
\begin{array}{cccc|cccc}
 & & & & 1d & 1c & 1b & 1a \\
 & & & & 2d & 2c & 2b & \\
 & & & & 3d & 3c & & \\
 & & & & 4d & & & \\
\hline
1u & 2t & 3r & 4o & & & & \\
2s & 3q & 4n & & & & & \\
3p & 4m & & & & & & \\
4h & & & & & & &
\end{array}
$$

where, as before, a number x followed by a letter y means to write x in y adjacent boxes. If $y' > y$, write an additional x in the *next* box, in its own space. Circle such a number. Note that every box has exactly one number, which may or may not be circled. Call this tableau T.

Example 4.3. Applying the bijection described to the puzzle results in the following tableau.

$$
\begin{array}{ccccccccccc|ccccccccccc}
 & & & & & & & & & & & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
 & & & & & & & & & & & 2 & 2 & 2 & 2 & 2 & 2 & 2 & 2 & & & \\
 & & & & & & & & & & & 3 & 3 & 3 & 3 & 3 & & & & & & \\
 & & & & & & & & & & & 4 & & & & & & & & & & \\
\hline
1 & 1 & 1 & 1 & 2 & 2 & \textcircled{2} & 3 & 3 & 4 & 4 & & & & & & & & & & & \\
2 & 2 & 2 & \textcircled{2} & 3 & 3 & \textcircled{3} & 4 & & & & & & & & & & & & & & \\
3 & 3 & 4 & 4 & 4 & 4 & 4 & & & & & & & & & & & & & & & \\
4 & & & & & & & & & & & & & & & & & & & & &
\end{array}
$$

We read off *exactly* the same equalities and inequalities from Figure 10. However, we interpret them differently.

<u>Content</u>. The top left picture shows that $\nu_2 - \lambda_2 = s + t$, leading to content$(T) = \nu$ where $\textcircled{i}$ is ignored.

<u>Shape</u>. The top right picture shows that $\mu_2 = s' + q' + n'$, showing that $\textcircled{i}$ shall occupy its own box.

Semistandard. The lower left picture shows that $u' + t' \geq s' + q' \geq p' + m'$. This directly translates to the semistandard condition of T, where ⓘ is treated as i.

Ballot. The lower right picture shows the final type of inequalities, whose interpretation is still slightly more complicated. Following the notation from the previous proof, we get $b + t \geq_s r + q$ as one of these inequalities. Let us see how this kind of inequalities interact with the ballot condition. Let w be an initial segment of $\mathrm{row}(T)$. As an example, let us compare the number of 2s and 3s. We may as well extend w with some more 3s without adding 2s. For example, suppose w ends between the 2s and 3s of row 2. There are at least as many (uncircled) 2s as (uncircled) 3s in w if and only if $b + t \geq r + q$. If there is a ② between the 2s and 3s of row 2, the incremented erasure of w would have an extra 3. Therefore we must have $b + t \geq_s r + q$. Other requirements of the ballot condition all amount to inequalities of this type.

This establishes one direction of the bijection. As before, reversing the bijection and proving correctness is straight-forward, so we omit the details.

4D. ***Bijection between puzzles and tableaux.*** Rather than repeat similar proofs over and over, we present in table form the inequalities that can be read off from puzzles and their corresponding interpretations in both skew and $\oplus$ tableaux rules.

For △, like for ⬢, we let $x' = x + 1$ if the added tile is above the x-beam; otherwise $x' = x$. For ▽ and ⏣, replace "above" in the definition above with "below." Consequently, u', s', p', h' are undefined for ▽ and ⏣.[3] As before, $x \geq_z y$ is a shorthand for $x \geq y + z' - z$.

We first redescribe ⬢ rules in Table 1 to help orient the reader.

The inequalities for ⏣, shown in Table 2, are very similar to those for ⬢. The main difference is seen in the last rows of the tables. Consider the semistandard condition of the skew rule. While the inequality $a \geq_u t$ dictates that ① in row 1 is to be written in the box *before* the 1s corresponding to u, the inequality $a \geq_t t$ instead dictates that ① in row 2 is to be written in the box *after* the 1s corresponding to t. Similarly, for the $\oplus$ rule's ballot condition, the erasure is not incremented. The other difference is marked with (▾) due to ⏣ being upside down. We see that the limited condition arises naturally in the $\oplus$ rule. Its counterpart in the skew rule is that the shape ν/λ cannot be enlarged by adding corners.

As compared to ⬢, the inequalities for ▽ (Table 3) look quite different on the surface. However, it turns out we are essentially swapping the skew and $\oplus$ rules with each other. Indeed, the only other difference is that ▽, being upside down,

[3]The ▽ and ⏣ are "upside down" in the sense that they replace the upside down 1-triangle ▾. Heuristically, since there are fewer opportunities to use these tiles, their corresponding set-valued tableaux have no option to fill a larger shape and circle tableaux have no ⓘ in row i. The rules in the tables where this manifests itself are marked with (▾).

⬢	ν/λ	$\mu \oplus \lambda$
$\nu_1 - \lambda_1 = u$ $\nu_2 - \lambda_2 = s + t$ $\nu_3 - \lambda_3 = p + q + r$ $\nu_4 - \lambda_4 = h + m + n + o$	Shape: ⓘ takes no space set-valued	Content: ignore ⓘ
$\mu_1 = u' + t' + r' + o'$ $\mu_2 = s' + q' + n'$ $\mu_3 = p' + m'$ $\mu_4 = h'$	Content: ⓘ $\mapsto i$	Shape: ⓘ takes a box
$u' \geq s' \geq p' \geq h'$ $u' + t' \geq s' + q' \geq p' + m'$ $u' + t' + r' \geq s' + q' + n'$	Ballot: ⓘ $\mapsto i$	Semistandard: ⓘ $\mapsto i$
$a \geq_u t, \quad b \geq_t r, \quad c \geq_r o, \quad d \geq_o 0$ $b + t \geq_s r + q, \; c + r \geq_q o + n, \; d + o \geq_n 0$ $c + r + q \geq_p o + n + m, \quad d + o + n \geq_m 0$ $d + o + n + m \geq_h 0$	Semistandard: ⓘ in previous box shape becomes ν/λ^-	Ballot: keep only last ⓘ ⓘ $\mapsto i + 1$

Table 1. ⬢ rules.

⬡	ν/λ	$\mu \oplus \lambda$
$\nu_1 - \lambda_1 = u$ $\nu_2 - \lambda_2 = s + t$ $\nu_3 - \lambda_3 = p + q + r$ $\nu_4 - \lambda_4 = h + m + n + o$	Shape: ⓘ takes no space set-valued	Content: ignore ⓘ
$\mu_1 = u + t' + r' + o'$ $\mu_2 = s + q' + n'$ $\mu_3 = p + m'$ $\mu_4 = h$	Content: ⓘ $\mapsto i$	Shape: ⓘ takes a box no ⓘ in row i (▾)
$u \geq s \geq p \geq h$ $u + t' \geq s + q' \geq p + m'$ $u + t' + r' \geq s + q' + n'$	Ballot: ⓘ $\mapsto i$	Semistandard: ⓘ $\mapsto i$
$a \geq_t t, \quad b \geq_r r, \quad c \geq_o o$ $b + t \geq_q r + q, \quad c + r \geq_n o + n$ $c + r + q \geq_m o + n + m$	Semistandard: ⓘ in next box stay within shape (▾)	Ballot: keep only last ⓘ ⓘ $\mapsto i$

Table 2. ⬡ rules.

▼	ν/λ	$\mu\oplus\lambda$
$\nu_1-\lambda_1=u$ $\nu_2-\lambda_2=s+t'$ $\nu_3-\lambda_3=p+q'+r'$ $\nu_4-\lambda_4=h+m'+n'+o'$	Shape: ⓘ takes a box no ⓘ in row i (▾)	Content: ⓘ $\mapsto i$
$\mu_1=u+t+r+o$ $\mu_2=s+q+n$ $\mu_3=p+m$ $\mu_4=h$	Content: ignore ⓘ	Shape: ⓘ takes no space set-valued
$u\geq_t s\geq_q p\geq_m h$ $u+t\geq_r s+q\geq_n p+m$ $u+t+r\geq_o s+q+n$	Ballot: keep only last ⓘ ⓘ $\mapsto i+1$	Semistandard: ⓘ in previous box stay within shape (▾)
$a\geq t',\quad b\geq r',\quad c\geq o'$ $b+t'\geq r'+q',\quad c+r'\geq o'+n'$ $c+r'+q'\geq o'+n'+m'$	Semistandard: ⓘ $\mapsto i$	Ballot: ⓘ $\mapsto i$

Table 3. ▼ rules.

is less frequently usable, as denoted by (▾) in two places. The first is the limited condition for the skew rule. However, any ⓘ in row i would violate the ballot condition, so the limited condition need not be explicitly stated in Theorem 3.6. The counterpart of the limited condition in the $\oplus$ rule is that the shape cannot be enlarged by adding corners, as in the case of ⬡.

The close relation between ▲ (shown in Table 4) and ▼ is similar to that between ⬢ and ⬡. Indeed, one difference of ▲ compared to ▼ is that its erasure is not incremented and ⓘ goes in the next box, just like ⬡. On the other hand, the other difference is that ▲ does not have (▾) restrictions,[4] like ⬢. The lack of perfect symmetry is somewhat puzzling.

4E. ***Correspondence to coefficients.*** In the previous section, we presented in table form the relevant parts of the bijection between the four puzzle rules given in Section 3B and the eight tableau rules given in Section 3C. What remains is to relate these to the coefficients defined in Section 3A.

Buch [2002] proved Theorem 3.5, establishing that the ▼ rules count $c^{\nu}_{\lambda\mu}$. We proved above that the ⬢ rules count $d^{\nu}_{\lambda\mu}$. In the following two section, we establish ▲ rules and ⬡ rules, respectively.

[4]So, in the $\oplus$ rule, ⓘ can be written in the next box, even protruding beyond the shape μ. However, if $\mu_2=\mu_3$, say, the inequalities $s\geq_p p$ and $s+q\geq_m p+m$ prohibit ③ and ④, respectively, from protruding in row 3. As such, μ^+ is μ with some *outer corners* added.

$\triangle$	ν/λ	$\mu \oplus \lambda$
$\nu_1 - \lambda_1 = u'$ $\nu_2 - \lambda_2 = s' + t'$ $\nu_3 - \lambda_3 = p' + q' + r'$ $\nu_4 - \lambda_4 = h' + m' + n' + o'$	Shape: ⓘ takes a box	Content: ⓘ $\mapsto i$
$\mu_1 = u + t + r + o$ $\mu_2 = s + q + n$ $\mu_3 = p + m$ $\mu_4 = h$	Content: ignore ⓘ	Shape: ⓘ takes no space set-valued
$u \geq_s s \geq_p p \geq_h h$ $u + t \geq_q s + q \geq_m p + m$ $u + t + r \geq_n s + q + n$	Ballot: keep only last ⓘ ⓘ $\mapsto i$	Semistandard: ⓘ in next box shape becomes μ^+
$a \geq t', \quad b \geq r', \quad c \geq o'$ $b + t' \geq r' + q', \quad c + r' \geq o' + n'$ $c + r' + q' \geq o' + n' + m'$	Semistandard: ⓘ $\mapsto i$	Ballot: ⓘ $\mapsto i$

Table 4. $\triangle$ rules.

4F. ***Proof of Theorem 3.7.*** Wheeler and Zinn-Justin [2017] proved Theorem 3.2, so we already know that the $\triangle$ rules count $\tilde{c}^{\nu}_{\lambda\mu}$. Regardless, here we provide a simple calculation as a way to establish the $\triangle$ rules from the $\triangledown$ rules, and that serves as an alternative proof to the result of Wheeler and Zinn-Justin.

By definition, we have

$$G_\mu \cdot G_1 = \sum_{\mu'} (-1)^{|\mu'|-|\mu|-1} c^{\mu'}_{\mu 1} G_{\mu'}.$$

By Theorem 3.5, the coefficient $c^{\mu'}_{\mu 1}$ is 1 if μ' is μ with a positive number of outer corners added,[5] and 0 otherwise. So

$$\begin{aligned} G_\lambda \cdot (G_\mu \cdot G_1) &= G_\lambda \sum_{\mu'} (-1)^{|\mu'|-|\mu|-1} G_{\mu'} \\ &= \sum_{\mu'} (-1)^{|\mu'|-|\mu|-1} \sum_{\nu} (-1)^{|\nu|-|\lambda|-|\mu'|} c^{\nu}_{\lambda\mu'} G_\nu \\ &= -\sum_{\nu,\mu'} (-1)^{|\nu|-|\lambda|-|\mu|} c^{\nu}_{\lambda\mu'} G_\nu, \end{aligned}$$

[5]Consider the shape $1 \oplus \mu$. The numbers filled in the lower box corresponds to the rows of μ'/μ.

where μ' runs over μ with a positive number of outer corners added. By definition, we have

$$\sum_{\nu}(-1)^{|\nu|-|\lambda|-|\mu|}\tilde{c}^{\nu}_{\lambda\mu}G_{\nu} = G_{\lambda}\cdot G_{\mu}\cdot(1-G_1)$$
$$= \sum_{\nu}(-1)^{|\nu|-|\lambda|-|\mu|}c^{\nu}_{\lambda\mu}G_{\nu} + \sum_{\nu,\mu'}(-1)^{|\nu|-|\lambda|-|\mu|}c^{\nu}_{\lambda\mu'}G_{\nu},$$

so

$$\tilde{c}^{\nu}_{\lambda\mu} = c^{\nu}_{\lambda\mu} + \sum_{\mu'} c^{\nu}_{\lambda\mu'}.$$

By Theorem 3.5, $\tilde{c}^{\nu}_{\lambda\mu}$ is the number of semistandard ballot set-valued tableaux of shape $\mu^{+}\oplus\lambda$ and content ν, where μ^{+} is either μ or μ with a positive number of outer corners added, as desired.

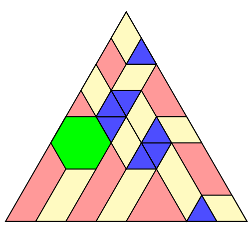
4G. ***Proof of Theorem 3.4.*** By Theorem 3.3, it suffices to show a bijection between -puzzles with boundary $\Delta^{\nu}_{\lambda\mu}$ and -puzzles with boundary $\Delta^{\nu'}_{\lambda'\mu'}$. The bijection is simple: mirror the puzzle across a vertical line and swap the 0 and 1 labels. This is clearly an involution. Each of the original puzzle pieces is mapped to a valid puzzle piece. The and pieces are mapped to each other. The boundary is mapped from $\Delta^{\nu}_{\lambda\mu}$ to $\Delta^{\nu'}_{\mu'\lambda'}$.[6] Finally, by definition, $d^{\nu}_{\lambda\mu} = d^{\nu}_{\mu\lambda}$, so we are done.

5. Final remarks

5A. Consider the example $\lambda = (2, 1)$, $\mu = (4, 2)$, and $\nu = (4, 3, 1)$. The skew tableau

	1	1	1
	2	2	
1			

corresponds to the -tiling



Since the shapes all fit in a 4×3 box, one might think $n = 7$ is sufficient side length for a puzzle. However, the piece will protrude to the left of the puzzle with side length 7.

[6]Indeed, recall that the binary string of a partition λ corresponds to the boundary of the diagram of λ. Reversing the string rotates (the boundary of) the diagram by 180°. Swapping 0 and 1 in the string flips the diagram across the line $x = y$. Composing these two transformations flips the diagram across the line $x + y = 0$.

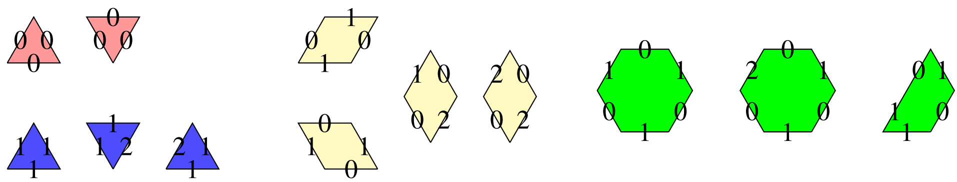
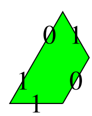


Figure 11. The complete set of tiles.

In Theorem 3.3, we dealt with this issue by increasing the puzzle side length by one. More precisely, puzzles of side length $n+1$ corresponds to using the standard ambient rectangle of size $(n-k)\times k$. So, to keep the side length of puzzles fixed at n, we must use a slightly narrower ambient rectangle of size $(n-1-k)\times k$ instead.

This is analogous for Theorem 3.4. As we can see from the bijection outlined in its proof, we need the transposed partitions to fit inside a slightly narrower ambient rectangle, so the partitions themselves must fit inside a slightly shorter ambient rectangle of size $(n-k)\times(k-1)$ instead.

5B. Another way to solve the protrusion issue outlined above is to add an additional trapezoid piece



as if to allow the hexagonal tile to protrude to the left. (By the way things are set up, the hexagon never needs to protrude to the right or below.) However, we do not want this piece used elsewhere. So we must make some more modifications. Figure 11 shows the complete set of tiles.

Consider the northeast–southwest slanting 1 edges. A 1-edge on the bottom-right side of pieces are now labeled with 2, so the new trapezoid piece cannot be used except at the left boundary. An old piece with a 1-edge on its top-left side must be duplicated, with a version for use at the left boundary and another for use in the interior.

Modification to is similar.

5C. Theorem 3.6 provides a skew tableau rule for calculating the K-theoretic Littlewood–Richardson coefficients $c^{\nu}_{\lambda\mu}$ using right circle tableaux. Pechenik and Yong [2017] give the same rule using *genomic* tableaux (definitions therein).

Theorem 5.1 (▼, [Pechenik and Yong 2017], K-theory, skew version). *The coefficient $c^{\nu}_{\lambda\mu}$ is the number of semistandard ballot* genomic *tableaux of shape ν/λ and content μ.*

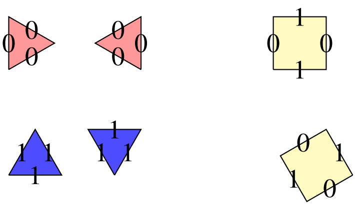
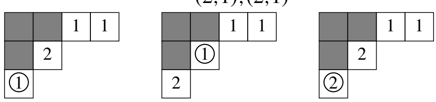


Figure 12. Mosaic version of the Knutson–Tao–Woodward tiles.

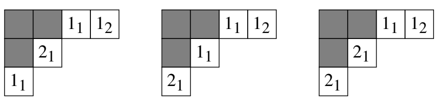
These two rules are virtually identical, as there is a simple bijection between right circle tableaux and genomic tableaux. Indeed, let a semistandard ballot right circle tableau of shape ν/λ and content μ be given. By semistandardness, the boxes filled with i and ⓘ form a horizontal strip. From left to right, rewrite these as i_1, i_2, i_3, and so on. Whenever ⓘ is encountered, the *next* subscript used is the same as the current subscript. By ballotness, the rightmost i in the tableau is not circled, so this rule is well-formed. It is easy to see that this yields a semistandard genomic tableau of the same shape and content. One can also check that the tableau is ballot.

Conversely, given a semistandard ballot genomic tableau, the boxes filled with i_j for a fixed i form a horizontal strip. From left to right, circle an entry if its subscript is the same as the next one. Erase all subscripts. The correctness of this bijection is straightforward and left as exercise to the reader.

Example 5.2. The structure constant $c^{(4,2,1)}_{(2,1),(2,1)}$ is computed by the circle tableaux



and by the corresponding genomic tableaux



5D. Purbhoo [2008] introduced mosaics, a useful variation of puzzles. These pieces do not need edge labels. Instead, edges labeled with 0 are rotated 30° anticlockwise. Below, the edge labels have been retained for clarity. Figure 12 shows the mosaic version of the ordinary Knutson–Tao–Woodward puzzle pieces.

Figure 13 shows the mosaic version of the four additional K-theoretic tiles. Note that the four tiles have the same geometric shape.

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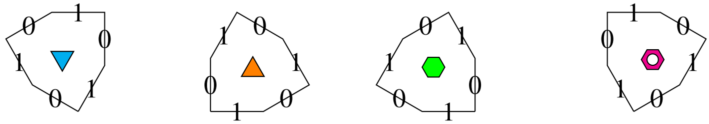

Figure 13. Mosaic version of the four additional K-theoretic tiles.

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LINEARLY DEPENDENT POWERS OF BINARY QUADRATIC FORMS

BRUCE REZNICK

Given an integer $d \geq 2$, what is the smallest r so that there is a set of binary quadratic forms $\{f_1, \dots, f_r\}$ for which $\{f_j^d\}$ is nontrivially linearly dependent? We show that if $r \leq 4$, then $d \leq 5$, and for $d \geq 4$, construct such a set with $r = \lfloor d/2 \rfloor + 2$. Many explicit examples are given, along with techniques for producing others.

1. Introduction

For a fixed positive integer k, let $H_k(\mathbb{C}^2)$ denote the $(k+1)$-dimensional vector space of binary forms of degree k with complex coefficients. We say that two such forms are *distinct* if they are not proportional, and we say that a set $\mathcal{F} = \{f_1, \dots, f_r\} \subset H_k(\mathbb{C}^2)$ is *honest* if its elements are pairwise distinct. For $d \in \mathbb{N}$, let $\mathcal{F}^d = \{f_1^d, \dots, f_r^d\}$; if $\mathcal{F}$ is honest, then so is $\mathcal{F}^d$.

When $k = 1$, there is a simple classical criterion for the linear dependence of $\mathcal{F}^d$; see, e.g., [Reznick 2013a, Theorem 4.2].

Theorem 1.1. *If $\mathcal{F} = \{f_1, \dots, f_r\} \subset H_1(\mathbb{C}^2)$ is honest, then $\mathcal{F}^d = \{f_1^d, \dots, f_r^d\}$ is linearly independent if and only if $r \leq d + 1$.*

A version of this criterion is generally true for $k \geq 2$; see, e.g., [Reznick 2013b, Theorem 1.8]. (The proofs of these theorems are given at the start of Section 2.)

Theorem 1.2. *If $\mathcal{F} = \{f_1, \dots, f_r\} \subset H_k(\mathbb{C}^2)$, then it is generally true that $\mathcal{F}^d$ is linearly independent if and only if $r \leq kd + 1$.*

But there are singular cases, and these will be the focus of this paper. It is easy to find smaller values of r for which $\mathcal{F}^d$ is linearly dependent; for example, the Pythagorean parametrization gives three quadratics whose squares are dependent:

$$(x^2 - y^2)^2 + (2xy)^2 = (x^2 + y^2)^2. \tag{1-1}$$

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There are other ways of finding small dependent sets: let $\{g_j(x, y)\}$ be an honest set of $d+2$ linear forms; then both $\{g_j(x^k, y^k)\}$ and $\{\ell(x, y)^{k-1} g_j(x, y)\}$ (for a fixed linear form ℓ) will be dependent sets in $H_k(\mathbb{C}^2)$.

Given $r, d \in \mathbb{N}$, we say that an honest set of forms $\{f_1, \dots, f_r\} \subseteq H_k(\mathbb{C}^2)$ is a $\mathcal{W}_k(r, d)$*-set* if $\{f_j^d\}$ is linearly dependent. For example, (1-1) presents the $\mathcal{W}_2(3, 2)$-set $\{x^2 - y^2, 2xy, x^2 + y^2\}$. Let $\Phi_k(d)$ denote the smallest r for which a $\mathcal{W}_k(r, d)$-set exists; clearly, $\Phi_k(d) \ge 3$. Theorem 1.1 implies that $\Phi_1(d) = d + 2$.

Our goal in this paper is twofold. First, we give upper and lower bounds for $\Phi_k(d)$ for $k \ge 2$. Second, we describe all $\mathcal{W}_2(\Phi_2(d), d)$-sets for $d \le 5$. In (5) and (6) below, we use a peculiar-looking function. If $e \mid d$, let

$$\Theta_e(d) := 1 + \min_{t \in \mathbb{N}} \Big(t \cdot \frac{d}{e} + \Big\lfloor \frac{e}{t} \Big\rfloor \Big).$$

We summarize our main results.

Theorem 1.3 (main theorem). (1) $\Phi_{k+1}(d) \le \Phi_k(d)$.

(2) $\Phi_k(2) = 3$.

(3) (Liouville) $\Phi_k(d) \ge 4$ *for* $d \ge 3$ *and all* k.

(4) (Hayman) $\Phi_k(d) > 1 + \sqrt{d+1}$ *for* $d \ge 3$ *and all* k.

(5) (Molluzzo, Newman, and Slater) $\Phi_d(d) \le \Theta_d(d) = 1 + \lfloor \sqrt{4d+1} \rfloor$.

(6) *If* $e \mid d$, *then* $\Phi_e(d) \le \min\{\Theta_k(d) : k \ge e,\ k \mid d\}$.

(7) $\Phi_k(d) = 4$ *for* $d = 3, 4, 5$ *and* $k \ge 2$.

(8) $\Phi_2(d) \ge 5$ *for* $d \ge 6$.

(9) $\Phi_2(d) = 5$ *for* $d = 6, 7$.

(10) $\Phi_2(14) \le 6$.

(11) $\Phi_2(d) \le \lfloor d/2 \rfloor + 2$ *for* $d \ge 4$.

All new parts of the main theorem except (8) and (11) have short proofs; these are given in Section 2. Examples give upper bounds for $\Phi_k(d)$; lower bounds are harder to find. The anomalous value in (10) for $d = 14$ is difficult to explain, and prevents us from conjecturing (11) as the exact value. This problem has been studied in [Gundersen and Hayman 2004; Newman and Slater 1979] without the degree condition on the summands. The recent [Nenashev et al. 2017] contains a generalization of this question, replacing f_i^d with $\prod_j f_{ij}^{a_j}$ for fixed tuples (a_j).

If $\mathcal{F}$ is a $\mathcal{W}_k(r, d)$-set, then there is an obvious way to transform the linear dependence of the d-th powers into a more natural expression for any m, $1 \le m \le r - 1$:

$$\sum_{j=1}^{r} \lambda_j f_j^d = 0 \quad (\lambda_j \ne 0) \quad \Longrightarrow \quad p = \sum_{j=1}^{m} \tilde{f}_j^d = \sum_{j=m+1}^{r} \tilde{f}_j^d, \tag{1-2}$$

where $\tilde{f}_j = (\pm\lambda_j)^{1/d} f_j$, for some p. In particular, a $\mathcal{W}_k(2m, d)$-set addresses the classical question of parametrizing two equal sums of m d-th powers. In this case, we say that (1-2) gives *two representations* of p as a sum of m d-th powers.

If $\alpha x + \beta y$ and $\gamma x + \delta y$ are distinct, then the map $M := (x, y) \mapsto (\alpha x + \beta y, \gamma x + \delta y)$ is an invertible change of variables (or *linear change* for short); let $(f \circ M)(x, y)$ denote $f(\alpha x + \beta y, \gamma x + \delta y)$. (This is a *scaling* if $\beta = \gamma = 0$.) If all members of $\mathcal{F}$ are subject to the same linear change, then the linear dependence of their d-th powers is unaltered. Any $\mathcal{W}_k(r, d)$-set can have its elements permuted and multiplied by various nonzero constants without essentially affecting the nature of the dependence.

So suppose $\mathcal{F}$ is a $\mathcal{W}_k(r, d)$-set and

$$\sum_{j=1}^{r} \lambda_j f_j^d = 0. \tag{1-3}$$

If $\pi \in S_r$ is a permutation of $\{1, \dots r\}$, $c = (c_1, \dots, c_r) \in (\mathbb{C} \setminus \{0\})^r$, M is a linear change, and $g_j = c_j(f_{\pi(j)} \circ M)$, $1 \le j \le r$, then (1-3) is equivalent to

$$\sum_{j=1}^{r} (\lambda_{\pi(j)} \cdot c_j^{-d}) g_j^d = 0. \tag{1-4}$$

In this situation, we say that $\mathcal{F} = \{f_j\}$ and $\mathcal{G} = \{g_j\}$ (and the corresponding identities (1-3) and (1-4)) are *cousins*. It is easy to show cousinhood by exhibiting M, π, and c. Proving that $\mathcal{F}$ and $\mathcal{G}$ are *not* cousins may require ad hoc arguments.

We aim to present identities as symmetrically as possible, often guided by an old idea of Felix Klein. Associate to each nonzero linear form $\ell(x, y) = sx - ty$ the image of $t/s \in \mathbb{C}^*$ on the unit sphere S^2 under the Riemann map. (Assign $\ell(x, y) = y$ to ∞ and $(0, 0, 1)$.) Then associate to the binary form $\phi(x, y) = \prod_{j=1}^{k}(s_j x - t_j y)$ the image under the Riemann map of $\{t_j/s_j\}$, and call it the *Klein set of* ϕ. Given (1-3), we shall be interested in the Klein set of $\prod_{j=1}^{r} f_j$. In (1-1), the Klein set of $(x^2 - y^2)(2xy)(x^2 + y^2)$ is the regular octahedron with vertices $\{\pm e_k\}$.

Under the linear change $M : (x, y) \mapsto (\alpha x + \beta y, \gamma x + \delta y)$, $t/s \mapsto T(t/s)$, where T is the Möbius transformation $T(z) = (\delta z - \beta)/(-\gamma z + \alpha)$. Every rotation of the sphere corresponds to a Möbius transformation of the complex plane, and so a rotation of the Klein set can be effected by imposing a linear change on the forms. (Unfortunately, not every Möbius transformation gives a rotation.) It often happens that $p = \sum f_j^d$ and $p = p \circ M$, but $\sum (f_j \circ M)^d$ gives a different representation for p.

A trivial remark is surprisingly useful:

$$p = f_1^d + f_2^d = f_3^d + f_4^d \quad \Longrightarrow \quad q = f_1^d - f_3^d = f_4^d - f_2^d$$

for suitable forms p, q; we call this a *flip*. For $k = 2$ and $d = 3, 4$, it can happen that q has a third representation as $q = f_5^d + f_6^d$, but that no such new expression exists for p. If $f_1^d + f_2^d = f_3^d + f_4^d$ and $g_1^d + g_2^d = g_3^d + g_4^d = g_5^d + g_6^d$, then $\mathcal{F} = \{f_1, \dots, f_4\}$ is a cousin of $\mathcal{G} = \{g_1, \dots, g_4\}$ and we say that $\mathcal{F}$ is a *subcousin* of $\mathcal{G}' = \{g_1, \dots, g_6\}$.

We now present some examples of small dependent sets of d-th powers. For integer $m \in \mathbb{N}$, let $\zeta_m = e^{2\pi i/m}$ be a primitive m-th root of unity, with the usual conventions that $\omega = \zeta_3$ and $i = \zeta_4$. A few interesting Klein sets will be noted.

The cubic identity with the simplest coefficients is probably

$$(x^2+xy-y^2)^3+(x^2-xy-y^2)^3 = 2(x^2)^3+2(-y^2)^3 = 2x^6-2y^6. \tag{1-5}$$

The right-hand side of (1-5) is unchanged by the scalings $y \to \omega y$ and $y \to \omega^2 y$, so (1-5) shows that $2x^6 - 2y^6$ is a sum of two cubes in four different ways. Under the linear change $(x, y) \mapsto (\alpha+\beta, \alpha-\beta)$, (1-5) is due to Gérardin in 1910 [Dickson 1966, p. 562]; in its present form, it was noted by Elkies [Darmon and Granville 1995, p. 542].

Here are two very simple quartic identities. The first generalizes to higher even degree (see (2-6)), and the second is in $\mathbb{Z}[x, y]$:

$$(x^2+y^2)^4+(\omega x^2+\omega^2 y^2)^4+(\omega^2 x^2+\omega y^2)^4 = 18(xy)^4. \tag{1-6}$$

$$(x^2+2xy)^4+(2xy+y^2)^4+(x^2-y^2)^4 = 2(x^2+xy+y^2)^4. \tag{1-7}$$

These are cousins. Upon making the linear change $(x, y) \mapsto (i(x-\omega y), (x-\omega^2 y))$ and division by $\sqrt{-3}$, (1-6) becomes (1-7) up to a permutation of terms. The Klein set of (1-6) is a regular hexagon at the equator plus the poles.

A remarkable identity for $d = 5$ was discovered independently by A. H. Desboves [1880; Dickson 1966, p. 684] and N. Elkies in 1995 [Darmon and Granville 1995, p. 542]:

$$\sum_{k=0}^{3}(-1)^k(i^k x^2+\sqrt{-2}xy+i^{-k}y^2)^5 = 0. \tag{1-8}$$

The Klein set of (1-8) is a cube with vertices $\left\{\left(\pm\sqrt{2/3}, 0, \pm\sqrt{1/3}\right), \left(0, \pm\sqrt{2/3}, \pm\sqrt{1/3}\right)\right\}$.

The next two examples appear to be new in detail, but are in the spirit of [Reznick 2003, §4]; the third explicitly appears there as (4.15); each is derived in Section 2:

$$\sum_{k=0}^{3} i^k (x^2 + i^k y^2)^6 = 80(xy)^6, \tag{1-9}$$

$$\sum_{k=0}^{3} \bigl(i^{-k} x^2 + \sqrt{-6/5}\, xy + i^k y^2\bigr)^7 = 26\sqrt{3} \cdot \bigl(-\sqrt{8/5}\, xy\bigr)^7, \tag{1-10}$$

$$\sum_{j=0}^{4} (\zeta_5^j x^2 + ixy + \zeta_5^{-j} y^2)^{14} = 5^7 (xy)^{14}. \tag{1-11}$$

The Klein set of (1-11) is the regular icosahedron, oriented so the vertices are the two poles plus two parallel regular pentagons at latitude $z = \pm\sqrt{1/5}$.

The second main focus of this paper is the characterization of $\mathcal{W}_2(\Phi_2(d), d)$-sets for $d = 3, 4, 5$. The characterization of $\mathcal{W}_k(3, 2)$-sets is classical, and can be proved by emulating the standard analysis of $a^2 + b^2 = c^2$ over $\mathbb{N}$.

Theorem 1.4. *If $p, q, r \in \mathbb{C}[x_1, \dots, x_n]$, $n \geq 1$, and $p^2 + q^2 = r^2$, then there exist $f, g, h \in \mathbb{C}[x_1, \dots, x_n]$ so that $p = f(g^2 - h^2)$, $q = f(2gh)$, and $r = f(g^2 + h^2)$.*

The proof of the following theorem will be found in the companion paper [Reznick 2020].

Theorem 1.5. *Every $\mathcal{W}_2(4, 3)$-set is a subcousin of a member of the $\mathcal{W}_2(6, 3)$ family given below, for some $\alpha \neq 0, \pm 1$:*

$$\begin{aligned}(\alpha x^2 - xy + \alpha y^2)^3 &+ \alpha(-x^2 + \alpha xy - y^2)^3 \\ &= (\omega^2 \alpha x^2 - xy + \omega \alpha y^2)^3 + \alpha(-\omega^2 x^2 + \alpha xy - \omega y^2)^3 \\ &= (\omega \alpha x^2 - xy + \omega^2 \alpha y^2)^3 + \alpha(-\omega x^2 + \alpha xy - \omega^2 y^2)^3 \\ &= (\alpha^2 - 1)(\alpha x^3 + y^3)(x^3 + \alpha y^3).\end{aligned} \tag{1-12}$$

If the first two lines of (1-12) are read as $f_1^3 + f_2^3 = f_3^3 + f_4^3$, then $f_1^3 - f_4^3 = f_3^3 - f_2^3$ also has a third representation as a sum of two cubes, but $f_1^3 - f_3^3 = f_4^3 - f_2^3$ does not.

(Put $(\alpha, x, y) \mapsto (i, \zeta_8^3 x, \zeta_8^5 y)$ in the first line of (1-12) to get (1-5).) After the linear change $(x, y) \mapsto (ix + \sqrt{3}y, ix - \sqrt{3}y)$, (1-12) becomes

$$\begin{aligned}((1-2\alpha)x^2 &+ 3(1+2\alpha)y^2)^3 + \alpha((2-\alpha)x^2 - 3(2+\alpha)y^2)^3 \\ &= ((1+\alpha)x^2 + 6\alpha xy + 3(1-\alpha)y^2)^3 + \alpha(-(1+\alpha)x^2 - 6xy + 3(1-\alpha)y^2)^3 \\ &= ((1+\alpha)x^2 - 6\alpha xy + 3(1-\alpha)y^2)^3 + \alpha(-(1+\alpha)x^2 + 6xy + 3(1-\alpha)y^2)^3.\end{aligned} \tag{1-13}$$

If $\alpha \in \mathbb{Q}$, then all forms in (1-13) are in $\mathbb{Q}[x, y]$, and if α is a rational cube, then (1-13) gives solutions to $f_1^3 + f_2^3 = f_3^3 + f_4^3$ in $\mathbb{Q}[x, y]$. Historically, these were used to parametrize solutions to the Diophantine equations $a^3 + b^3 = c^3 + d^3$ over $\mathbb{N}$.

Theorem 1.6. *Every* $\mathcal{W}_2(4, 4)$*-set is a cousin of* (1-6) *or a subcousin of* (1-14):

$$(x^2+\sqrt{3}xy-y^2)^4-(x^2-\sqrt{3}xy-y^2)^4 \\ =(\omega^2x^2+\sqrt{3}xy-\omega y^2)^4-(\omega^2x^2-\sqrt{3}xy-\omega y^2)^4 \\ =(\omega x^2+\sqrt{3}xy-\omega^2y^2)^4-(\omega x^2-\sqrt{3}xy-\omega^2y^2)^4 \\ =8\sqrt{3}xy(x^6-y^6). \tag{1-14}$$

In an earlier version of this work (see, e.g., [Reznick 2003, (3.9)]), the identity

$$(\sqrt{3}x^2+\sqrt{2}xy-\sqrt{3}y^2)^4+(\sqrt{3}x^2-\sqrt{2}xy-\sqrt{3}y^2)^4 \\ =(\sqrt{3}x^2+i\sqrt{2}xy+\sqrt{3}y^2)^4+(\sqrt{3}x^2-i\sqrt{2}xy+\sqrt{3}y^2)^4 \\ =18x^8-28x^4y^4+18y^8 \tag{1-15}$$

was given as an alternative in Theorem 1.6; (1-15) turns out to be a subcousin of (1-14); see Theorem 3.4. When scaled, (1-15) appears in [Desboves 1880, p. 243]. The set in (1-6) is not a subcousin of (1-14): three of the quadratics in (1-6) are linearly dependent, and no three quadratics in (1-14) are dependent.

The situation for quintics is simpler.

Theorem 1.7. *Every* $\mathcal{W}_2(4, 5)$*-set is a cousin of* (1-8).

Here is an outline of the rest of the paper. In Section 2, we prove Theorems 1.1 and 1.2 and Theorem 1.3 except (8). We also recall "synching" from [Reznick 2003] as a tool for finding "good" $\mathcal{W}_k(r, d)$-sets — the idea was inspired by a formula of Molluzzo [1972] — and use it to prove several parts of Theorem 1.3.

In Section 3, we recall two results familiar to nineteenth-century algebraists: a specialization of Sylvester's algorithm for determining the sums of two d-th powers of linear forms and a result on the simultaneous diagonalization of quadratic forms. We use these to lay out our strategy for proving Theorem 1.3(8). Suppose

$$p(x, y) = f_1^d(x, y) + f_2^d(x, y) = f_3^d(x, y) + f_4^d(x, y)$$

for an honest set $\{f_1, f_2, f_3, f_4\}$ of quadratics. There is a linear change which simultaneously diagonalizes f_1 and f_2 (making p even), but neither f_3 nor f_4 is even. We then make a systematic study of noneven $\{f_3, f_4\}$ for which $p = f_3^d + f_4^d$ is even, and check back to see whether p can be written as $f_1^d + f_2^d$. For $d \ge 3$, a shorter method can be used to prove Theorem 1.5; see the companion paper [Reznick 2020].

Section 4 is devoted to implementing in detail the strategy outlined above; this simultaneously proves Theorems 1.6 and 1.7, as well as Theorem 1.3(8). The proofs of Theorems 4.1 and 4.3 contain a great deal of "equation wrangling"; however, the reader should know that this has been greatly condensed from earlier drafts.

In Section 5, we do a brief review of the literature in the subject and derive the examples for $d \le 5$ via a priori constructions. We also give an explanation of (1-11), based on the properties of symmetric polynomials, which is similar to the derivation of (1-8) given in [Reznick 2003]. Corollaries 5.2 and 5.3 present the classification of forms which can be written as a sum of two d-th powers of quadratic forms and, for $d \ge 4$, those which have more than one representation. We suggest some further areas of exploration and finish with Conjecture 5.4 about the true growth of $\Phi_k(d)$.

2. Some proofs, and synching

We begin with proofs of Theorems 1.1 and 1.2.

Proof of Theorem 1.1. If $r > d+1 = \dim(H_d(\mathbb{C}^2))$, then $\mathcal{F}^d$ is dependent. Suppose $r \le d+1$, and let $f_i(x, y) = \alpha_i x + \beta_i y$. Define (if necessary) distinct f_j for $r+1 \le j \le d+1$ by $(\alpha_j, \beta_j) = (1, m_j)$, where $m_j\alpha_i \ne \beta_i$, $1 \le i \le r$, and express $\{f_1^d, \dots, f_{d+1}^d\}$ in terms of the basis $\left\{\binom{d}{v} x^{d-v} y^v\right\}$. The resulting $(d+1)\times(d+1)$ matrix, $[\alpha_i^{d-v}\beta_i^v]$, is Vandermonde with determinant $\prod_{1\le i<j\le d+1}(\alpha_i\beta_j - \alpha_j\beta_i) \ne 0$ since $\mathcal{F}$ is honest. □

Proof of Theorem 1.2. Again, if $r > kd+1$, then $\mathcal{F}^d$ is linearly dependent by dimension. Suppose $f_j(x, y) = \sum_{\ell=0}^k \binom{k}{\ell}\alpha_{\ell,j} x^{k-\ell} y^\ell$. If $r < kd+1$, again add pairwise distinct elements and assume that $r = kd+1$. Express $\{f_j^d\}$ in terms of the monomial basis $\left\{\binom{kd}{v} x^{kd-v} y^v\right\}$, obtaining a square matrix of order $kd+1$ whose entries are polynomials in the variables $\{\alpha_{\ell,j}\}$, and whose determinant is a polynomial $P(\{\alpha_{\ell,j}\})$. If we specialize to $f_j(x, y) = (x + jy)^k$, $1 \le j \le kd+1$, then $\alpha_{\ell,j} = j^\ell$, and $\mathcal{F}^d = \mathcal{G}^{kd}$ for $\mathcal{G} = \{x + jy\}$. By Theorem 1.1, $\mathcal{G}^{kd}$ is linearly independent; hence, $P(\{j^\ell\}) \ne 0$, and so P is not identically zero. That is, $\mathcal{F}^d$, generally, is linearly independent. □

We defer the proofs of Theorem 1.3(5), (6), and (11) until we have defined synching; (8) will require Sections 3 and 4.

Partial proof of Theorem 1.3. (1) If $g_j(x, y) = x f_j(x, y)$, then $\sum \lambda_j f_j^d = 0 \implies \sum \lambda_j g_j^d = 0$.

(2) This follows from (1-1) and (1).

(3) As noted in (1-2), the existence of a $\mathcal{W}_k(3, d)$-set for $d \ge 3$ would imply the existence of a nontrivial identity

$$f_1^d(x, y) + f_2^d(x, y) = f_3^d(x, y).$$

After a linear change, we may assume that $f_j(x, y)$ is not a multiple of y^k. Let $p_j(t) = f_j(t, 1)$. Then $p_1^d(t) + p_2^d(t) = p_3^d(t)$, where the p_j are nonconstant polynomials. In 1879, Liouville proved that the Fermat equation $X^d + Y^d = Z^d$ has no nonconstant solutions over $\mathbb{C}[t]$ for $d \ge 3$. (See [Ribenboim 1979, pp. 263–265] for a proof.)

(4) More generally, the elements of any $\mathcal{W}_k(r,d)$-set can be scaled as in (1-2) so that $\sum_{j=1}^{r-1} f_j^d(x,y) = f_r^d(x,y)$. Once again, by letting $p_j(t) = f_j(t,1)$ and $q_j(t) = f_j(t)/f_r(t)$ we obtain a set of $r-1$ rational functions so that $\sum_{j=1}^{r-1} q_j^d(t) = 1$. A theorem of Hayman [1985] says that if $\{\phi_j\}$, $1 \le j \le r-1$, are $r-1$ holomorphic functions in n complex variables, no two of which are proportional, and $\sum_{j=1}^{r-1} \phi_j^d = 1$, then $d < (r-1)^2 - 1$, so $r > 1 + \sqrt{d+1}$. This was the culmination of the work of Green [1975] and others; see [Gundersen and Hayman 2004, pp. 438–440] for a clear exposition and history.

(7) The equality for $k=2$ follows from combining (3) with (1-5), (1-6), and (1-8); for $k \ge 3$, apply (1).

(9) Subject to the as-yet unproved (8), this follows from (1-9) and (1-10).

(10) This follows from (1-11). □

Recall that for an integer $m \ge 2$ and for $s \in \mathbb{Z}$,

$$\frac{1}{m}\sum_{j=0}^{m-1} \zeta_m^{sj} = \begin{cases} 0 & \text{if } m \nmid s, \\ 1 & \text{if } m \mid s. \end{cases} \tag{2-1}$$

Synching was introduced in [Reznick 2003, §4] and is a generalization of the familiar formulas in which $\frac{1}{2}(f(x,y) \pm f(x,-y))$ give the even and odd parts of f.

Theorem 2.1. *Suppose $p(x,y) = \sum_{i=0}^{k} a_i x^{k-i} y^i \in H_k(\mathbb{C}^2)$ and $r \in \mathbb{Z}$. Then*

$$\frac{1}{m}\sum_{j=0}^{m-1} \zeta_m^{-rj} p(x, \zeta_m^j y) = \sum_{\substack{i \equiv r \pmod m \\ 0 \le i \le k}} a_i x^{k-i} y^i. \tag{2-2}$$

Proof. We expand the left-hand side of (2-2), switch the order of summation,

$$\frac{1}{m}\sum_{j=0}^{m-1} \zeta_m^{-rj} p(x, \zeta_m^j y) = \sum_{i=0}^{k} \biggl(\frac{1}{m}\sum_{j=0}^{m-1} \zeta_m^{-rj}\zeta_m^{ij}\biggr) a_i x^{k-i} y^i,$$

and then apply (2-1) to the inner sum of $\zeta_m^{(i-r)j}$. □

In our applications, $p = f^d$; for example, if $p(x,y) = (x+\alpha y)^d$, then

$$\frac{1}{m}\sum_{j=0}^{m-1} \zeta_m^{-rj} (x + \zeta_m^j \alpha y)^d = \sum_{-r/m \le i \le (d-r)/m} \binom{d}{r+im} \alpha^{r+im} x^{d-r-im} y^{r+im}. \tag{2-3}$$

Proof of Theorem 1.3(5) *and* (6). We generalize an identity found in Molluzzo's thesis [1972] (with $\ell = d$) and discussed in [Newman and Slater 1979, p. 485]; it follows from (2-3) with $r = 0$ that

$$\sum_{j=0}^{m-1}(x^\ell + \zeta_m^j y^\ell)^d = m \sum_{i=0}^{\lfloor d/m \rfloor} \binom{d}{im} x^{\ell d - im\ell} y^{im\ell}. \tag{2-4}$$

Suppose now that $d = ee'$, $\ell = e$, and $m = te'$ is a multiple of e'. Then the left-hand side of (2-4) is a sum of m d-th powers, and since $d \mid im\ell = itd$, the right-hand side is a sum of $1 + \lfloor d/m \rfloor$ d-th powers. Thus, the total number of summands is $1 + t \cdot d/e + \lfloor e/t \rfloor$. We choose t to minimize this sum, obtaining $\Theta_e(d)$.

Newman and Slater took $d = e$, so $e' = 1$ [1979, p. 485]; the minimum in $\Theta_d(d)$ is found by choosing $m \in \{\lfloor \sqrt{d} \rfloor, 1 + \lfloor \sqrt{d} \rfloor\}$, giving $\Phi_d(d) = 1 + \lfloor \sqrt{4d+1} \rfloor$.

If $e < d$, then $\Theta_e(d)$ is generally larger than $\Theta_d(d)$, since some m are skipped in computing the minimum; however, $\Theta_e(d)$ need not be monotone in e, so Theorem 1.3(1) need not be implemented. □

The first instance of nonmonotonicity in $\Theta_e(d)$ occurs at $d = 72$; in general, $\Theta_{8n}(72n^2) = \Theta_{9n}(72n^2) = 1 + 17n$, but $\Theta_{12n}(72n^2) = 1 + 18n$. This suggests interesting questions in combinatorial number theory which we hope to pursue elsewhere.

When d is even, we have a more symmetric specialization of (2-3):

Corollary 2.2. *We have*

$$\frac{1}{s+1} \cdot \sum_{j=0}^{s}(\zeta_{2s+2}^{-j}x + \zeta_{2s+2}^{j}y)^{2s} = \binom{2s}{s} x^s y^s. \tag{2-5}$$

Proof. Set $r = s$, $d = 2s$, and $m = s+1$ in (2-3). Since $|r/m| = |(d-r)/m| < 1$, the summation on the right-hand side has a single term, $i = 0$, and (2-3) becomes

$$\frac{1}{s+1} \cdot \sum_{j=0}^{s} \zeta_{s+1}^{-sj}(x + \zeta_{s+1}^{j}y)^{2s} = \binom{2s}{s} x^s y^s;$$

(2-5) follows from $\zeta_{s+1}^{-sj}(x+\zeta_{s+1}^{j}y)^{2s} = \zeta_{2s+2}^{-2sj}(x+\zeta_{2s+2}^{2j}y)^{2s} = (\zeta_{2s+2}^{-j}x+\zeta_{2s+2}^{j}y)^{2s}$. □

Proof of Theorem 1.3(11) *for even d.* Take $(x, y) \mapsto (x^2, y^2)$ in (2-5) to obtain

$$\sum_{j=0}^{s}(\zeta_{2s+2}^{-j}x^2 + \zeta_{2s+2}^{j}y^2)^{2s} = (s+1)\binom{2s}{s}(xy)^{2s}, \tag{2-6}$$

a linear dependence among $s+2$ $2s$-th powers of an honest set of quadratic forms. □

If $s = 2v$, we have $(\zeta_{4v+2}^{-j}, \zeta_{4v+2}^{-j}) = ((-\zeta_{2v+1}^{v})^j, (-\zeta_{2v+1}^{v+1})^j)$, so

$$\sum_{j=0}^{2v}((\zeta_{2v+1}^{v})^j x^2 + (\zeta_{2v+1}^{v+1})^j y^2)^{4v} = (2v+1)\binom{4v}{2v}(xy)^{4v}. \tag{2-7}$$

When $s = 1$, we have $\zeta_2 = -1$ and (2-7) reduces to (1-1); when $s = 2$ and 3, (2-7) becomes (1-6) and (1-9). Taking $(x, y) \mapsto (e^{-i\theta}(x+iy), e^{i\theta}(x-iy))$ in (2-5) (see [Reznick 2013a, (5.8)], which is incorrect — unfortunately missing the factor of 2^{-2s}) gives

$$\frac{1}{s+1}\sum_{j=0}^{s}\left(\cos\left(\frac{j\pi}{s+1}+\theta\right)x+\sin\left(\frac{j\pi}{s+1}+\theta\right)y\right)^{2s} = \frac{1}{2^{2s}}\binom{2s}{s}(x^2+y^2)^s, \quad \theta\in\mathbb{C}. \tag{2-8}$$

With $\theta \in \mathbb{R}$, (2-8) was a nineteenth-century quadrature formula; see the discussion after [Reznick 2013a, Corollary 5.6] for details. Taking $\theta \in \mathbb{R}$ and $(x, y) \mapsto (x^2 - y^2, 2xy)$, so that $x^2 + y^2 \mapsto (x^2 + y^2)^2$ in (2-8), gives a nice family of $\mathcal{W}_2(s+2, 2s)$ cousins in $\mathbb{R}[x, y]$.

There doesn't seem to be such a simple proof of Theorem 1.3(11) for odd d, and we need to introduce powers of trinomials as summands. More generally, it is useful to present two quadratic cases, which are corollaries of Theorem 2.1; note that

$$\zeta_m^{-rj}(\zeta_m^{-j}x^2+\alpha xy+\zeta_m^{j}y^2)^d = \zeta_m^{-(r+d)j}(x^2+\alpha\zeta_m^{j}xy+\zeta_m^{2j}y^2)^d$$

gives (2-9) the shape of Theorem 2.1 for $p(x, y) = (x^2+\alpha xy+y^2)^d$.

Corollary 2.3. *Suppose $d, m \in \mathbb{N}$, $v \in \mathbb{Z}$, and $\alpha \in \mathbb{C}$. Let*

$$\Psi(v, m, d; \alpha) := \frac{1}{m}\sum_{j=0}^{m-1}\zeta_m^{-vj}(\zeta_m^{-j}x^2+\alpha xy+\zeta_m^{j}y^2)^d. \tag{2-9}$$

(i) *If $m > d$, then*

$$\Psi(0, m, d; \alpha) = \left(\sum_{r=0}^{\lfloor d/2\rfloor}\frac{d!}{(r!)^2(d-2r)!}\alpha^{d-2r}\right)x^d y^d. \tag{2-10}$$

(ii) *If $2m > d \geq m$, then*

$$\Psi(0, m, d; \alpha) = \left(\sum_{r=0}^{\lfloor d/2\rfloor}\frac{d!}{(r!)^2(d-2r)!}\alpha^{d-2r}\right)x^d y^d + \left(\sum_{r=0}^{\lfloor (d-m)/2\rfloor}\frac{d!}{r!\,(r+m)!\,(d-m-2r)!}\alpha^{d-m-2r}\right)(x^{d+m}y^{d-m}+x^{d-m}y^{d+m}). \tag{2-11}$$

Proof. By the trinomial theorem,

$$(x^2+\alpha xy+y^2)^d = \sum_{r+s+t=d}\frac{d!}{r!\,s!\,t!}\alpha^s x^{2r+s}y^{s+2t};$$

note that $(2r+s, s+2t) = (2d-i, i) \iff r-t = d-i$; all sums can only be taken over $r, s, t \geq 0$. In each case, m is relatively large compared to d and very few terms will be nonzero. In (i), $x^{2d-i}y^i$ appears when $i \equiv d \pmod m$. Since $d < m$, this only occurs when $i = d$, so $r = t$ and the coefficient of $x^d y^d$ is found by summing $(d!/r!\,s!\,t!)\alpha^s$ over the set $\{(r, s, t) = (r, d-2r, r)\}$. Similarly, in (ii), $v = 0$ and $2m > d$, so we have three cases $r - t \in \{-m, 0, m\}$, and the terms sum as indicated. $\square$

We use (2-11) when $d - m \geq 2$ by choosing $\alpha = \alpha_0$ to be a nonzero root of the polynomial coefficient of $(x^{d+m}y^{d-m} + x^{d-m}y^{d+m})$, so that the terms on both sides of the expression are d-th powers. In general, the Klein set of $\Psi(v, m, d; \alpha)$ will consist of two parallel regular m-gons, whose altitude and relative orientation depends on α. If $(xy)^d$ appears in the identity, then the two poles are added.

Proof of Theorem 1.3(11) *for odd* d. Suppose $d = 2s + 1 \geq 5$. We have

$$\text{(2-12)}\quad \Psi(0, s+1, 2s+1; \alpha) = \sum_{j=0}^{s} (\zeta_{s+1}^{-j}x^2 + \alpha xy + \zeta_{s+1}^{j}y^2)^{2s+1}$$
$$= A_s(\alpha)x^{3s+2}y^s + B_s(\alpha)x^{2s+1}y^{2s+1} + A_s(\alpha)x^s y^{3s+2},$$
$$A_s(\alpha) = \binom{2s+1}{s}\alpha^s + (2s+1)\binom{2s}{s-2}\alpha^{s-2} + \cdots .$$

Let $\alpha = \alpha_0$ be a nonzero root of $A_s(\alpha)$; this exists because $s \geq 2$, so (2-12) becomes

$$\Psi(0, s+1, 2s+1; \alpha_0) = B(\alpha_0)(xy)^{2s+1},$$

which is a sum of $s+1$ $(2s+1)$-th powers equal to another $(2s+1)$-th power. $\square$

Alternate proof of Theorem 1.3(11) *for* $d = 2s$*,* $s \geq 3$. Suppose $s \geq 3$. Then

$$\text{(2-13)}\quad \Psi(0, s+1, 2s; \alpha) = \tilde{A}_s(\alpha)(x^{3s+1}y^{s-1} + x^{s-1}y^{3s+1}) + \tilde{B}_s(\alpha)x^{2s}y^{2s},$$
$$\tilde{A}_s(\alpha) = \binom{2s}{s-1}\alpha^{s-1} + (2s)\binom{2s-1}{s-3}\alpha^{s-3} + \cdots .$$

Again, choose $\alpha = \alpha_0$ to be a nonzero root of $\tilde{A}_s$. $\square$

By looking at the pattern of linear dependence among the elements, it is not hard to show that the families in (2-6) and (2-13) are not cousins.

Here are other synching examples; (2-10) requires $m > d$. We have $\Psi(0, 4, 3; \alpha) = (\alpha^3 + 6\alpha)x^3y^3$, so $\Psi(0, 4, 3, \sqrt{-6})$ gives a $\mathcal{W}_2(4, 3)$-set. In (ii) we need $d \in [m+2, 2m)$. For $m = 3$, this implies that $d = 5$, and we obtain a variant of [Reznick 2003, (4.12)]:

$$\text{(2-14)}\quad 3\Psi(0, 3, 5; \alpha) = \sum_{j=0}^{2} (\omega^k x^2 + \alpha xy + \omega^{-k}y^2)^5$$
$$= 15(1 + 2\alpha^2)(x^8y^2 + x^2y^8) + 3\alpha(\alpha^4 + 20\alpha^2 + 30)x^5y^5$$
$$\implies \quad \Psi\bigl(0, 3, 5; \sqrt{-1/2}\bigr) = \bigl(\sqrt{-9/2}\,xy\bigr)^5.$$

The linear change $(x, y) \mapsto (\sqrt{-2}x - (1+\sqrt{3})y, -(1+\sqrt{3})x + \sqrt{-2}y)$, applied to (2-14), gives $3(1+\sqrt{3})$ times a flip of (1-8). The Klein set here is again a cube, rotated so the vertices are the two poles and antipodal equilateral triangles at $z = \pm\frac{1}{3}$.

For $m = 4$, the possibilities are $d = 6, 7$; we have

$$4\Psi\big(0, 4, 6; \sqrt{-2/5}\big) = \sum_{k=0}^{3}\big(i^{-k}x^2 + \sqrt{-2/5}\,xy + i^k y^2\big)^6 = 11 \cdot \big(\sqrt{-8/5}\,xy\big)^6;$$

$\Psi\big(0, 4, 7; \sqrt{-6/5}\big)$ is just (1-10).

Two other examples show the range of Corollary 2.3. First,

$$4\Psi(2, 4, 4; \alpha) = \sum_{j=0}^{3}(-1)^k(i^{-k}x^2 + \alpha xy + i^k y^2)^4 = 8(2+3\alpha^2)(x^6y^2 + x^2y^6).$$

On taking $\alpha = \alpha_0 = \sqrt{-2/3}$, transposing two terms to get two equal sums of two fourth powers, and after multiplying through by $\sqrt{3}$, we obtain (1-15). For $d = 5$, we may recover (1-8) as $4\Psi(2, 4, 5, \sqrt{-2})$ from

$$4\Psi(2, 4, 5; \alpha) = \sum_{j=0}^{3}(-1)^k(i^{-k}x^2 + \alpha xy + i^k y^2)^5 = 40\alpha(2+\alpha^2)(x^7y^3 + x^3y^7).$$

An unusual phenomenon occurs with $\Psi(0, 5, 14; \alpha)$: by the general method,

$$\Psi(0, 5, 14; \alpha) = A(\alpha)(x^{24}y^4 + x^4y^{24}) + B(\alpha)(x^{19}y^9 + x^9y^{19}) + C(\alpha)x^{14}y^{14}.$$

It turns out that $A(\alpha)$ and $B(\alpha)$ have the common factor $1+\alpha^2$. Upon setting $\alpha = i$, we obtain (1-11). A computer search has not found other examples of this phenomenon. As noted earlier, the Klein form of (1-11) is an icosahedron, but an icosahedron can be rotated so that its vertices lie in four horizontal equilateral triangles. This suggests that (1-8) should be the cousin of a union of two $\Psi(v, 3, 14; \alpha)$. Indeed, with $\phi = (1+\sqrt{5})/2$ as usual,

$$\text{(2-15)} \quad \sum_{k=0}^{2}(\omega^k x^2 + \phi^2 xy - \omega^{-k}y^2)^{14} + \sum_{k=0}^{2}(\omega^k\phi x^2 - \phi^{-1}xy - \omega^{-k}\phi y^2)^{14} = 0.$$

The Schönemann coefficients of the icosahedron, $\{(\phi^2+1)^{-1/2}\cdot(\pm\phi, \pm 1, 0)\}$ and their cyclic images, lead to yet another cousin of (1-8):

$$\text{(2-16)} \quad \begin{aligned}&(x^2 + 2\phi xy - y^2)^{14} + (x^2 - 2\phi xy - y^2)^{14}\\ &\quad + \left((\phi+i)\left(x^2 - \frac{1-2i}{\sqrt{5}}y^2\right)\right)^{14} + \left((\phi-i)\left(x^2 - \frac{1+2i}{\sqrt{5}}y^2\right)\right)^{14}\\ &\qquad = (\phi x^2 + 2ixy + \phi y^2)^{14} + (\phi x^2 - 2ixy + \phi y^2)^{14}.\end{aligned}$$

The corresponding quadratics for a dodecahedron, alas, give a $\mathscr{W}_2(10, 14)$-set.

There is no reason for synching to be limited to trinomials. Here is an example of a $\mathscr{W}_4(4, 3)$-set of linearly independent elements:

$$\sum_{k=0}^{3}(-1)^k(x^4+i^k\sqrt{6}x^3y-6i^{2k}x^2y^2-\sqrt{6}i^{3k}xy^3+y^4)^3=0; \tag{2-17}$$

the quartics are linearly independent.

Finally, we compare Theorem 1.3(5), (6), and (11). The bound in (11) is linear in d and weaker than (5). This leads to the natural question: what is the smallest d so that $k \geq 2$ and $\Phi_{k+1}(d) < \Phi_k(d)$? Taking Theorem 1.3(7), (10), and (11) into account, we must have $d \geq 6$, and the smallest d for which (5) or (6) beats the bound for $k=2$ in (11) is $d=15$: $1+\lfloor\sqrt{61}\rfloor = 8 < 9 = 2+\lfloor\frac{15}{2}\rfloor$.

3. Overview of $\mathscr{W}_2(4, d)$-sets and tools.

In order to prove Theorem 1.3(8), we need an abbreviated version of Sylvester's algorithmic theorem from 1851 on the representation of forms as a sum of powers of linear forms. We refer the reader to [Reznick 2013a, Theorem 2.1] for the general theorem and proof.

Theorem 3.1 (after Sylvester). *Suppose $d \geq 3$ and*

$$p(x, y)=\sum_{j=0}^{d}\binom{d}{j}a_jx^{2d-2j}y^{2j}, \qquad q(x, y)=\sum_{j=0}^{d}\binom{d}{j}a_jx^{d-j}y^j. \tag{3-1}$$

Then p is a sum of d-th powers of two honest even quadratic forms if and only if there exists a nonsquare quadratic form $h(u, v)=c_0u^2+c_1uv+c_2v^2 \neq 0$ so that

$$\begin{pmatrix} a_0 & a_1 & a_2 \\ a_1 & a_2 & a_3 \\ \vdots & \vdots & \vdots \\ a_{d-2} & a_{d-1} & a_d \end{pmatrix} \cdot \begin{pmatrix} c_0 \\ c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}. \tag{3-2}$$

Sketch of the proof. A comparison of the coefficients of monomials in p and q shows that

$$p(x, y)=(\alpha_1x^2+\beta_1y^2)^d+(\alpha_2x^2+\beta_2y^2)^d \iff q(x, y)=(\alpha_1x+\beta_1y)^d+(\alpha_2x+\beta_2y)^d.$$

Assuming $\alpha_j \neq 0$, $q(x, y)=(\alpha_1x+\beta_1y)^d+(\alpha_2x+\beta_2y)^d$ implies that $a_j=\lambda_1\gamma_1^j+\lambda_2\gamma_2^j$, where $\lambda_i=\alpha_i^d$ and $\gamma_i=\beta_i/\alpha_i$, so (a_j) satisfies the linear recurrence given by (3-2) with $c_0=\gamma_1\gamma_2$, $c_1=-(\gamma_1+\gamma_2)$, and $c_2=1$; $h(u, v)=(\gamma_1u-v)(\gamma_2u-v)$. Conversely, any solution (a_j) to this recurrence has the indicated shape. If $\alpha_2=0$, then $\alpha_1 \neq 0$ by honesty; $a_j = \lambda_1 \gamma_1^j$ for $j \le d-1$ and (3-2) holds with $h(u, v) = u(\gamma_1 u - v)$. □

The matrix in (3-2) is called the 2-*Sylvester matrix* for p (or q). A necessary condition for p to be a sum of two d-th powers is that the 2-Sylvester matrix of p (with $d-2$ rows) has rank ≤ 2. As d increases, this becomes increasingly harder.

We also need a special case of a classical result about simultaneous diagonalization; there doesn't seem to be an easy-to-find modern proof.

Theorem 3.2 (diagonalization). *If f_1 and f_2 are relatively prime binary quadratic forms, then there is a linear change M so that $f_1 \circ M$ and $f_2 \circ M$ are both even.*

Proof. Suppose without loss of generality that $\operatorname{rank}(f_1) \ge \operatorname{rank}(f_2)$. If $\operatorname{rank}(f_1) = 1$, then $(f_1, f_2) = (\ell_1^2, \ell_2^2)$ and a linear change takes $(\ell_1, \ell_2) \mapsto (x, y)$. Otherwise, there exists M_1 so that $(f_1 \circ M_1)(x, y) = x^2 + y^2$ and $(f_2 \circ M_1)(x, y) = ax^2 + bxy + cy^2$. Since these are relatively prime, $a \pm ib - c \neq 0$.

Drop "M_1", and observe that for any $z \in \mathbb{C}$, f_1 is fixed by any orthogonal linear change $M_z : (x, y) \mapsto ((\cos z)x + (\sin z)y, -(\sin z)x + (\cos z)y)$, under which the coefficient of xy in $f_2 \circ M_z$ is $(a-c)\sin 2z + b \cos 2z$. If $a = c$, let $z = \pi/4$. Otherwise, choose z so that $\tan 2z = -b/(a-c)$; this is possible, since the range of $\tan z$ is $\mathbb{C} \setminus \{\pm i\}$. The coefficient of xy in $f_2 \circ M_z$ vanishes, so $f_1 \circ M_z$ and $f_2 \circ M_z$ are both even. □

Suppose $d \ge 3$ and we have a $\mathcal{W}_2(4, d)$-set, flipped and normalized so that

$$p(x, y) = f_1^d(x, y) + f_2^d(x, y) = f_3^d(x, y) + f_4^d(x, y), \tag{3-3}$$

for an honest set $\{f_1, f_2, f_3, f_4\}$ of binary quadratic forms.

Theorem 3.3. *If (3-3) holds, then there exists a linear change after which both f_1 and f_2 are even, so p is even. We have* $\gcd(f_1, f_2) = \gcd(f_3, f_4) = 1$, *but it is not true that f_3 and f_4 are both even.*

Proof. If $\gcd(f_1, f_2) = \ell$ for a linear form ℓ, so that $f_1 = \ell\ell_1$ and $f_2 = \ell\ell_2$, then

$$\ell^d \mid f_3^d + f_4^d = \prod_{k=0}^{d-1} (f_3 + \zeta_d^k f_4).$$

Since $d \ge 3$, ℓ must divide at least two different quadratic factors on the right, say $\ell \mid f_3 + \zeta_d^{k_1} f_4,\ f_3 + \zeta_d^{k_2} f_4$ for $k_1 \neq k_2$. This implies that $\ell \mid f_3, f_4$ and $f_3 = \ell\ell_3$ and $f_4 = \ell\ell_4$ for linear ℓ_3, ℓ_4. Hence, we can factor ℓ^d from (3-3) to obtain $\ell_1^d + \ell_2^d = \ell_3^d + \ell_4^d$, which contradicts Theorem 1.1, since $d \ge 3$. Similarly, $\gcd(f_3, f_4) = 1$.

Thus, f_1 and f_2 are relatively prime, and by Theorem 3.2, we may simultaneously diagonalize them, after which (dropping M),

$$p(x, y) = (\alpha_1 x^2 + \beta_1 y^2)^d + (\alpha_2 x^2 + \beta_2 y^2)^d = f_3^d(x, y) + f_4^d(x, y).$$

Suppose $f_3(x, y) = \alpha_3 x^2 + \beta_3 y^2$ and $f_4(x, y) = \alpha_4 x^2 + \beta_4 y^2$ are both even. Then

$$(\alpha_1 x^2 + \beta_1 y^2)^d + (\alpha_2 x^2 + \beta_2 y^2)^d = (\alpha_3 x^2 + \beta_3 y^2)^d + (\alpha_4 x^2 + \beta_4 y^2)^d \\ \implies \quad (\alpha_1 x + \beta_1 y)^d + (\alpha_2 x + \beta_2 y)^d = (\alpha_3 x + \beta_3 y)^d + (\alpha_4 x + \beta_4 y)^d. \tag{3-4}$$

Since $\{f_j\}$ is honest, (3-4) violates Theorem 1.1, so f_3 and f_4 are not both even. □

Here then is our strategy. We seek to find all pairs $\{f_3, f_4\}$ which are not both even but for which $f_3^d + f_4^d$ *is* even. Then, from among those, we need to find those which can *also* be written as a sum of two d-th powers of even quadratic forms.

How can it happen that $f_3^d + f_4^d$ is even when at least one of $\{f_3, f_4\}$ is not even? Two cases come readily to mind:

$$(ax^2 + bxy + cy^2)^d + (ax^2 - bxy + cy^2)^d, \tag{3-5}$$

and, if d is even,

$$(ax^2 + cy^2)^d + b(xy)^d. \tag{3-6}$$

We call (3-5) and (3-6) the *tame* cases; otherwise $\{f_3, f_4\}$ are in the *wild* case. There is an important practical distinction. The tame expressions are formally symmetric under $y \mapsto -y$, but wild expressions are not. Thus, any wild (3-3) implies the existence of a *third* representation for p a sum of two d-th powers.

The case $d = 3$ is best handled by other techniques and is covered in the companion paper [Reznick 2020]. In preparation for implementing this strategy, we calculate the tame and wild cases which might occur from the list of $\mathcal{W}_2(4, d)$-sets for $d \geq 4$ in Theorems 1.6 and 1.7. Each identity (3-3) has two flips $f_1^d - f_3^d = f_4^d - f_2^d$ and $f_1^d - f_4^d = f_3^d - f_2^d$, and since either side can be diagonalized, there are potentially six cases. (If there are three equal sums, there are potentially fifteen cases.) Fortunately, symmetry reduces the number of cases substantially.

Theorem 3.4. (i) *The diagonalizations of* (1-6) *are, up to scaling,*

$$(x^2 + y^2)^4 - 18(xy)^4 = -(\omega x^2 + \omega^2 y^2)^4 - (\omega^2 x^2 + \omega y^2)^4 \\ = x^8 + 4x^6 y^2 - 12x^2 y^2 + 4x^2 y^6 + y^8 \tag{3-7}$$

and

$$-(2x^2 + 2y^2)^4 + 18(x^2 - y^2)^4 \\ = (x^2 + 2\sqrt{-3}xy + y^2)^4 + (x^2 - 2\sqrt{-3}xy + y^2)^4 \\ = 2(x^8 - 68x^6 y^2 + 6x^4 y^4 - 68x^2 y^6 + y^8). \tag{3-8}$$

(ii) *The diagonalizations of* (1-14) *are, up to scaling,*

$$(\alpha x^2-\beta y^2)^4-(\beta x^2-\alpha y^2)^4 \tag{3-9}$$
$$= (\omega x^2-\sqrt{3}xy-\omega^2y^2)^4-(\omega^2x^2-\sqrt{3}xy-\omega y^2)^4$$
$$= (\omega x^2+\sqrt{3}xy-\omega^2y^2)^4-(\omega^2x^2+\sqrt{3}xy-\omega y^2)^4$$
$$= \sqrt{-3}(x^8-14x^6y^2+14x^2y^6-y^8),$$

where $\alpha=(2+\sqrt{-3})/2$ *and* $\beta=(2-\sqrt{-3})/2$, *and*

$$((1+\sqrt{-6})x^2+(1-\sqrt{-6})y^2)^4+((1-\sqrt{-6})x^2+(1+\sqrt{-6})y^2)^4 \tag{3-10}$$
$$= (x^2+2\sqrt{-6}xy+y^2)^4+(x^2-2\sqrt{-6}xy+y^2)^4$$
$$= 2(x^8-140x^6y^2+294x^4y^4-140x^2y^6+y^8).$$

(iii) *The diagonalization of* (1-8) *is, up to scaling,*

$$((1-\sqrt{-2})x^2+(1+\sqrt{-2})y^2)^5+((1+\sqrt{-2})x^2+(1-\sqrt{-2})y^2)^5 \tag{3-11}$$
$$= (x^2-2\sqrt{-2}xy+y^2)^5+(x^2+2\sqrt{-2}xy+y^2)^5$$
$$= 2(x^{10}-75x^8y^2+90x^6y^4+90x^4y^6-75x^2y^8+y^{10}).$$

Proof. (i) First, in (1-6), the summands on the left are cyclically permuted by $(x,y)\mapsto(\omega x,\omega^2y)$, so there is only one choice up to scaling. One is already diagonalized as in (3-7). To diagonalize the left-hand side in (3-7), take $(x,y)\mapsto(x+y,x-y)$ and multiply through by -1, to obtain (3-8).

(ii) It is convenient to name the forms from (1-14) in (3-12) . Let

$$\begin{aligned}
&f_{1,1}(x,y)=x^2+\sqrt{3}xy-y^2, && f_{1,2}(x,y)=x^2-\sqrt{3}xy-y^2,\\
&f_{1,3}(x,y)=f_{1,1}(\omega^2x,\omega y), && f_{1,4}(x,y)=f_{1,2}(\omega^2x,\omega y),\\
&f_{1,5}(x,y)=f_{1,1}(\omega x,\omega^2 y), && f_{1,6}(x,y)=f_{1,2}(\omega x,\omega^2 y),
\end{aligned} \tag{3-12}$$
$$f_{1,1}^4-f_{1,2}^4=f_{1,3}^4-f_{1,4}^4=f_{1,5}^4-f_{1,6}^4=8\sqrt{3}xy(x^6-y^6).$$

Let M_1 denote the linear change $(x,y)\mapsto(\omega^2x,\omega y)$, so that M_1 cycles $f_{1,1}\mapsto f_{1,3}\mapsto f_{1,5}\mapsto f_{1,1}$ and $f_{1,2}\mapsto f_{1,4}\mapsto f_{1,6}\mapsto f_{1,2}$. Let M_2 denote the linear change $(x,y)\mapsto\sqrt{1/2}(x+iy,ix+y)$, which has two nice properties. First, M_2 cycles $f_{1,3}\mapsto f_{1,5}\mapsto f_{1,6}\mapsto f_{1,4}\mapsto f_{1,3}$, but it also takes $(f_{1,1},f_{1,2})\mapsto(\alpha x^2-\beta y^2,\beta x^2-\alpha y^2)$. On the Riemann sphere, M_1 induces a $2\pi/3$ rotation on the axis of the poles, and M_2 induces the rotation taking $(a,b,c)\mapsto(a,c,-b)$.

By repeatedly using M_1 and M_2, the fifteen pairs $\{f_{1,i},f_{1,j}\}$ which might be simultaneously diagonalized given the identity $f_{1,3}^4-f_{1,4}^4=f_{1,5}^4-f_{1,6}^4$ reduce to two cases, after linear changes. We have already seen one: M_2 diagonalizes (1-14) into (3-9).

For the other, note that

$$f_{1,4}^4(x,y)+f_{1,5}^4(x,y)=f_{1,3}^4(x,y)+f_{1,6}^4(x,y) \\ =-(x^8+14x^6y^2+42x^4y^4+14x^2y^6+y^8). \tag{3-13}$$

An appeal to Theorem 3.1 shows that the octic in (3-13) is *not* a sum of two fourth powers of even quadratic forms. Under the linear change M_3, which takes $(x,y)\mapsto(x-(\sqrt{2}-1)y,\, i(\sqrt{2}-1)x+iy)$ and division by $\sqrt{2}-2$, (3-13) becomes (3-10).

(iii) We name the quadratics from (1-8) in (3-14). Let M_4 be the scaling $(x,y)\mapsto(\zeta_8x,\zeta_8^3y)$, which takes $(x^2,xy,y^2)\mapsto(ix^2,-xy,-iy^2)$, so that

$$\begin{aligned} f_{2,1}(x,y)&=x^2+\sqrt{-2}xy+y^2, &\quad f_{2,2}&=f_{2,1}\circ M_4,\\ f_{2,3}&=f_{2,2}\circ M_4, & f_{2,4}&=f_{2,3}\circ M_4,\end{aligned}$$
$$f_{2,1}^5+f_{2,2}^5+f_{2,3}^5+f_{2,4}^5=0. \tag{3-14}$$

Thus, M_4 cycles $f_{2,1}\mapsto f_{2,2}\mapsto f_{2,3}\mapsto f_{2,4}\mapsto f_{2,1}$. The symmetry of the Klein set for $\{f_{2,j}\}$ (the cube) suggests that we define M_5 to be the linear change $(x,y)\mapsto\sqrt{1/2}\cdot(-x+\zeta_8^5y,\,\zeta_8^3x+y)$. Then M_5 fixes $f_{2,1}$ and $f_{2,4}$ and permutes $f_{2,2}$ and $f_{2,3}$.

Thus, M_4 maps the flip $f_{2,1}^5+f_{2,2}^5=-f_{2,3}^5-f_{2,4}^5$ into $f_{2,2}^5+f_{2,3}^5=-f_{2,4}^5-f_{2,1}^5$ and M_5 maps it into $f_{2,1}^5+f_{2,3}^5=-f_{2,2}^5-f_{2,4}^5$, so up to cousin, we need only consider one flip. The easiest one to deal with is $f_{2,1}^5+f_{2,3}^5=-f_{2,2}^5-f_{2,4}^5$. This is

$$\begin{aligned}(x^2+\sqrt{-2}xy+y^2)^5&+(-x^2+\sqrt{-2}xy-y^2)^5\\ &=-(ix^2-\sqrt{-2}xy-iy^2)^5-(-ix^2-\sqrt{-2}xy+iy^2)^5\\ &=2\sqrt{-2}xy(5x^8-6x^4y^4+5y^8).\end{aligned} \tag{3-15}$$

Upon taking $(x,y)\mapsto(x+iy,x-iy)$, and dividing by $\sqrt{-2}$, (3-15) becomes (3-11). And under the linear change, $(x,y)\mapsto\sqrt{1/2}(x+iy,x-iy)$, (1-15) also becomes (3-11). The Klein set of the summands in (3-11) is a rotated cube lying in the planes $y=\pm\sqrt{1/3}$, so that the edge $\bigl(0,\pm\sqrt{1/3},\sqrt{2/3}\bigr)$ lies on top. □

4. Finishing the proof

We first make a simplifying observation in the tame case. If (f_3,f_4) is given in (3-5) or (3-6) and $a=0$ (or $c=0$), then f_3 and f_4 have a common factor of y (or x), violating Theorem 3.3. Similarly, we may assume that $b\neq0$. Thus, after scaling, we may assume that (3-5) and (3-6) take the shape

$$(x^2+bxy+y^2)^d+(x^2-bxy+y^2)^d,\quad b\neq0, \tag{4-1}$$

$$(x^2+y^2)^{2e}+b\binom{2e}{e}(xy)^{2e},\quad b\neq0. \tag{4-2}$$

Theorem 4.1. *The only $\mathcal{W}_2(4, d)$-sets which come from a tame representation for $d \ge 4$ are given in* Theorem 3.4 *by* (3-7), (3-8), (3-10), *and* (3-11). *These sets are all cousins or subcousins of the families in* Theorems 1.6 *and* 1.7.

Proof. We analyze (4-2) first. The 2-Sylvester matrix of $(x^2+y^2)^4+6b(xy)^4$ is

$$\begin{pmatrix} 1 & 1 & 1+b \\ 1 & 1+b & 1 \\ 1+b & 1 & 1 \end{pmatrix}, \tag{4-3}$$

which has rank 2 only if $-b^2(b+3)=0$; if $b=-3$, we obtain (3-7).

If $d=2s\ge 6$ and $p_{2s,b}(x, y)=(x^2+y^2)^{2s}+b\binom{2s}{s}(xy)^{2s}$, then the $(2s-1)\times 3$ 2-Sylvester matrix consists of (4-3), with $s-2$ rows of $(1, 1, 1)$ appended both at the top and the bottom. Such a matrix has rank 2 only if $b=0$.

For (4-1), we first observe that

$$(x^2+bxy+y^2)^d+(x^2-bxy+y^2)^d=2\sum_{0\le i\le d/2}\binom{d}{2i}(x^2+y^2)^{d-2i}(xy)^{2i}. \tag{4-4}$$

Suppose $d=4$. Then the sum in (4-4) becomes

$$2x^8+(8+12b^2)x^6y^2+(12+24b^2+2b^4)x^4y^4+(8+12b^2)x^2y^6+2y^8.$$

Apply Theorem 3.1: the 2-Sylvester matrix has discriminant $-\frac{1}{27}b^8(12+b^2)(24+b^2)$ and has rank 2 only if $b^2\in\{-12, -24\}$. These cases are presented in (3-8) and (3-10), and are a cousin of (1-6) and a subcousin of (1-14), respectively.

Suppose $d=5$. Then applying Theorem 3.1 to (4-4) gives a 4×3 matrix; computing the 3×3 minors shows that the matrix has rank 2 only when $b=0$ or $b^2=-8$. Taking $b=\sqrt{-8}$, we obtain (3-11), which is a cousin of (1-8).

Now suppose $d\ge 6$; (4-4) gives

$$\begin{aligned} a_0=a_d &= 2, \\ a_1=a_{d-1} &= 2+b^2(d-1), \\ a_2=a_{d-2} &= 2+b^2(d-2)(12+(d-3)b^2)/6, \\ a_3=a_{d-3} &= 2+b^2(d-3)(180+b^2(30d-120)+b^4(d^2-9d+20))/60. \end{aligned}$$

The submatrix of the 2-Sylvester matrix consisting of the first and last two rows is

$$\begin{pmatrix} a_0 & a_1 & a_2 \\ a_1 & a_2 & a_3 \\ a_3 & a_2 & a_1 \\ a_2 & a_1 & a_0 \end{pmatrix}.$$

The $1, 2, 4$ minor of this submatrix is

$$-\frac{b^8}{9(d-1)}\binom{d+1}{5}(12+b^2(d-3))(24+b^2(2d-7)).$$

If $b^2 = -12/(d-3)$, then the $1, 2, 3$ minor becomes

$$\frac{55296d^2(d+1)(d-4)}{25(d-3)^5} \neq 0.$$

However, if $b^2 = -24/(2d-7)$, then all four minors vanish. (Note that $d = 4, 5$ then give $b^2 = -24$ and $b^2 = -8$, which we have already seen.) We recompute the a_k for $b^2 = -24/(2d-7)$, and find that the first three rows of the 2-Sylvester matrix give

$$\begin{vmatrix} a_0 & a_1 & a_2 \\ a_1 & a_2 & a_3 \\ a_2 & a_3 & a_4 \end{vmatrix} = -\frac{3538944(d-5)(d-4)d(1+d)(2d-1)^2}{175(2d-7)^6} \neq 0.$$

Thus, no tame representations exist when $d \geq 6$. □

Suppose now that we have a wild representation

$$\begin{aligned} p(x, y) &= (a_1x^2 + b_1xy + c_1y^2)^d + (a_2x^2 + b_2xy + c_2y^2)^d \\ &= \sum_{i=0}^{2d} s_i(a_1, b_1, c_1, a_2, b_2, c_2; d)x^{2d-i}y^i, \end{aligned} \tag{4-5}$$

where $d \geq 4$, $s_{2j+1}(a_1, b_1, c_1, a_2, b_2, c_2; d) = 0$ for $0 \leq j \leq d-1$, $(b_1, b_2) \neq (0, 0)$, and (4-5) is not in the form (3-5) or (3-6).

Lemma 4.2. *Suppose $p \neq 0$ and (4-5) holds. Then, after a scaling of x and y,*

$$p(x, y) = p_{\lambda,\alpha,\beta}(x, y) := (x^2 - \lambda\alpha xy + y^2)^d + \lambda(x^2 + \alpha xy + \beta y^2)^d, \tag{4-6}$$

where $\alpha\lambda \neq 0$, $\beta^{d-1} = 1$, and $\lambda^2 \neq 1$.

Proof. First suppose $b_1 = 0$ in (4-5). Then $s_1 = da_2^{d-1}b_2$ and $s_{2d-1} = db_2c_2^{d-1}$. Since $(b_1, b_2) \neq (0, 0)$, we have $a_2 = c_2 = 0$ and $p(x, y) = (a_1x^2 + c_1y^2)^d + (b_2xy)^d$ is even, so d is even and we have (3-6). A similar argument lets us conclude that $b_2 \neq 0$.

Suppose now that $a_1 = 0$. Then $s_1 = da_2^{d-1}b_2 = 0$, and $b_2 \neq 0$ implies $a_2 = 0$. It then follows that y divides both f_3 and f_4, contradicting Theorem 3.3. Thus, $a_1 \neq 0$, and by similar arguments, we have $a_2c_1c_3 \neq 0$. That is, we may assume that all the coefficients in (4-5) are nonzero.

We now scale x and y so that $a_1 = c_1 = 1$ and let $\lambda = a_2^d$, so that, after renaming,

$$p(x, y) = (x^2 + \alpha_1xy + y^2)^d + \lambda(x^2 + \alpha_2xy + \beta y^2)^d, \tag{4-7}$$

where all parameters are nonzero. Returning to the computation,

$$s_1 = d(\alpha_1 + \lambda\alpha_2) = 0, \qquad s_{2d-1} = d(\alpha_1 + \lambda\alpha_2\beta^{d-1}) = 0.$$

It follows that $\alpha_1 = -\lambda\alpha_2$, and since $\lambda\alpha_2 \neq 0$, it also follows that $\beta^{d-1} = 1$. We now write $\alpha = \alpha_2$, so that $\alpha_1 = -\lambda\alpha$, and (4-7) becomes (4-6). Finally, if $\lambda^2 = 1$, then either $\lambda = 1$ (and (4-6) reduces to (3-5)), or $\lambda = -1$ (and (4-6) implies $p = 0$). □

Theorem 4.3. *For $d \geq 4$, the only $\mathcal{W}_2(4, d)$-set which comes from a wild representation is found in (3-10), and is a subcousin of (1-14).*

Proof. In view of Lemma 4.2, we simplify our notation: let

$$p_{\lambda,\alpha,\beta}(x, y) = \sum_{i=0}^{2d} a_i(\lambda, \alpha, \beta; d)x^{2d-i}y^i. \tag{4-8}$$

Since $p_{\lambda,\alpha,\beta}(x, y)$ is even, so is $p_{\lambda,\alpha,\beta}(y, x)$, as is their difference. For this reason, write

$$\begin{aligned}\lambda^{-1}(p_{\lambda,\alpha,\beta}(x, y) - p_{\lambda,\alpha,\beta}(y, x)) &= (x^2+\alpha xy+\beta y^2)^d - (\beta x^2+\alpha xy+y^2)^d \\ &= \sum_{i=0}^{2d} b_i(\alpha, \beta, d)x^{2d-i}y^i.\end{aligned} \tag{4-9}$$

We need to find the conditions under which $a_{2j+1}(\lambda, \alpha, \beta; d) = 0$ for $1 \leq 2j+1 \leq 2d-1$. Since $\lambda b_i(\alpha, \beta) = a_i(\lambda, \alpha, \beta; d) - a_{2d-i}(\lambda, \alpha, \beta; d)$ and $\lambda \neq 0$, it suffices to consider $a_{2j+1}(\lambda, \alpha, \beta; d) = b_{2j+1}(\alpha, \beta, d) = 0$ for $1 \leq 2j+1 \leq d$.

It follows from the definition and $\beta^{d-1} = 1$ that

$$p_{\lambda,\alpha,\beta}(x, y) = p_{\lambda,-\alpha,\beta}(x, -y), \qquad p_{\lambda,\alpha,\beta}(x, y) = p_{\lambda\beta,\alpha/\beta,1/\beta}(y, x), \tag{4-10}$$

so that, up to linear change, if $\alpha^2 = \kappa$ is known, then choosing $\alpha = \pm\sqrt{\kappa}$ gives two equations that are cousins. Also, any solution for a particular value $\beta = \beta_0$ will be a cousin of a solution in which $\beta = \beta_0^{-1}$. This reduces the number of choices to check.

We now have

$$\begin{aligned} a_1(\lambda, \alpha, \beta) &= -d\alpha\lambda + d\alpha\lambda = 0, \qquad b_1(\alpha, \beta) = d\alpha(\beta^{d-1} - 1) = 0, \\ a_3(\lambda, \alpha, \beta) &= \frac{\lambda\alpha d(d-1)}{6} \cdot ((d-2)\alpha^2(1-\lambda^2) + 6(\beta - 1)), \\ b_3(\alpha, \beta) &= \frac{\alpha d(d-1)}{6} \cdot (1 - \beta^{d-3})(6\beta + \alpha^2(d-2)). \end{aligned}$$

Now we claim that $\beta \neq 1$ and either

$$\beta = -1, \quad \alpha^2 = \frac{12}{(d-2)(1-\lambda^2)} \quad \text{(and } d \text{ is odd)}, \tag{4-11}$$

or

$$\beta = \frac{1}{\lambda^2}, \quad \alpha^2 = -\frac{6}{\lambda^2(d-2)}. \tag{4-12}$$

Indeed, since $\alpha(1-\lambda^2) \neq 0$, the equation $a_3 = 0$ implies that $\beta \neq 1$ and

$$\alpha^2 = \frac{6(1-\beta)}{(d-2)(1-\lambda^2)}. \tag{4-13}$$

The equation $b_3 = 0$ implies that $(1-\beta^{d-3})(6\beta + \alpha^2(d-2)) = 0$. If $\beta^{d-3} = 1$, then $\beta^{d-1} = 1$ implies $\beta^2 = 1$, and $\beta = 1$ is ruled out, so $\beta = -1$ and d is odd and (4-13) implies (4-11). Otherwise, we have by (4-13)

$$0 = 6\beta + \alpha^2(d-2) = 6\beta + \frac{6(1-\beta)}{(1-\lambda^2)} = \frac{6(1-\beta\lambda^2)}{1-\lambda^2},$$

so $1 = \beta\lambda^2$ and by (4-13),

$$\alpha^2 = \frac{6(1-\lambda^{-2})}{(d-2)(1-\lambda^2)} = -\frac{6}{\lambda^2(d-2)};$$

this is summarized as (4-12).

If $d = 4$, then only (4-12) can apply. Since $\beta^3 = 1$, $\beta \neq 1$, and $\omega \cdot \omega^2 = 1$, we can use (4-10) to assume that $\beta = \omega^2$. It follows from (4-12) that

$$\omega^2 = \frac{1}{\lambda^2}, \quad \alpha^2 = -\frac{3}{\lambda^2} \quad \implies \quad \lambda = \pm\omega^2, \quad \alpha^2 = -3\omega^2.$$

By (4-10), it suffices to take $\alpha = \sqrt{-3}\omega$, but there are two values for λ: $\lambda = \pm\omega^2$. There are two wild cases: since $\lambda\alpha = \pm\sqrt{-3}$ and $(\omega^2)^4 = \omega^2$, these are

$$\begin{aligned} p_{4,\pm}(x,y) &:= (x^2 \mp \sqrt{-3}xy + y^2)^4 \pm \omega^2(x^2 + \sqrt{-3}\omega xy + \omega^2 y^2)^4 \\ &= (x^2 \mp \sqrt{-3}xy + y^2)^4 \pm (\omega^2 x^2 + \sqrt{-3}xy + \omega y^2)^4. \end{aligned} \tag{4-14}$$

We scale the two cases of (4-14) to make them easier to work with. First

$$\begin{aligned} \omega^2 p_{4,+}(x, \omega i y) := q_1(x,y) &= -x^8 - 14x^6y^2 - 42x^4y^4 - 14x^2y^6 - y^8 \\ &= (\omega^2x^2 - \sqrt{3}xy - \omega y^2)^4 + (\omega x^2 + \sqrt{3}xy - \omega^2y^2)^4. \end{aligned} \tag{4-15}$$

The second line in (4-15) is $f_{1,4}^4 + f_{1,5}^4$, which gives a new representation after $y \mapsto -y$, namely, $f_{1,3}^4 + f_{1,6}^4$; see (3-13). However, the 2-Sylvester matrix of q_1 has rank 3, so this case does not fall under Theorem 3.3.

For the other case, we have

$$-\omega^2 p_{4,-}(x,\omega i y) := q_2(x,y) \tag{4-16}$$
$$= -(\omega^2x^2-\sqrt{3}xy-\omega y^2)^4+(\omega x^2-\sqrt{3}xy-\omega^2y^2)^4$$
$$= \sqrt{-3}(x^8-14x^6y^2+14x^2y^6-y^8).$$

The 2-Sylvester matrix of q_2 has rank 2, so it has a representation as a sum of two fourth powers. Indeed, (4-16) is embedded in (3-9), with two other representations of q_2: one from taking $y \mapsto -y$ in (4-16), and the other by applying Theorem 3.1.

Now suppose $d \geq 5$; more equations need to be satisfied. If (4-11) holds, then

$$a_5 = -\frac{8\sqrt{3}\lambda(1+\lambda^2)(d+1)d(d-1)(d-3)}{5((d-2)(1-\lambda^2))^{3/2}} = 0,$$

so $\lambda^2 = -1$, and (4-11) becomes

$$\beta = -1, \quad \lambda^2 = -1, \quad \alpha^2 = \frac{6}{d-2}. \tag{4-17}$$

If (4-12) holds, then

$$a_5 = -\frac{\sqrt{6}(\lambda^4-1)(2d+1)d(d-1)(d-4)}{10\lambda^4(d-2)^{3/2}}. \tag{4-18}$$

Since $\lambda^2 \neq 1$, (4-18) implies $\lambda^2 = -1$, and simplification yields (4-17) again. Observe that $\lambda = \pm i$ implies that $d \equiv 1 \pmod 4$.

If $d = 5$, then $\beta = -1$, $\lambda^2 = -1$, and $\alpha^2 = 2$. We choose $\alpha = \sqrt{2}$ and obtain two solutions, for $\lambda = i$ and $\lambda = -i$, which we rewrite in terms of the $f_{2,j}$, upon noting that $\pm i = (\pm i)^5$:

$$\begin{aligned} p_{5,+}(x,y) &= (x^2-i\sqrt{2}xy+y^2)^5+i(x^2+\sqrt{2}xy-y^2)^5 = -f_{2,3}^5-f_{2,4}^5 \\ &= (1+i)(x^{10}+15ix^8y^2-30x^6y^4+30ix^4y^6-15x^2y^8-iy^{10}), \\ p_{5,-}(x,y) &= (x^2+i\sqrt{2}xy+y^2)^5-i(x^2+\sqrt{2}xy-y^2)^5 = f_{2,1}^5+f_{2,4}^5 \\ &= (1-i)(x^{10}-15ix^8y^2-30x^6y^4-30ix^4y^6-15x^2y^8+iy^{10}). \end{aligned} \tag{4-19}$$

The expressions in (4-19) are close cousins; in fact, $p_{5,-}(x,y) = -ip_{5,+}(x,iy)$. Theorem 3.1 shows that neither has a representation as a sum of two even fifth powers; however, $p_{5,-}(x,y)+ip_{5,+}(x,iy) = 0$ is a cousin of (1-8).

Suppose now that $d \geq 6$; since $d \equiv 1 \pmod 4$, we have $d \geq 9$. It turns out that $b_5 = 0$ under the conditions of (4-17), but

$$a_7\left(\pm i, \sqrt{\frac{6}{d-2}}, -1, d\right) = \pm\frac{8i\sqrt{2}(2d-1)(d^3-d)(d-3)(d-5)}{35\sqrt{3}(d-2)^{5/2}} = 0 \tag{4-20}$$

is clearly impossible for $d \geq 9$, so we are finally done with the wild case. □

Proof of Theorems 1.3(8), 1.6*, and* 1.7. Combine Theorems 3.3, 4.1, and 4.3. □

5. Final remarks

Derivations and historical examples. It is foolhardy for a living author to claim priority for any polynomial identity which is verifiable by hand and so might well have been given as a school algebra assignment. We have given previous attributions when we could find them; the pre-1920 literature was scoured by Dickson [1966], but with Diophantine equations over $\mathbb{N}$ in mind: the coverage of parametrizations over $\mathbb{C}$ must be regarded as incomplete. For example, [Desboves 1880] includes both (1-15) and (1-8), and Dickson only cites the latter, perhaps because there were no real quintic parametrizations.

Any four binary quadratic forms are linearly dependent, so any $\mathscr{W}_2(4,d)$-set satisfies both $f_1^d + f_2^d = f_3^d + f_4^d$ and $c_1 f_1 + c_2 f_2 + c_3 f_3 + c_4 f_4 = 0$ for suitable c_i. It is remarkable that one can find the $\mathscr{W}_2(4,d)$-sets for $d = 4, 5$ by guessing a simple choice of c_i.

For example, Desboves [1880, p. 241] found his version of (1-8) by assuming $f_1 + f_2 = f_3 + f_4$ and $f_1^5 + f_2^5 = f_3^5 + f_4^5$ and parametrizing to get

$$0 = (f+g)^5 + (f-g)^5 - ((f+h)^5 + (f-h)^5) = 10f(g^2-h^2)(2f^2+g^2+h^2).$$

He then set $\{f, g, h\} = \{2xy, x^2-2y^2, i(x^2+2y^2)\}$ via Theorem 1.4, and by scaling via $y \mapsto \sqrt{-1/2}\,y$, this becomes essentially (1-8). Similarly, after noting that

$$(f+g)^4 + (f-g)^4 - ((f+h)^4 + (f-h)^4) = 2(g^2-h^2)(6f^2+g^2+h^2),$$

Desboves solved $6f^2 + g^2 + h^2 = 0$ and derived a cousin of (1-15).

One might also guess $f_1 + f_2 + f_3 = 0$; an old observation (at least back to Proth in 1878 [Dickson 1966, p. 657]) notes that

$$f_1^4 + f_2^4 + (-f_1 - f_2)^4 = 2(f_1^2 + f_1 f_2 + f_2^2)^2, \tag{5-1}$$

so if $f_1^2 + f_1 f_2 + f_2^2 = g^2$, we obtain a $\mathscr{W}_2(4,4)$-set. Take $f_1 = x^2 + y^2$ and $f_2 = \omega x^2 + \omega^2 y^2$; this implies $-(f_1+f_2) = \omega^2 x^2 + \omega y^2$ and $f_1^2 + f_1 f_2 + f_2^2 = 3x^2y^2$ and hence (1-6).

In 1904, Ferrari [Dickson 1966, p. 654] gave the ostensibly ternary identity

$$\begin{aligned}(a-b)^4(a+b+2c)^4 + (b+c)^4(b-c-2a)^4 + (c+a)^4(c-a+2b)^4 \\ = 2(a^2+b^2+c^2-ab+ac+bc)^4.\end{aligned} \tag{5-2}$$

Let $x = a - b$ and $y = b + c$, so that $x + y = a + c$. Then (5-2) becomes (1-7):

$$x^4(x+2y)^4 + y^4(-2x-y)^4 + (x+y)^4(y-x)^4 = 2(x^2+xy+y^2)^4.$$

One can derive (1-14) by guessing $(a+d)^4-(a-d)^4=(b+d)^4-(b-d)^4=(c+d)^4-(c-d)^4$ for quadratics a, b, c, d with a, b, c distinct and $d \neq 0$. Then routine computations lead to $a+b+c=0$ and $d^2=-(a^2+ab+b^2)$. Now set $a=x^2+y^2$, $b=\omega x^2+\omega^2 y^2$, and $c=\omega^2 x^2+\omega y^2$, with $d^2=-(a^2+ab+b^2)=-3x^2y^2$, and take $y \mapsto iy$ to get (1-14).

We derived (1-8) in [Reznick 2003, pp. 119–120] using Newton's theorem on symmetric polynomials. Every symmetric quaternary quintic polynomial p is contained in the ideal $\mathcal{I}=(t_1+t_2+t_3+t_4, t_1^2+t_2^2+t_3^2+t_4^2)$. In particular, $t_1^5+t_2^5+t_3^5+t_4^5 \in \mathcal{I}$, so

$$f_1+f_2+f_3+f_4=0,\ f_1^2+f_2^2+f_3^2+f_4^2=0 \quad \Longrightarrow \quad f_1^5+f_2^5+f_3^5+f_4^5=0.$$

Upon setting $f_4=-f_1-f_2-f_3$, the equation $f_1^2+f_2^2+f_3^2+(-f_1-f_2-f_3)^2=0$ can be analyzed as in Theorem 1.4 to obtain (1-8).

We present a similar ad hoc, post hoc derivation for (1-11).

Theorem 5.1. *Suppose $S(t_1, \dots, t_6)$ is a symmetric polynomial of degree 7. Then*

$$S \in \mathcal{I} := \left(\sum_{k=1}^{6} t_k, \sum_{k=1}^{6} t_k^2, \sum_{k=1}^{6} t_k^4 \right).$$

Proof. Let e_k denote the k-th elementary symmetric polynomial. We have $\sum_{k=1}^6 t_k^2 = e_1^2-e_2$ and $\sum_{k=1}^6 t_k^4 = e_1^4-4e_1^2e_2+2e_2^2+4e_1e_3-4e_4$. Thus, $\mathcal{I}=(e_1, e_2, e_4)$. By Newton's theorem, S is a linear combination of monomials in the e_k: $e_1^{a_1}e_2^{a_2}e_3^{a_3}e_4^{a_4}e_5^{a_5}e_6^{a_6}$, where $\sum ka_k=7$. But 7 cannot be written as a nonnegative linear combination of 3, 5, and 6, so each monomial in any such expression must contain one of $\{e_1, e_2, e_4\}$. □

Observe now that if we define $h_j=(\zeta_5^{j-1}x^2+ixy+\zeta_5^{-(j-1)}y^2)^2$ for $1 \le j \le 5$ and $h_6=-5x^2y^2$, then a synching computation shows that $\sum_{j=1}^6 h_j = \sum_{j=1}^6 h_j^2 = \sum_{j=1}^6 h_j^4 = 0$. Theorem 5.1 implies that $\sum_{j=1}^6 h_j^7=0$; that is, (1-11). The mystery now is *why* these particular squares work.

Jordan Ellenberg has suggested the following explanation to the author: the surface cut out by $\sum_{j=1}^6 X_j = \sum_{j=1}^6 X_j^2 = \sum_{j=1}^6 X_j^4$ is a Hilbert modular surface [Ellenberg 2005, Lemma 2.1]. He adds (personal communication, 2012), "Dollars to donuts the nice low-degree rational curve you find on this surface arises as a modular curve on this modular surface, parametrizing abelian surfaces isogenous to a product of elliptic curves."

Representations as a sum of at most two d-th powers of quadratic forms. Which forms $p \in H_{2d}(\mathbb{C}^2)$ can be written as a sum of two d-th powers of linear forms, and in how many ways? Let $A_{d,2}=\{(\alpha_1 x+\beta_1 y)^d+(\alpha_2 x+\beta_2 y)^d\}$. It is tautological to say that $p \in A_{d,2}$ if and only if there is a linear change taking p into x^d or $x^d + y^d$. (A practical test is given by Theorem 3.1.)

Corollary 5.2. *If $p \in H_{2d}(\mathbb{C}^2)$ is not a d-th power, then p is a sum of two d-th powers of quadratic forms if and only if either* (i) *$p = \ell^d q$, where $q \in A_{d,2}$, or* (ii) *after a linear change in p, $p(x, y) = q(x^2, y^2)$, where $q \in A_{d,2}$.*

Proof. Sufficiency is clear. Conversely, suppose $p = f_1^d + f_2^d$ and $\{f_1, f_2\}$ is honest. As in Theorem 3.2, there are two cases. If $\gcd(f_1, f_2) = \ell$ for a linear form ℓ, then $f_j = \ell\ell_j$, giving case (i). Otherwise, we make a linear change which simultaneously diagonalizes f_1, f_2, giving case (ii). □

If p is a sum of two d-th powers in more than one way, then the two representations together give a $\mathcal{W}_2(d, 4)$-set. The question is not interesting for $d = 2$, since $p = f^2 + g^2 \iff p = (f + ig)(f - ig)$, so two representations as a sum of two squares amount to two different factorizations into equal degrees. The situation for $d = 3$ is discussed in detail in [Reznick 2020]; by Theorem 1.3(8), it suffices now to consider $d = 4, 5$.

If p itself is a d-th power, then by Theorem 1.3(3), it does not have another representation as a sum of two d-th powers. In view of Theorems 1.6, 1.7, and 3.4, we have an immediate corollary. We choose even representatives (from Theorem 3.3), and they also happen to be symmetric (we have taken $y \mapsto \zeta_{16} y$ in (3-9)).

Corollary 5.3. (i) *The form $p \in H_8(\mathbb{C}^2)$ has exactly two different representations as a sum of two fourth powers of binary forms if and only if, after a linear change, it is $x^8 + 4x^6y^2 - 12x^4y^4 + 4x^2y^6 + y^8$, $x^8 - 68x^6y^2 + 6x^4y^4 - 68x^2y^6 + y^8$, or $x^8 - 140x^6y^2 + 294x^4y^4 - 140x^2y^4 + y^8$.*

(ii) *The form $p \in H_8(\mathbb{C}^2)$ has three different representations as a sum of two fourth powers of binary forms if and only if, after a linear change, it is $x^8 - 7\sqrt{2}(1+i)x^6y^2 - 7\sqrt{2}(1+i)x^2y^6 + y^8$.*

(iii) *The form $p \in H_{10}(\mathbb{C}^2)$ has two different representations as a sum of two fifth powers of binary forms if and only if, after a linear change, it is $x^{10} - 75x^8y^2 + 90x^6y^4 + 90x^4y^6 - 75x^2y^8 + y^{10}$.*

Open questions. We have already noted that there exist $k \geq 2$ and $d \geq 6$ so that $\Phi_k(d) > \Phi_{k+1}(d)$. Gundersen [1998] found three meromorphic (not rational) functions $g_j(t)$ so that $g_1^6 + g_2^6 + g_3^6 = 1$. It is unknown whether this can be achieved with rational functions. If so, a $\mathcal{W}_k(4, 6)$-set would exist for some $k > 2$.

In case $m = rs$, an m-synching on m can be viewed as r coordinated s-synchings. We have not found a useful instance in this when $r = s = 2$, although (2-15) shows what can happen with $(r, s) = (2, 3)$. We hope that improvements on the bounds may come from careful investigations in this direction.

Another natural question is to restrict our attention to forms with coefficients in a fixed subfield of $\mathbb{C}$, such as $\mathbb{Q}$ or $\mathbb{R}$. Real forms with even degree also lead to a discussion of "signatures". From the Diophantine point of view, the equations $A^4+B^4+C^4=D^4$ and $A^4+B^4=C^4+D^4$ are completely different questions. In this point of view, the real equation (1-7) is "(3, 1)". In 1772, Euler gave a famous (2, 2) "septic" example of a $\mathcal{W}_7(4,4)$-set [Dickson 1966, pp. 644–646; Hardy and Wright 1979, (13.7.11); Lander 1968]. So far as we have been able to determine there are no known real solutions of this kind of smaller degree, nor proofs that they cannot exist.

Theorem 1.4 shows that (1-1) is "universal" in presenting all $\mathcal{W}_k(3,2)$-sets; that is, projectively, all families come from the substitution $(x, y) \mapsto (g, h)$. Are the solutions given in Theorems 1.5, 1.6, and 1.7 also universal in this sense? The answers are "no" for $d = 3, 4$. These families are all linearly dependent. For $d = 3$, the family in (2-17) is linearly independent, as are the parametrizations of the Euler–Binet solutions to $x^3+y^3=u^3+v^3$ (see, e.g, [Hardy and Wright 1979, (13.7.8)]), when viewed as elements of $\mathbb{C}[a, b, \lambda]$. For $d = 4$, it can be checked that the Euler septics are also linearly independent. The case $d = 5$ is open. Can the $\mathcal{W}_k(4, d)$-sets themselves be parametrized for $k \geq 3$?

Finally, we note that the intricate calculations of Sections 3 and 4 suggest that new methods will be needed to study $\mathcal{W}_k(r, d)$-sets for $r > 4$ or $k > 2$. In their absence, we make a few remarks about the growth of $\Phi_k(d)$ for fixed k as $d \to \infty$. By Theorems 1.1 and 1.3, we have $\Phi_1(d) = d+2$ and $\Phi_2(d) \leq \lfloor d/2 \rfloor + 2$ for $d \geq 4$, with equality if $4 \leq d \leq 7$ and one exceptional value at $d = 14$. Furthermore, if $d = rk$ for integral r, then taking by setting $\ell = k$, $\ell' = m = r$, and $t = 1$ in (2-4), we see that $\Phi_k(d) \leq 1+r+k = d/k+k+1$. Based on this thin reed of information, we make the following conjecture.

Conjecture 5.4. *For fixed* k, $\Phi_k(d) = d/k + k + 1 + \mathbb{O}(1)$ *as* $d \to \infty$.

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STABILITY OF THE EXISTENCE OF A PSEUDO-EINSTEIN CONTACT FORM

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A pseudo-Einstein contact form plays a crucial role in defining some global invariants of closed strictly pseudoconvex CR manifolds. In this paper, we prove that the existence of a pseudo-Einstein contact form is preserved under deformations as a real hypersurface in a fixed complex manifold of complex dimension at least three.

1. Introduction

A pseudo-Einstein contact form, which was first introduced by Lee [1988], is necessary for defining some global CR invariants: the total Q-prime curvature [Case and Yang 2013; Hirachi 2014] and the boundary term of the renormalized Gauss–Bonnet–Chern formula [Marugame 2016]. When we consider the variation of such an invariant, the question arises whether the existence of a pseudo-Einstein contact form is preserved under deformations of a CR structure. In this paper, we will show this stability for deformations as a real hypersurface in a fixed complex manifold of complex dimension at least three. More precisely, we will prove:

Theorem 1.1. *Let Ω be a relatively compact strictly pseudoconvex domain in a complex manifold X of complex dimension at least three. Assume that its boundary $M = \partial\Omega$ admits a pseudo-Einstein contact form. Then there exists a neighborhood U of M in X such that its canonical bundle has a flat Hermitian metric.*

The stability for wiggles follows from this theorem and a necessary and sufficient condition to the existence of a pseudo-Einstein contact form (Proposition 2.1).

Corollary 1.2. *Let Ω, X, M, and U be as in Theorem 1.1. Then any strictly pseudoconvex real hypersurface M' in U admits a pseudo-Einstein contact form.*

Note that this stability may have been already known when an ambient complex manifold is a Stein manifold of dimension at least three; see Remark 4.2.

Here we give an outline of a proof of Theorem 1.1. Take a tubular neighborhood U of M in X. The existence of a pseudo-Einstein contact form on M implies that

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there is a flat Hermitian metric on the canonical bundle of $U \cap \Omega$ if we take U sufficiently small. By using the Bott–Chern class, we will show that K_U admits a flat Hermitian metric if the morphism

$$H^1(U, \mathscr{O}) \to H^1(U \cap \Omega, \mathscr{O}) \tag{1-1}$$

induced by the inclusion is injective (Lemma 3.1). On the other hand, a result of Andreotti and Grauert [1962] yields that (1-1) is an isomorphism; here we use the assumption that the complex dimension of X is at least three. A proof of this fact will be given in Section 4.

Before the end of the introduction, we remark a relation between our result and the Lee conjecture. Lee [1988, Proposition D] has proved that the first Chern class $c_1(T^{1,0}M)$ of $T^{1,0}M$ is equal to zero in $H^2(M, \mathbb{R})$ if M admits a pseudo-Einstein contact form, and conjectured that the converse also holds if M is closed; this is called the *Lee conjecture*. There are some affirmative results on this conjecture [Lee 1988; Dragomir 1994; Cao and Chang 2007; Chen et al. 2012; Chang et al. 2014], but it is still open. (Note that we need an extra assumption on the pseudo-Hermitian torsion in [Chang et al. 2014, Theorem 1.1], which has been pointed out in the erratum [Chang et al. 2016].) The stability of the existence of a pseudo-Einstein contact form follows from the Lee conjecture since the first Chern class of a CR structure is invariant under deformations of a CR structure. In other words, Corollary 1.2 can be considered as one of affirmative results on the Lee conjecture.

2. Preliminaries

We first recall some facts on strictly pseudoconvex domains; see [Grauert et al. 1994, Chapter V] for details. In what follows, the word "domain" means a relatively compact connected open set. Let Ω be a domain with smooth boundary M in an $(n+1)$-dimensional complex manifold X. A *defining function* of Ω is a smooth function on X such that $\Omega = \rho^{-1}((-\infty, 0))$, $M = \rho^{-1}(0)$, and $d\rho \neq 0$ on M. A domain Ω is said to be *strictly pseudoconvex* if we can take a defining function of Ω that is strictly plurisubharmonic near M. It is known that any strictly pseudoconvex domain Ω is holomorphically convex, and consequently, there exist a Stein space Z and a proper surjective holomorphic map $\varphi : \Omega \to Z$ having some good properties, called the *Remmert reduction* of Ω. In our setting, φ is described as follows. A compact analytic subset E of positive dimension at every point in Ω is called a *maximal compact analytic subset* of Ω if it is maximal among such subsets with respect to inclusion relations; this E is determined uniquely by Ω. The map φ contracts each connected component of E to a point, and induces a biholomorphism $\Omega \setminus E \to Z \setminus \varphi(E)$. In particular, Z has at most finite normal isolated singularities.

We next give a brief introduction to CR manifolds. Let M be a $(2n+1)$-dimensional manifold without boundary. A *CR structure* is an n-dimensional complex subbundle $T^{1,0}M$ of the complexified tangent bundle $TM \otimes \mathbb{C}$ satisfying the conditions

$$T^{1,0}M \cap T^{0,1}M = 0, \qquad [\Gamma(T^{1,0}M), \Gamma(T^{1,0}M)] \subset \Gamma(T^{1,0}M),$$

where $T^{0,1}M$ is the complex conjugate of $T^{1,0}M$ in $TM \otimes \mathbb{C}$. A typical example of a CR manifold is a real hypersurface M in a complex manifold X; it has the natural CR structure

$$T^{1,0}M = T^{1,0}X \cap (TM \otimes \mathbb{C}).$$

A CR structure $T^{1,0}M$ is said to be *strictly pseudoconvex* if there exists a nowhere-vanishing real one-form θ on M such that θ annihilates $T^{1,0}M$ and

$$-\sqrt{-1}d\theta(Z, \bar{Z}) > 0, \qquad 0 \neq Z \in T^{1,0}M;$$

we call such a one-form a *contact form*. Note that the boundary of a strictly pseudoconvex domain is a strictly pseudoconvex CR manifold with respect to its natural CR structure.

It is known that there is a canonical one-to-one correspondence between contact forms on M and Hermitian metrics on the canonical bundle of M. A contact form is said to be *pseudo-Einstein* if the corresponding Hermitian metric is flat; see [Hirachi et al. 2017, §2.3] for details. Note that this definition coincides with that given by Lee [1988] if $n \geq 2$. In this paper, however, we do not use this definition but the following necessary and sufficient condition to the existence of a pseudo-Einstein contact form in terms of a Hermitian metric on the canonical bundle of the ambient complex manifold.

Proposition 2.1 [Hirachi et al. 2017, Proposition 2.6]. *Let M be a strictly pseudoconvex real hypersurface in a complex manifold X. Then M admits a pseudo-Einstein contact form if and only if the canonical bundle K_X of X has a Hermitian metric that is flat on the pseudoconvex side near M.*

This proposition implies that any strictly pseudoconvex real hypersurface in a complex manifold X admits a pseudo-Einstein contact form if K_X has a flat Hermitian metric. Thus, we can derive Corollary 1.2 from Theorem 1.1. In the remainder of this paper, we will prove Theorem 1.1.

3. Bott–Chern class and the existence of a flat Hermitian metric

Let X be a complex manifold. The *real Bott–Chern cohomology* $H^{1,1}_{\mathrm{BC}}(X, \mathbb{R})$ *of bidegree* $(1,1)$ is defined by

$$H^{1,1}_{\mathrm{BC}}(X, \mathbb{R}) = \{d\text{-closed real } (1,1)\text{-forms on } X\}/\{\sqrt{-1}\partial\bar{\partial}\psi \mid \psi \in C^\infty(X, \mathbb{R})\}.$$

Let $f: Y \to X$ be a holomorphic map between complex manifolds. Then it defines the natural morphism $f^*: H^{1,1}_{\mathrm{BC}}(X, \mathbb{R}) \to H^{1,1}_{\mathrm{BC}}(Y, \mathbb{R})$ induced by the pullback of $(1, 1)$-forms.

For a holomorphic line bundle L over X, the *first Bott–Chern class* $c_1^{\mathrm{BC}}(L) \in H^{1,1}_{\mathrm{BC}}(X, \mathbb{R})$ is defined as follows. Take a Hermitian metric h of L. Then the curvature $(\sqrt{-1}/2\pi)\Theta_h = -(\sqrt{-1}/2\pi)\partial\bar{\partial}\log h$ is a d-closed real $(1, 1)$-form on X, and defines an element of $H^{1,1}_{\mathrm{BC}}(X, \mathbb{R})$. This cohomology class is independent of the choice of h, denoted by $c_1^{\mathrm{BC}}(L)$. From the definition, $c_1^{\mathrm{BC}}(L) = 0$ if and only if L admits a flat Hermitian metric. Note that c_1^{BC} is natural; that is, $f^*c_1^{\mathrm{BC}}(L) = c_1^{\mathrm{BC}}(f^*L)$ for any holomorphic map $f: Y \to X$.

The cohomology $H^{1,1}_{\mathrm{BC}}(X, \mathbb{R})$ has also a sheaf-theoretic interpretation. Let $\mathscr{A}^{p,q}$ be the sheaf of smooth (p, q)-forms and $\mathscr{P}$ be that of pluriharmonic functions. Then there exists the exact sequence of sheaves [Bigolin 1969, Teorema (2.1)]

$$0 \to \mathscr{P} \to \mathscr{A}^{0,0}_{\mathbb{R}} \xrightarrow{\sqrt{-1}\partial\bar{\partial}} \mathscr{A}^{1,1}_{\mathbb{R}} \xrightarrow{d} (\mathscr{A}^{2,1} \oplus \mathscr{A}^{1,2})_{\mathbb{R}}.$$

Here the subscript $\mathbb{R}$ means the subsheaf consisting of real forms. This exact sequence implies that $H^1(X, \mathscr{P})$ is isomorphic to $H^{1,1}_{\mathrm{BC}}(X, \mathbb{R})$. Note that a holomorphic map $f: Y \to X$ induces a natural morphism $f^*: H^1(X, \mathscr{P}) \to H^1(Y, \mathscr{P})$, which is compatible with $f^*: H^{1,1}_{\mathrm{BC}}(X, \mathbb{R}) \to H^{1,1}_{\mathrm{BC}}(Y, \mathbb{R})$ defined above.

This formulation gives a sufficient condition to the existence of a flat Hermitian metric.

Lemma 3.1. *Let X and Y be complex manifolds and $f: Y \to X$ be a holomorphic map. Assume that f induces injective morphisms $H^1(X, \mathbb{O}) \hookrightarrow H^1(Y, \mathbb{O})$ and $H^2(X, \mathbb{R}) \hookrightarrow H^2(Y, \mathbb{R})$, and a surjective morphism $H^1(X, \mathbb{R}) \twoheadrightarrow H^1(Y, \mathbb{R})$. Then, for any holomorphic line bundle L over X, it admits a flat Hermitian metric if so does f^*L.*

Proof. Assume that f^*L has a flat Hermitian metric. As we noted above, this is equivalent to $f^*c_1^{\mathrm{BC}}(L) = c_1^{\mathrm{BC}}(f^*L) = 0$. Hence, it is enough to prove the injectivity of $f^*: H^1(X, \mathscr{P}) \to H^1(Y, \mathscr{P})$. Consider the exact sequence of sheaves

$$0 \to \mathbb{R} \xrightarrow{\sqrt{-1}} \mathbb{O} \xrightarrow{\mathrm{Re}} \mathscr{P} \to 0.$$

This induces the following commutative diagram with exact rows:

$$\begin{array}{ccccccc}
H^1(X, \mathbb{R}) & \longrightarrow & H^1(X, \mathbb{O}) & \longrightarrow & H^1(X, \mathscr{P}) & \longrightarrow & H^2(X, \mathbb{R}) \\
\downarrow & & \downarrow & & \downarrow & & \downarrow \\
H^1(Y, \mathbb{R}) & \longrightarrow & H^1(Y, \mathbb{O}) & \longrightarrow & H^1(Y, \mathscr{P}) & \longrightarrow & H^2(Y, \mathbb{R})
\end{array}$$

The injectivity of $H^1(X, \mathscr{P}) \to H^1(Y, \mathscr{P})$ follows from an easy diagram chasing. $\square$

4. Proof of Theorem 1.1

Let X, Ω, and M be as in Theorem 1.1. We first reduce the problem on X to that on a Stein space. Take a defining function ρ of Ω that is strictly plurisubharmonic near the boundary. Without loss of generality, we may assume that $\rho : X \to \mathbb{R}$ is proper. Then, for sufficiently small $\delta > 0$, there exists a diffeomorphism

$$\chi : (-2\delta, 2\delta) \times M \to \rho^{-1}((-2\delta, 2\delta))$$

such that $\chi(0, p) = p$ and $\rho(\chi(t, p)) = t$. Replacing δ with a smaller one if necessary, we may assume that ρ is strictly plurisubharmonic on $\rho^{-1}((-2\delta, 2\delta))$. In particular, $\Omega' = \rho^{-1}((-\infty, \delta))$ is a strictly pseudoconvex domain in X containing Ω. Consider the Remmert reduction $\varphi : \Omega' \to Z$. From the strict plurisubharmonicity of ρ, it follows that the maximal compact analytic subset of Ω' cannot intersect with $\rho^{-1}((-\delta, \delta))$; in particular, φ is a biholomorphism on $\rho^{-1}((-\delta, \delta))$. Without loss of generality, we may assume that ρ descends to a smooth function $Z \to \mathbb{R}$; use the same letter ρ for abbreviation. It is sufficient to show the existence of a neighborhood $U \subset \rho^{-1}((-\delta, \delta))$ of $M = \rho^{-1}(0)$ such that K_U has a flat Hermitian metric. To this end, we need to construct a "good" exhaustion function on Z.

Lemma 4.1. *Fix $0 < \alpha < \delta$. There exists a smooth nonnegative strictly plurisubharmonic exhaustion function ϕ on Z satisfying the following conditions*:

- *$\phi^{-1}(0)$ coincides with the singular set A of Z,*
- *ϕ is of the form*

$$\phi(p) = \frac{\rho(p)}{\delta(\delta - \rho(p))} + K$$

  on $\rho^{-1}((-\alpha, \delta))$ for a constant $K > 0$,
- *$\phi < K$ on $\rho^{-1}((-\infty, -\alpha])$.*

The proof of this lemma is slightly complicated, and so will be given later. Now, we complete the proof of Theorem 1.1 using Lemmas 3.1 and 4.1. Note that our proof is similar in spirit to the proof of [Yau 1981, Theorem B].

Proof of Theorem 1.1. Set

$$\Omega(a, b) = \{K + a < \phi < K + b\}$$

for $-\infty \le a < b$. Note that $\phi^{-1}(K) = M$ and $\Omega(-K, b) = \Omega(-\infty, b) \setminus A$. It is enough to prove that the canonical bundle of $\Omega(-\epsilon, \epsilon)$ admits a flat Hermitian metric for some $\epsilon > 0$ if M has a pseudo-Einstein contact form. The existence of a pseudo-Einstein contact form on M implies that the canonical bundle of $\Omega(-\epsilon, 0)$ has a flat Hermitian metric for sufficiently small $\epsilon > 0$ by Proposition 2.1. We may also assume, by making ϵ small if necessary, the inclusion $\Omega(-\epsilon, 0) \hookrightarrow \Omega(-\epsilon, \epsilon)$ induces isomorphisms

$$H^1(\Omega(-\epsilon, \epsilon), \mathbb{R}) \xrightarrow{\simeq} H^1(\Omega(-\epsilon, 0), \mathbb{R}),$$
$$H^2(\Omega(-\epsilon, \epsilon), \mathbb{R}) \xrightarrow{\simeq} H^2(\Omega(-\epsilon, 0), \mathbb{R}).$$

According to Lemma 3.1, it suffices to prove that

$$H^1(\Omega(-\epsilon, \epsilon), \mathbb{O}) \to H^1(\Omega(-\epsilon, 0), \mathbb{O})$$

is also an isomorphism. Consider the following commutative diagram induced by inclusions:

$$\begin{tikzcd} H^1(\Omega(-K, \epsilon), \mathbb{O}) \arrow[r] \arrow[d] & H^1(\Omega(-\epsilon, \epsilon), \mathbb{O}) \arrow[d] \\ H^1(\Omega(-K, 0), \mathbb{O}) \arrow[r] & H^1(\Omega(-\epsilon, 0), \mathbb{O}) \end{tikzcd}$$

From [Andreotti and Grauert 1962, Théorème 15], it follows that each row is an isomorphism; here we use the assumption that the complex dimension of X is at least three. Hence, it is sufficient to show the left column is an isomorphism. Since $\Omega(-\infty, \epsilon)$ and $\Omega(-\infty, 0)$ are Stein spaces, we obtain the following commutative diagram whose rows are isomorphisms:

$$\begin{tikzcd} H^1(\Omega(-K, \epsilon), \mathbb{O}) \arrow[r, "\simeq"] \arrow[d] & H^2_A(\Omega(-\infty, \epsilon), \mathbb{O}) \arrow[d] \\ H^1(\Omega(-K, 0), \mathbb{O}) \arrow[r, "\simeq"] & H^2_A(\Omega(-\infty, 0), \mathbb{O}) \end{tikzcd}$$

On the other hand, the right column of the above diagram is also an isomorphism by the excision property of the local cohomology. This completes the proof. □

What is left is to show Lemma 4.1, the existence of a "good" exhaustion function ϕ on Z.

Proof of Lemma 4.1. As noted in Section 2, the singular set A of Z is finite, given by $A = \{p_1, \dots, p_k\} \subset Z$. We first construct a smooth nonnegative strictly plurisubharmonic exhaustion function ψ on Z with $\psi^{-1}(0) = A$. There exists a proper holomorphic regular embedding $f : Z \to \mathbb{C}^N$ for sufficiently large N [Narasimhan 1960, Theorem 6]; in what follows, we identify Z with the image of f. Then $\psi_0 = |z|^2 + \sum_{j=1}^k \log|z - p_j|^2$ is a strictly plurisubharmonic exhaustion function on $\mathbb{C}^N$ with $\psi_0^{-1}(-\infty) = A$. Hence, $\psi = \exp\psi_0 = \exp(|z|^2)\prod_{j=1}^k |z - p_j|^2$ is a smooth nonnegative strictly plurisubharmonic exhaustion function on $\mathbb{C}^N$ with $\psi^{-1}(0) = A$.

Choose $\beta \in \mathbb{R}$ with $\alpha < \beta < \delta$, and take a smooth function $\lambda : \mathbb{R} \to [0, 1]$ on $\mathbb{R}$ such that $\lambda \equiv 1$ on $(-\infty, -\beta)$ and $\lambda \equiv 0$ on $(-\alpha, \infty)$. Then the function

$$\phi_1(p) = \lambda(\rho(p))\psi(p)$$

is strictly plurisubharmonic on $\rho^{-1}((-\infty, -\beta))$ and identically zero on $\rho^{-1}((-\alpha, \delta))$.

Next, take a nonnegative smooth function g_1 on $\mathbb{R}$ with

$$\operatorname{supp} g_1 \subset ((2\delta)^{-1}, (\beta+\delta)^{-1}), \qquad \int_{\mathbb{R}} g_1(t)dt = 1,$$

and set

$$g_2(t) = \int_0^t \int_0^s g_1(r)\, dr\, ds.$$

This g_2 is a nonnegative and nondecreasing convex smooth function on $\mathbb{R}$ and vanishes identically on $(-\infty, (2\delta)^{-1}]$, and

$$g_2(t) = t - \delta^{-1} + g_2(\delta^{-1}) > 0$$

on a neighborhood of $[(\beta+\delta)^{-1}, \infty)$. The function

$$\phi_2(p) = g_2\left(\frac{1}{\delta - \rho(p)}\right)$$

vanishes identically on $\rho^{-1}((-\infty, -\delta])$ and is plurisubharmonic on $\rho^{-1}((-\delta, \delta))$, and

$$\phi_2(p) = \frac{\rho(p)}{\delta(\delta - \rho(p))} + g_2(\delta^{-1}) > 0$$

on a neighborhood of $\rho^{-1}([-\beta, \delta))$. Hence, for any $\epsilon > 0$, the sum $\phi = \epsilon\phi_1 + \phi_2$ is a nonnegative smooth exhaustion function on Z such that it is strictly plurisubharmonic on $\rho^{-1}((-\infty, -\beta) \cup (-\alpha, \delta))$, and satisfies $\phi^{-1}(0) = A$. Since ϕ_2 is strictly plurisubharmonic on the compact set $\rho^{-1}([-\beta, -\alpha])$, the function ϕ is also strictly plurisubharmonic there for sufficiently small ϵ. Replacing ϵ by a smaller one, we also have $\phi < g(\delta^{-1})$ on $\rho^{-1}((-\infty, -\alpha])$. □

Remark 4.2. Cao and Chang [2007, Main Theorem (2)] have stated that if M is the boundary of a strictly pseudoconvex domain in a Stein manifold of complex dimension at least three, then M admits a pseudo-Einstein contact form. However, as the author has pointed out in [Takeuchi 2018, Remark 4.3], there exists such an M satisfying $c_1(T^{1,0}M) \neq 0$ in $H^2(M, \mathbb{R})$; in particular, M has no pseudo-Einstein contact form. Here, we give a short proof of a corrected statement: "if M is the boundary of a strictly pseudoconvex domain in a Stein manifold of complex dimension at least three, and satisfies $c_1(T^{1,0}M) = 0$ in $H^2(M, \mathbb{R})$, then M admits a pseudo-Einstein contact form". A discussion in [Lee 1988, §6] gives that a closed strictly pseudoconvex CR manifold $(M, T^{1,0}M)$ of dimension greater than three admits a pseudo-Einstein contact form if $c_1(T^{1,0}M) = 0$ in $H^2(M, \mathbb{R})$ and the Kohn–Rossi cohomology $H^{0,1}(M)$ of bidegree (0, 1) vanishes. On the other hand, a result of Yau [1981, Theorem B] yields that $H^{0,1}(M) = 0$ if M is as in the statement. Hence, M admits a pseudo-Einstein contact form.

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