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RIPS CONSTRUCTION WITHOUT UNIQUE PRODUCT

GOULNARA ARZHANTSEVA AND MARKUS STEENBOCK

Given a finitely presented group Q, we produce a short exact sequence $1 \to N \hookrightarrow G \twoheadrightarrow Q \to 1$ such that G is a torsion-free hyperbolic group without the unique product property and N is without the unique product property and has Kazhdan's Property (T). Varying Q yields a wide diversity of concrete examples of hyperbolic groups without the unique product property. We also note, as an application of Ol'shanskiĭ's construction of torsion-free Tarski monsters, the existence of torsion-free Tarski monster groups without the unique product property.

1. Introduction

A group G has the *unique product property*, or is said to be a *unique product group*, whenever for all pairs of nonempty finite subsets A and B of G the set of products AB has an element $g \in G$ with a unique representation of the form $g = ab$ with $a \in A$ and $b \in B$. Unique product groups are torsion-free. They satisfy the Kaplansky zero-divisor conjecture [1957; 1970], which states that the group ring of a torsion-free group over an integral domain has no zero-divisors. Rips and Segev [1987] gave the first examples of torsion-free groups without the unique product property. In [Steenbock 2015], the second author proved that the (generalized) Rips–Segev groups are hyperbolic, and gave an uncountable family of nonunique product groups. Other examples of torsion-free groups without the unique product property are in [Promislow 1988; Carter 2014; Soelberg 2018].

Our goal is to provide new concrete examples of nonunique product groups with diverse algebraic and geometric properties. In fact, we produce a variety of strongly nonamenable examples.

Theorem 1.1. *Let Q be a finitely generated group. Then there exists a short exact sequence $1 \to N \hookrightarrow G \twoheadrightarrow Q \to 1$ such that*

- *G is a torsion-free group without the unique product property which is a direct limit of hyperbolic groups,*

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- *N is a finitely generated subgroup of G with Kazhdan's Property* (*T*) *and without the unique product property.*

If, *in addition*, *Q is finitely presented*, *then G is hyperbolic.*

Theorem 1.1 extends the result on Rips short exact sequence with Kazhdan's Property (T) kernel from [Ollivier and Wise 2007]. An alternative construction is in [Belegradek and Osin 2008].

Varying Q in Theorem 1.1 yields many new groups without the unique product property that have various algebraic and algorithmic properties, see Section 4. The examples obtained using Theorem 1.1 contrast the torsion-free groups without the unique product property from [Promislow 1988; Carter 2014; Soelberg 2018], which are infinite groups with the Haagerup property (= a-T-menable groups, in Gromov's terminology, see [Cherix et al. 2001]), and, hence, groups which do not have Kazhdan's Property (T). Indeed, the group in [Promislow 1988] is solvable, hence, a-T-menable; groups in [Carter 2014] are a-T-menable as they have $\mathbb{Z}^k \times \mathbb{F}_m$ as a finite index subgroup; the group in [Soelberg 2018] is a-T-menable as it has a central extension of $\mathbb{Z}$ by $\mathbb{Z}^2$ as a finite index subgroup, see [Soelberg 2018, p. 24].

2. Small cancellation theory over hyperbolic groups

A useful way to get novel nonunique product groups is to take quotients of free products of hyperbolic nonunique product groups with other suitably chosen groups. We will apply the following result:

Theorem 2.1 [Ol'shanskiĭ 1993, Theorem 2]. *Let $G = H_1 * H_2$ be the free product of two nonelementary torsion-free hyperbolic groups and $M \subseteq H_1$ be a finite subset. Then G has a nonelementary torsion-free hyperbolic quotient $\overline{G}$ such that the canonical projection $G \twoheadrightarrow \overline{G}$ is injective on M and restricts to a surjection $H_2 \twoheadrightarrow \overline{G}$.*

Theorem 2.1, together with [Steenbock 2015, Theorem 2], yields first examples of Kazhdan's Property (T) groups without the unique product property.

Corollary 2.2. *There are torsion-free hyperbolic groups with Kazhdan's Property* (*T*) *and without the unique product property.*

Proof. Take for H_1 a torsion-free hyperbolic group without the unique product property such that the unique product property fails for the sets A and B, see [Steenbock 2015]. Take for H_2 a hyperbolic group with Property (T) (e.g., a discrete subgroup of finite covolume in $\mathrm{Sp}(n, 1)$) and for M a finite subset of H_1 containing A, B, and AB. By Theorem 2.1, there exists a torsion-free hyperbolic quotient $\overline{G}$ of $H_1 * H_2$ with Property (T) such that M injects into this quotient. It follows that $\overline{G}$ is without the unique product property. □

Remark 2.3. The group H_1 can be generated by two letters, say, a_1 and a_2, and it can be defined using a finite set of relators that we denote by $\mathcal{RS}$. A procedure to obtain such a set of relators follows from [Rips and Segev 1987; Steenbock 2015]. Thus, H_1 can be given by an explicit presentation $H_1 = \langle a_1, a_2 \mid \mathcal{RS} \rangle$.

Let $H_2 = \langle Y \mid \mathcal{R}_T \rangle$, where $\mathcal{R}_T$ is a fixed finite set of relators. An explicit presentation of an infinite torsion hyperbolic group with Property (T) with 16 relators is given, for example, in [Caprace 2018]. To get a required torsion-free H_2, one can then take a subgroup of sufficiently large index in this Property (T) group. A finite presentation of such H_2 can be obtained from the group presentation given in [Caprace 2018], using Schreier's method.

Let g and h be hyperbolic elements of H_2 that do not generate an elementary subgroup. Let q, s, and t denote natural numbers. Let

$$\mathcal{R}_{q,s,t} := \{a_1^{-1} g^q h^s g^q h^{2s} \cdots g^q h^{ts},\ a_2^{-1} g^q h^{(t+1)s} g^q h^{(t+2)s} \cdots g^s h^{2ts}\}.$$

Following [Ol'shanskiĭ 1993], there are $s_0 > 0$, $t_0 > 0$, and $q_0 > 0$ such that

$$\overline{G} := \langle a_1, a_2, Y \mid \mathcal{RS} \sqcup \mathcal{R}_T \sqcup \mathcal{R}_{q_0,s_0,t_0} \rangle$$

defines a group, as required by Corollary 2.2. The numbers q_0, s_0, and t_0 depend only on A and B, the hyperbolicity constant and the size of the balls in the Cayley graph of H_2.

Moreover, we obtain torsion-free Tarski monster groups without the unique product property. These are the first examples of torsion-free groups without the unique product property, all of whose proper subgroups are unique product groups.

Corollary 2.4. *There are torsion-free Kazhdan's Property* (*T*) *groups G without the unique product property such that all proper subgroups of G are cyclic. Moreover, these groups have explicit recursive presentations.*

Proof. Let G be a noncyclic torsion-free hyperbolic group, and let M be a finite subset of G. It follows from [Ol'shanskiĭ 1993, Theorem 2] that there exists a nonabelian torsion-free quotient $\widetilde{G}$ such that all proper subgroups of $\widetilde{G}$ are cyclic, and such that $G \twoheadrightarrow \widetilde{G}$ is injective on M [Ol'shanskiĭ 1993, Corollary 1]. Moreover, an explicit presentation of G yields an explicit recursive presentation of $\widetilde{G}$. Applied to a finite subset containing A, B, and AB in a torsion-free hyperbolic group G without the unique product property for A and B from [Steenbock 2015], this immediately yields Tarski monster groups without the unique product property, that have explicit recursive presentations. □

3. Rips construction via small cancellation over hyperbolic groups

We now prove Theorem 1.1. The idea is to adapt [Belegradek and Osin 2008] by using Theorem 2.1 as in Remark 2.3. Recall that $H_1 := \langle a_1, a_2 \mid \mathcal{RS} \rangle$ is our torsion-free hyperbolic group without the unique product property for sets A and B (see [Steenbock 2015], we set $a_2 := b$) and M is a finite subset of H_1 containing A, B, and AB. Recall that $H_2 := \langle y_1, \dots, y_l \mid \mathcal{R}_T \rangle$ is a torsion-free hyperbolic group with Property (T).

Let $Q := \langle x_1, \dots, x_m \mid r_1, \dots, r_n, \dots \rangle$ be a finitely generated group. We produce the required G as a suitable quotient of the free product $H_1 * H_2 * \langle x_1, \dots, x_m \rangle$.

Let $g, h \in H_2$ be hyperbolic elements that do not generate an elementary subgroup. Let $s, t, q, q_1, \dots, q_i, \dots$ denote natural numbers, let $\bar{q} = \{q, q_1, \dots\}$, and let $\mathcal{R}_{\bar{q},s,t}$ be the set of words:

$$a_1^{-1} g^q h^s g^q h^{2s} \cdots g^q h^{ts} \text{ and } a_2^{-1} g^q h^{(t+1)s} g^q h^{(t+2)s} \cdots g^q h^{2ts}, \tag{1}$$

$$\begin{aligned} x_j a_1 x_j^{-1} g^q h^{((j+1)t+1)s} g^q h^{((j+1)t+2)s} \cdots g^q h^{(j+2)ts} \quad & \forall\, 1 \leqslant j \leqslant m, \\ x_j a_2 x_j^{-1} g^q h^{((j+m+1)t+1)s} g^q h^{((j+m+1)t+2)s} \cdots g^q h^{(j+m+2)ts} \quad & \forall 1 \leqslant j \leqslant m, \\ x_j^{-1} a_1 x_j g^q h^{((j+2m+1)t+1)s} g^q h^{((j+2m+1)t+2)s} \cdots g^q h^{(j+2m+2)ts} \quad & \forall\, 1 \leqslant j \leqslant m, \\ x_j^{-1} a_2 x_j g^q h^{((j+3m+1)t+1)s} g^q h^{((j+3m+1)t+2)s} \cdots g^q h^{(j+3m+2)ts} \quad & \forall\, 1 \leqslant j \leqslant m, \end{aligned} \tag{2}$$

$$\begin{aligned} & x_j y_k x_j^{-1} g^q h^{((j+(k-1)m+4m+1)t+1)s} g^q h^{((j+(k-1)m+4m+1)t+2)s} \\ & \qquad \cdots g^q h^{(j+(k-1)m+4m+2)ts} \quad \forall\, 1 \leqslant j \leqslant m,\ \forall\, 1 \leqslant k \leqslant l, \\ & x_j^{-1} y_k x_j g^q h^{((j+(k+l+3)m+1)t+1)s} g^q h^{((j+(k+l+3)m+1)t+2)s} \\ & \qquad \cdots g^q h^{(j+(k+l+3)m+2)ts} \quad \forall\, 1 \leqslant j \leqslant m,\ \forall\, 1 \leqslant k \leqslant l, \end{aligned} \tag{3}$$

$$r_i g^{q_i} h^s g^{q_i} h^{s+1} \cdots g^{q_i} h^{ts} \quad \forall\, i = 1, 2, \dots. \tag{4}$$

Following [Ol'shanskiĭ 1993, Lemma 4.2], there exist $s_0 > 0$, $t_0 > 0$, and $\bar{q}_0$ such that $\mathcal{R}_{\bar{q}_0,s_0,t_0}$ satisfies the C_1-condition of [Ol'shanskiĭ 1993, Section 4] with respect to $H_1 * H_2 * \langle x_1, \dots, x_m \rangle$. It follows from the proof of Theorem 2 of [Ol'shanskiĭ 1993] that the quotient

$$G := \langle a_1, a_2, y_1, \dots, y_l, x_1, \dots, x_m \mid \mathcal{RS} \sqcup \mathcal{R}_T \sqcup \mathcal{R}_{\bar{q}_0,s_0,t_0} \rangle$$

is a direct limit of torsion-free hyperbolic groups, that G is torsion-free, and that M injects into G. In particular, G does not have the unique product property.

Let N be the subgroup generated by $a_1, a_2, y_1, \dots, y_n$. By the relators (2) and (3), N is normal. By the relators (4), the map defined by sending the generators x_i onto themselves, and the a_1, a_2, y_k onto 1 is a projection onto Q, the kernel of which is the group N.

As M consists of words in a_1 and a_2, the set M injects into N as well, so that N does not have the unique product property. By the relators (1), N is a quotient of H_2, hence N has Property (T).

This finishes the proof of Theorem 1.1 and gives presentations of the groups G.

Remark 3.1. If Q is the trivial group, we recover Corollary 2.2 and the conclusion of Remark 2.3.

4. More examples of torsion-free groups without unique product

We now vary the quotient group Q. All examples of groups G below are not isomorphic to a free product. The following results are immediate generalizations of [Rips 1982]:

Proposition 4.1. *For each of the following, there exists a torsion-free hyperbolic group G without the unique product property and such that*:

1. *G has unsolvable generalized word problem*;
2. *there are finitely generated subgroups P_1 and P_2 of G such that $P_1 \cap P_2$ is not finitely generated*;
3. *there is a finitely generated, but not finitely presented, subgroup of G*;
4. *for any $r \geqslant 3$, there is an infinite strictly increasing sequence of r-generated subgroups of G.*

More algorithmic properties in the context of Rips construction are investigated in [Baumslag et al. 1994]. Applied to our situation they yield the following:

Proposition 4.2. *There is no algorithm to determine each of the following*:

1. *the rank of a torsion-free hyperbolic group without unique product*;
2. *whether an arbitrary finitely generated subgroup of a torsion-free hyperbolic group without unique product has finite index*;
3. *whether an arbitrary finitely generated subgroup of a torsion-free hyperbolic group without unique product is normal*;
4. *whether an arbitrary finitely generated subgroup of a torsion-free hyperbolic group without unique product is finitely presented*;
5. *whether an arbitrary finitely generated subgroup S of a torsion-free hyperbolic group without unique product has a finitely generated second integral homology group $H_2(S, \mathbb{Z})$.*

The proofs of (2)–(5) are by choosing a group Q with the required property, which then allows to pullback the property to the group G, see [Baumslag et al. 1994, Theorem 4]. To prove (1), one produces a family of groups G with the required properties as in the proof of [Baumslag et al. 1994, Theorem 2].

Remark 4.3. As pointed out by a referee, groups satisfying Proposition 4.1 or assertion (1), (4), or (5) of Proposition 4.2 could also be produced by taking free products of a hyperbolic group without the unique product property with a hyperbolic group with the respective properties, or more generally, by embedding them as peripheral subgroups in a relatively hyperbolic group.

5. Further remarks

We first proved Theorem 1.1 by a completely different method of graphical small cancellation theory over free products. The interested reader can find this proof in the arXiv version of this article, [Arzhantseva and Steenbock 2014]. It provides a variant of Theorem 1.1, where the group G has, moreover, a graphical presentation that satisfies the graphical $\mathrm{Gr}'_*\left(\frac{1}{6}\right)$-small cancellation condition over the free product.

This initial approach is independent of prior results from [Ol'shanskiĭ 1993; Belegradek and Osin 2008]. It combines, under this novel free product viewpoint, the Rips construction [1982], the construction by Rips and Segev [1987] of groups without the unique product property, and Gromov's construction [2003, Section 1.2.A and item (3) in Section 4.8] of graphical small cancellation groups with Property (T), based on his spectral characterization of this property [Silberman 2003; Ollivier and Wise 2007].

We observe, in particular, that Gromov's probabilistic construction of graph labelings defining groups with Property (T) is flexible under taking edge subdivisions.

Theorem 5.1 [Arzhantseva and Steenbock 2014, Theorem 4]. *For all $m > 64$, there exists a finite connected graph $\mathcal{T}$ labeled by $\{a_1, \dots, a_m\}$ such that the labeling satisfies the $\mathrm{Gr}'_*\left(\frac{1}{6}\right)$-small cancellation condition over the free product $\langle a_1\rangle * \cdots * \langle a_m\rangle$, the labeling satisfies the $\mathrm{Gr}'\left(\frac{1}{6}\right)$-small cancellation condition with respect to the word length metric, and the group with $a_1, \dots, a_m$ as generators and the labels of the cycles of $\mathcal{T}$ as relators has Kazhdan's Property (T).*

One can take $\mathcal{T}$ of arbitrarily large girth. Following the strategy of Ollivier and Wise [2007], the graph $\mathcal{T}$ is produced by assigning to every edge of an expander graph a letter and an orientation independently uniformly at random.

The intuition behind Theorem 5.1 is that the free product length in $\langle a_1\rangle * \cdots * \langle a_m\rangle$ approximates the word length on the free group on $a_1, \dots, a_m$ as $m \to \infty$. Indeed, the minimal cycle length in the free product length bounds the length of the minimal cycles in the word length from below. Pieces are words of finite length chosen uniformly at random. Let us evaluate the probability that the word length and the free product length of such a random word in letters $a_1^{\pm 1}, \dots, a_m^{\pm 1}$ coincide. Such a word is of word length equal to n if it is $a_{i_1}^{P_1} a_{i_2}^{P_2} \dots a_{i_j}^{P_j}$ with all coefficients $P_i \neq 0$, $a_{i_j} \neq a_{i_{j+1}}$, and $\sum_{i=1}^{j} |P_i| = n$. Its free product length is equal to n if, in addition, all exponents $P_i = \pm 1$. The probability that all $P_i = \pm 1$ in such a word is given by $((2m-2)/2m)^{n-1}$, which tends to 1 as $m \to \infty$.

For further details on the genericity aspects underlying Theorem 1.1 see [Arzhantseva and Steenbock 2014].

6. Open problems

Our constructions are motivated by two open problems.

Open problem 6.1. Do the Rips–Segev groups without the unique product property satisfy the Kaplansky zero-divisor conjecture?

Combining [Schreve 2014; Linnell et al. 2012; Agol 2013], we observe that the Kaplansky zero-divisor conjecture holds for all torsion-free CAT(0)-cubical[1] hyperbolic groups, over the field of complex numbers. The groups from Corollary 2.2 are not CAT(0)-cubical as they are infinite Property (T) groups. Thus, the CAT(0)-cubulation cannot solve the conjecture for all hyperbolic groups without the unique product property.

It is unknown whether or not any of the hyperbolic groups without the unique product from [Rips and Segev 1987; Steenbock 2015; Gruber et al. 2015] is CAT(0)-cubical [Martin and Steenbock 2017] or, more generally, a-T-menable.

Open problem 6.2. Is every hyperbolic group residually finite?

We mention this question as every residually finite hyperbolic group has a finite index subgroup with the unique product property by a result of Delzant [1997]. If Q is finite, then N in our construction is normal of finite index and without the unique product property. Then the following questions arise naturally:

- Does there exist a hyperbolic group all of whose normal finite index subgroups are without the unique product property?
- Does there exist a hyperbolic group all of whose subgroups of index at most k, for a given $k \geqslant 2$, are without the unique product property?

After we first announced our results in 2014, our last question has been answered in the affirmative [Gruber et al. 2015].

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[1] A group is *CAT(0)-cubical* if it admits a proper cocompact action on a CAT(0)-cubical complex.

Computation in Groups" and participants A. Minasyan and F. Dahmani, who, after they learned from our results, pointed out that Ol'shanskiĭ's small cancellation theory helps to produce more Property (T) groups without the unique product property.

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GOULNARA ARZHANTSEVA
FACULTY OF MATHEMATICS
UNIVERSITY OF VIENNA
VIENNA
AUSTRIA

goulnara.arzhantseva@univie.ac.at

MARKUS STEENBOCK
FACULTY OF MATHEMATICS
UNIVERSITY OF VIENNA
VIENNA
AUSTRIA

markus.steenbock@univie.ac.at

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NO PERIODIC GEODESICS IN JET SPACE

ALEJANDRO BRAVO-DODDOLI

The J^k space of k-jets of a real function of one real variable x admits the structure of a sub-Riemannian manifold, which then has an associated Hamiltonian geodesic flow, and it is integrable. As in any Hamiltonian flow, a natural question is the existence of periodic solutions. Does J^k have periodic geodesics? This study will find the action-angle coordinates in T^*J^k for the geodesic flow and demonstrate that geodesics in J^k are never periodic.

1. Introduction

This paper is the first attempt to prove that Carnot groups do not have periodic sub-Riemannian geodesics; Enrico Le Donne made this conjecture. Here, we will establish the first case we found, which also has a simple and elegant proof.

This work is the continuation of that done in [4; 5]. In [4], J^k was presented as a sub-Riemannian manifold, the sub-Riemannian geodesic flow was defined, and its integrability was verified. In [5], the sub-Riemannian geodesics in J^k were classified, and some of their minimizing properties were studied. The main goal of this paper is to prove:

Theorem A. *J^k does not have periodic geodesics.*

Following the classification of geodesics from [5, p. 5], the only candidates to be periodic are the ones called x-periodic (the other geodesics are not periodic on the x-coordinate); so we are focusing on the x-periodic geodesics.

An essential tool during this work is the bijection made by Monroy-Perez and Anzaldo-Meneses [2; 8; 9], also described in [5, p. 4], between geodesics on J^k and the pair (F, I) (module translation $F(x) \to F(x-x_0)$), where $F(x)$ is a polynomial of degree bounded by k and I is a closed interval, called the hill interval. Let us formalize its definition.

Definition 1. A closed interval I is called a hill interval of $F(x)$, if for each x inside I, then $F^2(x) < 1$ and $F^2(x) = 1$ if x is in the boundary of I.

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Keywords: Carnot group, jet space, integrable system, Goursat distribution, sub-Riemannian geometry, Hamilton–Jacobi, periodic geodesics.

By definition, the hill interval I of a constant polynomial $F^2(x) = c^2 < 1$ is $\mathbb{R}$, while the hill interval I of the constant polynomial $F(x) = \pm 1$ is a single point. Also, I is compact if and only if $F(x)$ is not a constant polynomial; in this case, if I is of the form $[x_0, x_1]$, then $F^2(x_1) = F^2(x_0) = 1$. This terminology comes from celestial mechanics, and I is the region where the dynamics governed by the fundamental equation (3-5) take place.

Geodesics corresponding to constant polynomials are called horizontal lines since their projection to (x, θ_0)-planes are lines. In particular, geodesics corresponding to $F(x) = \pm 1$ are abnormal geodesics (see [6], [10], or [11]). Then this work will be restricted to geodesics associated with nonconstant polynomials. Further, x-periodic geodesics correspond to the pair $(F, [x_0, x_1])$, where x_0 and x_1 are regular points of $F(x)$, which implies they are simple roots of $1 - F^2(x)$.

Outline of the paper. In Section 2, Proposition 2 is introduced and Theorem A is proved. The main purpose of Section 3 is to prove Proposition 2. In Section 3.1, the sub-Riemannian structure and the sub-Riemannian Hamiltonian geodesic function are introduced. In Section 3.2, a generating function is presented and a canonical transformation from traditional coordinates in T^*J^k to action-angle coordinates (μ, ϕ) for the Hamiltonian systems is shown. In Section 3.3, Proposition 2 is proved.

2. Proof of Theorem A

Throughout this work, the alternate coordinates $(x, \theta_0, \dots, \theta_k)$ will be used, the meaning of which is introduced in Section 3 and described in more detail in [2], [9], or [5]. Further, x-periodic geodesics have the property that the change undergone by the coordinates θ_i after one x-period is finite and does not depend on the initial point. We summarize the above discussion with the following proposition:

Proposition 2. *Let $\gamma(t) = (x(t), \theta_0(t), \dots, \theta_k(t))$ in J^k be an x-periodic geodesic corresponding to the pair (F, I). Then the x-period is*

$$L(F, I) = 2\int_I \frac{dx}{\sqrt{1-F^2(x)}}. \tag{2-1}$$

Moreover, it is twice the time it takes for the x-curve to cross its hill interval exactly once. After one period, the changes $\Delta\theta_i := \theta_i(t_0 + L) - \theta_i(t_0)$ for $i = 0, 1, \dots, k$ undergone by θ_i are given by

$$\Delta\theta_i(F, I) = \frac{2}{i!}\int_I \frac{x^i F(x)dx}{\sqrt{1 - F^2(x)}}. \tag{2-2}$$

In [5], a sub-Riemannian manifold $\mathbb{R}^3_F$, called magnetic space, was introduced, and a similar statement like Proposition 2 was proved, see [5, Proposition 4.1], with an argument of classical mechanics, see [7, (11.5)].

Proposition 2 implies that a x-periodic geodesic $\gamma(t)$ corresponding to the pair (F, I) is periodic if and only if $\Delta\theta_i(F, I) = 0$ for all i.

Because that period L from (2-1) is finite, we can define an inner product in the space of polynomials of degree bounded by k in the following way:

$$\langle P_1(x), P_2(x)\rangle_F := \int_I \frac{P_1(x)P_2(x)dx}{\sqrt{1 - F^2(x)}}. \tag{2-3}$$

This inner product is nondegenerate and will be the key to the proof of Theorem A.

2.1. *Proof of Theorem A.*

Proof. We will proceed by contradiction. Let us assume $\gamma(t)$ is a periodic geodesic on J^k corresponding to the pair (F, I), where $F(x)$ is not constant, then $\Delta\theta_i(F, I) = 0$ for all i in $0, \dots, k$.

In the context of the space of polynomials of degree bounded by k with inner product $\langle\ ,\ \rangle_F$, the condition $\Delta\theta_i(F, I) = 0$ is equivalent to $F(x)$ being perpendicular to x^i $\big(0 = \Delta\theta_i(F, I) = \langle x^i, F(x)\rangle_F\big)$, so $F(x)$ being perpendicular to x^i for all i in $0, 1, \dots, k$. However, the set $\{x^i\}$, with $0 \le i \le k$, is a base for the space of polynomials with degree bounded by k. Then $F(x)$ is perpendicular to any vector, so $F(x)$ is zero since the inner product is nondegenerate. However, $F(x)$ equals 0 contradicts the assumption that $F(x)$ is not a constant polynomial. ☐

Coming work: The proof of the conjecture in the meta-abelian group $\mathbb{G}$, that is, $\mathbb{G}$ is such that $0 = [[\mathbb{G}, \mathbb{G}], [\mathbb{G}, \mathbb{G}]]$.

3. Proof of Proposition 2

3.1. ***J^k as a sub-Riemannian manifold.*** The sub-Riemannian structure on J^k will be described here briefly. For more details, see [4; 5]. We see J^k as $\mathbb{R}^{k+2}$, using $(x, \theta_0, \dots, \theta_k)$ as global coordinates, then J^k is endowed with a natural rank 2 distribution $D \subset TJ^k$ characterized by the k Pfaffian equations

$$0 = d\theta_i - \frac{1}{i!}x^i d\theta_0, \quad i = 1, \dots, k. \tag{3-1}$$

D is globally framed by two vector fields

$$X_1 = \frac{\partial}{\partial x} \quad \text{and} \quad X_2 = \sum_{i=0}^{k} \frac{x^i}{i!}\frac{\partial}{\partial\theta_i}. \tag{3-2}$$

A sub-Riemannian structure on $\mathcal{J}^k$ is defined by declaring these two vector fields to be orthonormal. In these coordinates, the sub-Riemannian metric is given by restricting $ds^2 = dx^2 + d\theta_0^2$ to D.

3.1.1. *Sub-Riemannian geodesic flow.* Here it is emphasized that the projections of the solution curves for the Hamiltonian geodesic flow are geodesics, that is, if $(p(t), \gamma(t))$ is a solution for the Hamiltonian geodesic flow, then $\gamma(t)$ is a geodesic on J^k.

Let $(p_x, p_{\theta_0}, \dots, p_{\theta_k}, x, \theta_0, \dots, \theta_k)$ be the traditional coordinates on T^*J^k, or (p, q) for short. Let $P_1, P_2 : T^*J^k \to \mathbb{R}$ be the momentum functions of the vector fields X_1 and X_2, see [10, p. 8] or [1], in terms of the coordinates (p, q) given by

$$P_1(p,q) := p_x \quad \text{and} \quad P_2(p,q) := \sum_{i=0}^{k} p_{\theta_i} \frac{x^i}{i!}. \tag{3-3}$$

Then the Hamiltonian governing the geodesic on J^k is

$$H_{sR}(p,q) := \frac{1}{2}(P_1^2 + P_2^2) = \frac{1}{2}p_x^2 + \frac{1}{2}\left(\sum_{i=0}^{k} p_{\theta_i} \frac{x^i}{i!}\right)^2. \tag{3-4}$$

It is noteworthy that $h = \frac{1}{2}$ implies that the geodesic is parameterized by arc-length. It can be noticed that if H does not depend on θ_i for all i, then the p_θ define $k+1$ constants of motion.

Lemma 3. *The sub-Riemannian geodesic flow in J^k is integrable. If $(p(t), \gamma(t))$ is a solution, then*

$$\dot\gamma(t) = P_1(t)X_1 + P_2(t)X_2 \quad \textit{and} \quad (P_1(t), P_2(t)) = (p_x(t), F(x(t))),$$

where $p_{\theta_i} = i!\,a_i$ and $F(x) = \sum_{i=0}^{k} a_i x^i$.

Proof. H does not depend on t and θ_i for all i, so $h := H_{sR}$ and p_{θ_i} are constants of motion, thus the Hamiltonian system is integrable. A consequence of the first equation from Lemma 3 is that P_1 and P_2 are linear in p_x and p_θ. We denote by $(a_0, \dots, a_k)$ the level set $i!\,a_i = p_{\theta_i}$, then the result follows by the definitions of P_1 and P_2 given by (3-3). $\square$

3.1.2. *Fundamental equation.* The level set $(a_0, \dots, a_k)$ defines a fundamental equation

$$H_F(p_x, x) := \tfrac{1}{2}p_x^2 + \tfrac{1}{2}F^2(x) = H|_{(a_0,\dots,a_k)}(p,q) = \tfrac{1}{2}. \tag{3-5}$$

Here, $H_F(p_x, x)$ is a Hamiltonian function in the phase plane (p_x, x), where the dynamic of $x(s)$ takes place in the hill region $I = [x_0, x_1]$ and its solution $(p_x(t), x(t))$ with energy $h = \frac{1}{2}$ lies in an algebraic curve or loop given by

$$\alpha_{(F,I)} := \left\{(p_x, x) : \tfrac{1}{2} = \tfrac{1}{2}p_x^2 + \tfrac{1}{2}F^2(x) \text{ and } x_0 \le x \le x_1\right\}, \tag{3-6}$$

and $\alpha_{(F,I)}$ is closed and simple.

Lemma 4. *$\alpha(F, I)$ is smooth if and only if x_0 and x_1 are regular points of $F(x)$, in other words, $\alpha(F, I)$ is smooth if and only if the corresponding geodesic $\gamma(t)$ is x-periodic.*

Proof. A point $\alpha = (p_x, x)$ in $\alpha(F, I)$ is smooth if and only if

$$0 \neq \nabla H_F(p_x, x)|_{\alpha(F,I)} = \big(p_x, F(x)F'(x)\big).$$

Then α is smooth for all $p_x \neq 0$, and the points $\alpha(F, I)$ such that $p_x = 0$ correspond to endpoints of the hill interval I, since the condition $p_x = 0$ implies $F^2(x) = 1$. The point $\alpha = (0, x_0)$ is smooth if $F'(x_0) \neq 0$, and the point $\alpha = (0, x_1)$ is smooth if $F'(x_1) \neq 0$. Then $\alpha(F, I)$ is smooth if and only if x_0 and x_1 are regular points of $F(x)$. Also, $\alpha(F, I)$ is smooth is equivalent to $H_F(p_x, x)|_{\alpha(F,I)}$ is never zero, which is equivalent to the Hamiltonian vector field is never zero on $\alpha(F, I)$. ☐

3.1.3. *Arnold–Liouville manifold.* The Arnold–Liouville manifold $M|_F$ is given by

$$M_F := \big\{(p, q) \in T^*J^k : \tfrac{1}{2} = H_F(p_x, x),\ p_{\theta_i} = i!\, a_i\big\}.$$

In the case $\gamma(t)$ is x-periodic, M_F is diffeomorphic to $\mathbb{S}^1 \times \mathbb{R}^{k+1}$, where $\mathbb{S}^1$ is the simple, closed, and smooth curve $\alpha(F, I)$.

The curve $\alpha(F, I)$ has two natural charts using x as coordinates and is given by solving the equation $H_F = \frac{1}{2}$ with respect to p_x, namely $(p_x, x) = \big(\pm\sqrt{1 - F^2(x)}, x\big)$. With this in mind:

Lemma 5. *Let $d\phi_t$ be the closed one-form on $M_F \subset T^*J^k$ given by*

$$d\phi_h := \frac{p_x}{\Pi(F, I)}|_{M_F} dx = \frac{\sqrt{1 - F^2(x)}}{\Pi(F, I)} dx, \tag{3-7}$$

where $\Pi(F, I)$ is the area enclosed by $\alpha(F, I)$. Then,

$$\int_{\alpha(F,I)} d\phi_h = 1 \quad \textit{and} \quad \frac{\partial}{\partial h}\Pi(F, I) = L(F, I),$$

and as a consequence the inverse function $h(\Pi)$ exists.

Proof. Let $\Omega(F, I)$ be the closed region by $\alpha(F, I)$, then $d\phi_h$ can be extended to $\Omega(F, I)$ and Stokes' theorem implies

$$\Pi(F, I) := \int_{\alpha(F,I)} p_x\, dx = \int_{\Omega(F,I)} dp_x \wedge dx = 2\int_I \sqrt{2h - F^2(x)}\,\big|_{h=1/2}\, dx. \tag{3-8}$$

This shows that $\int_{\alpha(F,I)} d\phi_h = 1$, thus $d\phi_h$ is not exact.

Since $\Pi(F, I)$ is a function of h,

$$\frac{\partial}{\partial h}\Pi(F, I) = \frac{\partial}{\partial h}\int_I d\phi_h = \int_I \frac{2\, dx}{\sqrt{1 - F^2(x)}}. \tag{3-9}$$

☐

We note that $\Pi(F, I)$ is also called an adiabatic invariant, see [3, p. 297]. We will use Π when we use it as a variable, and we will use $\Pi(F, I)$ for the adiabatic invariant.

3.2. ***Action-angle variables in T^*J^k.*** We consider the action $\mu = (\Pi, a_0, \dots, a_k)$ and find its angle coordinates $\phi = (\phi_h, \phi_0, \dots, \phi_k)$, such that the set (μ, ϕ) of coordinates are action-angle coordinates in T^*J^k.

Lemma 6. *There exist a canonical transformation $\Phi(p, q) = (\mu, \phi)$, where ϕ_h is the local function defined by the close form $d\phi_h$ from Lemma 5 and*

$$\phi_i = -\int^x \frac{\tilde{x}^i F(\tilde{x})\, d\tilde{x}}{\sqrt{1 - F^2(\tilde{x})}} + i!\,\theta_i, \quad x \in I \text{ and } i = 0, \dots, k.$$

To construct the canonical transformation $\Phi(p, q)$, we will look for its generating function $S(\mu, q)$ of the second type that satisfies the three following conditions:

$$p = \frac{\partial S}{\partial q}, \quad \phi = \frac{\partial S}{\partial \mu}, \quad H\Big(\frac{\partial S}{\partial q}, q\Big) = h(\Pi) = \frac{1}{2}, \tag{3-10}$$

where $h(\Pi)$ is the function defined in Lemma 5. For more details on the definition of $S(\mu, q)$, see [3, Section 50] or [7].

To find $S(\mu, q)$, we will solve the sub-Riemannian Hamilton–Jacobi equation associated with the sub-Riemannian geodesic flow. For more details about the definition of this equation in sub-Riemannian geometry and its relation to the Eikonal equation, see [10, p. 8] or [5].

Proof. The sub-Riemannian Hamilton–Jacobi equation is given by

$$h|_{1/2} = \frac{1}{2}\Big(\frac{\partial S}{\partial x}\Big)^2 + \frac{1}{2}\Big(\sum_{i=0}^{k} \frac{x^i}{i!}\frac{\partial S}{\partial \theta_i}\Big)^2. \tag{3-11}$$

Take the ansatz

$$S(\mu, q) := f(x) + \sum_{i=0}^{k} i!\, a_i \theta_i$$

as a solution. The equation (3-11) becomes (3-5), and then the generating function is given by

$$S(\mu, q) = \int_{x_0}^{x} \sqrt{2h(\Pi) - F^2(\tilde{x})}\, d\tilde{x} + \sum_{i=0}^{n} i!\, a_i \theta_i. \tag{3-12}$$

Here, $h(\Pi) = \frac{1}{2}$ and $S(\mu, q)$ is a local function, since x must lay in the hill region I, that is, $S(\mu, q)$ is defined in the subset $\mu \times I \times \mathbb{R}^{k+1}$.

We can see that conditions 1 and 3 of (3-10) are satisfied: $p(\mu, q) = \partial S/\partial q$ and $H(p(\mu, q), q) = h$. To find the new coordinates ϕ, we use condition 2:

$$\frac{\partial S}{\partial h} = \int^x \frac{d\tilde{x}}{\sqrt{1-F^2(\tilde{x})}} = \phi_h,$$

$$\frac{\partial S}{\partial a_i} = -\int^x \frac{\tilde{x}^i F(\tilde{x})\, d\tilde{x}}{\sqrt{1-F^2(\tilde{x})}} + i!\,\theta_i = \phi_i. \qquad \square$$

Note that in [5] a projection $\pi_F : J^k \to \mathbb{R}^3_F$ was built, and the solution to the sub-Riemannian Hamilton–Jacobi equation on the magnetic space $\mathbb{R}^3_F$ was found. The solution given by (3-12) is the pull-back by π_F of the solution previously found in $\mathbb{R}_F$, where π_F is, in fact, a sub-Riemannian submersion.

Corollary 7. *The coordinates* (μ, ϕ) *are action-angle coordinates.*

Proof. Using the Hamilton equations for the new coordinates (μ, ϕ), we have $\phi_t = t$ and $\phi_i = \text{const}$. ☐

Note that h and ϕ_t are action-angles coordinates for the Hamiltonian H_F.

3.2.1. *Horizontal derivative.* A horizontal derivative ∇_{hor} of a function $S : J^k \to \mathbb{R}$ is the unique horizontal vector field that satisfies; for every q in J^k,

$$\langle \nabla_{\text{hor}} S, v\rangle_q = dS(v), \quad \text{for } v \in D_q, \tag{3-13}$$

where $\langle\ ,\ \rangle_q$ is the sub-Riemannian metric in D_q. For further details, see [10, pp. 14–15] or [1].

Lemma 8. *Let* $\gamma(t)$ *be a geodesic parameterized by arc length corresponding to the pair* (F, I) *and* S_F *be the solution given by* (3-12), *then*

$$dS_F(\dot{\gamma})(t) = 1.$$

Proof. Let us prove that $\dot{\gamma}(t) = (\nabla_{\text{hor}} S_F)_{\gamma(t)}$, which is just a consequence of S_F being a solution to the Hamilton–Jacobi equation, that is,

$$X_1(S_F)|_{\gamma(t)} = \frac{\partial S}{\partial x}\Big|_{\gamma(t)} = p_x(t).$$

However, Lemma 3 implies that $P_1(t) = p_x(t)$, so $P_1(t) = X_1(S_F)|_{\gamma(t)}$. As well,

$$X_2(S_F)|_{\gamma(t)} = \sum_{i=0}^{k} \frac{x^i(t)}{i!} \frac{\partial S}{\partial \theta_i}\Big|_{\gamma(t)} = \sum_{i=0}^{k} a_i x^i(t) = F(x(t)).$$

Also, Lemma 3 implies that $P_2(t) = F(x(t))$, so $P_2(t) = X_2(S_F)|_{\gamma(t)}$. As a consequence,

$$\nabla_{\text{hor}} S|_{\gamma(t)} := X_1(S_F)|_{\gamma(t)} X_1 + X_2(S_F)|_{\gamma(t)} X_2 = P_1(t) X_1 + P_2(t) X_2.$$

Lemma 3 implies $P_1(t)X_1 + P_2(t)X_2 = \dot{\gamma}(t)$. Thus, $\nabla_{\mathrm{hor}} S = \dot{\gamma}(t)$ and $dS_F(v)|_q = \langle \nabla_{\mathrm{hor}} S_F, v \rangle$ for all D_q. In particular,

$$dS_F(\dot{\gamma}) = \langle \dot{\gamma}(t), \dot{\gamma}(t) \rangle = 1,$$

since t is the arc length parameter. □

3.3. *Proof of Proposition 2.*

Proof. It is well known that the fundamental system H_F with energy $\frac{1}{2}$ has period $L(F, I)$ given by (2-1) and the relation between $\Pi(F, I)$ and $L(F, I)$ is given by Lemma 5, see [3, p. 281]. Let $\gamma(t)$ be an x-periodic corresponding to (F, I), we are interested in seeing the change suffered by the coordinates θ_i after one $L(I, F)$. For that, we consider the change in $S(\mu, q)$ after $\gamma(t)$ travel from t to $t + L(F, I)$, in other words,

$$L(F, I) = \int_t^{t+L(F,I)} dS(\dot{\gamma}(t))\, dt = \Pi(F, I) + \sum_{i=0}^{n} i!\, a_i \Delta\theta_i(F, I). \tag{3-14}$$

The left side of the equation is a consequence of Lemma 8, and the right side is the integration term by term. Taking the derivative of (3-14) with respect to a_i to find $-(\partial/\partial a_i)\Pi(F, I) = i!\, \Delta\theta_i$, which is equivalent to (2-2).

We differentiate $\Delta\theta_i := \theta_i(t + L) - \theta_i(t)$, with respect to t, to see that $\Delta\theta_i(F, I)$ is independent of the initial point. The derivative is

$$\frac{x^i(t+L)F(x(t+L))}{\sqrt{1 - F^2(x(t+L))}} - \frac{x^i(t)F(x(t))}{\sqrt{1 - F^2(x(t))}},$$

but $x(t + L) = x(t)$. □

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ALEJANDRO BRAVO-DODDOLI
DEPARTMENT OF MATHEMATICS
UNIVERSITY OF CALIFORNIA SANTA CRUZ
SANTA CRUZ, CA
UNITED STATES

abravodo@ucsc.edu

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COARSE GEOMETRY OF HECKE PAIRS AND THE BAUM–CONNES CONJECTURE

CLÉMENT DELL'AIERA

We study Hecke pairs using the coarse geometry of their coset space and their Schlichting completion. We prove new stability results for the Baum–Connes and the Novikov conjectures in the case where the pair is co-Haagerup. This allows to generalize previous results, while providing new examples of groups satisfying the Baum–Connes conjecture with coefficients. For instance, we show that for some S-arithmetic subgroups of $\mathrm{Sp}(5, 1)$ and $\mathrm{Sp}(3, 1)$ the conjecture with coefficients holds.

1. Overview and statement of the results

The Baum–Connes conjecture for a locally compact second countable group G predicts that the K-theory groups of the reduced C^*-algebra of a locally compact group, which is the norm closure of the complex algebra generated by the left regular representation of $L^1(G)$ on $L^2(G)$, are isomorphic to the equivariant K-homology of the group's classifying space for proper actions. One of its most spectacular applications is the descent principle, that allows to derive the Novikov conjecture from a certain form of injectivity of the Baum–Connes assembly map. See Section 4 for a reminder with references for both statements.

The conjectures are known to hold in many cases, and the Baum–Connes conjecture has various stability properties. For instance, groups with the Haagerup property satisfy the Baum–Connes conjecture with coefficients, and the conjecture is stable by extensions. Moreover, if a group acts by isometries on a tree with stabilizers that satisfy the Baum–Connes conjecture, then so does the group. Recall that the Haagerup property can be defined as the existence of a metrically proper action on a real affine Hilbert space by isometries.

This leads to the following question: if a group acts on a real affine Hilbert space by isometries, suppose that one orbit is a proper subspace, but possibly with infinite isotropy subgroups. Can we deduce the Baum–Connes conjecture for the group if the stabilizer satisfies it?

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In this setting, the typical stabilizer of the proper orbit is co-Haagerup in the ambient group, and this forces the subgroup to be almost normal, in the sense that it is commensurable to any of its conjugates. We answer our question in the affirmative.

Theorem 1.1. *Let $\Lambda < \Gamma$ be a co-Haagerup subgroup of a discrete countable group. Then, if all subgroups of Γ containing Λ as a subgroup of finite index satisfy the Baum–Connes conjecture with coefficients, so does Γ.*

Being almost normal is weaker than co-Haagerup. It is actually equivalent to Γ/Λ being of bounded geometry, if we equip Γ/Λ with the metric induced from a left proper metric on Γ. With this in mind, we deduce the following from the theorem.

Corollary 1.2. *Let $\Lambda < \Gamma$ be a Hecke pair. If Λ and Γ/Λ admit a coarse embedding into a Hilbert space, then Γ satisfies the Novikov conjecture.*

The paper is organized as follows. The second section gives a geometric characterization of Hecke pairs: a subgroup is almost normal if and only if the coset space with the quotient metric is of bounded geometry. In the third section, we review the construction of the Schlichting completion of a Hecke pair, a totally disconnected locally compact group that acts as a replacement of the quotient group when the subgroup is only almost normal, and prove that a subgroup is co-Haagerup if and only if the corresponding Schlichting completion has Haagerup's property. Here, we use implicitly that co-Haagerup subgroups are almost normal. The fourth section is devoted to the proof of the main theorem, and the fifth section to the proof of the corollary. In the last section, we apply these results to establish that the Baum–Connes conjecture with coefficients holds for some countable discrete groups. The first examples recover previous known results with a different proof, the second examples are, to the author's knowledge, new. For instance, we have the following.

Corollary 1.3. *Let G be an absolutely simple algebraic group over $\mathbb{Q}$ such that groups containing $G(\mathbb{Z})$ as a subgroup of finite index satisfy the Baum–Connes conjecture with coefficients. Let p be a prime number, and suppose that the $\mathbb{Q}_p$-rank of G is* 1, *then $G(\mathbb{Z}[1/p])$ satisfies the Baum–Connes conjecture with coefficients.*

This can be applied when $G(\mathbb{Z})$ is a uniform lattice in $\mathrm{Sp}(3, 1)$ and $\mathrm{Sp}(5, 1)$ (or $\mathrm{SO}(n, 1)$ for $n = 5, 7, 9$) since these are Gromov hyperbolic groups, and thus satisfies the Baum–Connes conjecture with coefficients.

2. Coarse geometry and Hecke pairs

Let Γ be a discrete group. A subgroup $\Lambda < \Gamma$ is *almost normal* if one of the following equivalent conditions is satisfied:

- For every $\gamma \in \Gamma$, Λ and $\Lambda^\gamma = \gamma\Lambda\gamma^{-1}$ are commensurable (i.e., they contain a common subgroup of finite index).
- The index $[\Lambda : \Lambda \cap \Lambda^\gamma]$ is finite for every $\gamma \in \Gamma$.
- The left action of Λ on Γ/Λ has finite orbits.
- Every double coset $\Lambda s \Lambda$ is a finite union of cosets $\gamma\Lambda$.

In this case, we call (Γ, Λ) a Hecke pair. The equivalence is easily seen since the cardinal of the orbit $\Lambda g \Lambda$ is the index $[\Lambda : \Lambda \cap g\Lambda g^{-1}]$. Let us fix a left Γ-invariant metric on Γ, given by a proper length $|\cdot|$. We endow $X = \Gamma/\Lambda$ with the left Γ-invariant metric

$$d(s\Lambda, t\Lambda) = \inf_{\lambda,\lambda' \in \Lambda} |\lambda s^{-1} t \lambda'|.$$

Recall that a metric space (X, d) is of *bounded geometry* if for every $r > 0$, $\sup_{x\in X} |B(x, r)|$ is finite.

Proposition 2.1. *The coset space $X = \Gamma/\Lambda$ is of bounded geometry if and only if (Γ, Λ) is a Hecke pair.*

Proof. The metric being left invariant and the action transitive, it is enough to show that any ball of finite radius is finite. But $d(g\Lambda, \Lambda) \leq r$ if and only if

$$g \in \bigcup_{|\gamma|\leq r} \Lambda\gamma\Lambda.$$

Γ is of bounded geometry, so that the latter is a finite union of double cosets $\Lambda\gamma\Lambda$, themselves being a finite union of left Λ-cosets by almost normality.

Now, if X is of bounded geometry, Γ acts by isometries, by left invariance of the metric. As Λ stabilizes the base point, it stabilizes all spheres, and thus its orbits are contained in those, which are finite. ☐

This gives a large class of examples of Hecke pairs. Let Γ be a discrete group acting by isometries on a locally finite metric space, then any stabilizer is almost normal. For instances, groups acting by isometries on locally finite trees, such as HNN extensions and amalgamated free products, have almost normal subgroups.

- If $\mathrm{BS}(m, n) = \langle a, b \mid a^{-1}b^m a = b^n\rangle$ is the Baumslag–Solitar group, then $\mathbb{Z} \cong \langle b\rangle$ is an almost normal subgroup.
- $\mathrm{SL}(2, \mathbb{Z})$ is almost normal in $\mathrm{SL}(2, \mathbb{Z}[1/p])$, by considering its restricted action on the Bass–Serre tree of $\mathrm{SL}(2, \mathbb{Q}_p)$.

Other examples do not readily come from isometric actions. The previous proposition gives a geometric interpretation to these pairs.

(1) If Γ is a discrete group acting on a set X, and $Y \subset X$ a commensurate subset, i.e., the symmetric difference $|Y \Delta \gamma Y| < \infty$ for every $\gamma \in \Gamma$, and F a finite group, then $\bigoplus_Y F$ is almost normal in the (generalized) wreath product $F \wr_X \Gamma = \left(\bigoplus_X F\right) \rtimes \Gamma$.

If one specifies $\Gamma = \mathbb{Z}$ and $Y = \mathbb{N} \subset X = \mathbb{Z}$, we get an almost normal subgroup of the Lamplighter group.

(2) $\mathrm{SL}(n, \mathbb{Z})$ is almost normal in $\mathrm{SL}(n, \mathbb{Q})$. More generally, arithmetic lattices in global fields have commensurate subgroups: if F is a global field, and $\mathcal{O}$ its ring of integers, let G be an absolutely simple, simply connected algebraic group over F. Let S and S' be sets of inequivalent valuations on F, containing all archimedean ones, and such that $S' \subset S$. We denote by $\mathcal{O}_S$ the ring of S-integers in F. A S-arithmetic group is a subgroup commensurable with $G(\mathcal{O}_S)$. Then if Γ is a S-arithmetic group, any S'-arithmetic group Λ is almost normal in Γ.

3. The Schlichting completion and coarse embeddings

Let (Γ, Λ) be a Hecke pair and $X = \Gamma/\Lambda$. There exists a locally compact totally discontinuous Hecke pair (G, K) where K is a compact open subgroup of G, and a homomorphism $\sigma : \Gamma \to G$ with dense image satisfying $\sigma^{-1}(K) = \Lambda$, hence inducing isomorphisms $\Gamma/\Lambda \cong G/K$ and $\Lambda\backslash\Gamma/\Lambda \cong K\backslash G/K$. This construction was introduced by Schlichting in [22] and used extensively by Tzanev in [27].

Let us recall the construction: we endow the group of permutations $\mathfrak{S}(X)$ with the topology induced from pointwise convergence in the space of maps from X to X. It is a standard fact that this makes $\mathfrak{S}(X)$ a Polish group. We denote by $\sigma : \Gamma \to \mathfrak{S}(X)$ the representation by permutation, and by G (respectively K) the closure of the image of Γ (respectively Λ) by σ. These are totally discontinuous groups.

From this follows that K is compact open if (Γ, Λ) is a Hecke pair, thus G is locally compact. Indeed, K is a closed subgroup of the group

$$\prod_{[g]\in\Lambda\backslash X} \mathfrak{S}(\Lambda g \Lambda/\Lambda),$$

which is compact as a product of finite groups (the topology of pointwise convergence coincides with the product topology). It is also the stabilizer of a point, $K = \mathrm{stab}_G(\Lambda)$, hence it is open since the finite intersections of stabilizers form a basis for the topology of pointwise convergence. The group G thus has a compact open neighborhood of the identity.

The following points are important.

- If Λ is normal, the pair (G, K) is $(\Gamma/\Lambda, 1)$.
- If Λ is finite, then $N = \bigcap_\gamma \Lambda^\gamma$ is a finite normal subgroup of Γ contained in Λ, and $(G, K) \cong (\Gamma/N, \Lambda/N)$.
- The definition of a Hecke pairs makes sense if Γ is locally compact and Λ is open (and closed) in Γ. Then the previous remarks remain true, if finite is replaced by compact. In general, Hecke pairs in totally disconnected locally compact groups are useful, with almost normal subgroups given by compact open subgroups.

We see that the biggest normal subgroup contained in Λ is $N = \bigcap_\gamma \Lambda^\gamma$. We will call N the core of Λ. The Hecke pair is a substitute for the quotient group in the absence of normality. It is thus natural to focus on *reduced Hecke pairs*, i.e., N is trivial. If a pair (Γ, Λ) is not reduced, its reduced pair will be $(\Gamma/N, \Lambda/N)$. A useful result to identify the Schlichting completion of a Hecke pair is the following.

Lemma 3.1 [23, Lemma 3.5]. *Let* (Γ, Λ) *a Hecke pair. Suppose there exist a locally compact group* G, *a compact open subgroup* $K < G$, *and a homomorphism* $\psi : \Gamma \to G$ *such that* $\psi(\Gamma)$ *is dense in* G *and* $\psi^{-1}(K) = \Lambda$. *Then the Schlichting completion of* (Γ, Λ) *and* (G, K) *coincide. In particular, that of* Γ *is isomorphic to* G/N, *where* N *is the largest normal subgroup contained in* K.

Here are some examples of computation of Schlichting completions.

- If $\Lambda = \bigoplus_Y F$ in $\Gamma = F \wr_X G$, as in (1) with F finite and Y commensurate in X, let us define $G = P \rtimes \Gamma$ where

$$P = \Big(\prod_X F\Big) \oplus \big(\bigoplus\nolimits_{\Gamma \setminus X} F\big) \subset \prod_\Gamma F.$$

Then $\Gamma \hookrightarrow G$ satisfies the hypothesis of the lemma, with $K = \prod_X F$. The core of K is easily seen to be $N = \prod_{\bigcap_\gamma \gamma \cdot X} F$, and G/N is the Schlichting completion in that case. Notice that in the case where the intersection of all translates of X is trivial, N also is, so that G is the Schlichting completion of Γ.

- By using $\mathrm{SL}(n, \mathbb{Z}[1/p]) \hookrightarrow \mathrm{SL}(n, \mathbb{Q}_p)$ for p prime, the Schlichting completion of $(\mathrm{SL}(n, \mathbb{Z}[1/p]), \mathrm{SL}(n, \mathbb{Z}))$ is $\mathrm{PSL}(n, \mathbb{Q}_p)$. With the help of the diagonal embedding $\mathrm{SL}(n, \mathbb{Q}) \hookrightarrow \mathrm{SL}(n, \mathbb{A})$, we also get that the Schlichting completion of $(\mathrm{SL}(n, \mathbb{Q}), \mathrm{SL}(n, \mathbb{Z}))$ is $\mathrm{PSL}(n, \mathbb{A})$.

This last example is a particular case of a general statement. With the notation of the second example at the end of the previous section, recall that $G(\mathcal{O}_S)$ is almost normal in $G(\mathcal{O}_{S'})$. Let $\mathbb{A}$ be the ring of adèles F, and $G(\mathbb{A}_S)$ be the subgroup of $G(\mathbb{A})$ obtained as a restricted product over places in S. If $\overline{G}(\mathcal{O}_S)$ denotes the closure of the image of $G(\mathcal{O}_S)$ under the diagonal embedding $G(F) \hookrightarrow G(\mathbb{A}_S)$, then the corresponding Schlichting completion is obtained as that of $(\overline{G}(\mathcal{O}_{S'}), \overline{G}(\mathcal{O}_S))$. If G is F-isotropic, the diagonal embedding has dense image, yielding that, if S_0 is the set of finite places in S, then the Schlichting completion of $(G(\mathcal{O}_S), G(\mathcal{O}))$ coincides with $G(\mathbb{A}_{S_0})$ quotiented by its center (see [23], Section 3).

Recall that a group is a-T-menable, also called Haagerup's property, if there exists a real valued continuous function on G that is proper and conditionally of negative-type (see [7], Chapter 1). We also recall that a metric space with bounded geometry:

- Admits a coarse embedding into Hilbert space if there exists a symmetric normalized kernel on X that is conditionally of negative-type and effectively proper (see [8], Definition 5.6).
- Has Yu's property (A) if for every positive numbers ε and r, there exists a symmetric normalized kernel on X of positive-type with finite propagation and (r, ε)-propagation (see [28], Theorem 1.2.4).

Furthermore, a subgroup $\Lambda < \Gamma$ is co-Følner if and only if Γ/Λ carries a Γ-invariant mean. Exactness of a locally compact group is defined as exactness of the reduced crossed-product. It is known to be equivalent to *amenability at infinity*, that is, G admits an amenable action on some compact Hausdorff space (see [3]).

From these definitions (which are actually theorems), we see that a discrete group is a-T-menable if and only if it admits a Γ-equivariant coarse embedding into Hilbert space, and that it is amenable if and only if it satisfies property (A)'s condition with the kernel being Γ-equivariant.

Proposition 3.2. *With the notation above*:

- *X admits a Γ-equivariant coarse embedding into a Γ-Hilbert space if and only if G has Haagerup's property.*
- *X admits a coarse embedding into a Hilbert space if and only if the action of G on βX is a-T-menable.*
- *Λ is co-Følner in Γ if and only if G is amenable.*
- *X has Yu's property (A) if and only if G is exact.*

Proof. The key fact is the correspondence between kernels on X and G. Indeed, the map quotient map $G \to X$ induces a map that takes kernels on X to kernels on G, respects properness and, if the original kernel is Γ-invariant, its image will be G-invariant. Thus, if we have a conditionally negative-type Γ-equivariant metrically proper kernel on X, we get a continuous conditionally negative-type proper function on G.

For the converse, if we have a continuous conditionally negative-type proper function $\phi : G \to \mathbb{R}$, then

$$\varphi(sK, tK) = \int_K \int_K \phi(k_1 s^{-1} t k_2)\, dk_1\, dk_2$$

defines a conditionally negative-type Γ-equivariant metrically proper kernel on X.

Remark that these two correspondences respects the support in the sense that $\operatorname{supp}\varphi \subset \{(x, y) \in X \times X : d(x, y) \leq r\}$ if and only if $\operatorname{supp}\phi \subset \bigcup_{|s|\leq r} K\sigma(s)K$. Thus kernels supported in an entourage[1] of X correspond to compactly supported kernels on G. This gives the two last points. □

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[1] In the sense of coarse geometry: for a metric space (X, d), a subset $E \subset X \times X$ is an entourage if $\sup_{(x,y)\in E} d(x, y) < +\infty$.

Let H be a subgroup of Γ. Recall that H is co-Haagerup in Γ if there exists a proper Γ-invariant kernel of conditionally negative-type on Γ/H, and is co-Følner if Γ/H carries a Γ-invariant mean. In general, co-Følner subgroups are not co-Haagerup (see Example 6.1 of [8]), but in the case of Hecke pairs, it follows from the previous proposition that this implication holds. Moreover, if $\Lambda < \Gamma$ is co-Haagerup, it is a Hecke pair (see Example 6.1 and Proposition B.2 of [8]) and the converse obviously does not hold. We easily see that Hecke pairs which admits a Γ-equivariant coarse embedding into a Hilbert space are thus exactly the co-Haagerup subgroups.

This relation between the large scale property of Γ/Λ and the dynamical properties of G yields a series of questions. The action of Γ on βX extends to a continuous action of G. In the case of a normal subgroup, the coarse groupoid $\mathcal{G}(X)$ of X (see [24]) is isomorphic to $\beta Q \rtimes Q$ with Q being the quotient group.

It is an interesting question to describe the coarse groupoid in general. A natural candidate would be $\beta X \rtimes G$, but G does not always act by bounded propagation on X.

Motivated by the case of a normal subgroup, we could also ask how are geometric property (T) of X (see [29]) and dynamical property (T) for the action of G on βX (see [9]) related; or, in the same spirit, the asymptotic dimension of X and the dynamical asymptotic dimension of G acting on βX (see [12]).

4. Stability of Baum–Connes conjecture for Hecke pairs

The goal of this section is to prove the next theorem.

Theorem 4.1. *Let* (Γ, Λ) *be a Hecke pair and* A *a* Γ*-algebra. If every subgroup of* Γ *that is commensurable with* Λ *satisfy the Baum–Connes conjecture with coefficients, and* Γ/Λ *admits a* Γ*-equivariant coarse embedding into Hilbert space, then* Γ *satisfies the Baum–Connes conjecture with coefficients.*

This generalizes previous results:

- If Λ is normal, the theorem reduces to a particular case of Oyono-Oyono's stability result of Baum–Connes by extensions (see [19]), namely the case where the quotient is a-T-menable.
- If Γ/Λ embeds into a locally finite tree, the theorem reduces to Oyono-Oyono's stability result of Baum–Connes for groups acting on trees (see [20]).

The theorem relies on the Higson–Kasparov result that a-T-menable groups satisfy the Baum–Connes conjecture with coefficients [14]. It implies that if a group admits an action by isometries on a real Hilbert space with an orbit that is proper as a metric space, and the commensurate class of the stabilizer satisfies the Baum–Connes conjecture with coefficients, then the group also does.

If Λ and Γ are discrete groups, let us say that Γ is a co-Haagerup extension if Λ is isomorphic to an almost normal subgroup of Γ such that the resulting quotient equivariantly coarsely embeds into a Hilbert space. We define $\mathcal{C}$ to be the smallest class of groups containing a-T-menable groups and Gromov hyperbolic groups, that is closed under co-Haagerup extensions. The theorem implies the following.

Corollary 4.2. *All groups of class $\mathcal{C}$ satisfies the Baum–Connes conjecture with coefficients.*

See Section 6 for a discussion on the class $\mathcal{C}$.

Preliminaries. We first establish general conventions and notations, then give an overview of the proof.

Let G be a locally compact group, and A a G-algebra, by which we mean a C^*-algebra endowed with an action $\alpha : G \to \mathrm{Aut}(A)$ of G by $*$-automorphisms. We suppose as usual that $g \mapsto \alpha_g(a)$ is continuous for every $a \in A$. We will often leave α implicit. We will denote the reduced-crossed product by $A \rtimes_r G$.

We say that G satisfies the Baum–Connes conjecture with coefficients in A if the Baum–Connes assembly map

$$\mu_{G,A} : K_\bullet^{\mathrm{top}}(G, A) \to K_\bullet(A \rtimes_r G)$$

is an isomorphism (see [1] for a definition). For convenience, we will write $\mathrm{BC}(G, A)$ for this statement. If the coefficients are not specified, they are meant to be the complex numbers with trivial G-action. The conjecture with coefficients means that $\mathrm{BC}(G, A)$ holds for all G-algebras A.

The Baum–Connes conjecture with coefficients is known to hold for:

- a-T-menable groups (Higson and Kasparov [14]).
- Gromov hyperbolic groups (Lafforgue [18]).
- Groups acting on trees with a-T-menable stabilizers (Oyono-Oyono [20]).

Counterexamples with nontrivial coefficients are known (see [15]). With complex coefficients, the Baum–Connes conjecture is still open, and it also holds for discrete cocompact subgroups of rank one real Lie groups or $\mathrm{SL}(3, F)$ for a local field F (Lafforgue [17]).

In the case of a product group $G = G_1 \times G_2$, $A \rtimes_r G_1$ is a G_2-algebra, $A \rtimes_r G \cong (A \rtimes_r G_1) \rtimes_r G_2$, and the assembly map can be factored by a partial assembly map. Indeed, let

$$\mu^{(G_2)}_{G_1,A} : K_\bullet^{\mathrm{top}}(G_1 \times G_2, A) \to K_\bullet^{\mathrm{top}}(G_2, A \rtimes_r G_1)$$

be the partial assembly map, first defined in [4] (see Definition 3.9, or Section 2 of [6]). Then the following diagram commutes:

$$\begin{tikzcd}
K_\bullet^{\mathrm{top}}(G, A) \arrow[r, "\mu^{(G_2)}_{G_1,A}"] \arrow[dr, "\mu_{G,A}"'] & K_\bullet^{\mathrm{top}}(G_2, A \rtimes_r G_1) \arrow[d, "\mu_{G_2, A\rtimes_r G_1}"] \\
 & K_\bullet(A \rtimes_r G)
\end{tikzcd}$$

We will use $\mathrm{BC}^{(G_2)}(G_1, A)$ to refer to the statement that $\mu^{(G_2)}_{G_1,A}$ is an isomorphism.

The second ingredient in the proof is the use of Morita invariance of the Baum–Connes assembly map. In our case, we can restrict to Shapiro's lemma, proved in [5].

Recall that if H is a closed subgroup of a locally compact group G, and A a H-algebra with H-action α, the induced algebra $\mathrm{ind}_H^G(A)$ is defined as the sub-C^*-algebra of the bounded continuous functions $f : G \to A$ satisfying $f(gh) = \alpha_h(f(g))$ for every $g \in G,\ h \in H$, and such that the function $gH \mapsto \|f(gH)\|$ belongs to $C_0(G/H)$. It is a G-C^*-algebra with the G-action $\alpha_g(f)(s) = f(g^{-1}s)$ for $f \in \mathrm{ind}_H^G(A)$ and $g, s \in G$.

Proposition 4.3 [5, Corollary 0.6]. *Let H be a closed subgroup of a locally compact group G and A a H-algebra. Then* $\mathrm{BC}(G, \mathrm{ind}_H^G(A))$ *holds if and only if* $\mathrm{BC}(H, A)$ *does.*

Our strategy to prove Theorem 4.1 is the following.

(1) We realize Γ as a closed subgroup of $\Gamma \times G$, where G is the Schlichting completion of the Hecke pair (Γ, Λ).

(2) We define a transitive continuous action of $\Gamma \times G$ on G, with stabilizers isomorphic to Γ. Shapiro's lemma ensures that $\mathrm{BC}(\Gamma, A)$ is equivalent to

$$\mathrm{BC}(\Gamma \times G, C_0(G, A)).$$

(3) If Γ/Λ admits a Γ-equivariant coarse embedding into a Hilbert space, then G is a-T-menable and thus satisfies the Baum–Connes conjecture with coefficients. Factorization by the partial assembly map ensures that it is enough to prove $\mathrm{BC}^{(G_2)}(\Gamma, C_0(G, A))$ in order to show $\mathrm{BC}(\Gamma \times G, C_0(G, A))$.

(4) We show that the Baum–Connes conjecture for all subgroups $L < \Gamma$ containing Λ as a subgroup of finite index implies $\mathrm{BC}^{(G_2)}(\Gamma, C_0(G, A))$.

Proof. Let A be a Γ-algebra. Define the action of $\Gamma \times G$ on $C_0(G, A)$ by

$$((\gamma, g) \cdot f)(x) = \gamma \cdot (f(\gamma x g^{-1})).$$

Proposition 4.4. *In the above setting, if $\mu^{(G)}_{\Gamma, C_0(G,A)}$ and $\mu_{G, C_0(G,A)\rtimes_r \Gamma}$ are isomorphisms, then Γ satisfies the Baum–Connes conjecture with coefficients in A.*

Proof. Let $\Gamma \times G$ act on G by

$$(\gamma, g) \cdot x = \sigma_\gamma x g^{-1}.$$

The action is transitive, and the stabilizer of e_G is isomorphic to Γ:

$$\operatorname{stab}(e_G) = \{(\gamma, \sigma_\gamma)\}_{\gamma \in \Gamma} \cong \Gamma.$$

Since G is Hausdorff, the stabilizer is closed, and by Corollary 0.6 of [5], for every $\Gamma \times G$ algebra (A, α),

$$\mathrm{BC}(\Gamma \times G, C_0(G, A)) \Leftrightarrow \mathrm{BC}(\widetilde{\Gamma}, A_{|\widetilde{\Gamma}}).$$

We denoted the stabilizer $\operatorname{stab}(e_G)$ by $\widetilde{\Gamma}$ to differentiate it from its isomorphic image Γ by the first projection. Here, $A_{\widetilde{\Gamma}}$ is the algebra A endowed with the action $\gamma \cdot a = \alpha_{\gamma, \sigma_\gamma}(a)$. In particular, if G acts trivially on A, and any Γ-algebra can be seen like this, we get that

$$\mathrm{BC}(\Gamma \times G, C_0(G, A)) \Leftrightarrow \mathrm{BC}(\Gamma, A),$$

where the action of $\Gamma \times G$ on $C_0(G, A)$ is given by

$$((\gamma, g) \cdot f)(x) = \gamma \cdot (f(\gamma x g^{-1})).$$

The factorization of the assembly map via the partial assembly gives

$$\mathrm{BC}^{(G)}(\Gamma, C_0(G, A)) \quad \text{and} \quad \mathrm{BC}(\Gamma, C_0(G, A) \rtimes_r \Gamma) \Longrightarrow \mathrm{BC}(\Gamma \times G, C_0(G, A))$$

for A a Γ-algebra, seen as a $\Gamma \times G$-algebra via the trivial action of G. ☐

Theorem 4.5. *Let* (Λ, Γ) *be a Hecke pair, and* (G, K) *its Schlichting completion, and* A *a* Γ*-algebra. If*

- G *satisfies the Baum–Connes conjecture with coefficients in* $C_0(G, A) \rtimes_r \Gamma$,
- *every subgroup* $L < \Gamma$ *containing a conjugate of* Λ *as a subgroup of finite index satisfies the Baum–Connes conjecture with coefficients in* A,

then Γ *satisfies the Baum–Connes conjecture with coefficients in* A.

Proof. Since G satisfies the Baum–Connes conjecture with coefficients in

$$C_0(G, A) \rtimes_r \Gamma,$$

Proposition 4.4 ensures that it is enough to show that the partial assembly map

$$\mu^{(G)}_{\Gamma, C_0(G,A)} : RK_\bullet^{\Gamma \times G}(\underline{E}\Gamma \times \underline{E}G, C_0(G, A)) \to RK_\bullet^{G}(\underline{E}G, C_0(G, A) \rtimes_r \Gamma)$$

is an isomorphism.

The space $\underline{E}G$ can be covered by open subset of the type $G \times_L U$, for L a compact subgroup of G and U a L-space. Moreover, G being totally disconnected, we can restrict to compact open subgroups L. By a standard Mayer–Vietoris argument, it is enough to show that

$$\mu^{(G)}_{\Gamma,C_0(G,A)} : RK^{\Gamma\times G}_{\bullet}(\underline{E}\Gamma\times(G\times_L U), C_0(G,A)) \to RK^{G}_{\bullet}(G\times_L U, C_0(G,A)\rtimes_r\Gamma)$$

is an isomorphism.

By restriction principle, this is equivalent to show that

$$\mu^{(L)}_{\Gamma} : RK^{\Gamma\times L}_{\bullet}(\underline{E}\Gamma\times U, C_0(G,A)_{|\Gamma\times L}) \to RK^{L}_{\bullet}\big(U, (C_0(G,A)\rtimes_r\Gamma)_{|L}\big)$$

is an isomorphism, i.e., $\mathrm{BC}\big(\Gamma\times L, (C_0(G,A)\rtimes_r\Gamma)_{|F}\big)$.

Now, up to replacing L by $L\cap K$, we can suppose $L<K$. As a $\Gamma\times L$-space, G is isomorphic to $G/L\times L$, where the L factor acts only on the right. Since L and K are compact open, the quotient is finite. Thus there are only finitely many $\Gamma\times L$-orbits: $[K:L]$ many. The typical stabilizer of an orbit is isomorphic to $H=\sigma^{-1}(L)$, so contains Λ as a subgroup of finite index.

Green's isomorphism thus entails that $\mathrm{BC}(\Gamma\times L, C_0(G,A)_{\Gamma\times L})$ holds since we supposed $\mathrm{BC}(H,A)$ for every such subgroup H.

We thus proved that

$$\forall H\in\mathcal{S}_\Lambda,\quad \mathrm{BC}(H,A)\Longrightarrow \mathrm{BC}^{(G)}(\Gamma, C_0(G,A))$$

and the proof is done. (We denoted by $\mathcal{S}_\Lambda$ the family of subgroups of Γ containing Λ as a subgroup of finite index.) □

The proof of Theorem 4.1 follows: by Proposition 3.2, if X admits a Γ-equivariant coarse embedding into a Hilbert space, G is a-T-menable, and hence satisfies the Baum–Connes conjecture with coefficients [14].

5. Application to the Novikov conjecture

In order to prove the Novikov conjecture, we use Roe's *descent principle* (see Chapter 8 of [21]): to show that the Novikov conjecture for a discrete group Γ holds, it is enough to construct a compact second-countable Γ-space X such that

- Γ satisfies the Baum–Connes conjecture for every coefficients $C(X,A)$, for every Γ-algebra A,
- X is F-contractible, for every finite subgroup $F<\Gamma$.

This method was extensively used, originally by Higson [13] and later by Chabert, Echterhoff and Oyono-Oyono [6, Theorem 1.9], and by Skandalis, Tu and Yu [24, Theorem 6.1]. They proved that the Novikov conjecture is satisfied if the discrete group admits a coarse embedding into a Hilbert space. We will proceed accordingly in the case of Hecke pairs where the subgroup and the coset space admits coarse embeddings into Hilbert spaces.

Let us denote by $\mathcal{S}_\Lambda$ the family of subgroups of Γ containing Λ as a subgroup of finite index. Recall that Deng [10, Section 4.1] proved the following result.

Theorem 5.1. *Let* Γ *be a group and* Λ *a subgroup. Suppose* Λ *is coarsely embeddable into a Hilbert space, then there exists a compact metrizable* Γ*-space* X *such that, for every* $L \in \mathcal{S}_N$*, the restricted action of* L *on* X *is a-T-menable, and* X *is* F*-contractible, for every finite subgroup* $F < \Gamma$.

We will need the following lemma.

Lemma 5.2. *Let* (G, K) *be the Schlichting completion of a Hecke pair* (Γ, Λ). *Suppose* G *is a-T-menable, then there exists a second countable compact* G*-space* Y *such that the action of* G *is a-T-menable and* Y*, and* Y *is* L*-contractible for every compact open subgroup* $L < G$.

Proof. The action of Γ on βX extends to an action of G, and since G is a-T-menable, so is the groupoid $\beta X \rtimes G$. As in [13] and [24], up to quotienting βX, there exists a compact Hausdorff and second-countable G-space Y such that $Y \rtimes G$ is a-T-menable. Let $\mathcal{Y}$ be the space $\mathrm{prob}(Y)$ of Borel probability measures, endowed with the weak-$*$ topology: it is compact Hausdorff and second-countable. Lemma 6.7 of [24] shows that $\mathcal{Y} \rtimes G$ is a-T-menable. The remaining assertion follows from the fact that G acts on $\mathcal{Y}$ by affine isometries. ☐

Tu [26] proved that if X is a second-countable compact G-space with an a-T-menable action of G, then $\mathrm{BC}(G, C(X, A))$ holds for every G-algebra A. Combining this with Deng's result and the lemma above, if (Γ, Λ) is a Hecke pair with Λ and Γ/Λ are coarsely embeddable into a Hilbert space, we know there exist:

- A second-countable compact metrizable Γ-space X such that
$$\mathrm{BC}(L, C(X, A)_{|L}) \quad \forall L \in \mathcal{S}_N, \forall \Gamma\text{-algebra } A$$
and X is F-contractible for every finite subgroup $F < \Gamma$.
- By a-T-menability of G, a second-countable compact metrizable G-space Y such that $\mathrm{BC}(G, C(Y, A))$ for all G-algebra A and Y is L-contractible for every compact subgroup $L < G$.

We are now able to prove the main result of this section. It generalizes a result of Deng [10, Theorem 1.1] to the case where the subgroup is not normal.

Theorem 5.3. *Let* (Γ, Λ) *be a Hecke pair such that* Λ *and* Γ/Λ *are coarsely embeddable into a Hilbert space, then Novikov's conjecture holds for* Γ.

Proof. It is enough to show that there exists a compact metrizable Γ-space Ω such that $\mu_{\Gamma, C(\Omega, A)}$ is an isomorphism for every Γ-C^*-algebra A.

Let X and Y be second-countable compact spaces as above, and let $\Omega = X \times Y$ with action of $\Gamma \times G$ given by $(\gamma, g) \cdot (x, y) = (\gamma \cdot x, g \cdot y)$. There is a G-equivariant isomorphism of C^*-algebras

$$C_0(G, C(\Omega, A)) \rtimes_r \Gamma \cong C(Y) \otimes (C_0(G \times X, A) \rtimes_r \Gamma),$$

which ensures that $\mu_{G,C_0(G,C(\Omega,A))\rtimes_r\Gamma}$ is an isomorphism.

It is thus enough to show that the partial assembly map $\mu^{(\Gamma\times G)}_{\Gamma,C_0(G,C(\Omega,A))}$ is an isomorphism, which reduces to show that $\mu^{(\Gamma\times L)}_{\Gamma,C_0(G,C(\Omega,A))}$ is an isomorphism, for every compact open subgroup $L < G$, by standard restriction principle. With the same argument as before, the restricted action of $\Gamma \times L$ is a finite union of transitive actions with typical stabilizer $H = \sigma^{-1}(L) \in S_\Lambda$. By Green's principle, $\mu^{(\Gamma\times L)}_{\Gamma,C_0(G,C(\Omega,A))}$ is equivalent to $\mu_{H,C(X,A)}$. The latter being an isomorphism, this concludes the proof. ☐

6. Rational and S-integers points of algebraic groups over algebraic number fields

We present two applications of Theorem 4.1. The first one recover known results, the second one is, to the author's knowledge, new.

SL₂ *of an algebraic number field and of S-integers.* The first application of Theorem 4.1 is to the groups $\mathrm{SL}(2, \mathbb{Z}[1/N])$ and $\mathrm{SL}(2, \mathbb{Q})$. Both have the a-T-menable group $\mathrm{SL}(2, \mathbb{Z})$ as almost normal subgroup, and their respective Schlichting completion can be obtained by Lemma 3.1 with the homomorphisms

$$\mathrm{SL}(2, \mathbb{Z}[1/N]) \to \prod_{p|N} \mathrm{PGL}(2, \mathbb{Q}_p) \quad \text{and} \quad \mathrm{SL}(2, \mathbb{Q}) \to \mathrm{PGL}(2, \mathbb{A}),$$

where $\mathbb{A}$ is the ring of adèles. As both Schlichting completions are a-T-menable, the Hecke pairs are co-Haagerup. This generalizes easily to the following setting: let F be a finite extension of $\mathbb{Q}$, S a set of inequivalent valuations and $\mathcal{O}$ (respectively $\mathcal{O}_S$) the ring of integers (respectively S-integers) of F. Denote by $\mathbb{A}_F$ the ring of adèles of F.

Corollary 6.1. *Let S be a set of primes and $\mathbb{Z}_S$ the ring of S-integers in $\mathbb{Q}$. Then* $\mathrm{SL}(2, \mathbb{Z}_S)$ *and* $\mathrm{SL}(2, \mathbb{Q})$ *satisfy the Baum–Connes conjecture with coefficients. More generally,* $\mathrm{SL}(2, \mathcal{O}_S)$ *and* $\mathrm{SL}(2, \mathbb{A}_F)$ *satisfy the Baum–Connes conjecture with coefficients.*

Let G be an absolutely simple, simply connected algebraic group over F.

Corollary 6.2. *Let Γ be either $G(\mathcal{O}_S)$ or $G(F)$, then Γ satisfies the Novikov conjecture.*

Proof. Let A be a Γ-algebra. Denote $\mathbb{A}_F$ be the ring of adèles of F and R its compact open ring of integers. Observe the almost normal subgroup $\Lambda = G(\mathcal{O})$: its Schlichting completion G will be that of $(G(\mathbb{A}_F), G(R))$ if $\Gamma = G(F)$, or that of

$$\Big(\prod_{v \in S} G(F_v), \prod_{v \in S} G(\mathcal{O}_v)\Big)$$

if $\Gamma = G(\mathcal{O}_S)$.

Every group $L < \Gamma$ containing Λ as a subgroup of finite index is exact, so that $\mu_{L,B}$ is injective for every coefficients B.

By Theorem 5.2 of [16], the map $\mu_{G,A}$ is injective. The diagram

$$\begin{tikzcd}
K_\bullet^{\mathrm{top}}(\Gamma \times G, C_0(G, A)) \arrow[r, "\mu_{\Gamma \times G, C_0(G,A)}"] & K_\bullet(C_0(G, A) \rtimes_r (\Gamma \times G)) \\
K_\bullet^{\mathrm{top}}(\Gamma, A) \arrow[u, "\cong"] \arrow[r, "\mu_{\Gamma,A}"] & K_\bullet(A \rtimes_r \Gamma) \arrow[u, "\cong"']
\end{tikzcd}$$

commutes, and by factorization via partial assembly maps, we have

$$\mu_{\Gamma \times G, C_0(G,A)} = \mu_{G, C_0(G,A) \rtimes_r \Gamma} \circ \mu^{(G)}_{\Gamma,A},$$

hence the map $\mu_{\Gamma,A}$ is injective. We conclude by descent principle. □

These two corollaries also follow from [11], where it is proven that, if K is a field, every countable subgroup of $\mathrm{GL}(n, K)$ is coarsely embeddable into Hilbert space, and if $n = 2$, actually a-T-menable. A different proof can also be found in [2, Theorem 1.5].

Lattices in mixed product groups. Theorem 4.1 and Corollary 4.2 allow to prove the Baum–Connes conjecture for groups in class $\mathcal{C}$, some of which are non-a-T-menable. For instance, the group $\mathbb{Z}^2 \rtimes \mathrm{SL}(2, \mathbb{Z}[1/p])$ is not Haagerup since $\mathbb{Z}^2 < \mathbb{Z}^2 \rtimes \mathrm{SL}(2, \mathbb{Z})$ has relative property (T). Moreover, $\mathbb{Z}^2 \rtimes \mathrm{SL}(2, \mathbb{Z})$ satisfies the Baum–Connes conjecture with coefficients, and is almost normal in $\mathbb{Z}^2 \rtimes \mathrm{SL}(2, \mathbb{Z}[1/p])$. The Schlichting completion of the pair is $\mathrm{PSL}(2, \mathbb{Q}_p)$, which is a-T-menable so that we are in the conditions of the theorem.

This result could have actually been proved by Oyono-Oyono's stability result of the Baum–Connes conjecture by extensions since it is a-T-menable by a-T-menable, or by Oyono-Oyono's result on group acting on trees, since it acts on the Bass–Serre tree of $\mathrm{SL}(2, \mathbb{Q}_p)$ with stabilizers that are finite by a-T-menable.

In order to show that the class $\mathcal{C}$ is interesting, we want to build examples of discrete groups in $\mathcal{C}$ that are not a-T-menable, or more generally, not an extension of a-T-menable by a-T-menable, nor hyperbolic, nor acting on trees with a-T-menable stabilizers.

Proposition 6.3. *Let $\Gamma < G$ be an irreducible lattice in a product $G = G_1 \times G_2$ of locally compact groups such that G_1 is not compact and has property* (*T*), *and G_2 is totally disconnected and a-T-menable. Then Γ is not a-T-menable and*, *for every compact open subgroup $K < G_2$, $\Lambda = \varphi^{-1}(K)$ is co-Haagerup in Γ* (*and thus almost normal*).

Proof. Let us show that Γ is not a-T-menable. Since Γ is of finite covolume in G, $L^\infty(G/\Gamma)$ admits a G-invariant state: it is co-Følner. By Proposition 6.1.5 of [7], if Γ was a-T-menable, so would G be. Since (G, G_1) has relative property (T) and G_1 is notcompact, this is impossible.

Consider the morphism $\varphi : \Gamma \to G_2$ given by the second projection: by irreducibility, we are in the situation of Lemma 3.1. This ensures that Λ is almost normal in Γ, and that the Schlichting completion of (Γ, Λ) is the quotient of G_2 by the largest normal subgroup contained in K, hence it is a-T-menable. Thus Γ/Λ admits an equivariant coarse embedding into Hilbert space (equivalently Λ is co-Haagerup in Γ). ☐

Let G be an absolutely simple algebraic group over $\mathbb{Q}$, and (Γ, Λ) be the Hecke pair $(G(\mathbb{Z}[1/p]), G(\mathbb{Z}))$. Since the Schlichting completion identifies with that of $(G(\mathbb{Q}_p), G(\mathbb{Z}_p))$, it is enough to know that $rk_{\mathbb{Q}_p} G(\mathbb{Q}_p) = 1$ to know that the pair is co-Haagerup. We thus have the following.

Corollary 6.4. *If all subgroups $L < \Gamma$ containing Λ with finite index satisfy the Baum–Connes conjecture with coefficients*, *and $rk_{\mathbb{Q}_p} G(\mathbb{Q}_p) = 1$*, *then Γ satisfy the Baum–Connes conjecture with coefficients.*

In general, the classification of rank 1 groups over nonarchimedean local fields has been completed and accounts can be found; see, for instance, [25]. If one looks at groups with Tits index $C^2_{2,1}$ and $C^2_{3,1}$, choose a $\mathbb{Q}$-form G such that $G(\mathbb{R})$ is isomorphic to $\mathrm{Sp}(n, 1)$, with $n = 3$ or 5. Let $G(\mathcal{O})$ be an arithmetic cocompact lattice: it is Gromov hyperbolic, thus any groups which contains it with finite index satisfies the Baum–Connes conjecture with coefficients by [18]. Moreover, any S-arithmetic group $G(\mathcal{O}_S)$ will contain Λ as a co-Haagerup almost normal subgroup, thus Γ satisfies the Baum–Connes conjecture with coefficients. This gives example of countable subgroups of $\mathrm{GL}(n, K)$ for $n \leq 3$, that satisfy the Baum–Connes conjecture with coefficients.

In both these examples, Γ is non-a-T-menable, since it is an irreducible lattice in $G(\mathbb{R}) \times G(\mathbb{Q}_p)$, and by the S-arithmetic version of Margulis almost normal subgroup theorem, every normal subgroup of Γ is either finite or commensurable to Γ, so that proving the Baum–Connes conjecture by expressing it as an extension will fail. Also, Γ does not admit an isometric action on a tree with stabilizers satisfying the conjecture, nor is it hyperbolic.

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CLÉMENT DELL'AIERA
DEPARTMENT OF MATHEMATICS
UNITÉ DE MATHÉMATIQUES PURES ET APPLIQUÉES (UMPA)
ENS DE LYON
LYON
FRANCE

clement.dellaiera@ens-lyon.fr

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ON HOMOLOGY THEORIES OF CUBICAL DIGRAPHS

ALEXANDER GRIGOR'YAN AND YURI MURANOV

We prove the equivalence of the singular cubical homology and the path homology on the category of cubical digraphs. As a corollary we obtain a new relation between the singular cubical homology of digraphs and simplicial homology.

1. Introduction

The path homology theory and the singular cubical homology theory for the category of digraphs were introduced in [1; 2; 3; 4; 5]. In this category, there is a natural mapping of the cubical homology theory to the path homology theory, that induces an isomorphism of homology groups in dimensions 0 and 1. However, in [5] an example of a digraph was constructed, for which the path homology is trivial in dimension 2 while the singular cubical homology is nontrivial in this dimension. Hence, in general, these two theories give different homologies in dimensions ≥ 2. A natural question arises whether these two theories are equivalent on some subclass of digraphs.

In this paper we present a class of cubical digraphs and prove the equivalence of the singular cubical homology and the path homology theories on this class. As the main technical tool for that, we prove that the image of every map of a digraph cube to a cubical digraph is contractible.

The paper is organized as follows. In Section 2, we recall the basic definitions from graph theory and describe some properties of singular cubical homology H_*^c and the path homology H_* on the category of digraphs using [1; 2; 3; 5]. In Section 3, we recall the definition of cubical digraph from [2] and prove the contractibility of the image of a digraph cube in a cubical digraph for any digraph map. In Section 4, we prove the main result of the paper:

Theorem 1.1. *On the category of cubical digraphs, the singular cubical homology theory is equivalent to the path homology theory.*

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In Corollary 4.6 we obtain a consequence about the relation between the singular cubical homology theory of digraphs and simplicial homology.

2. Singular cubical and path homology theories

In this section we give necessary preliminary material about digraphs and homology theories on the category of finite digraphs.

Definition 2.1. *A digraph G* is a pair (V_G, E_G) of a set $V = V_G$ of *vertices* and a subset $E_G \subset \{V_G \times V_G \setminus \text{diagonal}\}$ of ordered pairs (v, w) of vertices which are called *arrows* and are denoted $v \to w$. The vertex $v = \text{orig}(v \to w)$ is called the *origin* of the arrow and the vertex $w = \text{end}(v \to w)$ is called the *end* of the arrow.

For two vertices $v, w \in V_G$, we write $v \overset{=}{\to} w$ if either $v = w$ or $v \to w$.

A *subgraph* H of a digraph G is a digraph whose set of vertices is a subset of that of G and the set edges of H is a subset of the set of edges of G. In this case we write $G \subset H$.

A subgraph H of G is called *induced* if the edges of H are all those edges of G whose adjacent vertices belong to H. In this case we write $G \sqsubset H$.

A *directed path* $p = (a_1, \alpha_1, a_2, \alpha_2, \dots, \alpha_n, a_{n+1})$ in a digraph G is a sequence of vertices a_i and arrows α_i such that $\alpha_i = (a_i \to a_{i+1})$. The number n of arrows in path is called *length* of the path and is denoted by $|p|$. The vertex a_1 is called the *origin* of the path and the vertex a_{n+1} is called the *end* of the path.

Definition 2.2. A *digraph map* (or simply *map*) from a digraph G to a digraph H is a map $f : V_G \to V_H$ such that $v \overset{=}{\to} w$ in G implies $f(v) \overset{=}{\to} f(w)$ in H.

A digraph map f is *nondegenerate* if $v \to w$ in G implies $f(v) \to f(w)$ in H.

The set of all digraphs with digraph maps form the *category* of digraphs that will be denoted by $\mathcal{D}$.

Definition 2.3. For two digraphs G and H, the *box product* $\Pi = G \Box H$ is defined as a digraph with a set of vertices $V_\Pi = V_G \times V_H$ and a set of arrows E_Π given by the rule

$$(x, y) \to (x', y') \quad \text{if } x = x' \text{ and } y \to y', \text{ or } x \to x' \text{ and } y = y',$$

where $x, x' \in V_G$ and $y, y' \in V_H$.

Fix $n \geq 0$. Denote by I_n any digraph with the set of vertices $V = \{0, 1, \dots, n\}$ such that, for $i = 0, 1, \dots n-1$, there is exactly one arrow $i \to i+1$ or $i+1 \to i$ and there are no other arrows. Such a digraph is called a *line* digraph. It is called a *direct line* digraph if, additionally, all arrows have the form $i \to i+1$. We denote the digraph $0 \to 1$ by I.

For any $n \geq 0$, define a *standard n-cube digraph* I^n as follows. For $n = 0$ we put $I^0 = \{0\}$ which is an one-vertex digraph. For $n \geq 1$, the set of vertices of I^n

consists of all 2^n binary sequences $a = (a_1, \dots, a_n)$, and there is an arrow $a \to b$ between two such vertices if and only if the sequence $b = (b_1, \dots, b_n)$ is obtained from $a = (a_1, \dots, a_n)$ by replacing a digit 0 by 1 at exactly one position. It is easy to see that

$$I^n = \underbrace{I\Box I\Box I\Box \dots \Box I}_{n \text{ times}}.$$

For example, the digraph $0 \to 1$ is an 1-cube. Any digraph that is isomorphic to I^2 will be referred to as a *square*. Any digraph that is isomorphic to I_n and isomorphic to the standard n-cube will be referred to as an *n-cube digraph*.

Let us recall the notion of homotopy in the category of digraphs that was introduced in [1].

Definition 2.4. Two digraph maps $f, g : G \to H$ are called *homotopic* if there exists a line digraph I_n with $n \geq 1$ and a digraph map

$$F : G\Box I_n \to H$$

such that

$$F|_{G\Box\{0\}} = f \quad \text{and} \quad F|_{G\Box\{n\}} = g,$$

where we identify $G\Box\{0\}$ and $G\Box\{n\}$ with G in a natural way. In this case we shall write $f \simeq g$. The map F is called a *homotopy* between f and g.

In the case $n = 1$ we refer to the map F as an *one-step homotopy*.

Definition 2.5. Digraphs G and H are called *homotopy equivalent* if there exist digraph maps

$$f : G \to H, \quad g : H \to G$$

such that

$$f \circ g \simeq \mathrm{id}_H, \quad g \circ f \simeq \mathrm{id}_G.$$

In this case we shall write $H \simeq G$ and the maps f and g are called *homotopy inverses* of each other.

A digraph G is called *contractible* if $G \simeq \{*\}$ where $\{*\}$ is an one-vertex digraph.

Definition 2.6 [1, Definition 3.4]. Let G be a digraph and H be its subgraph.

(i) A *retraction* of G onto H is a map $r : G \to H$ such that $r|_H = \mathrm{id}_H$.

(ii) A retraction $r : G \to H$ is called a *deformation retraction* if $i \circ r \simeq \mathrm{id}_G$, where $i : H \to G$ is the natural inclusion.

Proposition 2.7 [1, Corollary 3.7]. *Let $r : G \to H$ be a retraction of a digraph G onto a subdigraph H and*

$$x \overrightarrow{=} r(x) \quad \text{for all } x \in V_G \qquad \text{or} \qquad r(x) \overrightarrow{=} x \quad \text{for all } x \in V_G. \tag{2-1}$$

Then r is a deformation retraction, the digraphs G and H are homotopy equivalent, and i, r are the homotopy inverses of each other.

Now we recall the definitions of path homology groups from [2] with the group of coefficients $\mathbb{Z}$. An *elementary p-path* on a finite set V is any (ordered) sequence $i_0, \dots, i_p$ of $p+1$ vertices of V that will be denoted by $e_{i_0 \dots i_p}$. By $\Lambda_p = \Lambda_p(V)$ we denote the free abelian group generated by all elementary p-paths $e_{i_0 \dots i_p}$. The elements of Λ_p are called *p-paths*. Thus, each p-path $v \in \Lambda_p$ has the form

$$v = \sum_{i_0, \dots, i_p \in V} v^{i_0 i_1 \dots i_p} e_{i_0 i_1 \dots i_p},$$

where $v^{i_0 i_1 \dots i_p} \in \mathbb{Z}$ are the coefficients of v.

For $p \geq 0$, define the *boundary* operator $\partial : \Lambda_{p+1} \to \Lambda_p$ on basic elements by

$$\partial e_{i_0 \dots i_{p+1}} = \sum_{q=0}^{p+1} (-1)^q e_{i_0 \dots \hat{i}_q \dots i_{p+1}}, \tag{2-2}$$

where $\hat{k}$ means omission of the corresponding index, and extend ∂ to Λ_{p+1} by linearity. Set also $\Lambda_{-1} = \{0\}$ and define $\partial : \Lambda_0 \to \Lambda_{-1}$ by $\partial v = 0$ for all $v \in \Lambda_0$. It follows from this definition that $\partial^2 v = 0$ for any p-path v.

An elementary p-path $e_{i_0 \dots i_p}$ for $p \geq 1$ is called *regular* if $i_k \neq i_{k+1}$ for all k. For $p \geq 1$, let $\mathcal{I}_p$ be the subgroup of Λ_p that is spanned by all irregular $e_{i_0 \dots i_p}$ and we set $\mathcal{I}_0 = \mathcal{I}_{-1} = 0$. Then $\partial \mathcal{I}_{p+1} \subset \mathcal{I}_p$ for $p \geq -1$. Consider the chain complex $\mathcal{R}_*$ with

$$\mathcal{R}_p = \mathcal{R}_p(V) = \Lambda_p / \mathcal{I}_p$$

and with the chain map that is induced by ∂.

Now we define allowed paths on a digraph $G = (V, E)$. A regular elementary path $e_{i_0 \dots i_p}$ in V is called *allowed* if $i_{k-1} \to i_k$ for any $k = 1, \dots, p$, and *nonallowed* otherwise. For $p \geq 1$, denote by $\mathcal{A}_p = \mathcal{A}_p(G)$ the subgroup of $\mathcal{R}_p$ spanned by the allowed elementary p-paths, that is,

$$\mathcal{A}_p = \operatorname{span}\{e_{i_0 \dots i_p} : i_0 \dots i_p \text{ is allowed}\}$$

and set $\mathcal{A}_{-1} = 0$. The elements of $\mathcal{A}_p$ are called *allowed* p-paths.

Consider the following subgroup of $\mathcal{A}_p$ for $p \geq 0$:

$$\Omega_p = \Omega_p(G) = \{v \in \mathcal{A}_p : \partial v \in \mathcal{A}_{p-1}\}. \tag{2-3}$$

The elements of Ω_p are called ∂-*invariant* p-paths. It is easy to see that $\partial \Omega_{p+1} \subset \Omega_p$ so that we obtain a chain complex

$$0 \longleftarrow \Omega_0 \xleftarrow{\partial} \Omega_1 \xleftarrow{\partial} \dots \xleftarrow{\partial} \Omega_{p-1} \xleftarrow{\partial} \Omega_p \xleftarrow{\partial} \dots. \tag{2-4}$$

The *path homology groups* $H_*(G)$ of the digraph G are defined as the homology groups of the chain complex (2-4), that is,

$$H_p(G) := \ker \partial|_{\Omega_p} / \operatorname{Im} \partial|_{\Omega_{p+1}}.$$

In what follows we will also need a natural augmentation $\varepsilon : \Omega_0 \to \mathbb{Z}$ defined by

$$\varepsilon\Big(\sum k_i e_i\Big) = \sum k_i, \quad k_i \in \mathbb{Z}.$$

Clearly, ε is an epimorphism and $\varepsilon \circ \partial = 0$.

Now we recall from [5] the construction of the cubical singular homology theory of digraphs.

Definition 2.8. *A singular n-cube* in a digraph G is a digraph map $\phi : I^n \to G$.

Fix $n \geq 1$. For any $1 \leq j \leq n$ and $\epsilon = 0, 1$, define the inclusion $F_{j\epsilon}^{n-1} : I^{n-1} \to I^n$ of digraphs as follows: if $n \geq 2$, then

$$F_{j\epsilon}^{n-1}(c_1, \dots, c_{n-1}) = \begin{cases} (\epsilon, c_1, \dots, c_{n-1}) & \text{for } j = 1, \\ (c_1, \dots, c_{j-1}, \epsilon, c_j, \dots, c_{n-1}) & \text{for } 1 < j < n, \\ (c_1, \dots, c_{n-1}, \epsilon) & \text{for } j = n \end{cases} \tag{2-5}$$

and if $n = 1$, then $F_{1\epsilon}^{n-1}(0) = (\epsilon)$. We shall write shortly $F_{j\epsilon}$ instead of $F_{j\epsilon}^{n-1}$ if the dimension $n-1$ is clear from the context. Denote by $I_{j\epsilon}^{n-1}$ the image of $F_{j\epsilon}^{n-1}$. We shall write $I_{j\epsilon}$ instead $I_{j\epsilon}^{n-1}$ if the dimension is clear from the context.

Let $Q_{-1} = 0$. For $n \geq 0$, denote $Q_n = Q_n(G)$ the free abelian group generated by all singular n-cubes in G, and denote by $\phi^{\square}$ the singular n-cube ϕ as the element of the group Q_n. For $n \geq 1$ and $1 \leq p \leq n$, denote

$$\phi_{p\epsilon}^{\square} = (\phi \circ F_{p\epsilon})^{\square} \in Q_{n-1}. \tag{2-6}$$

For any $n \geq 1$, define a homomorphism $\partial^c : Q_n \to Q_{n-1}$ on the basis elements $\phi^{\square}$ by the rule

$$\partial^c \phi^{\square} = \sum_{p=1}^{n} (-1)^p (\phi_{p0}^{\square} - \phi_{p1}^{\square}), \tag{2-7}$$

and $\partial^c = 0$ for $n = 0$. Then $(\partial^c)^2 = 0$ and the groups $Q_n(G)$ form a chain complex that we denote $Q_* = Q_*(G)$.

For $n \geq 1$ and $1 \leq p \leq n$, consider the natural projection $T^p : I^n \to I^{n-1}$ on the p-face I^{n-1} defined as follows. For $n = 1$, T^1 is the unique digraph map $I^1 \to I^0$. For $n \geq 2$, we have on the set of vertices

$$T^p(i_1, \dots, i_n) = (i_1, \dots, i_{p-1}, i_{p+1}, \dots, i_n).$$

The singular n-cube $\phi : I^n \to G$ is degenerate if there is $1 \leq p \leq n$ such that $\phi = \psi \circ T^p$ where $\psi : I^{n-1} \to G$ is a singular $(n-1)$-cube. Then an abelian group $B_n = B_n(G)$ that is generated by all degenerated n-cubes is a subgroup Q_n for $n \geq 1$. We put also $B_0 = 0$, $B_{-1} = 0$. Then the quotient group

$$\Omega_p^c(G) = Q_p(G)/B_p(G) \tag{2-8}$$

is defined for $p \geq 0$. We have $\partial(B_n) \subset B_{n-1}$, and hence $B_*(G) \subset Q_*(G)$. Hence the quotient complex $\Omega_*^c(G) = Q_*(G)/B_*(G)$ is defined. We continue to denote the boundary operator in this complex ∂^c. The homology group $H_k(\Omega_*^c(G))$ is called the *singular cubical homology group of digraph G in dimension k* and is denoted $H_k^c(G)$.

We have a natural augmentation homomorphism $\varepsilon : \Omega_0^c(G) \to \mathbb{Z}$, defined by

$$\varepsilon\Big(\sum k_i \phi_i\Big) = \sum k_i, \quad k_i \in \mathbb{Z}.$$

Then ε is an epimorphism and $\varepsilon \circ \partial^c = 0$.

Here are some basic properties of the path and the singular cubical homology groups from [2] and [5].

- The groups $H_*^c(X)$ and $H_*(X)$ are functors from the category $\mathcal{D}$ to the category of abelian groups.

- Let $f \simeq g : X \to Y$ be two homotopic digraph maps. Then the induced homomorphisms f_*, g_* of homology groups are equal for $k \geq 0$ for the both theories.

3. Maps from cube to cubical digraph

In this section we slightly reformulate the definition of a cubical digraph from [2] and prove Theorem 3.6 saying that an image of a cube in a cubical digraph is contractible.

Recall that any vertex of a a cube I^n is given by a sequence of binary numbers $(a_1, \dots, a_n)$. For any arrow $a \to b$ in a digraph cube I^n we have also the arrow

$$\gamma_i = (0, \dots, 0) \to (b_1 - a_1, \dots, b_n - a_n) \tag{3-1}$$

in I^n where the right sequence represents a vertex in I^n that has only one nontrivial element 1 at some position i. We say that two arrows $\alpha = (a \to b)$ and $\beta = (c \to d)$ of I^n are *parallel* and write $\alpha \parallel \beta$ if

$$(b_1 - a_1, \dots, b_n - a_n) = (d_1 - c_1, \dots, d_n - c_n).$$

In the opposite case we say that the arrows α and β are *orthogonal.*

An arrow $\alpha \in E_{I^n}$ defines two $(n-1)$-faces of I^n: the face $I_0 = I_0^\alpha$ which contains the origin vertices of the arrows that are parallel to α and the face $I_1 = I_1^\alpha$ which contains the end vertices of the arrows that are parallel to α. Note that any arrow that is orthogonal to α lies in I_0 or in I_1.

For the digraph cube I^n, there is a natural partial order on the set of its vertices V_{I^n} that is defined as follows: we write $a \leq b$ if there exists a path along the arrows with the origin vertex a and the end vertex b. Now we introduce the *distance* $\Delta(a, b)$ for a pair of vertex $a, b \in I^n$ that is defined only for comparable pair of vertices.

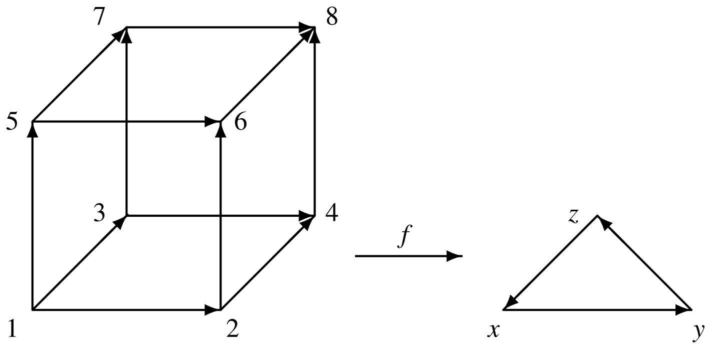

Figure 1. The map $f : I^3 \to G$ with noncontractible image.

Let a, b be two vertices of I^n such that $a \leq b$. As it follows from the definition of I^n, the length of the path p from a to b does not depend on the choice of the path, and we set

$$\Delta(a, b) = \Delta(b, a) := |p|.$$

We shall refer to the vertex $a = (0, \ldots, 0)$ of a cube as the *origin vertex* and to the vertex $d = (1, \ldots, 1)$ as the *end vertex*.

It follows immediately from the definition of I^n that, for any vertex x, the distances $\Delta(a, x)$ and $\Delta(x, d)$ are well defined. For an arrow $\alpha = (x \to y)$ we define $\Delta(\alpha, d) := \Delta(y, d)$.

Let $a \leq b$ be a pair of comparable vertices of I^n. Denote by $I_{a,b}$ the induced subgraph of I^n with the set of vertices $\{c \in V_{I^n} \mid a \leq c \leq b\}$. Clearly, $I_{a,b}$ is isomorphic to a digraph cube I^k, where $k = |p| = \Delta(a, b)$.

Definition 3.1. A subgraph G of I^n is called *cubical* if, for any two vertices $a, b \in V_G \subset V_{I^n}$ with $a \leq b$, we have $I_{a,b} \sqsubset G$.

Note that the set of all paths from a to b in $I_{a,b}$ coincides with the set of all paths from a to b in G. It is easy to see that cubical digraphs with digraph maps form a category. Now we prove that the image of a cube I^n in any cubical digraph is contractible. Note that this statement is not true for general digraphs.

Example 3.2. Consider a digraph map f (see Figure 1) that maps the cube I^3 onto the cycle digraph G and that is defined by $f(1) = f(8) = x$, $f(2) = f(3) = f(5) = y$, $f(4) = f(6) = f(7) = z$. Then the images of this map G is noncontractible.

Now consider a digraph map $f : I^n \to G$ where G is a cubical digraph. The image $f(I^n)$ is connected as the image of a connected digraph. Let $s = (0, \ldots, 0) \in V_{I^n}$ be the origin vertex and $z = (1, \ldots, 1) \in V_{I^n}$ be the end vertex of I^n. Then $f(s) \in V_G$, $f(z) \in V_G$ and $f(I^n) \subset I_{f(s),f(z)} \subset G$ where $I_{f(s),f(z)}$ is isomorphic to an m-dimensional cube which we denote $J = J^m \cong I^m$ where $m = \Delta(f(s), f(z))$. Hence, without loss of generality, we can assume that $G = I_{f(s),f(z)} = J$, that is,

$$f(s) = (0, \dots, 0) \in V_J, \quad f(z) = d = (1, \dots, 1) \in V_J.$$

For $m = 0, 1, 2$ the image $f(I^n) \subset G$ is contractible since all connected subgraphs of the digraphs J^0, J^1, and J^2 are contractible.

Consider the case $J = J^m$ where $m \geq 3$ and $d = (1, \dots, 1) \in V_J$ is the end vertex of the cube J. Since $d = f(z) \in \text{Image}(f)$, there exists a nonempty set of arrows $\Gamma \subset E_J$ defined by

$$[\tau \in \Gamma] \Leftrightarrow [\text{end}(\tau) = d \text{ and } \tau = f(\alpha), \alpha \in E_{I^n}].$$

The set Γ consists of arrows in E_J with the end vertex d that are lying in the image of the map f. Let $\gamma = (c \to d) \in \Gamma$ be an arrow satisfying

$$\begin{cases} f(\alpha) = f(x \to y) = (c \to d) = \gamma, \\ \Delta(\alpha, z) = \Delta(y, z) = k \geq 0 \text{ is minimal.} \end{cases} \tag{3-2}$$

Note that α is not uniquely defined.

Lemma 3.3. *For every vertex $v \in V_{I^n}$ with $\Delta(v, z) \leq k$ we have $f(v) = d$. Hence the cube $I_{y,z} \sqsubset I^n$ is mapped by f into the vertex d.*

Proof. It follows immediately from the definition of k in (3-2). ☐

The arrow γ defines two $(m-1)$-dimensional faces J_0 and J_1 of the cube J with $c \in V_{J_0}$, $d \in V_{J_1}$ and we have the natural projection $\pi : J \to J_0$ along the arrow γ. Let H be a subgraph of I^n. We define subgraphs $K_0, K_1, K \subset J$ that depend on the map $f : I^n \to J$ and $H \subset I^n$ such that

$$K := f(H) \subset J, \quad K_0 := f(H) \cap J_0 \subset J_0, \quad \text{and} \quad K_1 := f(H) \cap J_1 \subset J_1. \tag{3-3}$$

It is easy to see that for an arrow $(v \to w) \in E_J$ we have

$$[(v \to w) \parallel \gamma] \Leftrightarrow [(v \in J_0) \text{ and } (w \in J_1)]. \tag{3-4}$$

For technical reasons we introduce the following definition.

Definition 3.4. Let H be a subgraph of I^n and $f : I^n \to J$ be a digraph map. Let the digraphs $K_0, K_1, K \subset J$ be defined as above using (3-2) and (3-3). We say that the subgraph H satisfies the Π-*condition* if the following conditions are satisfied:

(1) For all $w \in V_{K_1}$ there is a vertex $v \in V_{K_0}$ such that $(v \to w) \in E_K$.

(2) For all $(w \to w') \in E_{K_1}$ we have $\pi(w \to w') \in E_{K_0}$.

The next statement is our key technical result.

Proposition 3.5. *Consider the map $f : I^n \to J = J^m$ with $m \geq 3$. Let k and γ are defined in (3-2). Then the cube I^n satisfies the Π-condition.*

Proof. Using induction on $k \geq 0$.

The base of induction, $k = 0$. Hence $y = z = (1, \dots, 1) \in V_{I^n}$ is the end vertex of I^n and $n \geq m \geq 3$. The arrow $\alpha = (x \to z) \in E_{I^n}$ with

$$f(\alpha) = f(x \to z) = \gamma = (c \to d) \tag{3-5}$$

defines $(n-1)$-face $I_0 = I_{s,x}$ and opposite $(n-1)$-face I_1 of the cube I^n. Let $a = (0, \dots, 0)$ be the origin vertex of J (and hence the origin vertex of J_0) and b the origin vertex of J_1. Then $a \to b$ is parallel to $\gamma = (c \to d)$. We have

$$f(I_0) = f(I_{s,x}) \subset I_{f(s), f(x)} = I_{a,c} = J_0 \tag{3-6}$$

and hence, by (3-3) for $H = I^n$, we have $f(I_0) \subset K_0$. Let t be a vertex of I_1 such that $w = f(t) \notin V_{K_0}$, that is, $w \in V_{K_1} \subset V_{J_1}$. There exists an unique vertex $r \in V_{I_0}$ such that $(r \to t) \in E_{I^n}$ is parallel to α and $f(r) = v \in K_0 \subset J_0$ by (3-6). Thus $f(r \to t) = v \to w$ with $v \in V_{K_0}$ and condition (1) of Definition 3.4 is satisfied.

Now let $\tau = (w \to w') \in E_{K_1}$ be an arrow such that $f(t \to t') = \tau$, that is,

$$f(t) = w, \quad f(t') = w', \qquad t, t' \in V_{I_1}.$$

The same line of arguments as above gives the vertices $r, r' \in V_{I_0}$ such that $(r \to t)$ and $r' \to t'$ are parallel to α and hence, $\pi(\tau) = f(r \to r')$ since $f(r), f(r') \in V_{K_0}$. This proves condition (2) of Definition 3.4. Thus Π-condition is satisfied for the cube I^n and $k = 0$.

We now consider the induction step. By inductive assumption we have that any map $f : I^n \to J$ satisfies the Π-condition if $\Delta(y, z) \leq k - 1 \geq 0$. Consider the case $\Delta(y, z) = k \geq 1$ and hence

$$\Delta(x, z) = \Delta(y, z) + 1 = k + 1 \geq 2$$

where

$$z = (\underbrace{1, \dots, 1}_{n}) \in V_{I^n}.$$

Thus, without loss of generality, we can suppose that

$$x = (\underbrace{1, \dots, 1}_{n-k-1}, \underbrace{0, 0, \dots, 0}_{k+1}), \qquad y = (\underbrace{1, \dots, 1}_{n-k-1}, 1, \underbrace{0, \dots, 0}_{k}). \tag{3-7}$$

From now we put $y_0 = y \in V_{I^n}$ and let the vertex y_i is obtained from y by replacing the last coordinate 1 in y by 0, and i-th coordinate 0 of y by 1 for $1 \leq i \leq k$. For example,

$$y_2 = (\underbrace{1, \dots, 1}_{n-k-1}, 0, \underbrace{0, 1, 0 \dots, 0}_{k}), \qquad y_k = (\underbrace{1, \dots, 1}_{n-k-1}, 0, \underbrace{0, 0, \dots, 0, 1}_{k}).$$

We also define

$$\alpha_i = (x \to y_i) \in E_{I^n} \quad \text{for } 0 \le i \le k.$$

By Lemma 3.3 we have

$$f(\alpha_i) = f(x \to y_i) = (c \to d) = \gamma \quad \text{for } 0 \le i \le k.$$

Let $I_0 = I_{s,x}$ be $(n-k-1)$-dimensional subcube of I^n. Then, as before, we have

$$f(I_0) \subset K_0 \subset J_0.$$

Consider a vertex $t \in V_{I^n}$ and $t \notin V_{I_0}$ that has the form

$$t = (a_1, \dots, a_{n-k-1}, b_0, \dots, b_k) \notin I_0, \quad a_i, b_j \in \{0, 1\},$$

where at least one coordinate b_j is 1. If at least one coordinate b_j is 0 we obtain that $t \in I_{s,z_j} \sqsubset I^n$ where

$$z_j = (\underbrace{1, \dots, 1}_{n-k-1}, \underbrace{1, \dots, \overset{j}{\hat{0}}, \dots, 1}_{k+1}).$$

The $(n-1)$-dimensional subcube $I_{s,z_j} \subset I^n$ contains the vertices x and t. Moreover, $\Delta(x, z_j) = k$ and there is an arrow

$$\alpha_i = (x \to y_i) \in E_{I_{s,z_j}}$$

with

$$f(\alpha_i) = \gamma \quad \text{and} \quad \Delta(\alpha_i, z_j) = k-1.$$

Hence, by the inductive assumption, the map

$$f|_{I_{s,z_j}} : I_{s,z_j} \to J$$

satisfies the Π-condition. Hence the conditions (1) and (2) of Definition 3.4 are satisfied for every $(n-1)$-dimensional subcube $I_{s,z_j} \subset I^n$.

Now consider a vertex t for which all $(k+1)$-coordinates b_j are equal to 1 such that $t \notin I_{x,z}$. This means that at least one of the first $(n-k-1)$-coordinates a_i is 0. Recall that $(k+1) \ge 2$. Thus, consider the vertices

$$t = (a_1, \dots, a_{n-k-1}, \underbrace{1, \dots, 1}_{k+1}) \notin I_0, \quad r = (a_1, \dots, a_{n-k-1}, \underbrace{0, \dots, 0}_{k+1}) \in I_0, \tag{3-8}$$

where $a_i \in \{0, 1\}$. Consider a directed path p in the digraph I_0 from the vertex $r \in V_{I_0}$ to the vertex $x \in V_{I_0}$ of the length $l = |p| \ge 1$ (since $t \notin I_{x,z}$). Write this path in the form

$$p = (r \to x_1 \to x_2 \to \cdots \to x_{l-1} \to x_l = x) \subset I_{r,x} \subset I_0.$$

Consider a directed path q from the vertex $r \in V_{I_0}$ to the vertex t of the length

$$k+1=|q|\geq 2.$$

Note that q lies in the digraph $I_{r,t}$ of dimension $k+1$. Write this path in the form

$$q=(r\to r^1\to r^2\to\cdots\to r^k\to r^{k+1}=t)\subset I_{r,t}.$$

Any such two paths p and q define a unique subgraph of the digraph I^n that has the form

$$\begin{tikzcd}
t=r^{k+1} \arrow[r] & r_1^{k+1} \arrow[r] & r_2^{k+1} \arrow[r] & \dots \arrow[r] & r_l^{k+1}=z \\
r^k \arrow[u] \arrow[r] & r_1^k \arrow[u] \arrow[r] & r_2^k \arrow[u] \arrow[r] & \dots \arrow[u] \arrow[r] & r_l^k \arrow[u] \\
\dots \arrow[u] \arrow[r] & \dots \arrow[u] \arrow[r] & \dots \arrow[u] \arrow[r] & \dots \arrow[u] \arrow[r] & \dots \arrow[u] \\
r^1 \arrow[u] \arrow[r] & r_1^1 \arrow[u] \arrow[r] & r_2^1 \arrow[u] \arrow[r] & \dots \arrow[u] \arrow[r] & r_l^1 \arrow[u] \\
r \arrow[u] \arrow[r] & x_1 \arrow[u] \arrow[r] & x_2 \arrow[u] \arrow[r] & \dots \arrow[u] \arrow[r] & x_l=x \arrow[u]
\end{tikzcd} \tag{3-9}$$

Now using induction in the length $l=|p|\geq 1$ we prove the following statement.

Statement A. For every path q and every path p, as above, there is a path

$$p'=(r\to x_1'\to x_2'\to\cdots\to x_{l-1}'\to x_l'=x)\subset I_{r,x}\subset I_0$$

(that may be equal to p) such that q and p' defines the subgraph (similarly as above)

$$\begin{tikzcd}
t=r^{k+1} \arrow[r] & r_1^{k+1'} \arrow[r] & r_2^{k+1'} \arrow[r] & \dots \arrow[r] & r_l^{k+1'}=z \\
r^k \arrow[u] \arrow[r] & r_1^{k'} \arrow[u] \arrow[r] & r_2^{k'} \arrow[u] \arrow[r] & \dots \arrow[u] \arrow[r] & r_l^{k'} \arrow[u] \\
\dots \arrow[u] \arrow[r] & \dots \arrow[u] \arrow[r] & \dots \arrow[u] \arrow[r] & \dots \arrow[u] \arrow[r] & \dots \arrow[u] \\
r^1 \arrow[u] \arrow[r] & r_1^{1'} \arrow[u] \arrow[r] & r_2^{1'} \arrow[u] \arrow[r] & \dots \arrow[u] \arrow[r] & r_l^{1'} \arrow[u] \\
r \arrow[u] \arrow[r] & x_1' \arrow[u] \arrow[r] & x_2' \arrow[u] \arrow[r] & \dots \arrow[u] \arrow[r] & x_l'=x \arrow[u]
\end{tikzcd} \tag{3-10}$$

and at least one of the following conditions is satisfied:

$$\text{(i) } f(t) = f(r^k), \quad \text{(ii) } f(t) = f(r_1^k), \quad \text{(iii) } f(t) = f(r_1^{k'}). \tag{3-11}$$

The base of induction for Statement A, the case $l = 1$. Consider the unique path $p = (r \to x) \subset I_0$ of the length $l = 1$ and a path q as above. We have the following subgraph of the digraph I^n:

$$\begin{tikzcd}
t = r^{k+1} \arrow[r] & r_1^{k+1} = z \\
r^k \arrow[u] \arrow[r] & r_1^k \arrow[u] \\
\vdots \arrow[u] \arrow[r] & \vdots \arrow[u] \\
r^1 \arrow[u] \arrow[r] & r_1^1 \arrow[u] \\
r \arrow[u] \arrow[r] & x_1 = x \arrow[u]
\end{tikzcd} \tag{3-12}$$

where

$$r, x \in V_{I_0} \quad \text{and} \quad f(r), f(x) \in V_{K_0},$$

and

$$f(r_1^i) = d \quad \text{for } 1 \leq i \leq k+1$$

since $k \geq 1$. Hence,

$$f(r_1^k) = f(r_1^{k+1}) = d$$

and thus at least one of the conditions (i) or (ii) in (3-11) is satisfied because there are no triangles in the digraph J. We put in this case $p' = p$, and hence the base of induction $l = 1$ is proved.

Inductive step of induction for Statement A. Consider vertices $t, r \in V_J$ given in (3-8) where

$$\Delta(t, r) = k + 1 \geq 2 \quad \text{and} \quad \Delta(r, x) \geq 2.$$

Let p be a path from r to x and q be a path from r to t as the above. Recall that

$$|q| = k + 1 \geq 2 \quad \text{and} \quad |p| = l \geq 2.$$

These paths define the subgraph of I^n given in (3-9). By the inductive assumption, for the vertex r_1^{k+1} at least one of the conditions

$$\text{(i) } f(r_1^{k+1}) = f(r_1^k), \quad \text{(ii) } f(r_1^{k+1}) = f(r_2^k), \quad \text{(iii) } f(r_1^{k+1}) = f(r_2^{k''}), \tag{3-13}$$

that is similar to (3-11) is realized. In (3-13) we have a path

$$r^k \to r_1^k \to r_2^{k''} \to \cdots \to r_l^k,$$

that is, from (3-9), similar to the path

$$r^k \to r_1^k \to r_2^k \to \cdots \to r_l^k.$$

If condition (i) is realized, that is, $f(r_1^{k+1}) = f(r_1^k)$, then for $f(t)$ at least one of the conditions (i) or (ii) in (3-11) is satisfied since there are no triangles in the digraph J (similar to the case $l = 1$).

If condition (ii) is realized and condition (i) is not realized, that is,

$$f(r_1^{k+1}) = f(r_2^k) \quad \text{and} \quad f(r_1^k) \neq f(r_2^k),$$

we can consider the subcube of I^n given in Figure 2 that is defined by the subgraph of (3-9) given by

$$\begin{tikzcd} t = r^{k+1} \arrow[r] & r_1^{k+1} \arrow[r] & r_2^{k+1} \\ r^k \arrow[u] \arrow[r] & r_1^k \arrow[u] \arrow[r] & r_2^k \arrow[u] \end{tikzcd} \tag{3-14}$$

We have

$$f(r_1^{k+1}) = f(r_2^k) \quad \text{and} \quad f(r_1^k) \neq f(r_2^k),$$

that is,

$$f(r_1^k \to r_1^{k+1}) = f(r_1^k \to r_2^k) \in E_J$$

is an arrow. If $f(r^k) = f(r_1^k)$, then the same line of above gives that

$$f(t) = f(r_1^k) \quad \text{or} \quad f(t) = f(r_2^k)$$

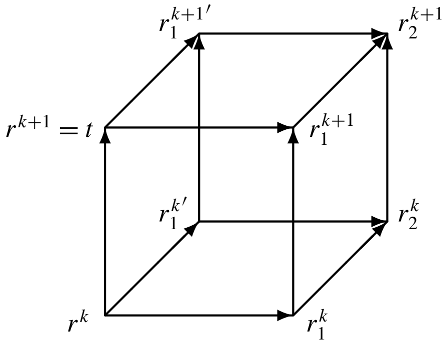

Figure 2. The subcube of I^n that is defined by the digraph in (3-13).

and the step of induction is proved. Let $f(r_k) \neq f(r_1^k)$, then

$$f(I_{r^k,r_2^k}) \subset f(I_{f(r^k),f(r_2^k)}) \quad \text{and} \quad f(I_{r^k,r_1^{k+1}}) \subset f(I_{f(r^k),f(r_2^k)}),$$

where $I_{f(r^k),f(r_2^k)}$ is the digraph square. Hence at least one of conditions

$$f(r^{k+1}) = f(r_1^k) \quad \text{or} \quad f(r^{k+1}) = f(r_1^{k'})$$

is satisfied and the inductive assumption is proved.

Consider the case when condition (iii) is realized and conditions (i) and (ii) are not realized. This case is the same as the case (ii). We must to start the consideration from the path

$$r^k \to r_1^k \to r_2^{k''} \to \cdots \to r_l^k$$

on the place of the path

$$r^k \to r_1^k \to r_2^k \to \cdots \to r_l^k$$

from (3-9). This finishes the proof of the inductive step as well as Statement A.

Since each of the vertices r^k, r_1^k, $r_1^{k'}$ lies in the image of a subcube I_{r,z_j} it follows from Statement A that image $w = f(t)$ lies in the image of a subcube I_{r,z_j} with

$$\Delta(x, z_j) = \Delta(r, z_j) = k,$$

which satisfies Π-condition by the inductive assumption in k. Hence condition (1) of Definition 3.4 is satisfied for every subcube $I_{r,t} \subset I^n$. By a similar way, it follows from Statement A that the image of every arrow with end or origin t lies in the image of a subcube I_{r,z_j} which satisfies Π-condition by the inductive assumption in k. Hence condition (2) of Definition 3.4 is satisfied for every subcube $I_{r,t} \subset I^n$. Hence every cube $I_{r,t}$ satisfies the Π-condition, and hence the cube I^n satisfies the Π-condition. This completes the proof of Proposition 3.5. □

Theorem 3.6. *Let $f : I^n \to G$ be a digraph map to a cubical digraph. Then the image $f(I^n) \subset G$ is contractible.*

Proof. The image $f(I^n)$ lies in the digraph $J = J^m$. Now we use the induction in m. For $m = 0, 1, 2$ the image $f(I^n)$ is contractible since all connected subgraphs of J are contractible. For $m \geq 3$ the digraph I^n satisfies the Π-condition, then (2-7) and conditions (1) and (2) of Definition 3.4 imply that restriction $\pi|_K$ of the projection $\pi : J^m \to J_0^{m-1}$ to the image K of the map f is well defined deformation retraction to K_0. But K_0 is contractible by the inductive assumption in m. □

4. Equivalence to homology theories on cubical digraphs

In this section we prove our main result, Theorem 1.1, stated below as Theorem 4.5. For that we use the acyclic carrier theorem from homology theory (see, for example, [6, Section 3.4] and [7, Section 1.2.1]). Recall that a chain complex C_* is called *nonnegative* if $C_p = 0$ for $p < 0$ and is called *free* if C_p are finitely generated free abelian groups for all p. We say that C_* is a *geometric chain complex* if it is nonnegative, free, and if a basis $\mathcal{B}_p$ is chosen in the group C_p for any $p \geq 0$. For example, any finite simplicial complex gives rise to a geometric chain complex, where $\mathcal{B}_p$ consists of all p-simplexes.

Let C_* be a geometric chain complex with fixed bases $\mathcal{B}_p$. For $b \in \mathcal{B}_{p-1}$ and $b' \in \mathcal{B}_p$, we write $b \prec b'$ if b enters with a nonzero coefficient into the expansion of $\partial b'$ in the basis $\mathcal{B}_{p-1}$. The *augmentation homomorphism* $\varepsilon : C_0 \to \mathbb{Z}$ is defined by

$$\varepsilon\Big(\sum_i k_i b_i\Big) = \sum_i k_i, \quad k_i \in \mathbb{Z},\ b_i \in \mathcal{B}_0,$$

and by $\widetilde{C}_*$ we denote the augmented complex

$$0 \longleftarrow \mathbb{Z} \xleftarrow{\varepsilon} C_0 \xleftarrow{\partial} C_1 \xleftarrow{\partial} \cdots.$$

A geometric chain complex C_* is called *acyclic* if all homology groups of the augmented complex $\widetilde{C}_*$ are trivial.

Let C_* and D_* be two geometric complexes with augmentation homomorphism ε and ε', respectively. A chain map $\phi_* : C_* \to D_*$ is called *augmentation preserving* if $\varepsilon'\phi_0(c) = \varepsilon(c)$ for any $c \in C_0$.

Definition 4.1. Let C_* and D_* be two geometric chain complexes.

(i) An *algebraic carrier* function from C_* to D_* is a mapping E that assigns to any basis element b in C_* a subcomplex $E_*(b) := E(b)$ of D_*, such that $b \prec b'$ implies $E_*(b) \subset E_*(b')$.

(ii) An algebraic carrier function E is called *acyclic* if each complex $E_*(b)$ is nonempty and acyclic.

(iii) A chain map $f_* : C_* \to D_*$ is *carried by E* if $f_n(b) \in E_*(b)$ for any basis element b in C_n.

We state the acyclic carrier theorem in the following form.

Theorem 4.2 [6, Section 3.4; 7, Section 1.2.1]. *Let C_* and D_* be two geometric chain complexes and E be an acyclic carrier function from C_* to D_*. If $f_*, g_* : C_* \to D_*$ are augmentation preserving chain maps that are carried by E, then f_* and g_* are chain homotopic.*

Before the proof of Theorem 1.1, we state and prove some technical results. We use the notations of [2; 5]. Let G be a cubical digraph. The free abelian groups $\Omega^c_p = \Omega^c_p(G)$ and $\Omega_p = \Omega_p(G)$ defined in (2-3) and (2-8) are finitely generated.

Let $I^0 = \{*\}$ be the one-vertex digraph. Any 0-dimensional singular cube $\phi : I^0 = \{*\} \to G$ is given by the vertex $\phi(*) \in V_G$ and thus we obtain the map $\tau_0 : \Omega^c_0(G) \to \Omega_0(G)$ which preserve augmentation.

For any digraph cube I^n $(n \geq 1)$ we denote by P the set of all directed paths of the length n going from the origin vertex

$$\underbrace{(0, \dots, 0)}_{n}$$

of the cube to the end vertex

$$\underbrace{(1, \dots, 1)}_{n}.$$

Every path $p \in P$ has the form

$$p = (a_0 \to a_1 \to a_2 \to \cdots \to a_n), \quad a_i \in V_{I_n}. \tag{4-1}$$

In (4-1) for $1 \leq i \leq n$ the vertex a_i differs from a_{i-1} only by one coordinate $1 \leq \pi(i) \leq n$ that equals 0 for a_{i-1} and 1 for a_i. Let $\sigma(p)$ be a sign of the permutation

$$\pi(p) = \begin{pmatrix} 1 & 2 & \dots & n \\ \pi(1) & \pi(2) & \dots & \pi(n) \end{pmatrix}.$$

Consider the path $w_n \in \Omega_n(I^n)$ given by

$$w_n = \sum_{p \in P} (-1)^{\sigma(p)} p, \tag{4-2}$$

which is the generator of the group $\Omega_n(I^n)$ (see [5] and [2]). For any singular n-dimensional cube $\phi : I^n \to G$, which gives a basic element $\phi^{\square} \in \Omega_n^c(G)$, we have a morphism of chain complexes defined in [5]

$$\tau_* : \Omega_*^c(G) \to \Omega_*(G), \quad \tau_n(\phi^{\square}) := \phi_*(w_n), \tag{4-3}$$

where $\phi_* : \Omega_*(I^n) \to \Omega_*(G)$ is the induced of ϕ morphism of chain complexes.

For $n \geq 0$ consider the set K_n of all subcubes G of dimension n that have the form $I_{s,t}$ with $s, t \in V_G$. By [2; 5], for every cube $I_{s,t} \in K_n$ there is an isomorphism $\chi_{s,t} : I^n \to I_{s,t}$ such that the set of elements

$$\{(\chi_{s,t})_*(w_n) : I_{s,t} \in K_n\}$$

gives the basis of $\Omega_n(G)$. For $n \geq 1$, define homomorphisms $\theta_n : \Omega_n(G) \to \Omega_n^c(G)$ on basic elements by

$$\theta_n((\chi_{s,t})_*(w_n)) = \chi_{s,t}^{\square}, \tag{4-4}$$

and then extend it by linearity. It is clear that θ_0 preserves the augmentation.

Proposition 4.3. *The homomorphisms θ_n define a morphism of chain complexes*

$$\theta_* : \Omega_*(G) \to \Omega_*^c(G), \tag{4-5}$$

which is a right inverse morphism to τ_*, *that is,*

$$\tau_*\theta_* = \mathrm{Id} : \Omega_*(G) \to \Omega_*(G).$$

Proof. Let us first prove that $\tau_n\theta_n = \mathrm{Id}$. For $n = 0, 1$ this is trivial. Let $n \geq 2$ and $(\chi_{s,t})_*(w_n) \in \Omega_n(G)$ be a basic element. By (4-4) and (4-3) we have

$$\tau_n\theta_n((\chi_{s,t})_*(w_n)) = \tau_n(\chi^{\square}_{s,t}) = \chi_{s,t*}(w_n). \tag{4-6}$$

Consider the diagram

$$\begin{tikzcd} \Omega_n(G) \arrow[r, "\theta_n"] \arrow[d, "\partial"] & \Omega^c_n(G) \arrow[r, "\tau_n"] \arrow[d, "\partial^c"] & \Omega_n(G) \arrow[d, "\partial"] \\ \Omega_{n-1}(G) \arrow[r, "\theta_{n-1}"] & \Omega^c_{n-1}(G) \arrow[r, "\tau_{n-1}"] & \Omega_{n-1}(G) \end{tikzcd} \tag{4-7}$$

where the horizontal compositions are identity homomorphisms by (4-6), the right square is commutative and the large square is evidently commutative. Now we prove that the left square is commutative. It follows from [2, Lemma 4] that, for

$$(\phi_{s,t})_*(w_n) \in \Omega_n(G),$$

we have

$$\begin{aligned} \theta_{n-1}\big(\partial((\phi_{s,t})_*(w_n))\big) &= \theta_{n-1}\Big(\sum_{I_{s',t'}\subset I_{s,t}} (-1)^{\sigma(I,I')}(\phi_{s',t'})_*(w_{n-1})\Big) \\ &= \sum(-1)^{\sigma(I,I')}\phi^{\square}_{s',t'}, \end{aligned} \tag{4-8}$$

where the sum is taken over all $(n-1)$-cubes $I' = I_{s',t'} \subset I_{s,t} = I$. By (2-7) and (4-4) for

$$(\phi_{s,t})_*(w_n) \in \Omega_n(G),$$

we have

$$\partial^c\big(\theta((\phi_{s,t})_*(w_n))\big) = \partial^c(\phi^{\square}_{s,t}) = \sum_{p=1}^{n}(-1)^p\big((\phi^{\square}_{s,t})_{p,0} - (\phi^{\square}_{s,t})_{p,1}\big), \tag{4-9}$$

where the sum consists of all singular $(n-1)$-subcubes of the cube I^n with coefficients. Since bottom row in (4-7) is the identity homomorphism we conclude from (4-3), (4-8) and (4-9) that the left square in (4-7) is commutative, which finishes the proof. □

Proposition 4.4. *There is a chain homotopy between* $\theta_*\tau_* : \Omega^c_*(G) \to \Omega^c_*(G)$ *and the identity map* $\mathrm{Id} : \Omega^c_*(G) \to \Omega^c_*(G)$.

Proof. The chain complex $\Omega^c_*(G)$ is geometric and the chain maps $\theta_*\tau_*$ and Id evidently preserve augmentation. For a singular cube $\phi : I^n \to G$ consider the subgraph $G_\phi \subset G$, that is, image of ϕ. This is a contractible cubical digraph by Theorem 3.6. Thus we assign to every basic element $\phi^\square \in \Omega^c_*(G)$ the subcomplex

$$E_*(\phi^\square) \overset{\text{def}}{=} \Omega^c_*(G_\phi) \subset \Omega^c_*(G), \tag{4-10}$$

which is acyclic since G_ϕ is contractible.

Now we check that E is an algebraic carrier function, that is, condition (i) of (4-1) is satisfied. Let $\phi^\square \in \Omega^c_*(G)$ be a basic element given by a singular cube $\phi : I^n \to G$ with $n \geq 0$. By (2-6) and (2-7), the element $\partial(\phi^\square)$ is given by the sum of the basic elements $(\phi \circ V_{p\epsilon})^\square$ with coefficients (± 1) where the maps $V_{p\epsilon} : I^{n-1} \to I^n$ are the inclusions. Hence the digraph $G_{\phi\circ V_{p\epsilon}}$ is a subgraph of G_ϕ, and hence the chain complex

$$E_*\big((\phi \circ V_{p\epsilon})^\square\big) = \Omega^c_*(G_{\phi\circ V_{p\epsilon}})$$

is a subcomplex of $E_*(\phi^\square)$. Thus for the basic singular cube $b \in \Omega^c_{n-1}(G)$ and $b \prec \phi^\square$ we obtain that $b = (\phi \circ V_{p\epsilon})^\square$ and

$$E_*(b) = E_*\big((\phi \circ V_{p\epsilon})^\square\big) \prec E_*(\phi^\square).$$

Hence we have the algebraic acyclic carrier function E from $\Omega^c_*(G)$ to itself.

Now we prove that the chain maps $\theta_*\tau_*$ and Id from $\Omega^c_*(G)$ to itself are carried by the function E. Consider a basic element $\phi^\square \in \Omega^c_n(G)$. Then

$$\mathrm{Id}(\phi^\square) = \phi^\square \in \Omega^c_*(G_\phi) = E_*(\phi^\square) \tag{4-11}$$

since image of ϕ is the digraph G_ϕ. Hence the chain map

$$\mathrm{Id} : \Omega^c_n(G) \to \Omega^c_n(G)$$

is carried by the algebraic carrier function E.

By (4-3) and (4-4), we have

$$\theta_n\tau_n(\phi^\square) = \theta_n(\phi_*(w_n)), \quad \phi : I^n \to G. \tag{4-12}$$

We have only two different possibilities for the $\phi_*(w_n)$. In the first case, ϕ is an isomorphism on its image $G_\phi = I_{s,t} \cong I^n$ with

$$s = \phi(0, \dots, 0), \quad t = \phi(1, \dots, 1),$$

where $(0, \dots, 0) \in V_{I^n}$ is the origin vertex and $(1, \dots, 1) \in V_{I^n}$ is the end vertex of the cube I^n. Note that for any isomorphism $\psi : I^n \to I^n$ we have $\psi_*(w_n) = \pm w_n$. Hence in this case subgraph $G_\phi \subset G$ coincides with the subgraph cube $G_{\chi_{s,t}} \subset G$ and by (4-4) we have

$$\theta_n\tau_n(\phi^\square) = \theta_n(\phi_*(w_n)) = \theta_n(\pm(\chi_{s,t})_*(w_n)) = \pm\chi^\square_{s,t}, \tag{4-13}$$

where

$$\chi_{s,t} : I^n \to D_{s,t} = G_\phi.$$

That is,

$$\theta_n \tau_n(\phi^{\square}) \in \Omega_n^c(G_{\chi_{s,t}}) = \Omega_n^c(G_\phi) = E_n(\phi^{\square}).$$

In the second case, the image of ϕ does not contain any cube of dimension n, and hence $\phi_*(w_n) = 0$. Consequently, we have

$$\theta_n \phi_*(w_n) = 0 \in E_*(\phi^{\square}).$$

Then the claim follows from the acyclic carriers Theorem 4.2. □

Theorem 4.5. *For any finite cubical digraph G, the chain maps τ_* and θ_* are homotopy inverses, and hence induce isomorphisms of homology groups*

$$H_*^c(G) \cong H_*(G).$$

Proof. Indeed, it follows from Propositions 4.3 and 4.4 that the chain maps τ_* and θ_* are homotopy inverses. □

Corollary 4.6. *Let Δ be a finite simplicial complex. Consider a digraph G_Δ (see [2]) with the set of vertices given by the set of all simplexes from Δ, and*

$$s \to t \,(t, s \in \Delta) \quad \textit{if and only if } s \supset t \textit{ and } \dim s = \dim t + 1.$$

Then the graph G_Δ is a cubical digraph and

$$H_*^c(G_\Delta) \cong H_*(\Delta),$$

where $H_*(\Delta)$ are the simplicial homology groups of Δ.

Proof. Indeed, it is proved in [2] that path homology groups $H_*(G_\Delta)$ are isomorphic to simplicial homology groups $H_*(\Delta)$. □

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ALEXANDER GRIGOR'YAN
DEPARTMENT OF MATHEMATICS
UNIVERSITY OF BIELEFELD
BIELEFELD
GERMANY

grigor@math.uni-bielefeld.de

YURI MURANOV
FACULTY OF MATHEMATICS AND COMPUTER SCIENCE
UNIVERSITY OF WARMIA AND MAZURY IN OLSZTYN
OLSZTYN
POLAND

muranov@matman.uwm.edu.pl

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THE GEOMETRY AND TOPOLOGY OF STATIONARY MULTIAXISYMMETRIC VACUUM BLACK HOLES IN HIGHER DIMENSIONS

VISHNU KAKKAT, MARCUS KHURI,
JORDAN RAINONE AND GILBERT WEINSTEIN

Extending recent work in 5 dimensions, we prove the existence and uniqueness of solutions to the reduced Einstein equations for vacuum black holes in $(n+3)$-dimensional spacetimes admitting the isometry group $\mathbb{R} \times \mathrm{U}(1)^n$, with Kaluza–Klein asymptotics for $n \geq 3$. This is equivalent to establishing existence and uniqueness for singular harmonic maps $\varphi : \mathbb{R}^3 \setminus \Gamma \to \mathrm{SL}(n+1, \mathbb{R})/\mathrm{SO}(n+1)$ with prescribed blow-up along Γ, a subset of the z-axis in $\mathbb{R}^3$. We also analyze the topology of the domain of outer communication for these spacetimes, by developing an appropriate generalization of the plumbing construction used in the lower-dimensional case. Furthermore, we provide a counterexample to a conjecture of Hollands–Ishibashi concerning the topological classification of the domain of outer communication. A refined version of the conjecture is then presented and established in spacetime dimensions less than 8.

1. Introduction

In several recent papers, harmonic maps into symmetric spaces were used to construct solutions of the 5-dimensional Einstein equations with symmetry group $\mathbb{R} \times \mathrm{U}(1)^2$. More precisely, in this situation the Einstein vacuum equations reduce to an axially symmetric harmonic map with prescribed singularities from $\mathbb{R}^3$ into the symmetric space $\mathrm{SL}(3, \mathbb{R})/\mathrm{SO}(3)$. In [16], solutions of this problem corresponding to spacetimes which are asymptotically flat were constructed, while in [15] a similar approach was applied to obtain solutions with Kaluza–Klein and locally Euclidean asymptotics. Furthermore, the absence of conical singularities on the two unbounded axes was also established in [15]. It is important to emphasize, however, that many of these solutions are expected to have conical singularities on at least one of the

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bounded components of the axis. In [1], existence and uniqueness results were produced for the stationary biaxisymmetric minimal supergravity equations, while in [17] plumbing of disk bundles was used to analyze the topology of the domain of outer communication (DOC) of these solutions. It is the purpose of the present work to extend these results to $(n+3)$-dimensional vacuum gravity with symmetry group $\mathbb{R} \times \mathrm{U}(1)^n$. Similarly, the Einstein vacuum equations in this setting reduce to an axially symmetric harmonic map with prescribed singularities from $\mathbb{R}^3$ to the symmetric space target $\mathrm{SL}(n+1, \mathbb{R})/\mathrm{SO}(n+1)$.

A significant motivation for this higher-dimensional study is to expand the availability of candidate regular solutions, as well as to expand the range of topologies exhibited. It is expected that in 4 dimensions, all asymptotically flat stationary and axially symmetric vacuum solutions with more than one horizon, the cross-sections of which must be 2-spheres, will have a conical singularity on some bounded component of the axis of rotation. Some results in this direction have been obtained [3; 9; 21; 40], but a complete resolution is still out of reach. On the other hand, in dimension 5, there are several known regular solutions other than the S^3-horizon Myers–Perry [30] black holes, namely the Emparan–Reall and Pomeransky–Sen'kov black rings [6; 38] having horizon topology $S^1 \times S^2$, the black saturns [4] of Elvang–Figueras, as well as the black birings [5] and dirings [7; 14] found by Elvang–Rodriguez, Evslin–Krishnan, and Iguchi–Mishima. Recent work by Lucietti–Tomlinson concerning the existence of conical singularities may be found in [24; 25], see also [18; 19]. It is reasonable to expect that many more regular solutions may be found in higher dimensions, other than trivial examples obtained for instance by taking products of known solutions with flat tori. The spacetimes that we produce provide a plethora of candidates having an increasing variety of topologies for the domain of outer communication. Moreover, even those solutions with a conical singularity should be of interest, since we expect that one could perturb time slices to obtain initial data, satisfying relevant energy conditions, with outermost apparent horizon and DOC having exotic topologies.

Motivation is also derived from questions regarding the topological classification of the domain of outer communication. Specifically, we address Conjecture 1 in [10], which postulates that under reasonable hypotheses, the topology of a Cauchy slice in the DOC can be obtained by removing the black hole region from the connected sum of a product of spheres with the asymptotic region. We provide a counterexample to this statement, and discuss why the spirit of the conjecture may nevertheless remain valid. We then offer a refined version of the conjecture, and present a proof for spacetime dimensions less than 8.

The methods used here parallel those employed in [15; 16; 17] with a number of notable differences which we now point out. The rod structure, an n-tuple of relatively prime integers associated with each axis rod, and which determines the combination of the Killing fields that degenerate on that rod, is much more complex than in the 5-dimensional setting where it was merely a pair of relatively prime integers. In particular, the admissibility condition at the corners (points where two axis rods meet), which ensures that the reconstructed spacetime has the structure of a manifold, now involves second determinant divisors. We are thus led to use Smith and Hermite normal forms. Also, the energy estimates for harmonic maps into higher rank symmetric spaces, needed to prove existence, require us to extend the construction of horocyclic coordinates to these more complicated spaces. Finally, the plumbing construction used to analyze the topology of the DOC in 5 dimensions must be generalized in higher dimensions, and involves in addition to the disk bundle integer invariants, a so-called "plumbing vector" which describes how neighboring bundles are glued together.

The paper is organized as follows. The next section presents necessary background and states the main results. In Section 3, we apply Smith and Hermite normal forms to describe the rod structures of T^n-manifolds. The model map, an approximate solution of the harmonic map problem, is constructed in Section 4. In Section 5, we produce horocyclic coordinates on the symmetric space target and use them to derive energy estimates. The domain of outer communication is analyzed in Section 6, using an adaptation of the technique of plumbing from the topology of disk bundles. We conclude with a study of the Hollands–Ishibashi conjecture in Section 7.

2. Background and main results

A connected asymptotically locally Kaluza–Klein stationary vacuum spacetime, with 3, 4, or 5 "large" asymptotically (locally) flat dimensions, will be referred to as *well-behaved* if the orbits of the stationary Killing field are complete, the domain of outer communication (DOC) is globally hyperbolic, and the DOC contains an acausal spacelike connected hypersurface which is asymptotic to the canonical slice in the asymptotic end and whose boundary is a compact cross-section of the horizon. These assumptions are used for the reduction of the stationary vacuum equations and are consistent with [10]. By *asymptotically locally Kaluza–Klein* we refer to a spacetime which asymptotes to the ideal geometry $(\mathbb{R}^{4-s,1}/G) \times T^{n+s-2}$, where T^{n+s-2} is a flat torus, $G \subset O(4-s)$ is a discrete subgroup of spatial rotations, and $s \in \{0, 1, 2\}$. If G is trivial, then the moniker "locally" is removed from the terminology.

Let $(\mathcal{M}^{n+3}, g)$, $n \geq 1$ be a well-behaved asymptotically Kaluza–Klein stationary n-axisymmetric vacuum spacetime, that is, it admits $\mathbb{R} \times \mathrm{U}(1)^n$ as a subgroup of its isometry group. As a consequence of topological censorship [2] the orbit space is simply connected, and hence the spacetime metric g may be written in Weyl–Papapetrou coordinates [10, Theorem 8] as

$$g = f^{-1}e^{2\sigma}(d\rho^2 + dz^2) - f^{-1}\rho^2\, dt^2 + f_{ij}(d\phi^i + v^i\, dt)(d\phi^j + v^j\, dt), \tag{2-1}$$

where (f_{ij}) is an $n \times n$ symmetric positive definite matrix with determinant f, and f_{ij}, v^j, σ are all functions of ρ and z. Let

$$g_3 = e^{2\sigma}(d\rho^2 + dz^2) - \rho^2\, dt^2, \quad A^{(j)} = v^j\, dt, \tag{2-2}$$

then the vacuum equations imply

$$d(f f_{ij} \star_3 dA^{(j)}) = 0, \tag{2-3}$$

where $\star_3$ represents the Hodge dual operator with respect to g_3. Thus, there exist globally defined *twist potentials* ω_i such that

$$d\omega_i = 2 f f_{ij} \star_3 dA^{(j)}. \tag{2-4}$$

The value of the twist potentials on axes adjacent to the horizons determines the angular momenta of the black holes. Next, note that we can write the 3-dimensional reduced Einstein–Hilbert action [27] as

$$S = \int_{\mathbb{R}\times(\mathcal{M}^{n+3}/[\mathbb{R}\times \mathrm{U}(1)^n])} R^{(3)} \star_3 1 + \tfrac{1}{4}\,\mathrm{Tr}(\Phi^{-1} d\Phi \wedge \star_3 \Phi^{-1} d\Phi), \tag{2-5}$$

where

$$\Phi = \begin{pmatrix} f^{-1} & -f^{-1}\omega_i \\ -f^{-1}\omega_i & f_{ij} + f^{-1}\omega_i\omega_j \end{pmatrix}, \quad i, j = 1, \dots, n \tag{2-6}$$

is symmetric, positive definite, and satisfies $\det(\Phi) = 1$. By varying the action with respect to Φ and applying $\mathbb{R}$-symmetry, a majority of the reduced Einstein vacuum equations may be obtained:

$$\begin{aligned} \tau^{f_{lj}} &= \Delta f_{lj} - f^{km}\nabla^\mu f_{lm}\nabla_\mu f_{kj} + f^{-1}\nabla^\mu \omega_l \nabla_\mu \omega_j = 0, \\ \tau^{\omega_j} &= \Delta\omega_j - f^{kl}\nabla^\mu f_{jl}\nabla_\mu \omega_k - f^{lm}\nabla^\mu f_{lm}\nabla_\mu \omega_j = 0. \end{aligned} \tag{2-7}$$

These are the equations for a harmonic map $\varphi : \mathbb{R}^3 \setminus \Gamma \to \mathrm{SL}(n+1, \mathbb{R})/\mathrm{SO}(n+1)$. Given a solution to this system, the remaining metric components v^i and σ may be found [13] by quadrature. Therefore, the stationary vacuum equations in the n-axially symmetric setting are equivalent to a harmonic map problem with prescribed singularities on Γ, a subset of the z-axis which represents the axes of the $\mathrm{U}(1)^n$-action or rather those points associated with a nontrivial isotropy group.

Consider the orbit space $\mathcal{M}^{n+3}/[\mathbb{R} \times \mathrm{U}(1)^n]$. It is homeomorphic to the right half plane $\{(\rho, z) : \rho > 0\}$ and its boundary $\rho = 0$ encodes the topology of the horizons [8; 11; 12]. The domain for the harmonic map is obtained from this observation by adding an ignorable angular coordinate $\phi \in [0, 2\pi)$, yielding $\mathbb{R}^3$ parametrized by the cylindrical coordinates (ρ, z, ϕ). The harmonic map itself is axisymmetric, as it does not depend on ϕ. Uniqueness theorems for higher-dimensional stationary n-axisymmetric black holes ultimately reduce to the uniqueness question for such harmonic maps [12], with prescribed axis behavior determined by invariants called *rod structures* as well as a set of *potential constants*; see Section 3 below for details. Together this information forms a *rod data set*, which may be encoded in an approximate solution referred to as a *model map*. We then say that the model map *corresponds* to the rod data set. If the rods that represent horizon cross-sections have nonzero length, then the rod structure is associated with nondegenerate black hole solutions [12, Lemma 7]. The prescribed harmonic map problem is solved by finding a solution which is *asymptotic* to the model map. A precise description of the properties required for the model map is given in Definition 4.1 and the notion of asymptotic maps is reviewed in Definition 5.1. Our first main result is a generalization of Theorem 1 in [16]. In particular, it extends the previous result to higher dimensions and removes the assumption of a compatibility condition for the rod data. However the notion of *admissibility*, which is explained in Section 3, is still retained since this is required to ensure that the total space arising from the rod structures is a manifold.

Theorem A. (a) *For any admissible rod data set, with nondegenerate horizon rods, there exists a model map* $\varphi_0 : \mathbb{R}^3 \setminus \Gamma \to \mathrm{SL}(n+1, \mathbb{R})/\mathrm{SO}(n+1)$ *which corresponds to the rod data set.*

(b) *There exists a unique harmonic map* $\varphi : \mathbb{R}^3 \setminus \Gamma \to \mathrm{SL}(n+1, \mathbb{R})/\mathrm{SO}(n+1)$ *which is asymptotic to the model map* φ_0.

(c) *A well-behaved asymptotically* (*locally*) *Kaluza–Klein solution of the* $(n+3)$-*dimensional vacuum Einstein equations admitting the isometry group* $\mathbb{R} \times \mathrm{U}(1)^n$ *can be constructed from* φ *if and only if the resulting metric coefficients are sufficiently smooth across* Γ, *and there are no conical singularities on any bounded axis rod.*

As indicated in the third part of this theorem, there are two possible regularity issues that may arise when constructing a spacetime from the harmonic map. Namely, these are the questions of analytic regularity and geometric regularity. Analytic regularity concerns differentiability properties of the harmonic map up to the orbit space boundary after removing the singular part, while geometric regularity concerns the possible presence of conical singularities [8, Section 3.3]. We note that in the 4-dimensional vacuum case analytic regularity was treated independently by Li–Tian [22; 23] and Weinstein [39], whereas the Einstein–Maxwell setting was addressed more recently by Nguyen [32].

Consider now the topology of the domain of outer communication. In 5 dimensions, we obtained a classification theorem [17, Theorem 1] in which the canonical slice was decomposed into a disjoint union of linearly plumbed disk bundles over 2-spheres, and a few other more simple pieces. There does not seem to be a direct natural generalization of linear plumbing which is applicable to the higher-dimensional setting of stationary n-axisymmetric vacuum spacetimes. In fact, a naive approach leads to a construction that is not unique, as there are various ways to glue the neighboring toroidal fibers together. In order to remedy this issue we define a generalized or *toric plumbing* with additional parameters $\mathfrak{p}_i \in \mathbb{Z}^n$ which are called *plumbing vectors*, see Definition 6.6. In the next result, the higher-dimensional generalization of [17, Theorem 1] is presented. This theorem applies beyond the realm of vacuum solutions, namely to those satisfying the null energy condition, which is a hypothesis included to ensure that the topological censorship theorem [2, Theorem 5.3; 10, Theorem 5] is valid.

We will use the following notation for the building blocks of the decomposition. The axis Γ is a union of intervals $\{\Gamma_{i,j}\}_{i=1}^{I_j+2}$, $j = 1, \dots, \mathfrak{J}$ called *axis rods*, each of which is defined by a particular isotropy subgroup of $\mathrm{U}(1)^n$. With each such rod that is flanked on both sides by another axis, we associate $\boldsymbol{\xi}_{i,j} = \xi_{i,j} \times T^{n-3}$ where $\xi_{i,j}$ is a (D^2) disk-bundle over either the 3-sphere S^3, the ring $S^1 \times S^2$, or a lens space $L(p, q)$ with $p > q$ relatively prime positive integers. A sequence of such product spaces may be glued together, with the help of plumbing vectors, to form the toric plumbing $\mathcal{P}(\boldsymbol{\xi}_{1,j}, \dots, \boldsymbol{\xi}_{I_j,j} \mid \mathfrak{p}_{2,j}, \dots, \mathfrak{p}_{I_j,j})$. The topologies of $\xi_{i,j}$, and the plumbing vectors themselves $\mathfrak{p}_{i,j}$, are completely determined by the rod structures of the axes involved.

Theorem B. *The topology of the domain of outer communication of an orientable well-behaved asymptotically Kaluza–Klein stationary n-axisymmetric spacetime, with* $n \geq 3$, *and satisfying the null energy condition is* $\mathcal{M}^{n+3} = \mathbb{R} \times M^{n+2}$ *where the Cauchy surface is given by a union of the form*

$$M^{n+2} = \bigcup_{j=1}^{J} \mathcal{P}(\boldsymbol{\xi}_{1,j}, \dots, \boldsymbol{\xi}_{I_j,j} \mid \mathfrak{p}_{2,j}, \dots, \mathfrak{p}_{I_j,j}) \bigcup_{k=1}^{N_1} C_k^{n+2} \bigcup_{m=1}^{N_2} B_m^4 \times T^{n-2} \bigcup M_{end}^{n+2}, \tag{2-8}$$

in which each constituent is a closed manifold with boundary and all are mutually disjoint expect possibly at the boundaries. Here C_k^{n+2} *is* $[0, 1] \times D^2 \times T^{n-1}$, B_m^4 *denotes a* 4*-dimensional ball, and the asymptotic end* M_{end}^{n+2} *is given by* $\mathbb{R}_+ \times Y \times T^{n-2}$ *where* Y *represents either* S^3 *or* $S^1 \times S^2$. *Furthermore* J, N_1, *and* N_2 *are the number of connected components of the axis which consist of three or more axis rods, one finite axis rod, and two axis rods, respectively.*

This result identifies the fundamental constituents of the DOC, and its proof shows how they may be computed from the rod structure of the torus action. On the other hand, it does not express the topology in a concise way. In order to achieve this goal, at least in low dimensions, we observe in the next result that a simplified expression may be obtained by filling in the horizons and capping off the asymptotic end with appropriately chosen toric plumbings. In particular, this produces a "compactified DOC" which is a simply connected $(n+2)$-manifold without boundary admitting an effective T^n-action. Classification results for such manifolds [33; 34; 35] may then be applied to obtain the following theorem, which generalizes [17, Theorem 2] where the case $n = 2$ was treated.

Theorem C. *Consider the domain of outer communication* $\mathcal{M}^{n+3} = \mathbb{R} \times M^{n+2}$ *of an orientable well-behaved asymptotically Kaluza–Klein stationary n-axisymmetric spacetime, with* $2 \le n \le 4$, *satisfying the null energy condition, and having H components of the horizon cross-section. There exists a choice of horizon fill-ins* $\{\overline{M}^{n+2}_h\}^H_{h=1}$ *and a cap for the asymptotic end* $\overline{M}^{n+2}_{end}$, *each of which is either the product of a* 4*-ball with a torus* $B^4 \times T^{n-2}$ *or a finite toric plumbing, such that the compactified Cauchy surface*

$$\overline{M}^{n+2} = (M^{n+2} \setminus M^{n+2}_{end}) \bigcup_{h=1}^{H} \overline{M}^{n+2}_h \bigcup \overline{M}^{n+2}_{end} \tag{2-9}$$

is homeomorphic to one of the following possibilities, where $k = b_2(\overline{M}^{n+2})$ *is the second Betti number and* $0 \le \ell \le k$.

$n=2$	$n=3$	$n=4$
S^4	S^5	$S^3 \times S^3$
$\#\frac{k}{2}(S^2 \times S^2)$	$\#k(S^2 \times S^3)$	$\#k(S^2 \times S^4)\#(k+1)(S^3 \times S^3)$
$\ell\mathbb{CP}^2\#(k-\ell)\overline{\mathbb{CP}}^2$	$(S^2 \tilde{\times} S^3)\#(k-1)(S^2 \times S^3)$	$(S^2 \tilde{\times} S^4)\#(k-1)(S^2 \times S^4)\#(k+1)(S^3 \times S^3)$

Moreover, the toric plumbings for each fill-in and cap may be computed algorithmically from the neighboring rod structures of each horizon and the asymptotic end.

In the chart above, the first row consists of the case when the compactified DOC is 2-connected, while the second and third rows consist of the spin and nonspin scenarios, respectively. In the second and third rows the second Betti number k is positive, and is even for dimension 4 with the spin property. The twisted product notation is used to denote the nontrivial (and nonspin) sphere bundles over S^2. Furthermore, note that $S^2 \tilde{\times} S^2 \cong \mathbb{CP}^2\#\overline{\mathbb{CP}}^2$ and $\mathbb{CP}^2\#\overline{\mathbb{CP}}^2\#\mathbb{CP}^2 \cong \mathbb{CP}^2\#(S^2 \times S^2)$ [35, Remark 5.8]. This together with [37, Theorem II.4.2, p. 313], shows that in the nonspin 4 dimensional case an alternate expression for the decomposition may be given in terms of a connected sum of a number of $S^2 \times S^2$'s, and either a single $S^2 \tilde{\times} S^2$ or a number of $\mathbb{CP}^2$'s. This is analogous to the result for dimensions 5 and 6 modulo the presence of the complex projective planes. Theorem C may be thought of as evidence towards a modified version of a conjecture made by Hollands and Ishibashi in [10, Conjecture 1], concerning the topological classification of the DOC under a spin assumption. In Section 7 we construct a spacetime which serves as a counterexample to the original conjecture, and this motivates the refinement below. Note that Theorem C shows that the following conjecture holds true for $n = 2, 3, 4$, if the compactified DOC is spin.

Conjecture D. *Consider the domain of outer communication* $\mathcal{M}^{n+3} = \mathbb{R} \times M^{n+2}$ *of an orientable well-behaved asymptotically Kaluza–Klein stationary* n*-axisymmetric spacetime*, *with* $n \geq 2$, *satisfying the null energy condition. If the Cauchy surface* M^{n+2} *is spin*, *then there exists a choice of horizon fill-in and a cap for the asymptotic end*, *such that the corresponding compactified DOC is homeomorphic to*

$$\#_{i=2}^{n} m_i \cdot S^i \times S^{n+2-i} \tag{2-10}$$

for some nonnegative integers m_i.

3. Topology and the rod structure

The topology of the spacetimes considered here will always be of the form $\mathbb{R} \times M^{n+2}$, due to the assumption of global hyperbolicity. The time slice M^{n+2} is assumed to admit an effective action by the torus T^n, and hence the quotient map $M^{n+2} \to M^{n+2}/T^n$ exhibits M^{n+2} as a T^n-bundle over a 2-dimensional base space with possibly degenerate fibers on the boundary. Fibers over interior points are n-dimensional, while fibers over points along the boundary can be $(n-1)$- or $(n-2)$-dimensional. The set of points where the fiber is $(n-1)$-dimensional are called *axis rods* while the points with an $(n-2)$-dimensional fiber are called *corners*. The set of corners is always discrete. If in addition topological censorship holds, as is the case under the hypotheses of the main theorems, then the base space M^{n+2}/T^n is homeomorphic to a half plane [12]. The boundary $\partial\mathbb{R}^2_+$ of this half-plane is divided into disjoint intervals separated by corners or *horizon rods* where the fibers do not degenerate. The boundary points of horizon rods are called *poles*. Associated to each axis rod interval $\Gamma_i \subset \partial\mathbb{R}^2_+$ is a vector $\boldsymbol{v}_i \in \mathbb{Z}^n$ called the *rod structure*, that defines the 1-dimensional isotropy subgroup $\mathbb{R}/\mathbb{Z} \cdot \boldsymbol{v}_i \subset \mathbb{R}^n/\mathbb{Z}^n \cong T^n$ for the action of T^n on points that lie over Γ_i. The topology of the DOC is determined by the rod structures, namely

$$M^{n+2} \cong (\mathbb{R}^2_+ \times T^n)/\sim, \tag{3-1}$$

where the equivalence relation $\sim$ is given by $(\boldsymbol{p}, \boldsymbol{\phi}) \sim (\boldsymbol{p}, \boldsymbol{\phi} + \lambda \boldsymbol{v}_i)$ with $\boldsymbol{p} \in \Gamma_i$, $\lambda \in \mathbb{R}/\mathbb{Z}$, and $\boldsymbol{\phi} \in T^n$. This setting is a special case of the following construction.

Definition 3.1. A *simple* T^n*-manifold* is an orientable smooth manifold M^k, $k \geq n$ with an effective T^n-action, in which the quotient space M^k/T^n is simply connected and the quotient map defines a trivial fiber bundle over the interior of the quotient.

If M^{n+2} is a simply connected T^n-manifold (it admits an effective T^n-action) such that $\partial(M^{n+2}/T^n) \neq \varnothing$, then it is necessarily a simple T^n-manifold, see Theorem 7.1. As above, the topology of an $(n+2)$-dimensional simple T^n-manifold is completely determined by the set of rod structures. A graphical representation of this information is called a *rod diagram*, see Figure 1 for examples. These are drawn as either a disk in the compact case, or a half plane in the noncompact case, in which the boundary is divided into segments with associated rod structure vectors indicating the linear combination of generators that degenerate at the axes. Black dots represent corners or poles where two rods meet, and the segments drawn with jagged lines are horizon rods along which the torus action is free. We will revisit this figure after Lemma 3.3.

It should be noted that the notion of rod structures given above does not guarantee a unique presentation. Indeed, the vectors $\boldsymbol{v}$ and $2\boldsymbol{v}$ both generate the same isotropy subgroup $\mathbb{R}/\mathbb{Z}\cdot\boldsymbol{v}$, and thus both can be used to describe the same rod structure. In order to identify a unique presentation (up to a choice of sign), it is natural to restrict attention to primitive elements. A vector or a set of vectors $\{\boldsymbol{v}_1, \dots, \boldsymbol{v}_k\} \subset \mathbb{Z}^n$ forms a *primitive set* if they are linearly independent and

$$\mathbb{Z}^n \cap \operatorname{span}_{\mathbb{R}}\{\boldsymbol{v}_1, \dots, \boldsymbol{v}_k\} = \operatorname{span}_{\mathbb{Z}}\{\boldsymbol{v}_1, \dots, \boldsymbol{v}_k\}. \tag{3-2}$$

For a single vector $\boldsymbol{v} = (v_1, \dots, v_n)$, this is equivalent to the components being relatively prime, that is, $\gcd\{v_1, \dots, v_n\} = 1$. Next, observe that the group $\mathrm{GL}(n, \mathbb{Z})$ of unimodular matrices provides the group of coordinate transformations for $T^n = \mathbb{R}^n/\mathbb{Z}^n$. Two rod diagrams are equivalent if every rod structure of one is obtained from the corresponding rod structure of the other by the action of the same unimodular matrix. Thus, quantities depending only on the T^n-structure will be invariant under $\mathrm{GL}(n, \mathbb{Z})$ transformations. The following proposition exhibits an example of such a quantity, Det_k, referred to as the k^{th} *determinant divisor* [31, Chapter II, Section 14]. In the statement we will use the multiindex notation I^n_k, for $k \le n$, to denote the set of k-tuples $\boldsymbol{i} = (i_1, \dots, i_k) \in \mathbb{Z}^k$ such that $1 \le i_1 < \dots < i_k \le n$.

Proposition 3.2. *Let* $\boldsymbol{v}_1, \dots, \boldsymbol{v}_m \in \mathbb{Z}^n$, $k \le \min\{m, n\}$, *and set*

$$\mathrm{Det}_k(\boldsymbol{v}_1, \dots, \boldsymbol{v}_m) = \gcd\{Q^{\boldsymbol{i}}_{\boldsymbol{j}} \mid \boldsymbol{i} \in I^n_k, \boldsymbol{j} \in I^m_k\}, \tag{3-3}$$

where $Q^{\boldsymbol{i}}_{\boldsymbol{j}}$ *is the determinant of the* $k \times k$ *minor obtained from the matrix defined by the column vectors* $\boldsymbol{v}_1, \dots, \boldsymbol{v}_m$, *by picking columns* $\boldsymbol{j}$ *and rows* $\boldsymbol{i}$. *Then* Det_k *is invariant under* $\mathrm{GL}(n, \mathbb{Z})$, *that is,*

$$\mathrm{Det}_k(\boldsymbol{v}_1, \dots, \boldsymbol{v}_m) = \mathrm{Det}_k(A\boldsymbol{v}_1, \dots, A\boldsymbol{v}_m) \tag{3-4}$$

for all $A \in \mathrm{GL}(n, \mathbb{Z})$.

Proof. Let $\omega \in \bigwedge^k \mathbb{Z}^n$ be a k-form on $\mathbb{Z}^n$. Each such form can be written as a linear combination of the basis elements $\{\boldsymbol{e}^{i_1} \wedge \dots \wedge \boldsymbol{e}^{i_k} \mid \boldsymbol{i} \in I^n_k\}$, where $\{\boldsymbol{e}^i\}$ is the basis of covectors dual to the standard basis $\{\boldsymbol{e}_j\}$ of $\mathbb{Z}^n$ so that $\boldsymbol{e}^i(\boldsymbol{e}_j) = \delta^i_j$. Thus

$$\omega = \sum_{\boldsymbol{i} \in I^n_k} a_{i_1 \dots i_k} \boldsymbol{e}^{i_1} \wedge \dots \wedge \boldsymbol{e}^{i_k}, \quad a_{\boldsymbol{i}} \in \mathbb{Z}, \tag{3-5}$$

where by definition $\boldsymbol{e}^{i_1} \wedge \cdots \wedge \boldsymbol{e}^{i_k}(\boldsymbol{v}_{j_1}, \ldots, \boldsymbol{v}_{j_k})$ is the minor determinant $Q^{\boldsymbol{i}}_{\boldsymbol{j}}$. Consider the $k \times k$ minor determinant $Q'^{\boldsymbol{i}}_{\boldsymbol{j}}$ of the matrix formed from the column vectors $A\boldsymbol{v}_{j_1}, \ldots, A\boldsymbol{v}_{j_k}$ and observe that $Q'^{\boldsymbol{i}}_{\boldsymbol{j}}$ is multilinear and antisymmetric in $\{\boldsymbol{v}_{j_1}, \ldots, \boldsymbol{v}_{j_k}\}$. Therefore it is a linear combination as in (3-5) and may be expressed as

$$Q'^{\boldsymbol{i}}_{\boldsymbol{j}} = \sum_{\boldsymbol{i}' \in I^n_k} a^{\boldsymbol{i}}_{\boldsymbol{i}'} Q^{\boldsymbol{i}'}_{\boldsymbol{j}}. \tag{3-6}$$

Observe that if $p \in \mathbb{Z}$ divides $Q^{\boldsymbol{i}'}_{\boldsymbol{j}}$ for all $\boldsymbol{i}' \in I^n_k$, then p also divides $Q'^{\boldsymbol{i}}_{\boldsymbol{j}}$ and hence

$$\begin{aligned} \text{Det}_k(A\boldsymbol{v}_1, \ldots, A\boldsymbol{v}_m) &= \gcd\{Q'^{\boldsymbol{i}}_{\boldsymbol{j}} \mid \boldsymbol{i} \in I^n_k, \boldsymbol{j} \in I^m_k\} \\ &\geq \gcd\{Q^{\boldsymbol{j}'}_{\boldsymbol{i}} \mid \boldsymbol{i}' \in I^n_k, \boldsymbol{j} \in I^m_k\} = \text{Det}_k(\boldsymbol{v}_1, \ldots, \boldsymbol{v}_m). \end{aligned} \tag{3-7}$$

Furthermore since $A^{-1} \in \text{GL}(n, \mathbb{Z})$, the same reasoning shows that

$$\begin{aligned} \text{Det}_k(\boldsymbol{v}_1, \ldots, \boldsymbol{v}_m) &= \text{Det}_k(A^{-1}(A\boldsymbol{v}_1), \ldots, A^{-1}(A\boldsymbol{v}_m)) \\ &\geq \text{Det}_k(A\boldsymbol{v}_1, \ldots, A\boldsymbol{v}_m). \end{aligned} \tag{3-8}$$

The desired invariance follows from these two inequalities. □

A corner point between two adjacent axis rods is *admissible* if the total space over a neighborhood of the corner is a manifold. The importance of the second determinant divisor in the current context arises from the fact that it determines whether or not a corner is admissible. Since the corner point represents an $(n-2)$-torus within the total space, a tubular neighborhood will be a manifold if and only if it is homeomorphic to $B^4 \times T^{n-2}$, or equivalently if its boundary is $S^3 \times T^{n-2}$. This last criteria occurs precisely when there is a matrix $Q \in \text{GL}(n, \mathbb{Z})$ such that $Q\boldsymbol{v} = \boldsymbol{e}_1$ and $Q\boldsymbol{w} = \boldsymbol{e}_2$, where $\boldsymbol{v}$, $\boldsymbol{w}$ are the rod structures of the axis rods forming the corner, and $\boldsymbol{e}_1$, $\boldsymbol{e}_2$ are members of the standard basis for $\mathbb{Z}^n$. Corollary 3.6 below, guarantees that such a Q exists if and only if $\text{Det}_2(\boldsymbol{v}, \boldsymbol{w}) = 1$. The statement of this result uses the *Hermite normal form*, whose properties are listed in the next lemma. A proof of this lemma can be found in [26]. The Hermite normal form may be viewed as the integer version of the reduced echelon form, or as the integer version of the QR decomposition for real matrices.

Lemma 3.3. *Let A be a $n \times k$ integer matrix. There exist integer matrices Q and H such that $QA = H$, where Q is unimodular and $H = (h_{ij})$ has the following properties.*

(1) *For some integer m, the rows 1 through m of H are nonzero, and the rows $m+1$ through n are rows of zeros.*

(2) *There is a sequence of integers $1 \leq r_1 < r_2 < \cdots < r_m \leq r = \text{rank}\, A$ such that the entries h_{ir_i} of H, called **pivots**, are positive for $i = 1, \ldots, m$. The pivot h_{ir_i} is the first nonzero element in the row i, that is, $h_{ij} = 0$ for $1 \leq j < r_i$.*

(3) *In each column of* H *that contains a pivot, the entries of the column are bounded between* 0 *and the pivot, that is, for* $i = 1, \ldots, m$ *and* $1 \leq j < i$ *we have* $0 \leq h_{jr_i} < h_{ir_i}$.

The matrix H *is unique and is known as the* ***Hermite normal form*** *of* A*. Furthermore, the Hermite normal form of* BA *is equal to the Hermite normal form of* A *whenever* B *is a unimodular matrix. Finally, the unimodular matrix* Q*, known as the* ***transformation matrix*** *of* A*, is unique when* A *is an invertible square matrix.*

It should be noted that if the first l columns of A are linearly independent, then the upper-left $l \times l$ block of the Hermite normal form of A is upper triangular with nonzero diagonal entries, namely $r_i = i$ for $i = 1, \ldots, l$. For our purposes, the matrix A will typically consist of a collection of k rod structures for rods which are not necessarily adjacent. An example of this is shown in Figure 1, where the 3×4 matrix A is assembled from the rod structures on the left (treated as column vectors), and sent to its Hermite normal form consisting of the rod structures on the right, via the transformation matrix that appears in the middle of the diagram.

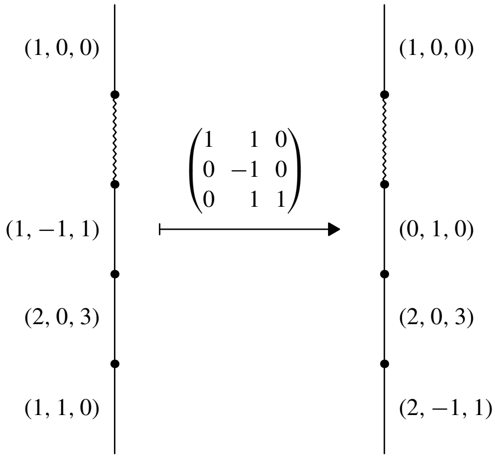

Figure 1. Two rod diagrams, separated by an arrow, both depicting $(5+1)$-dimensional spacetimes with a single black hole. Each rod diagram shows the 2-dimensional quotient space as the right-half-plane with the vertical lines being their boundaries. The jagged lines are black hole horizon rods, the interior of which correspond to the product of an open interval with T^3. The rod structures flanking the horizon rod yield horizon cross-sectional topology $S^1 \times S^3$. The two rod diagrams depict the same spacetime. The unimodular matrix in the middle represents a coordinate change on T^n. In particular, it is the transformation matrix from Lemma 3.3 which sends the rod structures on the left to their Hermite normal form on the right.

Remark 3.4. If rod structures $\{\boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3\}$ arise from three consecutive rods with admissible corners, then more information is known about their Hermite normal form $\{\boldsymbol{w}_1, \boldsymbol{w}_2, \boldsymbol{w}_3\}$. In particular $\boldsymbol{w}_1 = \boldsymbol{e}_1,\ \boldsymbol{w}_2 = \boldsymbol{e}_2$, and $\boldsymbol{w}_3 = (q, r, p, 0, \dots, 0)$ with $0 \le q < p,\ 0 \le r < p,\ p = \mathrm{Det}_3(\boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3)$, and $\gcd\{q, p\} = 1$ if the set of vectors is linearly independent. In the case of a linearly dependent triple, we have $p = 0$ and $q = 1$, while r is unconstrained. Furthermore, given any integers $\mu, \lambda \in \mathbb{Z}$ there exists a coordinate change which sends $\boldsymbol{v}_i$ to $\boldsymbol{w}_i'$ where

$$\begin{aligned} \boldsymbol{w}_1' &= (1, 0, \dots, 0), \\ \boldsymbol{w}_2' &= (0, 1, 0, \dots, 0), \\ \boldsymbol{w}_3' &= (q + \mu p, r + \lambda p, p, 0, \dots, 0). \end{aligned} \tag{3-9}$$

These observations will be utilized in Section 6.

In order to establish the relationship between the admissibility condition for corners and the second determinant divisor, we recall the *Smith normal form*. This may be considered as the integer matrix analog of the singular value decomposition, and is utilized in the classification of finitely generated Abelian groups. This latter fact will be employed when we compute the fundamental group of the DOC in Theorem 7.1. A proof of the following result can be found in [31].

Lemma 3.5. *Let A be an $n \times k$ integer matrix of rank l. There exist integer matrices U, V, and S such that $UAV = S$. The matrices U and V are unimodular, and S is diagonal with entries s_i such that $s_i | s_{i+1}$ for $1 \le i < l$. These entries, referred to as elementary divisors, satisfy $s_i = 0$ for $i > l$ with all others computed by*

$$s_i = \frac{\mathrm{Det}_i(A)}{\mathrm{Det}_{i-1}(A)}, \quad i \le l, \tag{3-10}$$

where we have set $\mathrm{Det}_0(A) = 1$. The matrix S is unique and is known as the ***Smith normal form*** *of A.*

The distinction between the Hermite and Smith normal forms, in the context of rod structures, is as follows. The transformations used to obtain Hermite normal form are always actions by $n \times n$ matrices on the left. Such an action corresponds to shuffling the Killing vectors around by linear combinations. This does not affect the topology of the total space nor its toric structure, only the representation of the torus $T^n \cong \mathbb{R}^n/\mathbb{Z}^n$ and thus the rod structures. By contrast, Smith normal form also includes actions on the right by $k \times k$ matrices. These actions correspond to shuffling the axis rods themselves. This changes the topology of our space, possibly no longer making it a manifold. Consequently, when seeking out a simpler presentation of the rod structures we will invoke the Hermite normal form in order to avoid changing the topology. Two exceptions to this are in the proof of Theorem 7.1, where only the integer span of the rod structures is significant and not their order, and in the proof of Corollary 3.6 below, where the Hermite and Smith normal forms coincide.

Corollary 3.6. *Let A be an $n \times k$ integer matrix of rank k. Then* $\operatorname{Det}_k(A) = 1$ *if and only if the upper $k \times k$ block of the Hermite normal form of A is the identity matrix.*

Proof. Assume that the upper $k \times k$ block of the Hermite normal form is the identity. By uniqueness, this matrix is also the Smith normal form. The diagonal entries are then $1 = s_i = \operatorname{Det}_i(A)/\operatorname{Det}_{i-1}(A)$, which implies that

$$\operatorname{Det}_k(A) = \operatorname{Det}_{k-1}(A) = \cdots = \operatorname{Det}_0(A) = 1.$$

Conversely, assume that $\operatorname{Det}_k(A) = 1$ and let

$$\begin{bmatrix} S \\ 0 \end{bmatrix} = UAV \tag{3-11}$$

be the Smith normal form of A, where $S = \operatorname{diag}(s_1, \dots, s_k)$. Consider the $n \times n$ matrix

$$B = U^{-1} \begin{bmatrix} S & 0 \\ 0 & \boldsymbol{I}_{n-k} \end{bmatrix} \begin{bmatrix} V^{-1} & 0 \\ 0 & \boldsymbol{I}_{n-k} \end{bmatrix} = [A \;\; E], \tag{3-12}$$

where E consists of the last $n-k$ columns of U^{-1}. It follows that

$$\begin{aligned} \det(B) &= \det(U^{-1}) \det(S) \det(V^{-1}) \\ &= s_1 \cdots s_k = \frac{\operatorname{Det}_1(A)}{\operatorname{Det}_0(A)} \cdots \frac{\operatorname{Det}_k(A)}{\operatorname{Det}_{k-1}(A)} = \operatorname{Det}_k(A). \end{aligned} \tag{3-13}$$

By assumption $\operatorname{Det}_k(A) = 1$, and thus B is invertible. Therefore

$$B^{-1}A = \begin{bmatrix} \boldsymbol{I}_k \\ 0 \end{bmatrix} \tag{3-14}$$

and by uniqueness this must be the Hermite normal form of A. □

As mentioned after the proof of Proposition 3.2, this corollary shows that a pair of adjacent rod structures $\boldsymbol{v}$, $\boldsymbol{w}$ is admissible if and only if $\operatorname{Det}_2(\boldsymbol{v}, \boldsymbol{w}) = 1$. Moreover, in a similar manner, a collection of k rod structures $\{\boldsymbol{v}_1, \dots, \boldsymbol{v}_k\}$ can be sent to the standard basis $\{\boldsymbol{e}_1, \dots, \boldsymbol{e}_k\}$, and thus forms a primitive set if and only if $\operatorname{Det}_k(\boldsymbol{v}_1, \dots, \boldsymbol{v}_k) = 1$. Another application of the Hermite normal form is to give a variant proof of Hollands and Yazadjiev's horizon topology theorem [12, Theorem 2]. It states that for $n \geq 2$, all closed $(n+1)$-manifolds with an effective T^n-action, whose quotient is not a circle, must be a product of T^{n-2} and either S^3, a lens space $L(p, q)$, or $S^1 \times S^2$. This is a generalization of a result by Orlik and Raymond for 3-manifolds, see [35, Section 2]. Observe that the $(n+1)$-dimensional case can be reduced to the 3-dimensional case by applying the transformation matrix from Lemma 3.3 to the matrix of rod structures defining the horizon, which we assume to be primitive vectors. In particular, the resulting Hermite normal form consists of the new rod structures $(1, 0, \dots, 0)$ and $(q, p, 0, \dots, 0)$, with $0 \le q < p$. With this representation of the T^n-action, the last $n-2$ coordinate Killing fields clearly never vanish. Therefore the total space is homeomorphic to a product of T^{n-2} and a 3-manifold Σ with an effective T^2 action. According to the possibilities given for the 3-dimensional case, we find that Σ is either S^3 if $p = 1$, $S^1 \times S^2$ if $p = 0$, or the lens space $L(p, q)$ if $p > 1$.

Remark 3.7. Given a horizon topology $\Sigma \times T^{n-2}$, it is possible to determine the topology of Σ directly from the second determinant divisor. Let $\boldsymbol{v}, \boldsymbol{w} \in \mathbb{Z}^n$ be primitive vectors that describe the flanking rod structures of the horizon, and compute $\mathrm{Det}_2(\boldsymbol{v}, \boldsymbol{w})$. If this value is 0, then $\boldsymbol{v} = \boldsymbol{w}$ and $\Sigma = S^1 \times S^2$. If it is 1, then the pair is admissible and $\Sigma = S^3$. If $\mathrm{Det}_2(\boldsymbol{v}, \boldsymbol{w}) = p > 1$ then $\Sigma = L(p, q)$ for some $q < p$. Moreover, q may be found from the relation $\boldsymbol{w} = q\boldsymbol{v} \mod p$.

Theorem 3.8. *Given any two (primitive) rod structures* $\boldsymbol{v}$ *and* $\boldsymbol{w}$, *it is always possible to find a finite number of additional rod structures that connect* $\boldsymbol{v}$ *to* $\boldsymbol{w}$ *in such a way that each corner in the resulting sequence of rods is admissible. That is, there exists a sequence of rod structures* $\{\boldsymbol{v}_1, \dots, \boldsymbol{v}_k\}$, *with* $\boldsymbol{v}_1 = \boldsymbol{v}$ *and* $\boldsymbol{v}_k = \boldsymbol{w}$, *having the property that* $\mathrm{Det}_2(\boldsymbol{v}_i, \boldsymbol{v}_{i+1}) = 1$ *for* $i = 1, \dots, k-1$.

Proof. By Lemma 3.3 there exists a unimodular matrix Q which transforms $\boldsymbol{v}$ and $\boldsymbol{w}$ into Hermite normal form, in particular $Q\boldsymbol{v} = (1, 0, \dots, 0)$ and $Q\boldsymbol{w} = (q, p, 0, \dots, 0)$ where $0 \le q < p$. If $q = 0$, then $p = 1$ since $\boldsymbol{w}$ is primitive, and hence $\mathrm{Det}_2(\boldsymbol{v}, \boldsymbol{w}) = 1$. So assume that $q \ge 1$. In [17, Section 3] an algorithm is presented that is based on the continued fraction decomposition of p/q, which produces a sequence of rod structures in $\mathbb{Z}^2$ connecting $(1, 0)$ to (q, p) such that each corner is admissible. We may then append zeros to each of the rod structures in this sequence, to obtain a sequence in $\mathbb{Z}^n$ that connects $(1, 0, \dots, 0)$ to $(q, p, 0, \dots, 0)$ with the same property. Applying Q^{-1} then produces the desired sequence. □

This result was used in [17], for $(4+1)$-dimensional spacetimes, to construct simply connected fill-ins for horizons. The simple connectivity of the fill-ins preserves the fundamental group of the DOC, and is not difficult to achieve since in this low dimensional setting admissible rod structures cannot contribute to the fundamental group. In higher dimensions this is not the case, and a more careful choice of rod structures is needed to achieve simply connected fill-ins. Moreover, since the boundary between the filled in region and the DOC now has a much larger fundamental group, there is a more complicated relation between the topologies of these regions. In the last section, we will study the fundamental group of the compactified domain of outer communication.

4. The model map

In this section we construct a model map $\varphi_0 : \mathbb{R}^3 \setminus \Gamma \to \mathrm{SL}(n+1, \mathbb{R})/\mathrm{SO}(n+1)$, which describes the singular behavior of the desired harmonic map near the axis Γ, as well as the asymptotics at infinity. The model map can be viewed as an approximate solution to the singular harmonic map problem near the axes and at infinity [16; 41]. We define a model map as follows.

Definition 4.1. A map $\varphi_0 : \mathbb{R}^3 \setminus \Gamma \to \mathrm{SL}(n+1, \mathbb{R})/\mathrm{SO}(n+1)$ is a *model map* if

(1) $|\tau(\varphi_0)|$ is bounded, where τ denotes the tension of φ_0, and

(2) there is a positive function $w \in C^2(\mathbb{R}^3)$ with $\Delta w \leq -|\tau(\varphi_0)|$ and $w \to 0$ at infinity.

It should be noted that if $|\tau(\varphi_0)| = O(r^{-\alpha})$ as $r \to \infty$, for some $\alpha > 2$, then this is sufficient to satisfy condition (2). In order to facilitate the construction of the model map, we will utilize the following parametrization of the target space. Namely, the target space is parametrized by (F, ω), where $F = (f_{ij})$ is a symmetric positive definite $n \times n$ matrix and $\omega = (\omega_i)$ is an n-tuple corresponding to the twist potentials. On each axis rod, the Dirichlet boundary data for ω_i is constant. These so-called *potential constants* determine the angular momenta of the horizons, and do not vary between adjacent axis rods which are separated by a corner. In (F, ω) coordinates, the metric on the target space $\mathrm{SL}(n+1, \mathbb{R})/\mathrm{SO}(n+1)$ may be expressed as (see [27])

$$\tag{4-1} \begin{aligned} &\tfrac{1}{4}\frac{df^2}{f^2} + \tfrac{1}{4} f^{ij} f^{kl}\, df_{ik}\, df_{jl} + \tfrac{1}{2}\frac{f^{ij}\, d\omega_i\, d\omega_j}{f} \\ &\qquad = \tfrac{1}{4}[\mathrm{Tr}(F^{-1} dF)]^2 + \tfrac{1}{4}\,\mathrm{Tr}(F^{-1} dF F^{-1} dF) + \tfrac{1}{2}\frac{d\omega^t F^{-1} d\omega}{f}, \end{aligned}$$

where $f = \det F$ and $F^{-1} = (f^{ij})$ is the inverse matrix. By setting

$$\tag{4-2} H = F^{-1}\nabla F, \quad G = f^{-1} F^{-1} (\nabla\omega)^2, \quad K = f^{-1} F^{-1} \nabla\omega,$$

it follows from (2-7) that the squared norm of the tension becomes

$$\tag{4-3} \begin{aligned} &|\tau|^2 \\ &= \tfrac{1}{4}[\mathrm{Tr}(\mathrm{div}\, H + G)]^2 + \tfrac{1}{4}\,\mathrm{Tr}[(\mathrm{div}\, H + G)(\mathrm{div}\, H + G)] + \tfrac{1}{2} f (\mathrm{div}\, K)^t F (\mathrm{div}\, K). \end{aligned}$$

It is clear from (4-3) that the tension norm is invariant under the transformation

$$\tag{4-4} F \mapsto hFh^t \quad \text{and} \quad \omega \mapsto h\omega$$

for any $h \in \mathrm{SL}(n, \mathbb{R})$. Note that $\det h = 1$ is not required for this to hold when ω is constant, since G and K are then zero. The next result generalizes the model map construction from lower dimensions that was presented in [15; 16].

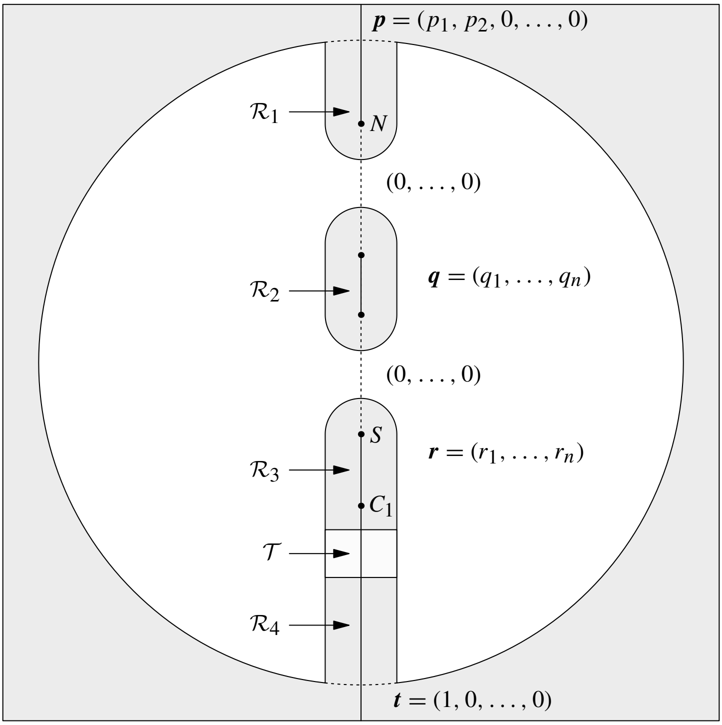

Figure 2. The various regions used in the construction of the model map. Axis rod structures are represented by $\boldsymbol{p}$, $\boldsymbol{q}$, $\boldsymbol{r}$, and $\boldsymbol{t}$, while horizon rods are indicated by dashed lines.

Lemma 4.2. *For any admissible rod data set, with nondegenerate horizons, there exists a corresponding model map* $\varphi_0 : \mathbb{R}^3 \setminus \Gamma \to \mathrm{SL}(n+1, \mathbb{R})/\mathrm{SO}(n+1)$, *for* $n \geq 2$, *having tension decay at infinity given by* $|\tau| = O(r^{-5/2})$.

Proof. We first present a proof for the rod data set corresponding to two horizons and a single corner, as shown in Figure 2. At the end of the proof, we will indicate the necessary adjustments for the general case. Observe that in the diagram there are four neighborhoods $\mathcal{R}_1$, $\mathcal{R}_2$, $\mathcal{R}_3$, and $\mathcal{R}_4$ associated with certain axis rods, having rod structures $\boldsymbol{p}$, $\boldsymbol{q}$, $\boldsymbol{r}$, and $\boldsymbol{t}$ respectively. The model map will be constructed separately in each of these regions. The following two harmonic functions on $\mathbb{R}^3 \setminus \Gamma$ will play an important role in the construction:

$$u_a = \log(r_a - (z-a)) = \log\bigl(2r_a \sin^2\bigl(\tfrac{1}{2}\theta_a\bigr)\bigr), \tag{4-5}$$
$$v_a = \log(r_a + (z-a)) = \log\bigl(2r_a \cos^2\bigl(\tfrac{1}{2}\theta_a\bigr)\bigr),$$

where $r_a = \sqrt{\rho^2 + (z-a)^2}$ is the Euclidean distance from the point $z = a$ on the z-axis, and θ_a is the polar angle.

Consider first the case in which the asymptotic end is modeled on $L(p,q)\times T^{n-2}$, where $0\le q<p$. By applying Lemma 3.3 if necessary, it may be assumed without loss of generality that the rod structures on the semiinfinite rods are $\boldsymbol{p}=(p_1,p_2,0,\dots,0)$ with $p_2>0$, and $\boldsymbol{t}=(1,0,\dots,0)$. The model map outside of a large ball (corresponding to the shaded region outside of the circle in Figure 2) and in the regions $\mathcal{R}_1$ and $\mathcal{R}_4$, may then be given by

$$F_1=h\tilde{F}_1h^t,\quad \omega=h\tilde{\omega}(\theta),\tag{4-6}$$

where $\tilde{\omega}$ is a function of $\theta=\theta_0$ alone described below and

$$\begin{aligned}\tilde{F}_1&=\operatorname{diag}(e^{u_0-\log 2},e^{v_0-\log 2},1,\dots,1),\\ h&=\begin{pmatrix}0&\sqrt{p_2}&0\\ 1/\sqrt{p_2}&-p_1/\sqrt{p_2}&0\\ 0&0&\boldsymbol{I}_{n-2}\end{pmatrix},\end{aligned}\tag{4-7}$$

with $\boldsymbol{I}_{n-2}$ representing the identity matrix. Notice that, up to multiplication by constants, h^t sends $\boldsymbol{t}\mapsto\boldsymbol{e}_2$ and $\boldsymbol{p}\mapsto\boldsymbol{e}_1$. Thus, the matrix F_1 possesses the appropriate kernel at the semiinfinite rods to encode the given rod structures. Moreover, since $\varphi_0=(F_1,\omega)$ is obtained from the map $(\tilde{F}_1,\tilde{\omega})$ by applying an isometry to the target space, and $\tilde{F}_1$ arises from the canonical flat metric on $\mathbb{R}^4\times T^{n-2}$, it follows that $\operatorname{div}H=\operatorname{div}F_1^{-1}\nabla F_1=0$. We may further choose $\tilde{\omega}(\theta)$ to be constant for $\theta\in[0,\epsilon]\cup[\pi-\epsilon,\pi]$, thus showing that (F_1,ω) is harmonic in $\mathcal{R}_1$ and $\mathcal{R}_4$. The constants are chosen to coincide with the prescribed potential constants on the axis rods. Within the remaining angular interval, $\tilde{\omega}(\theta)$ may be prescribed arbitrarily as long as it is smooth. In order to verify the decay of the tension for this map in the range $\theta\in[\epsilon,\pi-\epsilon]$, observe that since

$$F_1=O(r),\quad f=O(r^2),\quad |\nabla\omega|=O(r^{-1}),\quad\text{and}\quad \operatorname{div}K=O(r^{-4})$$

we have

$$f(\operatorname{div}K)^tF_1(\operatorname{div}K)=O(r^{-5}),\quad G=O(r^{-4}).\tag{4-8}$$

Hence $|\tau|$ decays like $r^{-5/2}$, which is sufficient. Similarly, in the case where the asymptotic end is modeled on $S^2\times T^{n-1}$, we can without loss of generality assume that the rod structures on both the semiinfinite rods are $(1,0,\dots,0)$. The model map outside of the large ball and in the regions $\mathcal{R}_1$ and $\mathcal{R}_4$ is now given by

$$F_1=\operatorname{diag}(e^u,1,\dots,1),\quad \omega=\omega(\theta),\tag{4-9}$$

where $u=2\log\rho$ and ω is constant on $\theta\in[0,\epsilon]\cup[\pi-\epsilon,\pi]$. As before, the tension decays as $|\tau|=O(r^{-5/2})$ when $r\to\infty$.

Next consider the compact region $\mathcal{R}_2$ below the first horizon. The poles in this region are located at $z = a$ and $z = b$, $a < b$, and the rod structure is $\boldsymbol{q} = (q_1, q_2, \ldots, q_n)$. The model map in this region is defined by

$$F_2 = h_2 \tilde{F}_2 h_2^t, \quad \omega = c_2, \tag{4-10}$$

where $\tilde{F}_2 = \operatorname{diag}(e^u, 1, \ldots, 1)$, $u = u_a - u_b$, and

$$h_2 = ([\boldsymbol{q}, \boldsymbol{e}_2, \ldots, \boldsymbol{e}_n]^t)^{-1}. \tag{4-11}$$

The constant vector c_2 is chosen to agree with the prescribed potential constants on the rod. As pointed out in the remark preceding the lemma, $\det h_2 = 1$ is not required here since ω is constant. It follows that the map $\varphi_0 = (F_2, \omega)$ is harmonic in region $\mathcal{R}_2$.

Now we will deal with the regions $\mathcal{R}_3$, $\mathcal{R}_4$ and the transition region $\mathcal{T}$ between them. Let the pole S be at $z = s > 0$ and the corner C_1 be at $z = 0$. The rod structure above the corner C_1 is $\boldsymbol{r} = (r_1, \ldots, r_n)$ and below the corner is $\boldsymbol{t} = (1, 0, \ldots, 0)$. Because of admissibility, we can without loss of generality assume that $r_2 > 0$. As above we set ω to be a constant c_3, agreeing with the prescribed potential constant on the rods, in the entire southern tubular neighborhoods $\mathcal{R}_3$ and $\mathcal{R}_4$. Let

$$\begin{gathered} \tilde{F}_3 = \operatorname{diag}(e^u, e^v, 1, \ldots, 1), \\ u = (u_0 - \log 2) - \lambda(z)(u_s - \log 2), \quad v = v_0 - \log 2, \end{gathered} \tag{4-12}$$

where $\lambda = \lambda(z)$ is a smooth cut-off function which is 1 near $\mathcal{R}_3$ and 0 near $\mathcal{R}_4$. Define the map in region $\mathcal{R}_3$ by

$$F_3 = h_3 \tilde{F}_3 h_3^t, \quad \omega = c_3, \tag{4-13}$$

where

$$h_3 = \sqrt{p_2}([\boldsymbol{r}, \boldsymbol{e}_1, \boldsymbol{e}_3, \ldots, \boldsymbol{e}_n]^t)^{-1}. \tag{4-14}$$

We have already given the map in $\mathcal{R}_4$. In order to define the map in $\mathcal{T}$, set $h_3(z)$ to be a smooth curve of invertible $n \times n$ matrices which connects h_3 in (4-14) to h in (4-7). Note that this is possible since both endpoint matrices have negative determinant, and that the curve may be chosen so that the second column of $(h_3(z)^t)^{-1}$ remains the constant vector $1/\sqrt{p_2}\,\boldsymbol{e}_1$. The map

$$F_3(z) = h_3(z) \tilde{F}_3(z) h_3^t(z)$$

then identifies the correct rod structures, and agrees with the previously defined map on $\mathcal{R}_4$. Since $\omega = c_3$, we have $G = K = 0$ in $\mathcal{R}_3 \cup \mathcal{R}_4$. It remains to show that $\operatorname{div} F_3^{-1} \nabla F_3$ is bounded on the transition region $\mathcal{T}$, since it vanishes on the complement. To see this, compute

$$\begin{aligned}\text{(4-15)}\quad \operatorname{div} F_3^{-1}\nabla F_3 &= [\nabla(\tilde{F}_3 h_3^t)^{-1}]\cdot(h_3^{-1}\nabla h_3)\tilde{F}_3 h_3^t + (\tilde{F}_3 h_3^t)^{-1}\operatorname{div}(h_3^{-1}\nabla h_3)\tilde{F}_3 h_3^t\\ &\quad + (\tilde{F}_3 h_3^t)^{-1}(h_3^{-1}\nabla h_3)\cdot\nabla(\tilde{F}_3 h_3^t) + (\nabla h_3^{-t})\cdot(\tilde{F}_3^{-1}\nabla\tilde{F}_3)h_3^t\\ &\quad + h_3^{-t}\operatorname{div}(\tilde{F}_3^{-1}\nabla\tilde{F}_3)h_3^t + h_3^{-t}(\tilde{F}_3^{-1}\nabla\tilde{F}_3)\cdot\nabla h_3^t + \operatorname{div}(h_3^{-t}\nabla h_3).\end{aligned}$$

Note that $|\nabla u|$ and $\partial_z v = 1/r$ are clearly bounded in $\mathcal{T}$. Moreover, the second row of $h_3^{-1}\nabla h_3$ vanishes, and this leads to the desired boundedness of $\operatorname{div} F_3^{-1}\nabla F_3$. Indeed, consider the first term on the right-hand side of (4-15), namely

$$\begin{aligned}\text{(4-16)}\quad &[\nabla(\tilde{F}_3 h_3^t)^{-1}]\cdot(h_3^{-1}\nabla h_3)\tilde{F}_3 h_3^t\\ &\qquad = [(h_3^t)^{-1}\partial_z\tilde{F}_3^{-1} + \partial_z(h_3^t)^{-1}\cdot\tilde{F}_3^{-1}](h_3^{-1}\partial_z h_3)\tilde{F}_3 h_3^t.\end{aligned}$$

The only potential difficulty in bounding this expression on $\mathcal{T}$ arises from the function e^{-v}, in $\tilde{F}_3^{-1}$ and $\partial_z\tilde{F}_3^{-1}$. However, since $h_3^{-1}\partial_z h_3$ has a vanishing second row, the products

$$\text{(4-17)}\qquad \tilde{F}_3^{-1}\cdot(h_3^{-1}\partial_z h_3),\qquad \partial_z\tilde{F}_3^{-1}\cdot(h_3^{-1}\partial_z h_3),$$

no longer contain e^{-v} and the first term of (4-15) is controlled. The remaining terms may be handled analogously. It follows that (4-15) is bounded, and hence the model map $\varphi_0 = (F_3, \omega)$ has bounded tension in a tubular neighborhood of the two southern most rods. This treats the case in which the asymptotic end is modeled on $L(p,q)\times T^{n-2}$, and a similar procedure may be used in the case that the asymptotic end is modeled on $S^2\times T^{n-1}$.

We will now address the multiple corner case. Any connected component of the axis consists of a consecutive sequence of axis rods. To construct the model map in a tubular neighborhood of such a component, first divide this region into neighborhoods centered at corners and transition regions between corners. The basic block consists of two such neighborhoods around adjacent corners C_n and C_s, and the transition region $\mathcal{T}$ between them. It suffices to illustrate the map construction in such blocks, as the full map may then be obtained by combining the individual pieces to handle any rod structure configuration.

Consider a basic block with rod structures $\boldsymbol{p}$, $\boldsymbol{q}$, and $\boldsymbol{r}$ on axis rods Γ_1, Γ_2, and Γ_3 respectively, moving from north to south. Note that $\boldsymbol{p}$ and $\boldsymbol{q}$, as well as $\boldsymbol{q}$ and $\boldsymbol{r}$, must be linearly independent since the corners C_n and C_s are admissible. It follows that there is a collection of standard basis vectors $\{\boldsymbol{e}_{i_1},\dots,\boldsymbol{e}_{i_{n-2}}\}$ that complete $\{\boldsymbol{p},\boldsymbol{q}\}$ to a basis, and similarly for $\{\boldsymbol{q},\boldsymbol{r}\}$. We may then form the matrices

$$\text{(4-18)}\quad h_{\boldsymbol{p},\boldsymbol{q}} = ([\boldsymbol{p},\boldsymbol{q},\boldsymbol{e}_{i_1},\dots,\boldsymbol{e}_{i_{n-2}}]^t)^{-1},\quad h_{\boldsymbol{r},\boldsymbol{q}} = ([\boldsymbol{r},\boldsymbol{q},\boldsymbol{e}_{j_1},\dots,\boldsymbol{e}_{j_{n-2}}]^t)^{-1}.$$

Next define $F_0 = \operatorname{diag}(e^u, e^v, 1, \dots, 1)$ where u and v are harmonic, with e^u vanishing on Γ_1 and Γ_3, and e^v vanishing on Γ_2. These functions may be given as the sum of logarithms of the form (4-5). Then F_0 corresponds to the rod structures $\boldsymbol{e}_1$, $\boldsymbol{e}_2$, and $\boldsymbol{e}_1$ on Γ_1, Γ_2, and Γ_3 respectively. Consider a smooth curve of invertible $n \times n$ matrices $h_{\boldsymbol{p}|\boldsymbol{r},\boldsymbol{q}}(z)$ which agrees with $h_{\boldsymbol{p},\boldsymbol{q}}$ on Γ_1 and in a neighborhood of C_n, and transitions over $\mathcal{T} \subset \Gamma_2$ so that it agrees with $h_{\boldsymbol{r},\boldsymbol{q}}$ on Γ_3 and in a neighborhood of C_s. The existence of such a curve is possible since we may assume that the determinants of $h_{\boldsymbol{p},\boldsymbol{q}}$ and $h_{\boldsymbol{r},\boldsymbol{q}}$ have the same sign by replacing $\boldsymbol{r}$ with $-\boldsymbol{r}$ if necessary. Moreover, the curve may be designed such that the second column of $(h_{\boldsymbol{p}|\boldsymbol{r},\boldsymbol{q}}(z)^t)^{-1}$ is the constant vector $\boldsymbol{q}$. This implies that the second row of $h^{-1}_{\boldsymbol{p}|\boldsymbol{r},\boldsymbol{q}} \nabla h_{\boldsymbol{p}|\boldsymbol{r},\boldsymbol{q}}$ vanishes, so that with the help of (4-15) we find that $\operatorname{div} F^{-1}\nabla F$ remains bounded along $\mathcal{T}$, where $F = h_{\boldsymbol{p}|\boldsymbol{r},\boldsymbol{q}} F_0\, h^t_{\boldsymbol{p}|\boldsymbol{r},\boldsymbol{q}}$. The model map $\varphi_0 = (F, \omega)$ on the basic block, with ω constant, then has bounded tension.

Lastly, it remains to treat the case of multiple blocks within an axis component. To accomplish this, take u and v harmonic so that e^u and e^v vanish in an alternating fashion on the string of axis rods. The diagonal matrix F_0 is then defined along the entire string. We will inductively construct the model map on basic block assemblies. As a demonstration of this, consider adding an additional rod Γ_4, with rod structure $\boldsymbol{w}$, to the sequence of three rods discussed above which we call basic block $\mathcal{B}_1$. We may view the Γ_2, Γ_3, Γ_4 string, with rod structures $\boldsymbol{q}$, $\boldsymbol{r}$, $\boldsymbol{w}$, as a basic block $\mathcal{B}_2$; the corner between the third and fourth rod will be denoted by C_w. The map has already been defined into a neighborhood of Γ_3, and may be extended into a neighborhood of Γ_4 as follows. Recall that the maps

$$F_1 = h_{\boldsymbol{p}|\boldsymbol{r},\boldsymbol{q}} F_0\, h^t_{\boldsymbol{p}|\boldsymbol{r},\boldsymbol{q}}, \qquad F_2 = h_{\boldsymbol{r},\boldsymbol{q}|\boldsymbol{w}} F_0\, h^t_{\boldsymbol{r},\boldsymbol{q}|\boldsymbol{w}} \tag{4-19}$$

are defined on the basic blocks $\mathcal{B}_1$ and $\mathcal{B}_2$ respectively, and identify the desired rod structures. However, they do not necessarily coincide on the overlap regions. In order to remedy this situation, let $h_4(z)$ be a smooth curve of invertible $n \times n$ matrices connecting $h_{\boldsymbol{r},\boldsymbol{q}}$ to $h_{\boldsymbol{r},\boldsymbol{w}}$ with a transition over $\widetilde{\mathcal{T}} \subset \Gamma_3$. This is possible since by replacing $\boldsymbol{w}$ with $-\boldsymbol{w}$ if necessary, we may assume that both endpoint matrices have determinants of the same sign. Moreover, this curve may be chosen such that the first column of $(h_4(z)^t)^{-1}$ remains the constant vector $\boldsymbol{r}$. Set $F = h_4(z) F_0\, h_4(z)^t$ on Γ_3, and observe that this agrees with F_1 and F_2 near the corners C_s and C_w, respectively, so that F is naturally defined on all of $\mathcal{B}_1 \cup \mathcal{B}_2$. Since the first row of $h_4^{-1}\nabla h_4$ vanishes, we find with the aid of (4-15) that $\operatorname{div} F^{-1}\nabla F$ remains bounded along Γ_3. The model map $\varphi_0 = (F, \omega)$ on the two basic blocks, with ω constant, then has bounded tension. We may continue this process inductively to treat any number of consecutive axis rods. ☐

Remark 4.3. In [15; 16] an additional technical assumption on the rod structures, known as the compatibility condition, was used for the construction of the model map. The condition, which is not required for Lemma 4.2, states that given three adjacent rod structures with admissible corners, say (m, n), (p, q), and (r, s), the following inequality must hold:

$$mr(mq-np)(ps-rq)\leq 0\,. \tag{4-20}$$

This turns out not to be a geometric condition, as it can always be achieved by a change of coordinates. To see this, first assume without loss of generality that the determinants $(mq-np)$ and $(ps-rq)$ are 1, by possibly replacing (p, q) or (r, s) or both with the vector of the same length and opposite direction. Note that this operation does not alter the isotropy subgroup prescribed by the rod structure. Next apply the unimodular matrix

$$A=\begin{pmatrix} q & -p\\ -n & m\end{pmatrix} \tag{4-21}$$

to obtain the rod structures $A\cdot\{(m, n), (p, q), (r, s)\}=\{(1, 0), (0, 1), (r', s')\}$ for some $r', s'\in\mathbb{Z}$. Then (4-20) is clearly satisfied for the new set of rod structures.

Remark 4.4. Lemma 4.2 and Remark 4.3 provide the proof of part (a) from Theorem A.

5. Horocyclic coordinates and energy estimates

In this section we show how the energy estimates based on horocyclic coordinates can be generalized from the lower-rank target space setting that was treated in [16, Section 6]. The target space is now $\mathrm{SL}(n+1,\mathbb{R})/\mathrm{SO}(n+1)$, which is a noncompact symmetric space of dimension $\frac{1}{2}(n(n+3))$ and rank n. For convenience we denote $G=\mathrm{SL}(n+1,\mathbb{R})$, $K=\mathrm{SO}(n+1)$, and $\boldsymbol{X}=G/K$. The Iwasawa decomposition is given by $G=NAK$, where A is the abelian group

$$A=\left\{\mathrm{diag}(e^{\lambda_1},\dots,e^{\lambda_{n+1}})\mid \prod_{i=1}^{n+1}e^{\lambda_i}=1\right\} \tag{5-1}$$

and N is the nilpotent subgroup of upper triangular matrices with diagonal entries set to 1. Thus, given $g\in G$ there are unique elements $m\in N$, $a\in A$, and $k\in K$ with $g=mak$, and the symmetric space $\boldsymbol{X}$ may be identified with the subgroup NA. Denote $x_0=[Id]\in\boldsymbol{X}$ and note that the orbits $A\cdot x_0=:\mathfrak{F}_{x_0}$ and $N\cdot x_0$ are respectively a maximal flat and a horocycle. The former is an n-dimensional totally geodesic submanifold with vanishing sectional curvature, and the latter is an $\frac{1}{2}(n(n+1))$-dimensional submanifold with the property that each flat which is asymptotic to the same Weyl chamber at infinity has an orthogonal intersection with the horocycle in a single point. Furthermore, since each point $x\in\boldsymbol{X}$ may be uniquely expressed as $ma\cdot x_0$, the assignment $x\mapsto\mathfrak{F}_x=ma\cdot\mathfrak{F}_{x_0}$ yields a smooth foliation whose leaves are the flats $\{m\cdot\mathfrak{F}_{x_0}\}_{m\in N}$; the flat $\mathfrak{F}_x$ orthogonally interacts the horocycle $N\cdot x$ only at x. In this manner, the pair (a, m) gives rise to a horocyclic orthogonal coordinate system for $\boldsymbol{X}$.

A Euclidean coordinate system $r=(r_1,\dots,r_n)$ may be introduced on $\mathfrak{F}_{x_0}$, and can then be pushed forward to each flat $m\cdot\mathcal{F}_{x_0}$ so that the horocyclic coordinates (a, m) may be represented by (r, m). Furthermore, each r' defines a diffeomorphism (translation) $(r, m)\mapsto(r+r', m)$ that preserves the m-coordinates, and for each $m'\in N$ there is an isometry that preserves the r-coordinates $(r, m)\mapsto(r, m'm)$. These r-translations map horocycles to horocycles, and therefore may be used to push forward a system of global coordinates $\theta=(\theta^1,\dots,\theta^{n(n+1)/2})$ on $N\cdot x_0\cong\mathbb{R}^{n(n+1)/2}$ to all horocycles. It follows that (r,θ) form a set of global coordinates on $\boldsymbol{X}$ in which the coordinate fields ∂_{r_i} and ∂_{θ^j} are orthogonal, and such that the G-invariant Riemannian metric on $\boldsymbol{X}$ is expressed as

$$\boldsymbol{g}=dr^2+Q(d\theta,d\theta)=\sum_{i=1}^{n}dr_i^2+\sum_{j,l=1}^{n(n+1)/2}Q_{jl}\,d\theta^j\,d\theta^l, \tag{5-2}$$

where the coefficients $Q_{jl}(r,\theta)$ are smooth functions. Moreover, the proof of [16, Lemma 8] generalizes in a direct manner to the current setting to yield the uniform bounds

$$bQ(\xi,\xi)\le\partial_{r_i}Q(\xi,\xi)\le cQ(\xi,\xi) \tag{5-3}$$

for all $i=1,\dots,n$ and $\xi\in\mathbb{R}^{n(n+1)/2}$ where $0<b<c$. With the help of (5-3), by expressing the harmonic map equations in the horocyclic parametrization we may establish energy bounds on compact subsets away from the axis. In particular, if $\varphi:\mathbb{R}^3\setminus\Gamma\to\boldsymbol{X}$ is a harmonic map and $\Omega\subset\mathbb{R}^3\setminus\Gamma$ is a bounded domain then the harmonic energy restricted to Ω satisfies

$$E_\Omega(\varphi)\le\mathcal{C}, \tag{5-4}$$

where the constant $\mathcal{C}$ depends only on the maximum distance $\sup_{y\in\Omega}d_{\boldsymbol{X}}(\varphi(y),x_0)$.

Definition 5.1. Two maps $\varphi_1,\varphi_2:\mathbb{R}^3\setminus\Gamma\to\boldsymbol{X}$ are *asymptotic* if there exists a constant C such that $d_{\boldsymbol{X}}(\varphi_1,\varphi_2)\le C$ and $d_{\boldsymbol{X}}(\varphi_1(y),\varphi_2(y))\to0$ as $|y|\to\infty$.

The distance between the model map and solutions to the harmonic map Dirichlet problem on an exhausting sequence of domains may be estimated via a maximum principle argument [41], which is based on convexity of the distance function in the nonpositively curved target. This supremum bound together with the energy bound, allow for an application of standard elliptic theory to control all higher-order derivatives. The sequence of harmonic maps on exhausting domains will then subconverge to the desired solution, see [16, Sections 6 and 7] for details. We record this conclusion as the following result.

Lemma 5.2. *Let φ_0 be a model map. Then there exists a unique harmonic map $\varphi : \mathbb{R}^3 \setminus \Gamma \to \boldsymbol{X}$ such that φ is asymptotic to φ_0.*

This lemma establishes part (b) of Theorem A. Since φ is asymptotic to φ_0, it can be shown in the same way as [16, Theorem 11], that the two maps respect the same rod data set. Furthermore, part (c) of Theorem A may be established analogously to [16, Section 8]. This completes the proof of Theorem A.

6. Plumbing and topology of the domain of outer communication

There are two methods that can be used to characterize the domain of outer communication. One method consists of filling in horizons and cross-sections in the asymptotic end to obtain a simply connected compact manifold. In the next section we use this method for spatial dimensions 4, 5, and 6, where a complete list of possible topologies is available. The other approach involves breaking up the domain of outer communication into simpler pieces, and then classifying the individual components. This is the method of plumbing constructions which will be discussed in the current section and will yield the proof of Theorem B. Throughout this section we will assume that $n \geq 3$.

In Theorem B the domain of outer communication is broken up into components determined by the number of corners that they contain. The pieces which contain no corners are either the asymptotic end M^{n+2}_{end}, or a piece which is homeomorphic to $[0, 1] \times D^2 \times T^{n-1}$ which we denote by C^{n+2}_k. When a piece contains a single corner, the admissibility condition may be used to show that it is the product of a ball with a torus $B^4 \times T^{n-2}$. This part of the analysis is identical to the (spatial) 4-dimensional case that is covered in [17, Theorem 1]. However, a significant difference occurs in higher dimensions when analyzing components that contain at least two corners. A component with exactly two corners will turn out to be the product of a torus T^{n-3} with a disk bundle over a 3-manifold, rather than a 2-sphere. Moreover, for components with more than two corners, we will have to define a generalization of plumbing where the fibers and base space are not of the same dimension.

Theorem 6.1. *Let M^{n+2} be a simple T^n-manifold, and consider a neighborhood N^2 in the orbit space of a portion of the axis with two corners and no horizon rods. The total space over N^2 is homeomorphic to $\xi \times T^{n-3}$, where the action of $T^n \cong T^3 \times T^{n-3}$ acts componentwise. Here ξ is a D^2-bundle over $X \in \{S^3, L(p, q), S^1 \times S^2\}$. The topologies of X and ξ may be read off from the Hermite normal form of the rod structures.*

Proof. The rod diagram of N^2 has three axis rods separated by two admissible corners. Using Remark 3.4 we can, without changing the topology, transform our rod structures into the form of (3-9), where the last $n-3$ entries of each rod structure are zero. The last $n-3$ Killing fields then do not vanish over N^2, and hence the total space is a product manifold $\xi \times T^{n-3}$, where the T^n-action splits naturally into T^3 acting on ξ and T^{n-3} acting on itself. Here ξ denotes the manifold represented by the rod diagram $\{(1,0,0), (0,1,0), (q,r,p)\}$ with $0 \le q < p,\ 0 \le r < p$, and $\gcd\{q,p\} = 1$ if the vectors are linearly independent. In the case that they are linearly dependent, we instead have $q = 1,\ p = 0$, and $r \in \mathbb{Z}$.

The middle axis rod, where the second Killing field vanishes, is a deformation retract of the space ξ. This rod represents a closed manifold $X \in \{S^3, L(p,q), S^1 \times S^2\}$. Fibers over this space correspond to rays extending out from the middle axis rod, see Figure 4. Each point in the interior of the middle axis rod corresponds to an entire T^2, while a ray terminating at that point corresponds to $D^2 \times T^2$. Moreover, each of the two corners corresponds to an S^1 in the base space X, while the adjacent axis rods correspond to $D^2 \times S^1$. It follows that ξ has the structure of a D^2-bundle over X.

To determine the topology of X and ξ, we look at the rod structures. If they are linearly dependent, then the rod structures must be $\{(1,0,0), (0,1,0), (1,r,0)\}$ by admissibility. There is then a free S^1 action, and after factoring this out, it remains to analyze the 4-dimensional disk bundle generated by the diagram with rod structures $\{(1,0), (0,1), (1,r)\}$. The base space of this latter disk-bundle is S^2, and its zero-section self-intersection number, or equivalently the characteristic number of its Euler class is r, see [17]. Moreover, we have $X = S^1 \times S^2$.

If the rod structures $\{(1,0,0), (0,1,0), (q,r,p)\}$ are linearly independent, the base space $X = L(p,q)$. Recall that $L(1,q) = S^3$ for all q. The number of distinct disk bundles, or equivalently SO(2)-bundles, over X is determined by the homotopy classes of maps $[X, \mathbb{CP}^\infty]$. Moreover, the classifying space $BS^1 = \mathbb{CP}^\infty$ is an Eilenberg–Mac Lane space of type $K(\mathbb{Z}, 2)$, so the homotopy classes of based maps from X to $K(\mathbb{Z}, 2)$ is in bijection with $H^2(X; \mathbb{Z}) \cong \mathbb{Z}_p$. The element of this cohomology group which corresponds to a specific bundle ξ is called the *Euler class* $e(\xi)$.

By uniqueness of the Hermite normal form, the $r \in \mathbb{Z}_p \cong H^2(L(p,q); \mathbb{Z})$ in the rod structure is uniquely determined for each equivariant homeomorphism class of ξ. Conversely, for each class in $H^2(L(p,q); \mathbb{Z})$ there is a unique disk bundle over $L(p,q)$. Each of these disk bundles admits an effective T^3 action, with T^1 acting on the fibers, and a T^2 acting on the base $L(p,q)$. Thus, to each of these disk bundles corresponds a rod diagram with three axis rods and two admissible corners. This gives a one-to-one correspondence between integers

$$r \in [0, p) \quad \text{and} \quad e(\xi) \in H^2(L(p,q), \mathbb{Z}).$$

Furthermore, for the trivial disk bundle $L(p,q) \times D^2$ both $r = 0$ and $e(\xi) = 0$. To see this, note that the quotient of $L(p,q)$ by its T^2-action can be represented as an interval where the $(1,0)$ and the (q,p) circles degenerate at the end points. Similarly, the quotient of D^2 by S^1 can be represented by a half open interval where the circle degenerates at the one end point. Taking the product of these two spaces produces the rod diagram $\{(1, 0, 0), (0, 1, 0), (q, 0, p)\}$, from which we deduce that $r = 0$. ☐

The above theorem shows that the total space over a neighborhood of three consecutive axis rod structures $\{\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}\}$, satisfying the admissibility condition, is $\xi \times T^{n-3}$ where ξ is a disk bundle over either a lens space or a ring. Observe that there is a subtorus T^3 which leaves the slices $\xi \times \{\boldsymbol{\varphi}\} \in \xi \times T^{n-3}$ invariant, and is spanned by the rod structures $\{\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}\} \subset \mathbb{Z}^n$ as

$$T^3 \cong \operatorname{span}_{\mathbb{R}}\{\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}\}/\mathbb{Z}^n \subset \mathbb{R}^n/\mathbb{Z}^n \cong T^n. \tag{6-1}$$

Although $\{\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}\}$ may not necessarily be a primitive set, this can be rectified by employing an integral version of the Gram–Schmidt process, which will lead to the formulation of generalized plumbing.

Lemma 6.2. *Let $\{\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}\} \subset \mathbb{Z}^n$ be a consecutive sequence of rod structures satisfying the admissibility condition and with a neighborhood that lifts to $\xi \times T^{n-3}$ in the total space. If ξ is a D^2-bundle over $L(p, q)$, $0 \le q < p$ with Euler class determined by $r \in [0, p)$, then there exists a unique primitive vector $\mathfrak{p} \in \mathbb{Z}^n$ satisfying*

$$\boldsymbol{w} = q\boldsymbol{u} + r\boldsymbol{v} + p\mathfrak{p}. \tag{6-2}$$

Furthermore, $\{\boldsymbol{u}, \boldsymbol{v}, \mathfrak{p}\} \subset \mathbb{Z}^n$ forms a primitive set. In addition, if ξ is a D^2-bundle over $S^1 \times S^2$, then (6-2) is satisfied with $\mathfrak{p} = 0$.

Proof. First consider the case in which ξ is a D^2-bundle over $L(p, q)$, $0 \le q < p$ with Euler class determined by $r \in [0, p)$. Let Q be the unimodular matrix that transforms $\{\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}\}$ into Hermite normal form, that is, $Q\boldsymbol{u} = \boldsymbol{e}_1$, $Q\boldsymbol{v} = \boldsymbol{e}_2$, and $Q\boldsymbol{w} = q\boldsymbol{e}_1 + r\boldsymbol{e}_2 + p\boldsymbol{e}_3$. We may then set $\mathfrak{p} = Q^{-1}\boldsymbol{e}_3$ and observe that (6-2) is satisfied. Since the Hermite normal form is unique, and $p \neq 0$, it is clear that $\mathfrak{p} \in \mathbb{Z}^n$ is the unique solution to the equation. Furthermore, since Q^{-1} is unimodular and $\boldsymbol{e}_3$ is a primitive vector we find that $\mathfrak{p}$ is primitive as well. Next note that $\{\boldsymbol{u}, \boldsymbol{v}, \mathfrak{p}\}$ is a primitive set if and only if $\operatorname{Det}_3(\boldsymbol{u}, \boldsymbol{v}, \mathfrak{p}) = 1$. Moreover, by multilinearity of the determinant together with (6-2), it follows that

$$\operatorname{Det}_3(\boldsymbol{u}, \boldsymbol{v}, \mathfrak{p}) = p^{-1} \operatorname{Det}_3(\boldsymbol{u}, \boldsymbol{v}, \boldsymbol{w}) = p^{-1} \operatorname{Det}_3(\boldsymbol{e}_1, \boldsymbol{e}_2, q\boldsymbol{e}_1 + r\boldsymbol{e}_2 + p\boldsymbol{e}_3) = 1, \tag{6-3}$$

where the second equality follows from the coordinate invariance of Det_3. Lastly, if ξ is a D^2-bundle over $S^1 \times S^2$, then $q = 1$ and $p = 0$ so that (6-2) is satisfied with $\mathfrak{p} = 0$. ☐

We will now consider portions of the axis having more than two consecutive corners in a simple T^n-manifold. The total space over neighborhoods of these regions of the axis, with $l + 1$ corners, will be shown to consist of l disk bundle-torus products that are glued together in a fashion that may be viewed as a generalization of the linear plumbing construction. This higher-dimensional plumbing, which we will refer to as *toric plumbing*, is not a straightforward generalization of 4-dimensional procedure due to the various ways that the extra toroidal dimensions may be conjoined. For each pair of neighboring disk bundles we will define a *plumbing vector*, which distinguishes the different ways that the two disk bundles can be plumbed together. Figure 3 provides examples of the same two disk bundles being plumbed together in different ways to form nonhomeomorphic total spaces.

Consider a section of the axis rod, having admissible corners, with rod structures $\{\boldsymbol{v}_1, \dots, \boldsymbol{v}_{l+2}\}$. From Theorem 6.1, a neighborhood of each consecutive triple of rod structures $\{\boldsymbol{v}_i, \boldsymbol{v}_{i+1}, \boldsymbol{v}_{i+2}\}$ lifts to the total space as a product $\boldsymbol{\xi}_i \cong \xi_i \times T^{n-3} \subset M^{n+2}$, where ξ_i is a disk bundle with Euler class determined by r_i over either $L(p_i, q_i)$, or $S^1 \times S^2$ if $p_i = 0$. With the aid of a unimodular transformation matrix Q, we can arrange the rod structures into Hermite normal form $\{\boldsymbol{w}_1, \dots, \boldsymbol{w}_{l+2}\}$ so that $Q\boldsymbol{v}_i = \boldsymbol{w}_i$. Recall that the $\boldsymbol{w}_i$ are uniquely determined, although Q may not have this property. By Remark 3.4, the first three elements are given by $\boldsymbol{w}_1 = \boldsymbol{e}_1$, $\boldsymbol{w}_2 = \boldsymbol{e}_2$, and $\boldsymbol{w}_3 = (q_1, r_1, p_1, 0, \dots, 0)$. For each i such that $p_i \neq 0$, Lemma 6.2 ensures the existence of a unique primitive vector $\boldsymbol{\mathfrak{p}}_i \in \mathbb{Z}^n$ satisfying

$$\boldsymbol{w}_{i+2} = q_i \boldsymbol{w}_i + r_i \boldsymbol{w}_{i+1} + p_i \boldsymbol{\mathfrak{p}}_i. \tag{6-4}$$

When $p_i = 0$ we define $\boldsymbol{\mathfrak{p}}_i = \boldsymbol{0}$, and (6-4) is trivially satisfied.

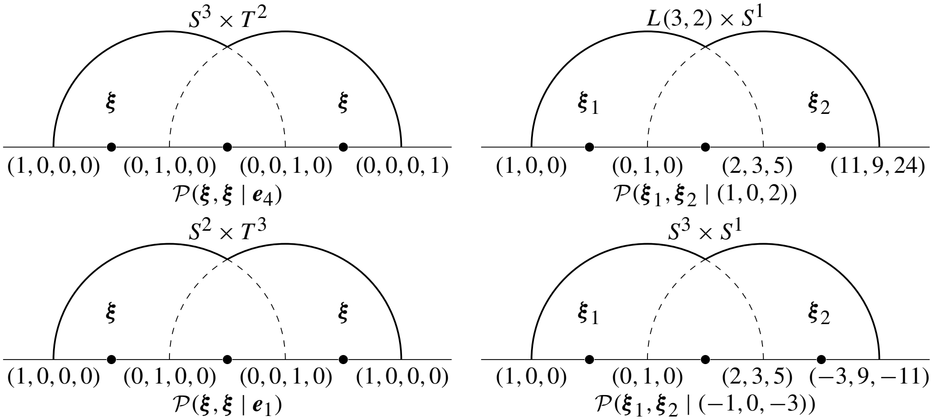

Figure 3. Left: Toric plumbings of the trivial bundle $\boldsymbol{\xi} = S^3 \times D^2 \times S^1$ with itself for the plumbing vector $\boldsymbol{\mathfrak{p}}_2 = \boldsymbol{e}_4$ (top) and $\boldsymbol{\mathfrak{p}}_2 = \boldsymbol{e}_1$ (bottom). Right: Toric plumbings of $\boldsymbol{\xi}_1$ over $L(5, 2)$ with Euler class determined by 3 and $\boldsymbol{\xi}_2$ over $L(7, 3)$ with Euler class determined by 2 for the plumbing vector $\boldsymbol{\mathfrak{p}}_2 = (1, 0, 2)$ (top) and $\boldsymbol{\mathfrak{p}}_2 = (-1, 0, -3)$ (bottom). For each pair the topology and toric structure of the total space is different, as a consequence of having different plumbing vectors. The notation $\mathcal{P}(\boldsymbol{\xi}_1, \boldsymbol{\xi}_2, \boldsymbol{\mathfrak{p}})$ refers to the toric plumbing of $\boldsymbol{\xi}_1$ and $\boldsymbol{\xi}_2$ with plumbing vector $\boldsymbol{\mathfrak{p}}$ (see Definition 6.6).

Definition 6.3. The vectors $\mathfrak{p}_i$ satisfying (6-4) are referred to as *plumbing vectors*.

Remark 6.4. If $\overline{Q}$ is a unimodular matrix, then $\{\boldsymbol{v}_1, \dots, \boldsymbol{v}_{l+2}\}$ and $\{\overline{Q}\boldsymbol{v}_1, \dots, \overline{Q}\boldsymbol{v}_{l+2}\}$ have the same Hermite normal form and thus the same plumbing vectors. Therefore, plumbing vectors do not depend on the choice of coordinates, but rather depend only on the toric structure of the total space.

While the set of plumbing vectors is uniquely determined by a set of rod structures, they are not uniquely determined by the topologies of ξ_i. In Figure 3, we present two pairs of examples in which the same disk bundles are being plumbed with different plumbing vectors. From Remark 6.4 we know that the total spaces will have different toric structures, and will not simply differ by a change of coordinates. Furthermore, in these examples the boundaries of the total spaces have different fundamental groups. Thus, plumbing vectors can affect the topology of the total space.

Plumbing vectors satisfy a number of relations, the first of which is the collection of recursion equations that are used in the definition

$$\boldsymbol{w}_1 = \boldsymbol{e}_1, \quad \boldsymbol{w}_2 = \boldsymbol{e}_2,$$

$$\boldsymbol{w}_{i+2} = q_i \boldsymbol{w}_i + r_i \boldsymbol{w}_{i+1} + p_i \mathfrak{p}_i \quad \text{if } p_i \neq 0, \text{ and} \tag{6-5a}$$

$$\mathfrak{p}_i = 0 \quad \text{if } p_i = 0$$

for $i = 1, \dots, l$. The next two conditions arise from are admissibility of the corners, and primitivity of the triples containing the plumbing vector. More precisely, adjacent rods $\{\boldsymbol{w}_{i+1}, \boldsymbol{w}_{i+2}\}$ are assumed to have an admissible corner, that is, $\mathrm{Det}_2(\boldsymbol{w}_{i+1}, \boldsymbol{w}_{i+2}) = 1$. By using the recursion relations and the multilinearity of determinants, this can be reexpressed as

$$\mathrm{Det}_2(\boldsymbol{w}_{i+1}, q_i \boldsymbol{w}_i + p_i \mathfrak{p}_i) = 1. \tag{6-5b}$$

Furthermore, the primitivity condition that is guaranteed by Lemma 6.2 asserts that

$$\mathrm{Det}_3(\boldsymbol{w}_i, \boldsymbol{w}_{i+1}, \mathfrak{p}_i) = 1, \tag{6-5c}$$

when $\mathfrak{p}_i \neq 0$. If $\mathfrak{p}_i = 0$ then this condition does not apply. Finally, we obtain two conditions from the fact that $\{\boldsymbol{w}_0, \dots, \boldsymbol{w}_{l+2}\}$ is in Hermite normal form. The first describes conditions under which certain entiees must vanish. That is, if $\mathfrak{p}_{ij} = 0$ for all $j \geq m$ and $1 \leq i < k$, where $\mathfrak{p}_i = (\mathfrak{p}_{i1}, \dots, \mathfrak{p}_{in})$, then

$$\mathfrak{p}_{kj} = 0 \quad \text{for all } j > m. \tag{6-5d}$$

The second condition indirectly restricts the size of certain components in the plumbing vectors. Write $\boldsymbol{w}_i = (w_{i1}, \dots, w_{in})$ and denote the last nonzero entry of $\mathfrak{p}_k$ by $\mathfrak{p}_{km_k}$. If $\mathfrak{p}_{im_k} = 0$ for all $1 \leq i < k$, then $w_{(k+2)m_k}$ is a pivot in the Hermite normal form so that

$$0 \leq w_{(k+2)j} < w_{(k+2)m_k} \quad \text{for all } j < m_k. \tag{6-5e}$$

These relations will be collectively referred to as the *plumbing relations*.

The first plumbing vector $\mathfrak{p}_1$ takes a simple form in all cases, depending only on whether p_1 vanishes. Namely, if the base space of ξ_1 is $S^1 \times S^2$ then $p_1 = 0$, and we have $\mathfrak{p}_1 = 0$. If $p_1 \neq 0$ then note that Remark 3.4 implies $\boldsymbol{w}_3 = (q_1, r_1, p_1, 0, \dots, 0)$. This immediately shows that $\mathfrak{p}_1 = \boldsymbol{e}_3$ solves (6-5a), and by uniqueness of plumbing vectors it follows that $\mathfrak{p}_1$ must take this form. In what follows, since $\mathfrak{p}_1$ is determined only by the topology of ξ_1 and not by plumbing information, we do not include it when describing the toric plumbing of ξ_1 and ξ_2. Thus, only $l-1$ plumbing vectors are needed to describe the gluing for a string of $l+2$ rod structures.

Proposition 6.5. *There is a one-to-one correspondence between collections of admissible rod structures* $\{\boldsymbol{w}_1, \dots, \boldsymbol{w}_{l+2}\} \subset \mathbb{Z}^n$ *in Hermite normal form, and collections of bundles* $\{\boldsymbol{\xi}_1, \dots, \boldsymbol{\xi}_l\}$ *paired with a set of primitive vectors* $\{\mathfrak{p}_2, \dots, \mathfrak{p}_l\} \subset \mathbb{Z}^n$ *satisfying* (6-5).

Proof. Let $\{\boldsymbol{w}_1, \dots, \boldsymbol{w}_{l+2}\} \subset \mathbb{Z}^n$ be a collection of admissible rod structures in Hermite normal. The proof of Theorem 6.1 shows that from each successive triple $\{\boldsymbol{w}_i, \boldsymbol{w}_{i+1}, \boldsymbol{w}_{i+2}\}$, there is a unique bundle $\boldsymbol{\xi}_i$ which is the lift of a (orbit space) neighborhood of these three rods to the total space M^{n+2}. The rod structures also give the integers q_i, r_i, and p_i used in Definition 6.3 to obtain the plumbing vectors $\mathfrak{p}_i$. By construction, together with the admissibility condition, these vectors satisfy the full set of plumbing relations (6-5).

Conversely, let $\{\boldsymbol{\xi}_1, \dots, \boldsymbol{\xi}_l\}$ be a collection of bundles and let $\{\mathfrak{p}_2, \dots, \mathfrak{p}_l\} \subset \mathbb{Z}^n$ be a collection of vectors satisfying (6-5). According to the discussion preceding this proposition, we may append to this list $\mathfrak{p}_1 = 0$ if the base of $\boldsymbol{\xi}_1$ is $S^1 \times S^2$, or $\mathfrak{p}_1 = \boldsymbol{e}_3$ if the base of $\boldsymbol{\xi}_1$ is a lens space. Equation (6-5a) then uniquely determines the rod structures $\{\boldsymbol{w}_1, \dots, \boldsymbol{w}_{l+2}\}$, since the integers q_i, r_i, and p_i are uniquely defined by each $\boldsymbol{\xi}_i$ as in the proof of Theorem 6.1. By hypothesis, the vectors $\{\boldsymbol{w}_1, \dots, \boldsymbol{w}_{l+2}\}$ satisfy (6-5b) which can be rewritten as $\mathrm{Det}_2(\boldsymbol{w}_{i+1}, \boldsymbol{w}_{i+2}) = 1$, thus establishing admissibility. Lastly, we note that (6-5a) and (6-5e) imply that the matrix composed of column vectors $\boldsymbol{w}_i$ satisfies the conditions of Lemma 3.3. Thus, the collection of rod structures is in Hermite normal form. □

Definition 6.6. Let $\boldsymbol{\xi}_i \cong \xi_i \times T^{n-3}$, $i = 1, \dots, l$ where each ξ_i is a D^2-bundle over either a 3-dimensional lens space or $S^1 \times S^2$, and let $\{\mathfrak{p}_2, \dots, \mathfrak{p}_l\} \subset \mathbb{Z}^n$ be a collection of primitive vectors satisfying the plumbing relations (6-5). We define the *toric plumbing* of $\boldsymbol{\xi}_1, \dots, \boldsymbol{\xi}_l$ along the plumbing vectors $\mathfrak{p}_2, \dots, \mathfrak{p}_l$ to be the $(n+2)$-dimensional simple T^n-manifold given by rod structures $\{\boldsymbol{w}_1, \dots, \boldsymbol{w}_l\}$, where the $\boldsymbol{w}_i$ are determined by (6-5a). This simple T^n-manifold is denoted by $\mathcal{P}(\boldsymbol{\xi}_1, \dots, \boldsymbol{\xi}_l \mid \mathfrak{p}_2, \dots, \mathfrak{p}_l)$.

Toric plumbing may be considered as a generalization of standard equivariant plumbing. In the latter construction the base and the fiber have the same dimension,

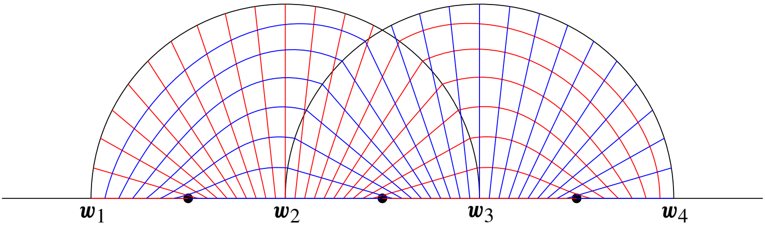

Figure 4. We have $\boldsymbol{w}_1 = \boldsymbol{e}_1$, $\boldsymbol{w}_2 = \boldsymbol{e}_2$, $\boldsymbol{w}_3 = (q_1, r_1, p_1)$, and $\boldsymbol{w}_4 = q_2\boldsymbol{w}_2 + r_2\boldsymbol{w}_3 + p_2\mathfrak{p}_2$ in accordance with (6-5a). The diagram shows a toric plumbing of two disk bundle-torus products $\boldsymbol{\xi}_1$ and $\boldsymbol{\xi}_2$ over lens spaces $L(p_1, q_1)$ and $L(p_2, q_2)$, along plumbing vector $\mathfrak{p}_2$. The fibers of $\boldsymbol{\xi}_1$ are given by rays emanating from $\boldsymbol{w}_2$, while the fibers of $\boldsymbol{\xi}_2$ are given by rays emanating from $\boldsymbol{w}_3$. Note that in the overlap, the fibers and sections switch roles between $\boldsymbol{\xi}_1$ and $\boldsymbol{\xi}_2$.

while in the former they do not. In order to elucidate the similarity between the two notions of plumbing, we restrict attention to $n = 3$ and consider a simple T^3-manifold $\mathcal{P}(\boldsymbol{\xi}_1, \boldsymbol{\xi}_2 \mid \mathfrak{p}_2)$. First note that this represents a gluing of $\boldsymbol{\xi}_1$ and $\boldsymbol{\xi}_2$. Indeed, the inclusion $\boldsymbol{\xi}_1 \hookrightarrow \mathcal{P}(\boldsymbol{\xi}_1, \boldsymbol{\xi}_2 \mid \mathfrak{p}_2)$ is manifested by the fact that $\{\boldsymbol{w}_1, \boldsymbol{w}_2, \boldsymbol{w}_3\}$ gives the canonical (Hermite normal form) rod diagram for $\boldsymbol{\xi}_1$. Furthermore, the inclusion of $\boldsymbol{\xi}_2$ may be observed by applying a unimodular transformation Q which sends $\boldsymbol{w}_2$ to $\boldsymbol{e}_1$, $\boldsymbol{w}_3$ to $\boldsymbol{e}_2$, and sends $\mathfrak{p}_2$ to $\boldsymbol{e}_3$ if $\mathfrak{p}_2 \neq 0$, to obtain the rod structures $\{Q\boldsymbol{w}_2, Q\boldsymbol{w}_3, Q\boldsymbol{w}_4\}$ which give the canonical rod diagram for $\boldsymbol{\xi}_2$; the primitivity condition from (6-5c) guarantees that existence of the matrix Q.

Consider now the gluing map between the two bundles. This map will operate between the subsets of $\boldsymbol{\xi}_1$ and $\boldsymbol{\xi}_2$ which are depicted by the overlap in Figure 4. This region is an open neighborhood of a single corner and thus is homeomorphic to $B^4 \times S^1$. In both $\boldsymbol{\xi}_1$ and $\boldsymbol{\xi}_2$ the corner represents a single (polar) circle in the base 3-manifold. The overlap region can further be viewed as a trivialization $B^2 \times D^2 \times S^1$ of the D^2-bundles $\boldsymbol{\xi}_1$, $\boldsymbol{\xi}_2$ over a neighborhood of a polar circle. Here we use B^2 to denote a disk in the base, and D^2 to denote a disk in the fiber. Just as in standard equivariant plumbing, Figure 4 shows that the D^2 fibers in say $\boldsymbol{\xi}_1$, which are represented by rays emanating from $\boldsymbol{w}_2$, switch roles in the overlap with the B^2 sections in the base of $\boldsymbol{\xi}_2$. The gluing map is an automorphism on the overlap $B^2 \times D^2 \times S^1$, and we have observed that the base and fiber disks B^2 and D^2 are exchanged in the gluing process. This leaves the circle S^1 unaccounted for. Since the automorphism must respect the action of T^3 on $B^2 \times D^2 \times S^1$, the image of this S^1 can be represented uniquely by an element of $\pi_1(T^3) \cong \mathbb{Z}^3$. Note, however, that the image of S^1 in $\mathbb{Z}^3$ does not necessarily coincide with the polar circle, but rather an $S^1 \subset T^3$ which acts upon it. These circle actions are not unique as there are two Killing fields, the ones associated to B^2 and D^2, which vanish on the polar circle. The Lie group homomorphism from T^3 to T^3 arising from these circle actions should be an isomorphism. This is the same as requiring that the image of the polar S^1, together with the circle actions on B^2 and D^2, forms an integral basis for $\mathbb{Z}^3$. The plumbing vector $\mathfrak{p}_2 \in \mathbb{Z}^3$ may then be interpreted as representing the image of the polar circle, with the integral basis criteria being equivalent to the primitivity property (6-5c).

Writing a simple T^n-manifold as a toric plumbing of disk bundles

$$\mathcal{P}(\boldsymbol{\xi}_1, \dots, \boldsymbol{\xi}_l \mid \mathfrak{p}_2, \dots, \mathfrak{p}_l)$$

facilitates the analysis of rod diagrams. Indeed

$$\mathcal{P}(\boldsymbol{\xi}_1, \dots, \boldsymbol{\xi}_l \mid \mathfrak{p}_2, \dots, \mathfrak{p}_l) \quad \text{and} \quad \mathcal{P}(\boldsymbol{\xi}'_1, \dots, \boldsymbol{\xi}'_l \mid \mathfrak{p}'_2, \dots, \mathfrak{p}'_l)$$

can be distinguished easily, as they are equivariantly homeomorphic if and only if $\boldsymbol{\xi}_j \cong \boldsymbol{\xi}'_j$ and $\mathfrak{p}_k = \mathfrak{p}'_k$ for all j and k. To see this, use Proposition 6.5 to obtain rod structures $\{\boldsymbol{w}_1, \dots, \boldsymbol{w}_{l+2}\}$ and $\{\boldsymbol{w}'_1, \dots, \boldsymbol{w}'_{l+2}\}$ from the disk bundles and plumbing vectors. These rod structures are automatically in their unique Hermite normal form, and therefore the two simple T^n-manifolds are equivariantly homeomorphic if and only if the rod structures are identical.

Remark 6.7. Given a set of bundles $\{\boldsymbol{\xi}_1, \dots, \boldsymbol{\xi}_l\}$, it may be difficult to determine all possible sets of vectors $\{\mathfrak{p}_2, \dots, \mathfrak{p}_l\}$ for which the plumbing relations (6-5) are satisfied. However, it is straightforward to check if a given set of vectors $\{\mathfrak{p}_2, \dots, \mathfrak{p}_l\}$ satisfies the plumbing relations for the bundles $\{\boldsymbol{\xi}_1, \dots, \boldsymbol{\xi}_l\}$. Namely, first confirm that each $\mathfrak{p}_i$ is a primitive vector. Then simply follow the recursion equations (6-5a) to find all the $\boldsymbol{w}_i$. If each successive pair $\{\boldsymbol{w}_i, \boldsymbol{w}_{i+1}\}$ is admissible, that is, if their second determinant divisor is 1, then $\{\boldsymbol{w}_1, \dots, \boldsymbol{w}_{l+2}\}$ does indeed give a well defined rod diagram for a manifold. Lastly, check that $\{\boldsymbol{w}_1, \dots, \boldsymbol{w}_{l+2}\}$ is in Hermite normal form. If so, then $\{\mathfrak{p}_2, \dots, \mathfrak{p}_l\}$ are valid plumbing vectors for the manifold arising from $\{\boldsymbol{w}_1, \dots, \boldsymbol{w}_{l+2}\}$.

The strategy to establish Theorem B is illustrated in Figure 5. More precisely, consider the orbit space of the domain of outer communication, and remove neighborhoods of the horizon rods (corresponding to the gray areas in the diagram). The axis is then broken into connected components, whose neighborhoods in the orbit space lift to one of the pieces in the total space of the decomposition (2-8). In particular, if the neighborhood contains no corners, one corner, or multiple corners then it is represented by C_k^{n+2}, $B_m^4 \times T^{n-2}$, or $\mathcal{P}(\boldsymbol{\xi}_{1,j}, \dots, \boldsymbol{\xi}_{I_j,j} \mid \mathfrak{p}_{2,j}, \dots, \mathfrak{p}_{I_j,j})$ respectively. The remaining portion of the orbit space lifts to the asymptotic end. Clearly any rod diagram that arises from a DOC, with the current hypotheses, can be organized into such pieces. This completes the proof of Theorem B.

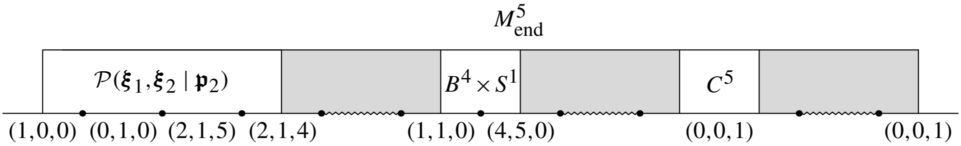

Figure 5. An example of the decomposition of the domain of outer communication described in Theorem B. The black hole horizons, represented by jagged intervals, are deformation retracts of the gray areas. In the leftmost piece of the decomposition, $\boldsymbol{\xi}_1$ is formed by a disk bundle over $L(5, 2)$ with Euler class determined by 1, while $\boldsymbol{\xi}_2$ is formed by a disk bundle over $L(2, 1)$ with Euler class 0; the plumbing vector is $\mathfrak{p}_2 = (1, 0, 2)$. The remaining pieces include a neighborhood of a corner $B^4 \times S^1$, a region centered on the interior of an axis rod $C^5 = [0, 1] \times D^2 \times T^2$, and the asymptotic end M^5_{end} which is homeomorphic to $\mathbb{R}_+ \times S^3 \times S^1$.

7. Classification of compact spaces

Theorem C arises from the classification of compact simply connected T^n-manifolds of cohomogeneity two in dimensions 4, 5, and 6. In dimensions 7 and higher, a complete classification is not known, and the technique used by Oh [33; 34] in the lower-dimensional cases does not appear to generalize to higher dimensions. On the other hand, the fundamental groups of $(n+2)$-dimensional T^n-manifolds can be readily computed in all dimensions by the Seifert–Van Kampen theorem, as recorded in the next result. Note that a portion of part (i) was established within the proof of Theorem 4 in [12].

Theorem 7.1. (i) *Let M^{n+2}, $n \geq 1$ be a closed orientable manifold with an effective T^n-action. If M^{n+2} is simply connected then it is either the* 3*-sphere*, *or a simple T^n-manifold where the integral span of its rod structures is $\mathbb{Z}^n$.*

(ii) *Let M^{n+2} be a connected simple T^n-manifold*, *possibly with boundary. Suppose that the rod diagram representing M^{n+2} is given by rod structures $\{\boldsymbol{v}_1, \dots, \boldsymbol{v}_m\} \subset \mathbb{Z}^n$. Then the fundamental group takes the form*

$$\pi_1(M^{n+2}) \cong \mathbb{Z}^n/\mathrm{span}_{\mathbb{Z}}\{\boldsymbol{v}_1, \dots, \boldsymbol{v}_m\} \cong \mathbb{Z}^{n-l} \oplus \mathbb{Z}_{s_1} \oplus \cdots \oplus \mathbb{Z}_{s_l}, \tag{7-1}$$

where $s_i\,|\,s_{i+1}$ and s_i is the i-th entry in the Smith normal form of the matrix composed of column vectors $\boldsymbol{v}_i$, *and $l = \dim \mathrm{span}_{\mathbb{R}}\{\boldsymbol{v}_1, \dots, \boldsymbol{v}_m\}$.*

Proof. Consider part (i). The fundamental group of a T^n-manifold of dimension $n+2$ can be calculated from the topology of the quotient space and the bundle structure, using the Seifert–Van Kampen theorem. This was carried out by Orlik and Raymond [36, p. 94] in the case when the quotient space is an orbifold without boundary, yielding the group presentation

$$\begin{aligned}(7\text{-}2)\qquad \pi_1(M^{n+2}) \cong \big\langle \tau_1, \dots, \tau_n, \alpha_1, \dots, \alpha_a, \gamma_1, \dots, \gamma_g, \delta_1, \dots, \delta_g \mid& \\ [\tau_i, \tau_j], [\tau_i, \alpha_j], [\tau_i, \gamma_j], [\tau_i, \delta_j] \quad \text{for all } i \text{ and } j;& \\ [\gamma_1, \delta_1] \cdots [\gamma_g, \delta_g] \cdot \alpha_1 \cdots \alpha_a \cdot \tau_1^{c_1} \cdots \tau_n^{c_n};& \\ \alpha_l^{q_l} \cdot \tau_1^{p_{l1}} \cdots \tau_n^{p_{ln}} \quad \text{for } l = 1, \dots, a\big\rangle.&\end{aligned}$$

The generators τ arise from the torus fibers, the α's represent loops around each of the a orbifold points, and the γ's and δ's are generators associated with each of the g handles. In the first line of relations we see that the τ's commute with themselves as they are the generators of a torus, and commute with the α's, γ's, and δ's since the former are generators of the fiber and the latter are generators in base space M^{n+2}/T^n. In analogy with the presentation of the fundamental group of a genus g surface, the second line of relations represents the obstruction to contractibility of the circumscribing loop around all of the handles and orbifold points. That loop is homotopic to the loop around the fibers described by $\boldsymbol{c} = (c_1, \dots, c_n) \in \mathbb{Z}^n \cong \pi_1(T^n)$. The last line of relations indicates how each orbifold point singularity is to be resolved, namely, going around the i-th orbifold point $q_i \neq 1$ times is equivalent to going around each of the torus fibers p_{ij} times.

We wish to show in this case that $M^{n+2} \cong S^3$. To do that, let the list of generators in (7-2) be denoted by $\mathcal{G}$ and the list of relations by $\mathcal{R}$, so that $\pi_1(M^{n+2}) \cong \langle \mathcal{G} \mid \mathcal{R} \rangle$ is trivial. Clearly then the group $\mathcal{H}_1 = \langle \mathcal{G} \mid \mathcal{R} \cup \{[\alpha_i, \alpha_j], \gamma_k, \delta_k\} \rangle$ is also trivial. This is an abelian group which can be presented as

$$(7\text{-}3)\qquad \mathcal{H}_1 = (\mathbb{Z}^a \oplus \mathbb{Z}^n)/\operatorname{span}_{\mathbb{Z}}\{(\mathbf{1}, \boldsymbol{c}), (q_1\boldsymbol{e}_1, \boldsymbol{p}_1), \dots, (q_a\boldsymbol{e}_a, \boldsymbol{p}_a)\},$$

where $\mathbf{1} \in \mathbb{Z}^a$ is the vector consisting of all 1's and $\boldsymbol{p}_l = (p_{l1}, \dots, p_{ln}) \in \mathbb{Z}^n$. The number of generators is $a + n$, and the number of relations is $a + 1$, hence $\mathcal{H}_1$ can only be trivial if $n \leq 1$. If $n = 1$ then M^{n+2} is a simply connected closed 3-manifold, and thus is homeomorphic to S^3.

We now consider the case where the quotient has boundary, i.e., $\partial(M^{n+2}/T^n) \neq \varnothing$. The fundamental group in this case was calculated by Hollands and Yazadjiev [12, Theorem 3] which takes the form

$$\begin{aligned}(7\text{-}4)\quad \pi_1(M^{n+2}) \cong \big\langle \tau_1, \dots, \tau_n, \alpha_1, \dots, \alpha_a, \beta_1, \dots, \beta_b, \gamma_1, \dots, \gamma_g, \delta_1, \dots, \delta_g \mid& \\ [\tau_i, \tau_j], [\tau_i, \alpha_j], [\tau_i, \beta_j], [\tau_i, \gamma_j], [\tau_i, \delta_j] \quad \text{for all } i \text{ and } j;& \\ [\gamma_1, \delta_1] \cdots [\gamma_g, \delta_g] \cdot \alpha_1 \cdots \alpha_a \cdot \beta_1 \cdots \beta_b;& \\ \alpha_l^{q_l} \cdot \tau_1^{p_{l1}} \cdots \tau_n^{p_{ln}} \quad \text{for } l = 1, \dots, a;& \\ \tau_1^{v_{k1}} \cdots \tau_n^{v_{kn}} \quad \text{for } k = 1, \dots, m\big\rangle.&\end{aligned}$$

The extra generators β represent the b boundary components of the orbit space which are homeomorphic to circles; on these components the torus action does not degenerate. Additional relations are included for these generators showing that they commute with the generators of the torus fibers. Moreover, the last line of relations is given by rod structures $\{\boldsymbol{v}_1, \dots, \boldsymbol{v}_m\}$ for M^{n+2} where each $\boldsymbol{v}_k = (v_{k1}, \dots, v_{kn})$ represents a generator of the isotropy subgroup along the corresponding rod. As before denote the generators of (7-4) by $\mathcal{G}$ and the list of relations by $\mathcal{R}$. We can immediately determine that $g = 0$ by examining $\langle \mathcal{G} \mid \mathcal{R} \cup \{\tau_i, \alpha_j, \beta_\ell\}\rangle$, which is in fact the fundamental group of a genus g surface. Next consider the subgroup $\langle \mathcal{G} \mid \mathcal{R} \cup \{\tau_i, \alpha_j\}\rangle = \langle \beta_1, \dots, \beta_b \mid \beta_1 \cdots \beta_b\rangle$, and observe that it is trivial only when all $\beta_i = 1$, or rather $b = 1$. Now consider the abelian group $\mathcal{H}_2 = \langle \mathcal{G} \mid \mathcal{R} \cup \{\tau_i, [\alpha_i, \alpha_j]\}\rangle$, which may be presented as

$$\mathcal{H}_2 = \mathbb{Z}^a/\operatorname{span}_{\mathbb{Z}}\{\mathbf{1}, q_1\boldsymbol{e}_1, \dots, q_a\boldsymbol{e}_a\}. \tag{7-5}$$

This group cannot be trivial unless $q_1 = \cdots = q_a = 1$, however this contradicts the nature of q_i, and thus $a = 0$. We then find that

$$\langle \mathcal{G} \mid \mathcal{R}\rangle = \mathbb{Z}^n/\operatorname{span}_{\mathbb{Z}}\{\boldsymbol{v}_1, \dots, \boldsymbol{v}_m\} \tag{7-6}$$

and note that this is trivial only if the integral span of the rod structures is $\mathbb{Z}^n$.

Lastly, we will establish part (ii). Notice that (7-4) reduces to the first equality in (7-1) when M^{n+2} is a simple T^n-space, since in this situation M^{n+2}/T^n has no holes, handles, or orbifold points. Furthermore, recall that the Smith normal form of the matrix $(\boldsymbol{v}_1, \boldsymbol{v}_2, \dots, \boldsymbol{v}_m)$ is obtained by both left and right actions using unimodular matrices. This does not alter the integral span of the columns. Thus, as in the classification of finitely generated abelian groups, by a change of basis given by these unimodular matrices, we obtain the second equality in (7-1). □

Theorem 7.1 may be used as a tool to analyze the topology of the domain of outer communication for stationary vacuum n-axisymmetric spacetimes. A conjecture providing a topological classification of the DOCs in the asymptotically Kaluza–Klein setting, and under a spin assumption, has been put forth by Hollands–Ishibashi in [10, Conjecture 1]. We now recall the original statement.

Conjecture (Hollands–Ishibashi). *Assume that $\mathcal{M}^{n+3}$, $n \geq 2$ is the domain of outer communication of a well-behaved asymptotically flat or asymptotically Kaluza–Klein spacetime which is spin, has Ricci tensor satisfying the null-convergence condition, and admits an effective* $\mathrm{U}(1)^n$ *action. Then any Cauchy surface M^{n+2} can be decomposed as*

$$M^{n+2} \cong (\#_{i=2}^{n} m_i \cdot (S^i \times S^{n+2-i})\#(\textit{asymptotic region})) \setminus (\textit{black holes}), \tag{7-7}$$

where the asymptotic region depends on the precise boundary conditions, e.g., in the standard Kaluza–Klein setup $\mathbb{R}^3 \times T^{n-1}$.

This conjecture implies that the fundamental group for the Cauchy surface always agrees with the fundamental group of the asymptotic region. Indeed, recall that taking a connected sum with simply connected space $S^k \times S^{n+2-k}$ does not affect the fundamental group, and neither does removing the black hole regions as can be seen from topological censorship, or alternatively by using Theorem 7.1. The next proposition provides an explicit static vacuum counterexample to the above conjecture.

Proposition 7.2. *There exists a well-behaved asymptotically Kaluza–Klein static biaxisymmetric vacuum spacetime* $\mathcal{M}^5 = \mathbb{R} \times M^4$, *which is devoid of conical singularities and has two spherical horizons. The domain of outer communication is spin and simply connected, while its asymptotic region is not simply connected. In particular, the Cauchy surface* M^4 *violates Conjecture* 1 *of* [10].

Proof. Consider the rod diagram consisting of rod structures $\{(1,0), (0,0), (0,1), (0,0), (1,0)\}$. According to Theorem A, there exists a well-behaved asymptotically Kaluza–Klein static biaxisymmetric vacuum spacetime $\mathcal{M}^5 = \mathbb{R} \times M^4$, whose orbit space M^4/T^2 is a half-plane admitting this rod diagram. In fact, in this static setting with a relatively simple rod structure, the existence result may be obtained through the superposition of harmonic functions and is in particular analytically regular, see [18; 20]. The two $(0,0)$ rods represent S^3 horizons, and the two semiinfinite rods $(1,0)$ give rise to the asymptotically Kaluza–Klein end $M^4_{\text{end}} \cong \mathbb{R}^3 \times S^1$. Moreover, in [15, Section 6] it is shown that there are no conical singularities on the two semiinfinite rods. The spacetime metric may be expressed in Weyl–Papapetrou form as in (2-1). Furthermore, since the Killing field ∂_{ϕ^2} that degenerates on the middle axis rod $(0,1)$ does not affect the cone angle at the two semiinfinite rods, or the asymptotics in M^4_{end} other than the size of the S^1 factor, we may scale the ϕ^2 coordinate appropriately to relieve any angle defect on this rod. The spacetime is then regular.

We will now analyze the topology of the domain of outer communication. First observe that Theorem 7.1 implies that M^4 is simply connected, while clearly $\pi_1(M^4_{\text{end}}) = \mathbb{Z}$. Next, fill in each S^3 horizon with a 4-ball B^4. This may be accomplished in the rod diagram by connecting the rods flanking the horizons with a single corner. As for the asymptotic end, a cross-section has the topology $S^1 \times S^2$, and thus may be filled in with an $S^1 \times B^3$. The asymptotic end is flanked by the rods $(1,0)$ and $(1,0)$, and thus the filling may be achieved in the rod diagram by extending one of these semiinfinite axis rods until it reaches the other, so that a single axis rod with the same rod structure is formed out of the two semiinfinite rods. Note that these fill-ins respect the T^2-structure by construction. After filling in the horizons and capping off the asymptotic end, we are left with a closed simple T^2-manifold having a rod diagram consisting of only two axis rods of rod structures $(1, 0)$ and $(0, 1)$, which meet at two admissible corners. This is the rod diagram for S^4. Therefore, the DOC M^4 is homeomorphic to $S^4 \setminus (B^4 \sqcup B^4 \sqcup S^1 \times B^3)$ which is homotopic to $\mathbb{R}^4 \setminus (\{\text{pt.}\} \sqcup S^1)$, which is a spin manifold.

Now assume by way of contradiction that Conjecture 1 of [10] is true. Although the black hole region is unknown, it cannot intersect the asymptotic region, by definition. We can therefore rearrange terms in (7-7) to find

$$M^4 \cong ((\#m_2 \cdot S^2 \times S^2) \setminus (\text{black holes}))\#(\text{asymptotic region}).$$

Recall that in three or more dimensions, the fundamental group of a connected sum is the free product of the fundamental groups of its components. Moreover, as stated in the conjecture, the asymptotic region for the standard Kaluza–Klein setup is $\mathbb{R}^3 \times S^1$. Therefore, there is an injective homomorphism $\mathbb{Z} \cong \pi_1(\mathbb{R}^3 \times S^1) \hookrightarrow \pi_1(M^4)$. This leads to a contradiction, since we have already seen that $M^4 \cong \mathbb{R}^4 \setminus (\{\text{pt.}\} \sqcup S^1)$, which is simply connected. □

Even though Conjecture 1 of [10] is not true as stated, the spirit of the conjecture which suggests that in the spin case Cauchy surfaces are primarily comprised of connected sums of products of spheres, may nevertheless remain valid. In fact Theorem C, which will be proven at the end of this section, confirms this sentiment in low dimensions. We are thus motivated to formulate a refined version, Conjecture D, and will give a proof of this conjecture for spacetime dimensions 5, 6, and 7. The primary difference between the revised and original versions is that instead of removing the black hole regions and including a connected sum to the asymptotic end, we consider closed extensions $\overline{M}^{n+2} \supset M^{n+2} \setminus M^{n+2}_{\text{end}}$. These extensions, which may be viewed as compactified domains of outer communication, fill in the asymptotic region as well as every horizon to form a closed manifold. Theorems 3.8 and 7.1 show that it is always possible to perform such fill-ins and obtain a closed, simply connected T^n-manifold, albeit the compactified DOC $\overline{M}^{n+2}$ may not be spin.

Proposition 7.3. *Conjecture D is valid when* $n = 2$, 3, *or* 4, *if the compactified domain of outer communication is spin.*

Proof. Let M^{n+2} be a Cauchy surface for the domain of outer communication of the spacetime $\mathcal{M}^{n+3}$ satisfying the desired hypotheses. Since all Cauchy surfaces are homeomorphic, we can without loss of generality assume that M^{n+2} admits a $\mathrm{U}(1)^n$ symmetry. This, together with the topological censorship theorem, shows that M^{n+2} is a simple T^n-manifold [10, Theorem 9]. To construct the compactified DOC $\overline{M}^{n+2} \supset M^{n+2} \setminus M^{n+2}_{\text{end}}$, we cap off the asymptotic region and fill in all of the horizons in such a way that the total space is simply connected, by adding additional rods. Theorem 3.8 describes how to construct the fill-ins from the rod diagram, while (7-1) explains how to make the total space simply connected. If $n = 2$, 3, or 4, and if $\overline{M}^{n+2}$ is spin, then by Theorem C it is homeomorphic to a connect sum of products of spheres. □

It is likely the case that a spin DOC yields a spin compactified DOC in the proof of this proposition, in which case Conjecture D would be fully verified for $n = 2$, 3, or 4. Furthermore, Proposition 7.3 can be generalized to include the nonspin case where $\overline{M}^{n+2}$ will instead be homeomorphic to a manifold in the third row of the table from Theorem C. In addition, it should be noted that the refined conjecture can be extended to the setting where geometric regularity of the spacetime metric is not required. This is relevant to applications of Theorem A, since generic spacetimes produced by this result may include conical singularities on the axes.

Remark 7.4. A slightly modified version of Proposition 7.3 holds true when the spacetime $\mathcal{M}^{n+3}$ has conical singularities on its axis rods. To see this, observe that the only place where geometric regularity of the metric becomes relevant, is when the topological censorship theorem is utilized. Thus, the regularity assumption as well as the null energy condition may be removed from the hypotheses of Conjecture D, if the topological censorship principle is added in their place. This principle, together with the $\mathrm{U}(1)^n$ symmetry, guarantees that the Cauchy surface M^{n+2} is a simple T^n-manifold. The remaining portion of the proof then proceeds without change. In fact, the conjecture is at its core a purely topological statement.

Conjecture E. *Let $n \geq 1$. Any closed, spin, simply connected $(n+2)$-manifold with an effective T^n-action is homeomorphic to either S^3, S^4, S^5, or $\#_{i=2}^{n} m_i \cdot S^i \times S^{n+2-i}$.*

It does not appear that this conjecture has previously been recorded in the literature. However, it should be noted that McGavran claimed in [29, Theorem 3.6] (see also [28]) to have proven a similar statement. Oh [34] pointed out flaws in McGavran's argument, and in fact provided counterexamples to his claims. Oh's work on this topic [33; 34], along with Orlik and Raymond's classification [35] in the 4-dimensional case, remains the best evidence towards Conjecture E.

Proof of Theorem C. We may follow the same line of argument as in the proof of Proposition 7.3. In particular, by applying Theorems 3.8 and 7.1 to cap-off the asymptotic end and fill-in the horizons, we arrive at a compactified domain of outer communication $\overline{M}^{n+2}$ which is closed, simply connected, and admits an effective T^n-action. Moreover, this process of capping-off and filling-in may be accomplished in an algorithmic manner, as explained in the proof of Theorem 3.8. We may then apply the classification results for such manifolds given in [33; 34; 35] for $n = 2, 3, 4$, to obtain the chart presented in Theorem C. □

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VISHNU KAKKAT
DEPARTMENT OF MATHEMATICS AND DEPARTMENT OF PHYSICS
ARIEL UNIVERSITY
ARIEL
ISRAEL
vishnuka@ariel.ac.il

MARCUS KHURI
DEPARTMENT OF MATHEMATICS
STONY BROOK UNIVERSITY
STONY BROOK, NY
UNITED STATES
khuri@math.sunysb.edu

JORDAN RAINONE
DEPARTMENT OF MATHEMATICS
STONY BROOK UNIVERSITY
STONY BROOK, NY
UNITED STATES
jordan.rainone@stonybrook.edu

GILBERT WEINSTEIN
DEPARTMENT OF MATHEMATICS AND DEPARTMENT OF PHYSICS
ARIEL UNIVERSITY
ARIEL
ISRAEL
gilbertw@ariel.ac.il

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QUASILINEAR SCHRÖDINGER EQUATIONS: GROUND STATE AND INFINITELY MANY NORMALIZED SOLUTIONS

HOUWANG LI AND WENMING ZOU

We study the normalized solutions for the following quasilinear Schrödinger equations:

$$-\Delta u - u\Delta u^2 + \lambda u = |u|^{p-2}u \quad \text{in } \mathbb{R}^N,$$

with prescribed mass

$$\int_{\mathbb{R}^N} u^2 = a^2.$$

We first consider the mass-supercritical case $p > 4 + \frac{4}{N}$, which has not been studied before. By using a perturbation method, we succeed to prove the existence of ground state normalized solutions, and by applying the index theory, we obtain the existence of infinitely many normalized solutions. We also obtain new existence results for the mass-critical case $p = 4 + \frac{4}{N}$ and remark on a concentration behavior for ground state solutions.

1. Introduction

We consider the equation

$$\begin{cases} i\partial_t \phi = -\Delta\phi - \sigma|\phi|^{p-2}\phi - \kappa\phi\Delta(|\phi|^2) & \text{in } \mathbb{R}^+ \times \mathbb{R}^N, \\ \phi(0,x) = \phi_0(x) & \text{in } \mathbb{R}^N, \end{cases} \tag{1-1}$$

where $N \geq 1$ is the space dimension, $2 < p < 2N/(N-2)^+$ and σ, κ are constants.

Equation (1-1) arises in the study of superfluid helium films (see [28; 46]), which describes the thickness and superfluid velocity of the helium films. More precisely, consider a superfluid helium film adsorbed on a substrate. Let $\psi(t,x)$ denote the condensate wave function, which is chosen proportionally so that the film thickness d and the superfluid velocity v can be defined by

$$n_0 \cdot d(t,x) = a + |\psi(t,x)|^2, \quad v(t,x) = \mathrm{Re}\left[\frac{\hbar}{M}\frac{\psi^*\nabla\psi}{|\psi(t,x)|^2}\right], \tag{1-2}$$

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where n_0 is the density number, M is the mass of helium atoms and a is the density of solid layer. Then the energy density of this quantum state consists of

$$\text{kinetic term} = \tfrac{1}{2} i\hbar(\psi^*\dot{\psi} - \dot{\psi}^*\psi),$$

the potential terms:

$$\text{bending energy term} = \frac{\hbar^2}{2M}|\nabla\psi|^2, \quad \text{chemical potential term} = -\mu|\psi|^2,$$

the van der Waals force term [2; 3]

$$\text{van der Waals term} \propto \frac{1}{d^2} - \frac{1}{d_{\min}^2} \propto \frac{1}{(a+|\psi|^2)^2} - \frac{1}{a^2},$$

and finally the surface energy term [46]

$$\text{surface term} \propto |\nabla d|^2 \propto \big|\nabla|\psi|^2\big|^2.$$

The Lagrangian density is the sum of these terms (we omit the constant $-1/a^2$, since it is irrelevant for our discussion):

$$L = \frac{1}{2} i\hbar(\psi^*\dot{\psi} - \dot{\psi}^*\psi) - \frac{\hbar^2}{2M}|\nabla\psi|^2 + \mu|\psi|^2 - \frac{A}{2(a+|\psi|^2)^2} - \frac{B}{2}\big|\nabla|\psi|^2\big|^2.$$

From the variational principle

$$\delta \int dt \int dx L = 0,$$

we write the equation of motion of the condensate wavefunction, which is a Schrödinger equation describing the nonlinear dynamics of the superfluid condensate

$$i\hbar\partial_t\phi = -\frac{\hbar^2}{2M}\Delta\phi - \mu\phi - \frac{A\phi}{(1+|\phi|^2)^3} - B\phi\Delta(|\phi|^2). \tag{1-3}$$

Equation (1-3) was already obtained in [28; 46]. To solve (1-3), expanding the van der Waals term in $|\psi|^2$ to the lowest order, and simplifying as in [28], we obtain the following special case of (1-1):

$$i\partial_t\phi = -\Delta\phi - \sigma|\phi|^2\phi - \kappa\phi\Delta(|\phi|^2), \tag{1-4}$$

where σ, κ are constants.

Except superfluid helium films, equation (1-4) also appears in plasmas, see [30; 52] for more physical information. If $\kappa = 0$, equation (1-4) reduces essentially to the ordinary nonlinear Schrödinger equation, which arises in the study of standing wave solutions of the nonlinear Gross–Pitaevskii equations proposed by Gross [22] and Pitaevskii [44], and its soliton solutions have been studied widely in physics and mathematics. But when $\kappa \neq 0$, the term $\kappa(\Delta|\phi|^2)\phi$ brings new difficulties to the theoretical analysis of soliton solution of (1-4). In [28; 46], the numerical simulations of soliton solutions to (1-4) and (1-3) was given, but the theoretical research is far from clear due to the appearance of the term $\kappa(\Delta|\phi|^2)\phi$. So in this paper, we focus on the theoretical research. In the following, we will analyze the reason why the term $\kappa(\Delta|\phi|^2)\phi$ is hard to handle, and we will use some techniques to overcome these difficulties to study soliton solutions.

We set $\sigma = 1$ and $\kappa = 1$. By considering soliton wave solutions, substituting $\phi(t,x) = e^{i\lambda t}u(x)$ into (1-5), we obtain

$$-\Delta u - u\Delta u^2 + \lambda u = |u|^{p-2}u \quad \text{in } \mathbb{R}^N, \tag{1-5}$$

which is usually called the modified nonlinear Schrödinger equation. Usually, to study (1-5) one always considers this equation for a given parameter λ. But now we introduce a second approach.

From (1-2), we know that $|\phi(t,x)|^2$ represents the superfluid film thickness and the total quasiparticle number

$$M \propto \int_{\mathbb{R}^N} |\phi(t,x)|^2 \, \mathrm{d}x.$$

Multiplying (1-1) with ϕ^*, subtracting the complex conjugate, and integrating over space, we find

$$\partial_t M = 0,$$

which means that the total quasiparticle number remains the same constant as t changes, i.e., the law of conservation of mass. So it is natural to assume

$$\int_{\mathbb{R}^N} |\phi(t,x)|^2 \, \mathrm{d}x = \text{constant}, \tag{1-6}$$

when considering soliton wave solutions. Combining (1-5) and (1-6), we obtain

$$\begin{cases} -\Delta u - u\Delta u^2 + \lambda u = |u|^{p-2}u \quad \text{in } \mathbb{R}^N, \\ \int_{\mathbb{R}^N} |u|^2 \, \mathrm{d}x = a, \end{cases} \tag{1-7}$$

and the aim is to find $u \in \mathcal{H}$ with a $\lambda \in \mathbb{R}$ such that (u, λ) satisfies (1-7) for a given $a > 0$. Here

$$\mathcal{H} = \left\{ u \in W^{1,2}(\mathbb{R}^N) : \int_{\mathbb{R}^N} |u|^2 |\nabla u|^2 < +\infty \right\}.$$

Solutions of (1-7) are often referred to as normalized solutions, and the search for such solutions has became a hot direction in recent years. We have to admit that although the physical motivation of searching for such solutions is described as above, we don't know much about its physical meaning and application. We point out that the barrier exponent $4 + \frac{4}{N}$ is also the threshold of the stability and instability of soliton solutions. Roughly speaking, it was shown in [17] that the standing wave of (1-1) is stable for $p < 4 + \frac{4}{N}$, while it is unstable for $p \geq 4 + \frac{4}{N}$. Later in [15] the results about stability was extended to equations with $u\Delta u^2$ replaced by general quasilinear terms $u^{\alpha-1}\Delta u^{\alpha}$. Now we give the mathematical motivation of normalized solutions. Formally, to obtain the normalized solutions of (1-5), one needs to consider the corresponding energy functional

$$I(u) := \tfrac{1}{2}\int_{\mathbb{R}^N} |\nabla u|^2 + \int_{\mathbb{R}^N} |u|^2 |\nabla u|^2 - \tfrac{1}{p}\int_{\mathbb{R}^N} |u|^p \tag{1-8}$$

on a L^2 sphere

$$\tilde{\mathcal{S}}(a) := \Big\{ u \in \mathcal{H} : \int_{\mathbb{R}^N} |u|^2 = a \Big\}, \tag{1-9}$$

which has particular difficulties. To derive the Palais–Smale sequence, one needs new variational methods. The derived Palais–Smale sequence may not be bounded; even if the Palais–Smale sequence is bounded, the weak limit may not be contained in the L^2 sphere (even in the radial case). Such difficulties make the study of normalized solutions of (1-7) much more complicated than the study of (1-5) with prescribed $\lambda \in \mathbb{R}$. So the search for normalized solutions is a challenging and interesting problem, and needs new variational methods.

We introduce some results about the existence of normalized solutions to the semilinear Schrödinger equation

$$-\Delta u + \lambda u = g(u) \quad \text{in } \mathbb{R}^N. \tag{1-10}$$

L. Jeanjean [24] obtained a normalized solution of (1-10) using an auxiliary functional and a minimax theorem from [19]. The existence of infinitely many normalized solutions of (1-10) was later proved by T. Bartsch and S. de Valeriola [4] using a new linking geometry for the auxiliary functional. After that, N. Ikoma and K. Tanaka [23] constructed a deformation theorem suitable for the auxiliary functional, and then obtained infinitely many normalized solutions of (1-10) through Krasnoselskii index under a weaker condition on $g(u)$. Soon later, L. Jeanjean and S. S. Lu [25] obtained infinitely many normalized solutions of (1-10) under a totally different assumption on $g(u)$ which permits $g(u)$ to be just continuous. As for the least energy normalized solutions, N. Soave [48; 49] obtained the existence of ground state normalized solutions with $g(u) = |u|^{p-2}u + \mu |u|^{q-2}u$ by restraining the energy functional on a smaller manifold. For more results on normalized solutions for scalar equations and systems, we refer to [5; 6; 7; 8; 9; 20; 21; 31].

Now back to the modified nonlinear Schrödinger equation (1-5), we analyze the difficulties induced by the term $\kappa(\Delta|\phi|^2)\phi$. When considering (1-5) with $\lambda \in \mathbb{R}$ fixed, one would always study the functional

$$E_\lambda(u) := \tfrac{1}{2}\int_{\mathbb{R}^N} (|\nabla u|^2 + \lambda |u|^2) + \int_{\mathbb{R}^N} |u|^2 |\nabla u|^2 - \tfrac{1}{p}\int_{\mathbb{R}^N} |u|^p \tag{1-11}$$

on the space $\mathcal{H}$. It is easy to check that u is a weak solution of (1-5) if and only if

$$E'_\lambda(u)\phi = \lim_{t\to 0^+} \frac{E_\lambda(u+t\phi) - E_\lambda(u)}{t} = 0$$

for every $\phi \in \mathcal{C}_0^\infty(\mathbb{R}^N)$. We recall, see [37] for example, that the value 22^* with

$$2^* := \begin{cases} \frac{2N}{N-2}, & N \geq 3, \\ +\infty, & N \leq 2 \end{cases}$$

corresponds to a critical exponent. Compared to (1-10), the search for solutions of (1-5) presents a major difficulty: the functional associated with the term $u\Delta u^2$

$$V(u) = \int_{\mathbb{R}^N} |u|^2 |\nabla u|^2$$

is nondifferentiable in $\mathcal{H}$ when $N \geq 2$. To overcome this difficulty, various arguments have been developed, such as the minimization methods [35] where the nondifferentiability of E_λ does not come into play, the methods of a Nehari manifold approach [38; 39], the methods of changing variables [16; 37] which transform problem (1-5) into a semilinear one (1-10), and a perturbation method in a series of papers [36; 40; 41] which recovers the differentiability by considering a perturbed functional on a smaller function space.

However, when considering the normalized solution problem (1-7), one would find that the methods of Nehari manifold approach and changing variables are no longer applicable, since the parameter λ is unknown and the L^2-norm $\|u\|_2$ must be equal to a given number. So there are very few results on problem (1-7). Formally, a normalized solution of (1-7) can be obtained as a critical point of $I(u)$ defined by (1-8) on the set $\tilde{\mathcal{S}}(a)$. That is, a normalized solution of (1-7) is a $u \in \tilde{\mathcal{S}}(a)$ such that there exists a $\lambda \in \mathbb{R}$ satisfying

$$\text{(1-12)} \quad \int_{\mathbb{R}^N} \nabla u \cdot \nabla \phi + 2\int_{\mathbb{R}^N} (u\phi|\nabla u|^2 + |u|^2 \nabla u \cdot \nabla \phi) + \lambda \int_{\mathbb{R}^N} u\phi - \int_{\mathbb{R}^N} |u|^{p-2} u\phi = 0$$

for any $\phi \in \mathcal{C}_0^\infty(\mathbb{R}^N)$. To proceed our paper, we introduce a sharp Gagliardo–Nirenberg inequality [1]:

$$\text{(1-13)} \qquad \int_{\mathbb{R}^N} |u|^{\frac{p}{2}} \leq \frac{C(p,N)}{\|Q_p\|_1^{(p-2)/(N+2)}} \Big(\int_{\mathbb{R}^N} |u|\Big)^{\frac{4N-(N-2)p}{2(N+2)}} \Big(\int_{\mathbb{R}^N} |\nabla u|^2\Big)^{\frac{N(p-2)}{2(N+2)}}$$

for all $u \in \mathcal{E}^1$ where $2 < p < 22^*$,

$$C(p,N) = \frac{p(N+2)}{[4N-(N-2)p]^{\frac{4-N(p-2)}{2(N+2)}} \, [2N(p-2)]^{\frac{N(p-2)}{2(N+2)}}},$$

and the space $\mathcal{E}^q$ for $q \geq 1$ is defined by

$$\mathcal{E}^q := \{u \in L^q(\mathbb{R}^N) : \nabla u \in L^2(\mathbb{R}^N)\},$$

with norm $\|u\|_{\mathcal{E}^q} := \|\nabla u\|_2 + \|u\|_q$. For embedding theorems and related properties of $\mathcal{E}^q$, we refer to [29]. Moreover, Q_p optimizes (1-13) and the unique nonnegative radially symmetric solution of the following equation [47]:

$$-\Delta u + 1 = u^{\frac{p}{2}-1} \quad \text{in } \mathbb{R}^N. \tag{1-14}$$

Strictly speaking, it has been proved in [47, Theorem 1.3] that Q_p has a compact support in $\mathbb{R}^N$ and it exactly satisfies a Dirichlet–Neumann free boundary problem. Namely, there exists an $R > 0$ such that Q_p is the unique positive solution of

$$\begin{cases} -\Delta u + 1 = u^{\frac{p}{2}-1} & \text{in } B_R, \\ u = \frac{\partial u}{\partial n} = 0 & \text{on } \partial B_R. \end{cases} \tag{1-15}$$

In what follows, if we say that u is a nonnegative solution of (1-14), then we mean that u is a solution of (1-15). By replacing u with u^2 in (1-13), one immediately obtains the following Gagliardo–Nirenberg-type inequality:

$$\int_{\mathbb{R}^N} |u|^p \le \frac{C(p,N)}{\|Q_p\|_1^{(p-2)/(N+2)}} \Big(\int_{\mathbb{R}^N} |u|^2\Big)^{\frac{4N-p(N-2)}{2(N+2)}} \Big(4\int_{\mathbb{R}^N} |u|^2 |\nabla u|^2\Big)^{\frac{N(p-2)}{2(N+2)}}. \tag{1-16}$$

Now we collect some known results about normalized solutions of (1-7). First, to avoid the nondifferentiability of $V(u)$, M. Colin, L. Jeanjean and M. Squassina [17] (see also [15] for general quasilinear terms) and L. Jeanjean and T. J. Luo [26] considered the minimization problem

$$\tilde{m}(a) = \inf_{u \in \tilde{S}(a)} I(u),$$

with $2 < p \le 4 + \frac{4}{N}$. Using inequality (1-16), one can find that $\tilde{m}(a) > -\infty$ when $2 < p < 4 + \frac{4}{N}$ and $\tilde{m}(a) = -\infty$ when $p > 4 + \frac{4}{N}$, since

$$\frac{N(p-2)}{2(N+2)} < 1 \quad \text{if and only if } p < 4 + \frac{4}{N}.$$

These considerations show that the exponent $4 + \frac{4}{N}$ for (1-7) plays the role of $2 + \frac{4}{N}$ in (1-10). After that, X. Y. Zeng and Y. M. Zhang [53] studied the existence and asymptotic behavior of the minimizers to

$$\inf_{u \in \tilde{S}(a)} I(u) + \int_{\mathbb{R}^N} a(x)|u|^2,$$

where $a(x)$ is an infinite potential well. In addition to these minimization approaches, L. Jeanjean, T. J. Luo and Z. Q. Wang [27] obtained another mountain-pass-type normalized solution of (1-7) through the perturbation method. We remark that all of these results on normalized solution of (1-7) have considered either the mass-subcritical or mass-critical case, i.e., $2 < p \le 4 + \frac{4}{N}$.

In this paper, we consider the mass-critical and mass-supercritical cases, i.e., $p \ge 4 + \frac{4}{N}$. To the best of our knowledge, the case of mass-supercritical has not been considered before. Actually, we obtain:

Theorem 1.1. *Assume that one of the following conditions holds*:

(H1) $N = 1, 2,\ p > 4 + \frac{4}{N},\ a > 0.$

(H2) $N = 3,\ 4 + \frac{4}{N} < p < 2^*,\ a > 0.$

Then there exists a radially symmetric positive ground state normalized solution $u \in W^{1,2}(\mathbb{R}^N) \cap L^\infty(\mathbb{R}^N)$ *of* (1-7) *in the sense that*

$$I(u) = \inf\{I(v) : v \in \tilde{\mathcal{S}}(a),\ I|'_{\tilde{\mathcal{S}}(a)}(v) = 0,\ v \neq 0\}.$$

Theorem 1.2. *Assume that one of the following conditions holds*:

(H1′) $N = 2,\ p > 4 + \frac{4}{N},\ a > 0.$

(H2) $N = 3,\ 4 + \frac{4}{N} < p < 2^*,\ a > 0.$

Then there exists a sequence of normalized solutions $u^j \in W^{1,2}(\mathbb{R}^N) \cap L^\infty(\mathbb{R}^N)$ *of* (1-7) *with increasing energy* $I(u^j) \to +\infty$.

Remark 1.3. (1) We state that the dimension is limited due to a lemma limitation used to control the Lagrange multipliers, see Lemma 2.2 and Remark 4.2.

(2) The difference between Theorems 1.1 and 1.2 is that we cannot prove the existence of infinitely many solutions when $N = 1$, because the failure of the compact embedding $W^{1,2}(\mathbb{R}) \hookrightarrow L^q(\mathbb{R})$ for $2 < q < 2^*$. When considering the ground state, however, we are able to recover the compactness of bounded sequences using the symmetric decreasing arrangement, due to the advantage of the associated minimization $m_\mu(a)$ defined in (3-8).

Now we turn to the mass-critical case, i.e., $p = 4 + \frac{4}{N}$. Let $a_* = \|Q_{4+\frac{4}{N}}\|_1$.

Theorem 1.4. *Assume that one of the following conditions holds*:

(H3) $N \leq 3,\ p = 4 + \frac{4}{N},\ a > a_*;$

(H4) $N \geq 4,\ p = 4 + \frac{4}{N},\ a_* < a < \left(\frac{N-2}{N-2-(4/N)}\right)^{\frac{N}{2}} a_*,$

Then there exists a radially symmetric positive ground state normalized solution $u \in W^{1,2}(\mathbb{R}^N) \cap L^\infty(\mathbb{R}^N)$ *of* (1-7) *in the sense that*

$$I(u) = \inf\{I(v) : v \in \tilde{\mathcal{S}}(a),\ I|'_{\tilde{\mathcal{S}}(a)}(v) = 0,\ v \neq 0\}.$$

Remark 1.5. Recently H. Y. Ye and Y. Y. Yu [51] obtained the existence of ground state normalized solution of (1-7) under assumption (H3). As one can see, although Theorem 1.4 contains their existence result, the method we used in the current paper is totally different from theirs, while as they said in [51, Remark 1.3], they are unable to handle the case $N \geq 4$. Moreover, they also consider an asymptotic behavior, but our Theorem 1.8 is more accurate, since we give a description of u_n when $a \to a_*$.

We observe that when $p = 4 + \frac{4}{N}$, the value a_* is a threshold of the existence of normalized solution of (1-7). Actually, we have:

Proposition 1.6. *Let* $p = 4 + \frac{4}{N}$ *and* $N \geq 1$. *Then*:

(1) $\tilde{m}(a) = \begin{cases} 0, & 0 < a \leq a_*, \\ -\infty, & a > a_*. \end{cases}$

(2) *Equation (1-7) has no solutions for any* $0 < a \leq a_*$.

(3) *Equation (1-7) has at least one radially symmetric positive solution for* $a > a_*$ *and* a *is close to* a_*.

Remark 1.7. We state that (1) is a direct conclusion of [17, Theorem 1.9] and (3) is a direct conclusion of Theorem 1.4 above. Now we prove (2). Since u is a solution of (1-7), there holds (see Lemma 2.1)

$$\int_{\mathbb{R}^N} |\nabla u|^2 + (2+N) \int_{\mathbb{R}^N} |u|^2 |\nabla u|^2 - \frac{N(2+N)}{4(N+1)} \int_{\mathbb{R}^N} |u|^{4+\frac{4}{N}} = 0.$$

Combining with (1-16), we obtain

$$\int_{\mathbb{R}^N} |\nabla u|^2 + (2+N) \int_{\mathbb{R}^N} |u|^2 |\nabla u|^2 \leq (2+N) \Big(\frac{a}{a_*}\Big)^{\frac{2}{N}} \int_{\mathbb{R}^N} |u|^2 |\nabla u|^2,$$

from which we get $u = 0$ for any $0 < a \leq a_*$, a contradiction since $\|u\|_2 = a$.

Inspired by Proposition 1.6, we enlighten a concentration behavior of the radially symmetric positive solution of (1-7) when $p = 4 + \frac{4}{N}$ and $a \to a_*$.

Theorem 1.8. *Let* $p = 4 + \frac{4}{N}$, $N \geq 1$, *and let* u_n *be a radially symmetric positive solution of (1-7) for* $a = a_n$ *with* $a_n > a_*$ *and* $a_n \to a_*$. *Then there exists a sequence* $y_n \in \mathbb{R}^N$ *such that up to a subsequence, we have*

$$\left[\Big(\frac{Na_*}{N}\Big)^{\frac{1}{2+N}} \varepsilon_n\right]^N u_n^2\Big(\Big(\frac{Na_*}{N}\Big)^{\frac{1}{2+N}} \varepsilon_n x + \varepsilon_n y_n\Big) \to Q_{4+\frac{4}{N}} \quad \text{in } L^q(\mathbb{R}^N) \tag{1-17}$$

for $1 \leq q < 2^*$, *where*

$$\varepsilon_n = \Big(\int_{\mathbb{R}^N} u_n^2 |\nabla u_n|^2\Big)^{-(2+N)} \to 0.$$

Remark 1.9. Theorem 1.8 gives a description of radially symmetric positive solution of (1-7) as the mass a_n approaches to a_* from above. Roughly speaking, it shows that for n large enough, we have

$$u_n(x) = \left[\Big(\frac{Na_*}{N}\Big)^{\frac{1}{2+N}} \varepsilon_n\right]^{-\frac{N}{2}} Q_{4+\frac{4}{N}}\Big(\Big(\frac{Na_*}{N}\Big)^{-\frac{1}{2+N}} \varepsilon_n^{-1}(x - \varepsilon_n^{-1} y_n)\Big).$$

The paper is organized as follows. In Section 2, we give perturbation settings and an important lemma. In Section 3A, we give some properties of the associated Pohozaev manifold. In Sections 3B and 3C, we prove the existence of ground state and infinitely many critical points for perturbed functional. In Section 4, we study the convergence of the critical points for the perturbed functional as $\mu \to 0^+$. And Theorem 1.1 for $N = 1$ is proved in Section 3B; Theorem 1.1 for $N \geq 2$ and Theorem 1.2 are proved in Section 4. Finally, in Section 5, we study the mass-critical case, and prove Theorems 1.4 and 1.8. In the Appendix, we prove some valuable results.

Throughout the paper, we use standard notations. For simplicity, we write $\int_{\mathbb{R}^N} f$ to mean the Lebesgue integral of $f(x)$ over $\mathbb{R}^N$ and $\|\cdot\|_p$ denotes the standard norm of $L^p(\mathbb{R}^N)$. We use $\to$ and $\rightharpoonup$, respectively, to denote the strong and weak convergences in the related function spaces. By $C, C_1, C_2, \dots$ we denote positive constants unless specified otherwise.

2. Preliminary

2A. *Perturbation setting.* Let $I(u)$ be defined by (1-8). Observe that when $N = 1$, $I(u)$ is of class $\mathcal{C}^1$ in $W^{1,2}(\mathbb{R})$, so there is no need to perturb $I(u)$, and in this case the proof will be stated separately in the last of part Section 3B. Thus we assume $N \geq 2$. To avoid the nondifferentiability, we take the perturbation method, which has been applied firstly to unconstrained situation in [40; 41] and then to constrained situation in [27]. For $\mu \in (0, 1]$, we define

$$I_\mu(u) := \frac{\mu}{\theta}\int_{\mathbb{R}^N} |\nabla u|^\theta + I(u) \tag{2-1}$$

on the space $\mathcal{X} := W^{1,\theta}(\mathbb{R}^N) \cap W^{1,2}(\mathbb{R}^N)$ for some fixed θ satisfying

$$\frac{4N}{N+2} < \theta < \min\left\{\frac{4N+4}{N+2}, N\right\}, \quad \text{when } N \geq 3 \qquad \text{and} \qquad 2 < \theta < 3, \quad \text{when } N = 2.$$

Then $\mathcal{X}$ is a reflexive Banach space. And Lemma A.1 implies $I_\mu \in \mathcal{C}^1(\mathcal{X})$. We will consider I_μ on the constraint

$$\mathcal{S}(a) := \left\{u \in \mathcal{X} : \int_{\mathbb{R}^N} |u|^2 = a\right\}. \tag{2-2}$$

Recalling the L^2-norm preserved transform [24]

$$u \in \mathcal{S}(a) \mapsto s \star u(x) = e^{\frac{N}{2}s} u(e^s x) \in \mathcal{S}(a), \tag{2-3}$$

we define

$$\begin{aligned} Q_\mu(u) &:= \frac{\mathrm{d}}{\mathrm{d}s}\bigg|_{s=0} I_\mu(s \star u) \\ &= (1+\gamma_\theta)\mu \int_{\mathbb{R}^N} |\nabla u|^\theta + \int_{\mathbb{R}^N} |\nabla u|^2 + (2+N)\int_{\mathbb{R}^N} |u|^2 |\nabla u|^2 - \gamma_p \int_{\mathbb{R}^N} |u|^p, \end{aligned}$$

where $\gamma_p = N(p-2)/2p$. And again Lemma A.1 implies $Q_\mu \in \mathcal{C}^1(\mathcal{X})$. Then we define the manifold

$$\mathcal{Q}_\mu(a) := \{u \in \mathcal{S}(a) : Q_\mu(u) = 0\}. \tag{2-4}$$

We observe that:

Lemma 2.1. *Any critical point u of $I_\mu|_{\mathcal{S}(a)}$ is contained in $\mathcal{Q}_\mu(a)$.*

Proof. By [11, Lemma 3], there exists a $\lambda \in \mathbb{R}$ such that

$$I'_\mu(u) + \lambda u = 0 \quad \text{in } \mathcal{X}^*. \tag{2-5}$$

On one hand, testing (2-5) with $x \cdot \nabla u$ (see [10, Proposition 1] for details), we obtain

$$\begin{aligned} 0 = \frac{\theta - N}{\theta}\mu \int_{\mathbb{R}^N} |\nabla u|^\theta + \frac{2-N}{2}\int_{\mathbb{R}^N} |\nabla u|^2 \\ + (2-N)\int_{\mathbb{R}^N} |u|^2|\nabla u|^2 + \frac{N}{p}\int_{\mathbb{R}^N} |u|^p - \frac{N}{2}\lambda \int_{\mathbb{R}^N} |u|^2. \end{aligned} \tag{2-6}$$

On the other hand, testing (2-5) with u, we obtain

$$0 = \mu \int_{\mathbb{R}^N} |\nabla u|^\theta + \int_{\mathbb{R}^N} |\nabla u|^2 + 4\int_{\mathbb{R}^N} |u|^2|\nabla u|^2 - \int_{\mathbb{R}^N} |u|^p + \lambda \int_{\mathbb{R}^N} |u|^2. \tag{2-7}$$

Combining (2-6) and (2-7), we have $Q_\mu(u) = 0$. Then $u \in \mathcal{Q}_\mu(a)$. ☐

2B. *An important lemma.* We need the following result, which is crucially used to control the possible values of the Lagrange parameters.

Lemma 2.2. *Suppose $u \neq 0$ is a critical point of $I_\mu|_{\mathcal{S}(a)}$ with $0 \leq \mu \leq 1$, that is, there exists a $\lambda \in \mathbb{R}$ such that*

$$I'_\mu(u) + \lambda u = 0 \quad \textit{in } \mathcal{X}^*.$$

And assume that one of the following conditions holds:

(a) $1 \leq N \leq 2,\ p \geq 4 + \frac{4}{N},\ a > 0.$

(b) $N = 3,\ 4 + \frac{4}{N} \leq p \leq 2^*,\ a > 0.$

(c) $N \geq 4,\ p = 4 + \frac{4}{N},\ 0 < a < \left(\frac{N-2}{N-2-(4/N)}\right)^{\frac{N}{2}} a_*.$

Then $\lambda > 0$.

Proof. By combining $Q_\mu(u) = 0$ and (2-7), we obtain

$$\begin{aligned} \frac{\lambda N(p-2)}{2p} a = \left(1 + \frac{N(p-\theta)}{p\theta}\right)\mu \int_{\mathbb{R}^N} |\nabla u|^\theta \\ + \frac{2N-(N-2)p}{2p}\int_{\mathbb{R}^N} |\nabla u|^2 + \frac{4N-(N-2)p}{2p}\int_{\mathbb{R}^N} u^2|\nabla u|^2. \end{aligned}$$

So if condition (a) holds, we immediately get $\lambda > 0$. Now suppose condition (b) holds. Again from $Q_\mu(u) = 0$ and (2-7), and using inequality (1-16), we obtain

$$\begin{aligned}\lambda a &= \frac{N(\theta-2)}{2\theta}\mu\int_{\mathbb{R}^N}|\nabla u|^\theta + (N-2)\int_{\mathbb{R}^N}u^2|\nabla u|^2 - \frac{N^2-2N-4}{4(N+1)}\int_{\mathbb{R}^N}|u|^{4+\frac{4}{N}}\\ &\geq \Bigl[(N-2) - \Bigl(N-2-\frac{4}{N}\Bigr)\Bigl(\frac{a}{a_*}\Bigr)^{\frac{2}{N}}\Bigr]\int_{\mathbb{R}^N}u^2|\nabla u|^2 > 0,\end{aligned}$$

which gives $\lambda > 0$. □

3. The critical points of perturbed functional

Throughout this section we assume $p > 4 + \frac{4}{N}$.

3A. *Properties of $\mathcal{Q}_\mu(a)$.*

Lemma 3.1. *Let $0 < \mu \leq 1$, then $\mathcal{Q}_\mu(a)$ is a $\mathcal{C}^1$-submanifold of codimension 1 in $\mathcal{S}(a)$, and hence a $\mathcal{C}^1$-submanifold of codimension 2 in $\mathcal{X}$.*

Proof. As a subset of $\mathcal{X}$, the set $\mathcal{Q}_\mu(a)$ is defined by the two equations $G(u) = 0$ and $Q_\mu(u) = 0$, where

$$G(u) = a - \int_{\mathbb{R}^N}|u|^2,$$

and clearly $G \in \mathcal{C}^1(\mathcal{X})$. We have to check that

$$\mathrm{d}(Q_\mu, G) : \mathcal{X} \to \mathbb{R}^2 \quad \text{is surjective.} \tag{3-1}$$

If this is not true, $\mathrm{d}Q_\mu(u)$ and $\mathrm{d}G(u)$ are linearly dependent, i.e., there exists $\nu \in \mathbb{R}$ such that

$$\begin{aligned}&\theta(1+\gamma_\theta)\mu\int_{\mathbb{R}^N}|\nabla u|^{\theta-2}\nabla u\cdot\nabla\phi + 2\int_{\mathbb{R}^N}\nabla u\cdot\nabla\phi\\ &\quad + (2+N)2\int_{\mathbb{R}^N}(|u|^2\nabla u\cdot\nabla\phi + u\phi|\nabla u|^2) - p\gamma_p\int_{\mathbb{R}^N}|u|^{p-2}u\phi = 2\nu\int_{\mathbb{R}^N}u\phi\end{aligned} \tag{3-2}$$

for any $\phi \in \mathcal{X}$. Similar to Lemma 2.1, taking $\phi = x\cdot\nabla u$ and $\phi = u$, we obtain

$$\begin{aligned}&\theta(1+\gamma_\theta)^2\mu\int_{\mathbb{R}^N}|\nabla u|^\theta\\ &\qquad + 2\int_{\mathbb{R}^N}|\nabla u|^2 + (2+N)^2\int_{\mathbb{R}^N}|u|^2|\nabla u|^2 - p\gamma_p^2\int_{\mathbb{R}^N}|u|^p = 0.\end{aligned} \tag{3-3}$$

Since $Q_\mu(u) = 0$, we get

$$\begin{aligned}&(p\gamma_p - \theta - \theta\gamma_\theta)(1+\gamma_\theta)\mu\int_{\mathbb{R}^N}|\nabla u|^\theta + (p\gamma_p - 2)\int_{\mathbb{R}^N}|\nabla u|^2\\ &\qquad + (p\gamma_p - 2 - N)(2+N)\int_{\mathbb{R}^N}|u|^2|\nabla u|^2 = 0,\end{aligned} \tag{3-4}$$

which means $u = 0$ since $p\gamma_p > \theta + \theta\gamma_\theta$ and $p\gamma_p > 2 + N$. That contradicts with $u \in \mathcal{S}(a)$. □

Lemma 3.2. *For any $0 < \mu \leq 1$ and any $u \in \mathcal{X} \setminus \{0\}$, the following statements hold.*

1. *There exists a unique number $s_\mu(u) \in \mathbb{R}$ such that $Q_\mu(s_\mu(u) \star u) = 0$.*
2. *$I_\mu(s \star u)$ is strictly increasing in $s \in (-\infty, s_\mu(u))$ and is strictly decreasing in $s \in (s_\mu(u), +\infty)$, then*
$$\lim_{s\to-\infty} I_\mu(s \star u) = 0^+, \qquad \lim_{s\to+\infty} I_\mu(s \star u) = -\infty, \qquad I_\mu(s_\mu(u) \star u) > 0.$$
3. *$s_\mu(u) < 0$ if and only if $Q_\mu(u) < 0$.*
4. *The map $u \in \mathcal{X} \setminus \{0\} \mapsto s_\mu(u) \in \mathbb{R}$ is of class $\mathcal{C}^1$.*
5. *$s_\mu(u)$ is an even function with respect to $u \in \mathcal{X} \setminus \{0\}$.*

Proof. (1) By direct computation, one can check that

$$\begin{aligned}
\text{(3-5)}\quad Q_\mu(s\star u) &:= \frac{\mathrm{d}}{\mathrm{d}s} I_\mu(s\star u) \\
&= (1+\gamma_\theta)\mu e^{\theta(1+\gamma_\theta)s}\int_{\mathbb{R}^N}|\nabla u|^\theta + e^{2s}\int_{\mathbb{R}^N}|\nabla u|^2 \\
&\qquad + (2+N)\, e^{(2+N)s}\int_{\mathbb{R}^N}|u|^2|\nabla u|^2 - \gamma_p e^{p\gamma_p s}\int_{\mathbb{R}^N}|u|^p \\
&= e^{p\gamma_p s}\Big[(1+\gamma_\theta)\mu e^{-(p\gamma_p-\theta-\theta\gamma_\theta)s}\int_{\mathbb{R}^N}|\nabla u|^\theta + e^{-(p\gamma_p-2)s}\int_{\mathbb{R}^N}|\nabla u|^2 \\
&\qquad + (2+N)\, e^{-(p\gamma_p-2-N)s}\int_{\mathbb{R}^N}|u|^2|\nabla u|^2 - \gamma_p\int_{\mathbb{R}^N}|u|^p\Big].
\end{aligned}$$

Since $p\gamma_p > \theta + \theta\gamma_\theta$ and $p\gamma_p > 2 + N$ when $p > 4 + \frac{4}{N}$, $Q_\mu(s \star u) = 0$ has only one solution $s_\mu(u) \in \mathbb{R}$.

(2) From (1), $Q_\mu(s \star u) > 0$ when $s < s_\mu(u)$ and $Q_\mu(s \star u) < 0$ when $s > s_\mu(u)$. So $I_\mu(s \star u)$ is strictly increasing in $s \in (-\infty, s_\mu(u))$ and is strictly decreasing in $s \in (s_\mu(u), +\infty)$. Obviously,

$$\lim_{s\to-\infty} I_\mu(s \star u) = 0^+, \qquad \lim_{s\to+\infty} I_\mu(s \star u) = -\infty,$$

which implies that

$$I_\mu(s_\mu(u) \star u) = \max_{s\in\mathbb{R}} I_\mu(s \star u) > 0.$$

(3) It can be obtained directly from (2).

(4) Let $\Phi_\mu(s, u) = Q_\mu(s \star u)$. Then $\Phi_\mu(s_\mu(u), u) = 0$. Moreover,

$$\begin{aligned}
\text{(3-6)}\quad \frac{\partial}{\partial s}\Phi_\mu(s, u) &= \theta(1+\gamma_\theta)^2\mu e^{\theta(1+\gamma_\theta)s}\int_{\mathbb{R}^N}|\nabla u|^\theta + 2e^{2s}\int_{\mathbb{R}^N}|\nabla u|^2 \\
&\qquad + (2+N)^2 e^{(2+N)s}\int_{\mathbb{R}^N}|u|^2|\nabla u|^2 - p\gamma_p^2 e^{p\gamma_p s}\int_{\mathbb{R}^N}|u|^p.
\end{aligned}$$

Combining with $Q_\mu(s_\mu(u)\star u)=0$, we obtain

$$\begin{aligned}\text{(3-7)}\quad &\frac{\partial}{\partial s}\Phi_\mu(s_\mu(u),u)\\ &=-(p\gamma_p-\theta-\theta\gamma_\theta)(1+\gamma_\theta)\mu\int_{\mathbb{R}^N}|\nabla u|^\theta-(p\gamma_p-2)\int_{\mathbb{R}^N}|\nabla u|^2\\ &\qquad-(p\gamma_p-2-N)(2+N)\int_{\mathbb{R}^N}|u|^2|\nabla u|^2\\ &<0.\end{aligned}$$

Then the implicit function theorem [14] implies that the map $u\mapsto s_\mu(u)$ is of class $\mathcal{C}^1$.

(5) Since

$$Q_\mu(s_\mu(u)\star(-u))=Q_\mu(-s_\mu(u)\star u)=Q_\mu(s_\mu(u)\star u)=0,$$

by the uniqueness, there is $s_\mu(-u)=s_\mu(u)$. □

3B. ***Ground state critical point of*** $I_\mu|_{\mathcal{S}(a)}$**.** In this subsection, we consider a minimization problem

$$m_\mu(a):=\inf_{u\in\mathcal{Q}_\mu(a)}I_\mu(u). \tag{3-8}$$

From Lemma 2.1, we know that if $m_\mu(a)$ is achieved, then the minimizer is a ground state critical point of $I_\mu|_{\mathcal{S}(a)}$. We have:

Lemma 3.3. (1) $\mathcal{D}(a):=\inf_{0<\mu\le1,u\in\mathcal{Q}_\mu(a)}\int_{\mathbb{R}^N}|u|^2|\nabla u|^2>0$ *is independent of* μ.

(2) *If* $\sup_{n\ge1}I_\mu(u_n)<+\infty$ *for* $u_n\in\mathcal{Q}_\mu(a)$, *then*

$$\sup_{n\ge1}\max\Bigl\{\mu\int_{\mathbb{R}^N}|\nabla u_n|^\theta,\ \int_{\mathbb{R}^N}|u_n|^2|\nabla u_n|^2,\ \int_{\mathbb{R}^N}|\nabla u_n|^2\Bigr\}<+\infty.$$

Proof. (1) For any $u\in\mathcal{Q}_\mu(a)$, by the inequality (1-16), there holds

$$\begin{aligned}\text{(3-9)}\quad &(2+N)\int_{\mathbb{R}^N}|u|^2|\nabla u|^2\\ &\le\gamma_p\int_{\mathbb{R}^N}|u|^p\le K(p,N)\gamma_p\,a^{\frac{4N-p(N-2)}{2(N+2)}}\Bigl(\int_{\mathbb{R}^N}|u|^2|\nabla u|^2\Bigr)^{\frac{N(p-2)}{2(N+2)}}.\end{aligned}$$

Since $\frac{N(p-2)}{2(N+2)}>1$, we obtain $\mathcal{D}(a)>0$.

(2) For any $u\in\mathcal{Q}_\mu(a)$, there is

$$\begin{aligned}\text{(3-10)}\quad I_\mu(u)&=I_\mu(u)-\frac{1}{p\gamma_p}Q_\mu(u)\\ &=\frac{p\gamma_p-\theta-\theta\gamma_\theta}{\theta p\gamma_p}\mu\int_{\mathbb{R}^N}|\nabla u|^\theta+\frac{p\gamma_p-2}{2p\gamma_p}\int_{\mathbb{R}^N}|\nabla u|^2\\ &\qquad+\frac{p\gamma_p-2-N}{p\gamma_p}\int_{\mathbb{R}^N}|u|^2|\nabla u|^2.\end{aligned}$$

So the conclusion holds. □

Remark 3.4. Form (3-10), we see that

$$m_\mu(a) \geq \mathcal{D}_0(a) := \frac{p\gamma_p - 2 - N}{p\gamma_p}\mathcal{D}(a) > 0 \quad \text{for all } \mu \in (0, 1].$$

Then we have:

Lemma 3.5. *There exists a small* $\rho > 0$ *independent of* μ *such that for any* $0 < \mu \leq 1$, *we have that*

$$0 < \sup_{u \in B_\mu(\rho, a)} I_\mu(u) < \mathcal{D}_0(a) \qquad \textit{and} \qquad I_\mu(u),\, Q_\mu(u) > 0 \quad \textit{for all } u \in B_\mu(\rho, a),$$

where

$$B_\mu(\rho, a) = \left\{u \in \mathcal{S}(a) : \mu \int_{\mathbb{R}^N} |\nabla u|^\theta + \int_{\mathbb{R}^N} |\nabla u|^2 + \int_{\mathbb{R}^N} |u|^2 |\nabla u|^2 \leq \rho\right\}.$$

Proof. From the definition of I_μ, we have

$$\sup_{u \in B_\mu(\rho, a)} I_\mu(u) \leq \max\left\{\frac{1}{\theta}, \frac{1}{2}, 1\right\}\rho < \mathcal{D}_0(a), \tag{3-11}$$

where $\rho > 0$ is small and is independent of μ. On the other hand, by inequality (1-16), for any $u \in \partial B_\mu(r, a)$ with $0 < r < \rho$ for a smaller $\rho > 0$, we have

$$\begin{aligned} \inf_{\partial B_\mu(r,a)} I_\mu(u) &\geq \frac{\mu}{\theta}\int_{\mathbb{R}^N} |\nabla u|^\theta + \frac{1}{2}\int_{\mathbb{R}^N} |\nabla u|^2 + \int_{\mathbb{R}^N} |u|^2 |\nabla u|^2 \\ &\qquad - \frac{K(p, N)}{p} a^{\frac{4N - p(N-2)}{2(N+2)}} \left(\int_{\mathbb{R}^N} |u|^2 |\nabla u|^2\right)^{\frac{N(p-2)}{2(N+2)}} \\ &\geq \frac{\mu}{\theta}\int_{\mathbb{R}^N} |\nabla u|^\theta + \frac{1}{2}\int_{\mathbb{R}^N} |\nabla u|^2 + C\int_{\mathbb{R}^N} |u|^2 |\nabla u|^2 \\ &\geq C_1(a, \theta, p, N) r > 0, \\ \inf_{\partial B_\mu(r,a)} Q_\mu(u) &\geq C_2(a, \theta, p, N) r > 0. \end{aligned}$$

□

To find a Palais–Smale sequence, we consider an auxiliary functional as the one in [24]:

$$J_\mu(s, u) := I_\mu(s \star u) : \mathbb{R} \times \mathcal{X} \to \mathbb{R}. \tag{3-12}$$

We study J_μ on the radial space $\mathbb{R} \times \mathcal{S}_r(a)$ with

$$\mathcal{S}_r(a) := \mathcal{S}(a) \cap \mathcal{X}_r, \quad \mathcal{X}_r = W^{1,\theta}_{\text{rad}}(\mathbb{R}^N) \cap W^{1,2}_{\text{rad}}(\mathbb{R}^N).$$

Notice that J_μ is of class $\mathcal{C}^1$. By the symmetric critical point principle [43], a Palais–Smale sequence for $J_\mu|_{\mathbb{R}\times\mathcal{S}_r(a)}$ is also a Palais–Smale sequence for $J_\mu|_{\mathbb{R}\times\mathcal{S}(a)}$. Denoting the closed sublevel set by

$$I^c_\mu = \{u \in \mathcal{S}(a) : I_\mu(u) \leq c\}, \tag{3-13}$$

we introduce the minimax class

$$\Gamma_\mu := \big\{\gamma = (\alpha, \beta) \in \mathcal{C}([0,1], \mathbb{R} \times \mathcal{S}_r(a)) : \gamma(0) \in \{0\} \times B_\mu(\rho, a), \gamma(1) \in \{0\} \times I_\mu^0\big\},$$

with the associated minimax level

$$\sigma_\mu(a) := \inf_{\gamma \in \Gamma_\mu} \sup_{t \in [0,1]} J_\mu(\gamma(t)). \tag{3-14}$$

Lemma 3.6. *For any* $0 < \mu \le 1$, *we have* $m_\mu(a) = \sigma_\mu(a)$.

Proof. For any $\gamma = (\alpha, \beta) \in \Gamma_\mu$, let us consider the function

$$f_\gamma(t) := Q_\mu(\alpha(t) \star \beta(t)).$$

We have $f_\gamma(0) = Q_\mu(\beta(0)) > 0$ by Lemma 3.5. We *claim* that $f_\gamma(1) = Q_\mu(\beta(1)) < 0$: indeed, since $I_\mu(\beta(1)) < 0$, we have that $s_\mu(\beta(1)) < 0$, which by Lemma 3.2 means that $Q_\mu(\beta(1)) < 0$. Moreover, f_γ is continuous, and hence we deduce that there exists $t_\gamma \in (0,1)$ such that $f_\gamma(t_\gamma) = 0$, namely $\alpha(t_\gamma) \star \beta(t_\gamma) \in \mathcal{Q}_\mu(a)$. So

$$\max_{t \in [0,1]} J_\mu(\gamma(t)) \ge I_\mu(\alpha(t_\gamma) \star \beta(t_\gamma)) \ge m_\mu(a)$$

and consequently $\sigma_\mu(a) \ge m_\mu(a)$.

On the other hand, if $u \in \mathcal{Q}_\mu(a) \cap \mathcal{X}_r$, then

$$\gamma_u(t) := \big(0, ((1-t)s_0 + ts_1) \star u\big) \in \Gamma_\mu,$$

where $s_0 \ll -1$ and $s_1 \gg 1$. Since

$$I_\mu(u) \ge \max_{t \in [0,1]} I_\mu\big(((1-t)s_0 + ts_1) \star u\big) \ge \sigma_\mu(a),$$

there holds

$$m_\mu^r(a) := \inf_{u \in \mathcal{Q}_\mu(a) \cap \mathcal{X}_r} I_\mu(u) \ge \sigma_\mu(a).$$

Finally the inequality $m_\mu(a) \ge m_\mu^r(a)$ can be obtained easily by using the symmetric decreasing rearrangement, see [33]. □

Remark 3.7. For any $0 < \mu_1 < \mu_2 \le 1$, since $I_{\mu_2}(u) \ge I_{\mu_1}(u)$ and $\Gamma_{\mu_2} \subset \Gamma_{\mu_1}$, there holds

$$\begin{aligned}\sigma_{\mu_2}(a) = \inf_{\gamma \in \Gamma_{\mu_2}} \sup_{t \in [0,1]} J_{\mu_2}(\gamma(t)) &\ge \inf_{\gamma \in \Gamma_{\mu_2}} \sup_{t \in [0,1]} J_{\mu_1}(\gamma(t)) \\ &\ge \inf_{\gamma \in \Gamma_{\mu_1}} \sup_{t \in [0,1]} J_{\mu_1}(\gamma(t)) = \sigma_{\mu_1}(a),\end{aligned}$$

i.e., $\sigma_\mu(a)$ is nondecreasing with respect to $\mu \in (0,1]$.

Definition A [19, Definition 3.1]. Let B be a closed subset of X. We say that a class $\mathcal{F}$ of compact subsets of X is a homotopy stable family with boundary B provided:

(a) Every set in $\mathcal{F}$ contains B.

(b) For any set A in $\mathcal{F}$ and any $\eta \in \mathcal{C}([0,1] \times X, X)$ satisfying $\eta(t,x) = x$ for all (t,x) in $(\{0\} \times X) \cup ([0,1] \times B)$ we have that $\eta(1, A) \subset \mathcal{F}$.

We remark that the case $B = \varnothing$ is admissible.

Theorem B [19, Theorem 5.2]. *Let ϕ be a $\mathcal{C}^1$-functional on a complete connected C^1-Finsler manifold X and consider a homotopy stable family $\mathcal{F}$ with an extended closed boundary B. Set $c = c(\phi, \mathcal{F})$ and let F be a closed subset of X satisfying*

$$A \cap F \setminus B \neq \varnothing \quad \text{for all } A \in \mathcal{F} \tag{3-15}$$

and

$$\sup \phi(B) \leq c \leq \inf \phi(F). \tag{3-16}$$

Then for any sequence of sets $A_n \subset \mathcal{F}$ such that $\lim_{n\to\infty} \sup_{A_n} \phi = c$, there exists a sequence $x_n \subset X \setminus B$ such that

(1) $\lim_{n\to\infty} \phi(x_n) = c$,

(2) $\lim_{n\to\infty} \|\mathrm{d}\phi(x_n)\| = 0$,

(3) $\lim_{n\to\infty} \operatorname{dist}(x_n, F) = 0$,

(4) $\lim_{n\to\infty} \operatorname{dist}(x_n, A_n) = 0$.

Now we establish a technical result showing the existence of a Palais–Smale sequence of $\sigma_\mu(a)$ with an additional property.

Lemma 3.8. *For any fixed $\mu \in (0,1]$, there exists a sequence $u_n \in \mathcal{S}_r(a)$ such that*

$$I_\mu(u_n) \to \sigma_\mu(a), \quad I_\mu|'_{\mathcal{S}(a)}(u_n) \to 0, \quad Q_\mu(u_n) \to 0 \quad \text{and} \quad u_n^- \to 0 \text{ a.e. in } \mathbb{R}^N.$$

Proof. Using Definition A, it is easy to check that $\mathcal{F} = \{A = \gamma([0,1]) : \gamma \in \Gamma_\mu\}$ is a homotopy stable family of compact subsets of $X = \mathbb{R} \times \mathcal{S}_\mu^r$ with boundary $B = (\{0\} \times B_\mu(\rho, a)) \cup (\{0\} \times I_\mu^0)$. Set $F = \{J_\mu \geq \sigma_\mu(a)\}$, then the assumptions (3-15) and (3-16) with $\phi = J_\mu$ and $c = \sigma_\mu(a)$ are satisfied. Therefore, taking a minimizing sequence $\{\gamma_n = (0, \beta_n)\} \subset \Gamma_\mu$ with $\beta_n \geq 0$ a.e. in $\mathbb{R}^N$, there exists a Palais–Smale sequence $\{(s_n, w_n)\} \subset \mathbb{R} \times \mathcal{S}_r(a)$ for $J_\mu|_{\mathbb{R}\times\mathcal{S}_r(a)}$ at level $\sigma_\mu(a)$, that is,

$$\partial_s J_\mu(s_n, w_n) \to 0 \quad \text{and} \quad \partial_u J_\mu(s_n, w_n) \to 0 \qquad \text{as } n \to \infty, \tag{3-17}$$

with the additional property that

$$|s_n| + \operatorname{dist}_{\mathcal{X}}(w_n, \beta_n([0,1])) \to 0 \quad \text{as } n \to \infty. \tag{3-18}$$

Let $u_n = s_n \star w_n$. The first condition in (3-17) reads $Q_\mu(u_n) \to 0$, while the second condition gives

$$\begin{aligned}\text{(3-19)}\qquad \|\mathrm{d}I_\mu|_{\mathcal{S}(a)}(u_n)\| &= \sup_{\psi\in T_{u_n}\mathcal{S}(a),\,\|\psi\|_{\mathcal{X}}\le 1} |\mathrm{d}I_\mu(u_n)[\psi]| \\ &= \sup_{\psi\in T_{u_n}\mathcal{S}(a),\,\|\psi\|_{\mathcal{X}}\le 1} |\mathrm{d}I_\mu(s_n\star w_n)[s_n\star(-s_n)\star\psi]| \\ &= \sup_{\psi\in T_{u_n}\mathcal{S}(a),\,\|\psi\|_{\mathcal{X}}\le 1} |\partial_u J_\mu(s_n, w_n)[(-s_n)\star\psi]| \\ &\le \|\partial_u J_\mu(s_n, w_n)\| \sup_{\psi\in T_{u_n}\mathcal{S}(a),\,\|\psi\|_{\mathcal{X}}\le 1} |(-s_n)\star\psi| \\ &\le C\|\partial_u J_\mu(s_n, w_n)\| \to 0 \quad \text{as } n\to\infty.\end{aligned}$$

Finally, (3-18) implies that $u_n^- \to 0$ a.e. in $\mathbb{R}^N$. □

Now we show the compactness of the Palais–Smale sequence obtained in Lemma 3.8.

Lemma 3.9. *For any fixed $\mu \in (0, 1]$, let u_n be a sequence obtained in Lemma 3.8. Then there exists a $u_\mu \in \mathcal{X}\setminus\{0\}$ and a $\lambda_\mu \in \mathbb{R}$ such that up to a subsequence,*

$$\text{(3-20)}\qquad u_n \rightharpoonup u_\mu \ge 0 \quad \textit{in } \mathcal{X},$$

$$\text{(3-21)}\qquad I_\mu(u_\mu) = \sigma_\mu(a) \quad \textit{and} \quad I'_\mu(u_\mu) + \lambda_\mu u_\mu = 0.$$

Moreover, if $\lambda_\mu \ne 0$, we have that

$$u_n \to u_\mu \quad \textit{in } \mathcal{X}.$$

Proof. From Lemma 3.3 and Remark 3.7, we know that u_n is bounded in $\mathcal{X}_r$. Thus by [13, Propositon 1.7.1], we conclude that up to a subsequence, there exists a $u_\mu \in \mathcal{X}_r$ such that

$$\begin{aligned} u_n &\rightharpoonup u_\mu && \text{in } \mathcal{X} \text{ and in } L^2(\mathbb{R}^N), \\ u_n &\to u_\mu && \text{in } L^q(\mathbb{R}^N) \text{ for all } q \in (2, 2^*), \\ u_n &\to u_\mu \ge 0 && \text{a.e. in } \mathbb{R}. \end{aligned}$$

By interpolation and inequality (1-16), we have that

$$u_n \to u_\mu \quad \text{in } L^q(\mathbb{R}^N) \text{ for all } q \in (2, 22^*).$$

We claim that $u_\mu \ne 0$. Assume $u_\mu = 0$. Then as $n \to \infty$, we write

$$\begin{aligned}(1+\gamma_\theta)\mu\int_{\mathbb{R}^N}|\nabla u_n|^\theta + \int_{\mathbb{R}^N}|\nabla u_n|^2 + (2+N)\int_{\mathbb{R}^N}|u_n|^2|\nabla u_n|^2 \\ = Q_\mu(u_n) + \gamma_p\int_{\mathbb{R}^N}|u_n|^p \to 0,\end{aligned}$$

which implies that $I_\mu(u_n) \to 0$, in contradiction with Remark 3.4. So $u_\mu \neq 0$. By [11, Lemma 3], it follows from $I_\mu|'_{\mathcal{S}(a)}(u_n) \to 0$ that there exists a sequence $\lambda_n \in \mathbb{R}$ such that

$$I'_\mu(u_n) + \lambda_n u_n \to 0 \quad \text{in } \mathcal{X}^*. \tag{3-22}$$

Hence $\lambda_n = \frac{1}{a} I'_\mu(u_n)[u_n] + o_n(1)$ is bounded in $\mathbb{R}$, and we assume, up to a subsequence, $\lambda_n \to \lambda_\mu$. Since u_n is bounded, we have $I'_\mu(u_n) + \lambda_\mu u_n \to 0$. From Lemma A.2, we see that

$$I'_\mu(u_\mu) + \lambda_\mu u_\mu = 0. \tag{3-23}$$

Then testing (3-23) with $x \cdot \nabla u$ and u, we obtain $Q_\mu(u_\mu) = 0$. It follows that

$$Q_\mu(u_n) + \gamma_p \int_{\mathbb{R}^N} |u_n|^p \to Q_\mu(u_\mu) + \gamma_p \int_{\mathbb{R}^N} |u_\mu|^p.$$

Then using the weak lower semicontinuous property (see [17, Lemma 4.3]) there must be

$$\mu \int_{\mathbb{R}^N} |\nabla u_n|^\theta \to \mu \int_{\mathbb{R}^N} |\nabla u_\mu|^\theta, \tag{3-24}$$

$$\int_{\mathbb{R}^N} |\nabla u_n|^2 \to \int_{\mathbb{R}^N} |\nabla u_\mu|^2, \tag{3-25}$$

$$\int_{\mathbb{R}^N} |u_n|^2 |\nabla u_n|^2 \to \int_{\mathbb{R}^N} |u_\mu|^2 |\nabla u_\mu|^2. \tag{3-26}$$

That gives $I_\mu(u_\mu) = \lim_{n\to\infty} I_\mu(u_n) = \sigma_\mu(a)$. Moreover, from (3-24)–(3-26):

$$I'_\mu(u_n)[u_n] \to I'_\mu(u_\mu)[u_\mu]. \tag{3-27}$$

Thus combining (3-27) with (3-22) and (3-23), there holds $\lambda_\mu \|u_n\|_2^2 \to \lambda_\mu \|u_\mu\|_2^2$. So $\lambda_\mu \neq 0$ implies that $u_n \to u_\mu$ in $\mathcal{X}$. □

Based on the above preliminary works, we conclude that:

Theorem 3.10. *For any fixed $\mu \in (0, 1]$, there exists a $u_\mu \in \mathcal{X}_r \setminus \{0\}$ and a $\lambda_\mu \in \mathbb{R}$ such that*

$$I'_\mu(u_\mu) + \lambda_\mu u_\mu = 0,$$

$$I_\mu(u_\mu) = m_\mu(a), \quad Q_\mu(u_\mu) = 0, \qquad 0 < \|u_\mu\|_2^2 \le a, \quad u_\mu \ge 0.$$

Moreover, if $\lambda_\mu \neq 0$, we have that $\|u_\mu\|_2^2 = a$, i.e., $m_\mu(a)$ is achieved, and u_μ is a ground state critical point of $I_\mu|_{\mathcal{S}(a)}$.

Proof of Theorem 1.1 for $N = 1$. When $N = 1$, there is $W^{1,2}(\mathbb{R}) \hookrightarrow \mathcal{C}^{0,\alpha}(\mathbb{R})$, so $V(u)$ and hence $I(u)$ is of class $\mathcal{C}^1(W^{1,2}(\mathbb{R}))$. Then one can follow the process in this subsection to prove Theorem 1.1 by taking $\mu = 0$, but we claim that there needs some modifications, since the compact embedding $W^{1,2}_{\text{rad}}(\mathbb{R}^N) \hookrightarrow L^q(\mathbb{R}^N)$ for $2 < q < 2^*$ does not hold when $N = 1$. However, the compactness still holds for bounded sequences of radially decreasing functions (see, e.g., [13, Propositon 1.7.1]). So we need to confirm that the Palais–Smale sequence obtained in Lemma 3.8 consists of radially decreasing functions. Then it is natural to replace the minimizing sequence $\gamma_n = (0, \beta_n)$ chosen in Lemma 3.8 with $\bar{\gamma}_n := (0, \bar{\beta}_n)$, where $\bar{\beta}_n(t) = |\beta_n(t)|^*$ is the symmetric decreasing rearrangement of $\beta_n(t)$ at every $t \in [0, 1]$. This is a natural candidate to be minimizing sequence, with $\bar{\beta}_n(t) \geq 0$, radially symmetric and decreasing for every $t \in [0, 1]$. In order to check that $\bar{\gamma}_n \in \Gamma_0$, we have to check that each $\bar{\beta}_n$ is continuous on [0, 1], which has been proved in [18] (for more argument we refer to [48, Remark 5.2]). As a result, Theorem 3.10 with $\mu = 0$ holds, and combining with Lemma 2.2, we obtain Theorem 1.1 immediately. ☐

3C. ***Infinitely many critical points of $I_\mu|_{\mathcal{S}(a)}$.*** This subsection concerns the existence of infinitely many radial critical points of $I_\mu|_{\mathcal{S}(a)}$. Denote $\tau(u) = -u$ and let $Y \subset \mathcal{X}$. A set $A \subset Y$ is called τ-invariant if $\tau(A) = A$. A homotopy $\eta : [0, 1] \times Y \to Y$ is τ-equivariant if $\eta(t, \tau(u)) = \tau(\eta(t, u))$ for all $(t, u) \in [0, 1] \times Y$.

Definition C [19, Definition 7.1]. Let B be a closed τ-invariant subset of Y. A class $\mathcal{G}$ of compact subsets of Y is said to be a τ-homotopy stable family with boundary B provided:

(a) Every set in $\mathcal{G}$ is τ-invariant.

(b) Every set in $\mathcal{G}$ contains B.

(c) For any set $A \in \mathcal{G}$ and any τ-equivariant homotopy $\eta \in \mathcal{C}([0, 1] \times Y, Y)$ satisfying $\eta(t, x) = x$ for all (t, x) in $(\{0\} \times Y) \cup ([0, 1] \times B)$ we have that $\eta(1, A) \subset \mathcal{G}$.

Following [25, Section 5], we consider the functional $K_\mu : \mathcal{X} \setminus \{0\} \to \mathbb{R}$ defined by

$$K_\mu(u) := I_\mu(s_\mu(u) \star u) = \tfrac{\mu}{\theta} e^{\theta(1+\gamma_\theta) s_\mu(u)} \int_{\mathbb{R}^N} |\nabla u|^\theta + \tfrac{1}{2} e^{2 s_\mu(u)} \int_{\mathbb{R}^N} |\nabla u|^2 + e^{(2+N) s_\mu(u)} \int_{\mathbb{R}^N} |u|^2 |\nabla u|^2 - \tfrac{1}{p} e^{p \gamma_p s_\mu(u)} \int_{\mathbb{R}^N} |u|^p, \tag{3-28}$$

where $s_\mu(u)$ is given by Lemma 3.2. Then we see that $K_\mu(u)$ is τ-invariant. Moreover, inspired by [50, Proposition 2.9], there holds:

Lemma 3.11. *The functional K_μ is of class $\mathcal{C}^1$ and*

$$\begin{aligned} K'_\mu(u)[\phi] &= \mu e^{\theta(1+\gamma_\theta) s_\mu(u)} \int_{\mathbb{R}^N} |\nabla u|^{\theta-2} \nabla u \cdot \nabla \phi + e^{2 s_\mu(u)} \int_{\mathbb{R}^N} \nabla u \cdot \nabla \phi \\ &\quad + 2 e^{(2+N) s_\mu(u)} \int_{\mathbb{R}^N} (u \phi |\nabla u|^2 + |u|^2 \nabla u \cdot \nabla \phi) - e^{p \gamma_p s_\mu(u)} \int_{\mathbb{R}^N} |u|^{p-2} u \phi \\ &= I'_\mu(s_\mu(u) \star u)[s_\mu(u) \star \phi] \end{aligned}$$

for any $u \in \mathcal{X} \setminus \{0\}$ and $\phi \in \mathcal{X}$.

Proof. Let $u \in \mathcal{X} \setminus \{0\}$ and $\phi \in \mathcal{X}$. We estimate the term

$$K_\mu(u_t) - K_\mu(u) = I_\mu(s_t \star u_t) - I_\mu(s_0 \star u),$$

where $u_t = u + t\phi$ and $s_t = s_\mu(u_t)$ with $|t|$ small enough. By the mean value theorem, we have

$$\begin{aligned} &I_\mu(s_t \star u_t) - I_\mu(s_0 \star u) \\ &\quad \le I_\mu(s_t \star u_t) - I_\mu(s_t \star u) \\ &\quad = \mu e^{\theta(1+\gamma_\theta)s_t} \int_{\mathbb{R}^N} |\nabla u_{\eta_t}|^{\theta-2}(\nabla u \cdot \nabla\phi + \eta_t|\nabla\phi|^2)t + e^{2s_t}\int_{\mathbb{R}^N}\Big(\nabla u \cdot \nabla \phi + \frac{t}{2}|\nabla\phi|^2\Big)t \\ &\qquad\qquad + 2e^{(2+N)s_t}\int_{\mathbb{R}^N}\big(u_{\eta_t}\phi|\nabla u_{\eta_t}|^2 + |u_{\eta_t}|^2(\nabla u \cdot \nabla\phi + \eta_t|\nabla\phi|^2)\big)t \\ &\qquad\qquad - e^{p\gamma_p s_t}\int_{\mathbb{R}^N}|u_{\eta_t}|^{p-2}\Big(u\phi + \frac{\eta_t}{2}\phi^2\Big)t, \end{aligned}$$

where $|\eta_t| \in (0, |t|)$. Similarly,

$$\begin{aligned} &I_\mu(s_t \star u_t) - I_\mu(s_0 \star u) \\ &\quad \ge I_\mu(s_0 \star u_t) - I_\mu(s_0 \star u) \\ &\quad = \mu e^{\theta(1+\gamma_\theta)s_0} \int_{\mathbb{R}^N} |\nabla u_{\xi_t}|^{\theta-2}(\nabla u \cdot \nabla\phi + \xi_t|\nabla\phi|^2)t + e^{2s_0}\int_{\mathbb{R}^N}\Big(\nabla u \cdot \nabla \phi + \frac{t}{2}|\nabla\phi|^2\Big)t \\ &\qquad\qquad + 2e^{(2+N)s_0}\int_{\mathbb{R}^N}\big(u_{\xi_t}\phi|\nabla u_{\xi_t}|^2 + |u_{\xi_t}|^2(\nabla u \cdot \nabla\phi + \xi_t|\nabla\phi|^2)\big)t \\ &\qquad\qquad - e^{p\gamma_p s_0}\int_{\mathbb{R}^N}|u_{\xi_t}|^{p-2}\Big(u\phi + \frac{\xi_t}{2}\phi^2\Big)t, \end{aligned}$$

where $|\xi_t| \in (0, |t|)$. Since $s_t \to s_0$ as $t \to 0$, it follows from the last two inequalities that

$$\begin{aligned} &\lim_{t\to 0}\frac{K_\mu(u_t) - K_\mu(u)}{t} \\ &\quad = \mu e^{\theta(1+\gamma_\theta)s_\mu(u)}\int_{\mathbb{R}^N}|\nabla u|^{\theta-2}\nabla u \cdot \nabla\phi + e^{2s_\mu(u)}\int_{\mathbb{R}^N}\nabla u \cdot \nabla\phi \\ &\qquad + 2e^{(2+N)s_\mu(u)}\int_{\mathbb{R}^N}(u\phi|\nabla u|^2 + |u|^2\nabla u \cdot \nabla\phi) - e^{p\gamma_p s_\mu(u)}\int_{\mathbb{R}^N}|u|^{p-2}u\phi. \end{aligned}$$

Then similarly as Lemma A.1, we see that the Gâteaux derivative of K_μ is bounded linear and continuous. Therefore K_μ is of class $\mathcal{C}^1$, see [14]. In particular, by changing variables in the integrals, we have

$$K'_\mu(u)[\phi] = I'_\mu(s_\mu(u) \star u)[s_\mu(u) \star \phi]. \qquad \square$$

To get the particular Palais–Smale sequence of $I_\mu|_{\mathcal{S}(a)}$ as in Lemma 3.8, we need:

Lemma 3.12. *Let $\mathcal{G}$ be a τ-homotopy stable family of compact subsets of $Y = \mathcal{S}_r(a)$ with boundary $B = \varnothing$, and set*

$$d := \inf_{A\in\mathcal{G}}\max_{u\in A} K_\mu(u).$$

If $d > 0$, then there exists a sequence $u_n \in \mathcal{S}_r(a)$ such that

$$I_\mu(u_n) \to d, \quad I_\mu|'_{\mathcal{S}(a)}(u_n) \to 0, \quad Q_\mu(u_n) = 0.$$

Proof. Let $A_n \in \mathcal{G}$ be a minimizing sequence of d. We define the mapping

$$\eta : [0, 1] \times \mathcal{S}(a) \to \mathcal{S}(a), \quad \eta(t, u) = (ts_\mu(u)) \star u,$$

which is continuous and satisfies $\eta(t, u) = u$ for all $(t, u) \in \{0\} \times \mathcal{S}(a)$. Thus, by the definition of $\mathcal{G}$, one has

$$D_n := \eta(1, A_n) = \{s_\mu(u) \star u : u \in A_n\} \in \mathcal{G}.$$

In particular, $D_n \subset \mathcal{Q}_\mu(a)$ for any $n \in \mathbb{N}^+$. For any $u \in \mathcal{S}(a)$ and $s \in \mathbb{R}$, we see that

$$Q_\mu\big((s_\mu(u) - s) \star (s \star u)\big) = Q_\mu\big((s_\mu(u) \star u)\big) = 0,$$

that is, $s_\mu(s \star u) = s_\mu(u) - s$, which gives $K_\mu(s \star u) = K_\mu(u)$. Then it is clear that $\max_{D_n} K_\mu = \max_{A_n} K_\mu \to d$ and thus D_n is another minimizing sequence of d. Now, using the minimax principle [19, Theorem 7.2], we obtain a Palais–Smale sequence $v_n \in \mathcal{S}(a)$ for K_μ at the level d such that

$$\operatorname{dist}_{\mathcal{X}}(v_n, D_n) \to 0.$$

Finally, a similar argument as the one in Lemma 3.8 gives $u_n = s_n \star v_n$ satisfying that

$$I_\mu(u_n) \to d, \quad I_\mu|'_{\mathcal{S}(a)}(u_n) \to 0, \quad Q_\mu(u_n) = 0. \qquad \square$$

To construct a sequence of τ-homotopy stable families of compact subsets of $\mathcal{S}_r(a)$ with boundary $B = \varnothing$, we proceed as in [11, Section 8]. Since $\mathcal{X}$ is separable, there exists a nested sequence of finite dimensional subspaces of $\mathcal{X}$, $W_1 \subset W_2 \subset \cdots \subset W_i \subset W_{i+1} \subset \cdots \subset \mathcal{X}$ such that $\dim(W_i) = i$ and the closure of $\bigcup_{i \in \mathbb{N}^+} W_i$ in $\mathcal{X}$ is equal to $\mathcal{X}$. Note that since $\mathcal{X}$ is dense in $W^{1,2}(\mathbb{R}^N)$, the closure in $W^{1,2}(\mathbb{R}^N)$ is also equal to $W^{1,2}(\mathbb{R}^N)$. Since $W^{1,2}(\mathbb{R}^N)$ is a Hilbert space, we denote by P_i the orthogonal projection from $W^{1,2}(\mathbb{R}^N)$ onto W_i. We also recall the definition of the genus of τ-invariant sets due to M. A. Krasnoselskii and refer the reader to [45, Section 7].

Definition D (Krasnoselskii genus). For any nonempty closed τ-invariant set $A \subset \mathcal{X}$, the genus of A is defined by

$$\operatorname{Ind}(A) := \min\big\{k \in \mathbb{N}^+ : \exists \phi : A \to \mathbb{R}^k \setminus \{0\}, \phi \text{ is odd and continuous}\big\}.$$

We set $\operatorname{Ind}(A) = +\infty$ if such ϕ does not exist, and set $\operatorname{Ind}(A) = 0$ if $A = \varnothing$.

Let $\mathcal{A}(a)$ be the family of compact τ-invariant subsets of $\mathcal{S}_r(a)$. For each $j \in \mathbb{N}^+$:

$$\mathcal{A}_j(a) := \{A \in \mathcal{A}(a) : \operatorname{Ind}(A) \geq j\} \quad \text{and} \quad c^j_\mu(a) := \inf_{A \in \mathcal{A}_j(a)} \max_{u \in A} K_\mu(u).$$

Concerning $\mathcal{A}_j(a)$ and $c_\mu^j(a)$, we have:

Lemma 3.13. (1) *$\mathcal{A}_j(a) \neq \varnothing$ for any $j \in \mathbb{N}^+$, and $\mathcal{A}_j(a)$ is a τ-homotopy stable family of compact subsets of $\mathcal{S}_r(a)$ with boundary $B = \varnothing$.*

(2) *$c_\mu^{j+1}(a) \geq c_\mu^j(a) \geq \mathcal{D}_0(a) > 0$ for any $\mu \in (0, 1]$ and $j \in \mathbb{N}^+$.*

(3) *$c_\mu^j(a)$ is nondecreasing with respect to $\mu \in (0, 1]$ for any $j \in \mathbb{N}^+$.*

(4) *$b_j(a) := \inf_{0<\mu\leq 1} c_\mu^j(a) \to +\infty$ as $j \to +\infty$.*

Proof. (1) For any $j \in \mathbb{N}^+$, $\mathcal{S}_r(a) \cap W_j \in \mathcal{A}(a)$. By the basic properties of the genus, one has

$$\operatorname{Ind}(\mathcal{S}_r(a) \cap W_j) = j$$

and thus $\mathcal{A}_j(a) \neq \varnothing$. The rest is clear by the properties of the genus.

(2) For any $A \in \mathcal{A}_j(a)$, using the fact that $s_\mu(u) \star u \in \mathcal{Q}_\mu(a)$ for all $u \in A$, we have

$$\max_{u\in A} K_\mu(u) = \max_{u\in A} I_\mu(s_\mu(u) \star u) \geq m_\mu(a) \geq \mathcal{D}_0(a)$$

and thus $c_\mu^j(a) \geq \mathcal{D}_0(a) > 0$. Since $\mathcal{A}_{j+1}(a) \subset \mathcal{A}_j(a)$, it is clear that $c_\mu^{j+1}(a) \geq c_\mu^j(a)$.

(3) For any $0 < \mu_1 < \mu_2 \leq 1$ and $u \in A \in \mathcal{A}_j(a)$, there holds

$$K_{\mu_2}(u) = I_{\mu_2}(s_{\mu_2}(u) \star u) \geq I_{\mu_2}(s_{\mu_1}(u) \star u) > I_{\mu_1}(s_{\mu_1}(u) \star u) = K_{\mu_1}(u),$$

which means $c_{\mu_2}^j(a) \geq c_{\mu_1}^j(a)$, i.e., $c_\mu^j(a)$ is nondecreasing with respect to $\mu \in (0, 1]$.

(4) The proof is inspired by that of [11, Theorem 9]. First, we claim that:

Claim. *For any $M > 0$, there exists a small $\delta_0 = \delta_0(a, M) > 0$, a small $r_0 = r_0(a, M) > 0$ and a large $k_0 = k_0(a, M) \in \mathbb{N}^+$ such that for any $0 < \mu < \delta_0$ and any $k \geq k_0$, one has*

$$I_\mu(u) \geq M \quad \text{if } \|P_k u\|_{\mathcal{X}} \leq r_0 \text{ and } u \in \mathcal{Q}_\mu^r(a).$$

Now we check it. By contradiction, we assume that there exists $M_0 > 0$ such that for any $0 < \delta \leq 1$, any $r > 0$ and any $k \in \mathbb{N}^+$ one can always find $\mu \in (0, \delta]$, $l \geq k$ and $u \in \mathcal{Q}_\mu^r(a)$ such that

$$\|P_k u\|_{\mathcal{X}} \leq r \quad \text{but} \quad I_\mu(u) < M_0.$$

As a result, one can obtain the sequences $\mu_n \to 0^+$, $k_n \to +\infty$ and $u_n \in \mathcal{Q}_{\mu_n}^r(a)$ such that

$$\|P_{k_n} u_n\|_{\mathcal{X}} \leq \tfrac{1}{n} \quad \text{and} \quad I_{\mu_n}(u_n) < M_0$$

for any $n \in \mathbb{N}^+$. From Lemma 3.3, we know that u_n is bounded in $W^{1,2}(\mathbb{R}^N)$. Since $P_{k_n} u_n$ is also bounded in $\mathcal{X}$, we assume that up to a subsequence

$$u_n \rightharpoonup u \quad \text{in } W^{1,2}(\mathbb{R}^N) \qquad \text{and} \qquad P_{k_n} u_n \rightharpoonup v \quad \text{in } \mathcal{X}.$$

We show that $u = v$. Indeed, one also has $P_{k_n} u_n \rightharpoonup v$ in $W^{1,2}(\mathbb{R}^N)$ and

$$\begin{aligned}\|u - v\|^2_{W^{1,2}(\mathbb{R}^N)} &= \lim_{n\to\infty} \langle u_n - P_{k_n} u_n, u - v\rangle_{W^{1,2}(\mathbb{R}^N)} \\ &= \lim_{n\to\infty} \langle u_n, u - v\rangle_{W^{1,2}(\mathbb{R}^N)} - \lim_{n\to\infty} \langle P_{k_n} u_n, u - v\rangle_{W^{1,2}(\mathbb{R}^N)} \\ &= \langle u, u - v\rangle_{W^{1,2}(\mathbb{R}^N)} - \lim_{n\to\infty} \langle u_n, P_{k_n} u - P_{k_n} v\rangle_{W^{1,2}(\mathbb{R}^N)} \\ &= \langle u, u - v\rangle_{W^{1,2}(\mathbb{R}^N)} - \langle u, u - v\rangle_{W^{1,2}(\mathbb{R}^N)} = 0,\end{aligned}$$

where we use the fact that $P_{k_n} u \to u$ and $P_{k_n} v \to v$ in $W^{1,2}(\mathbb{R}^N)$. Therefore $u = v$ and $u \in \mathcal{X}$. Since $\|P_{k_n} u_n\|_{\mathcal{X}} \to 0$, there must be $u = 0$. Then combining the interpolation inequality and the fact that $\sup_{n\in\mathbb{N}^+} \int_{\mathbb{R}^N} |u_n|^2 |\nabla u_n|^2 < +\infty$, we obtain $\|u_n\|_p \to 0$. Further, $u_n \in \mathcal{Q}_{\mu_n}(a)$ gives that

$$\mu_n \int_{\mathbb{R}^N} |\nabla u_n|^\theta \to 0, \quad \int_{\mathbb{R}^N} |\nabla u_n|^2 \to 0, \quad \int_{\mathbb{R}^N} |u_n|^2 |\nabla u_n|^2 \to 0,$$

which is in contradiction with Lemma 3.3. So we prove the claim.

Then we can prove the conclusion (4). By contradiction, we assume that

$$\liminf_{j\to\infty} b_j < M \quad \text{for some } M > 0.$$

Then there exist $\mu \in (0, \delta_0)$ for $k > k_0$ such that $c^k_\mu(a) < M$. By the definition of $c^k_\mu(a)$, one can find $A \in \mathcal{A}_k(a)$ such that

$$\max_{u\in A} I_\mu(s_\mu(u) \star u) = \max_{u\in A} K_\mu(u) < M.$$

As Lemma 3.2 implies that the mapping $\varphi : A \to \mathcal{Q}^r_\mu(a)$ defined by $\varphi(u) = s_\mu(u) \star u$ is odd and continuous, we have $\bar{A} := \varphi(A) \subset \mathcal{Q}^r_\mu(a)$, $\max_{u\in\bar{A}} I_\mu(u) < M$ and

$$\operatorname{Ind}(\bar{A}) \geq \operatorname{Ind}(A) \geq k > k_0. \tag{3-29}$$

On the other hand, it follows from the claim that $\inf_{u\in\bar{A}} \|P_{k_0} u_n\|_{\mathcal{X}} \geq r_0 > 0$. Setting

$$\psi(u) = \frac{P_{k_0} u}{\|P_{k_0} u_n\|_{\mathcal{X}}} \quad \text{for any } u \in \bar{A},$$

we obtain an odd continuous mapping $\psi : \bar{A} \to \psi(\bar{A}) \subset W_{k_0} \setminus \{0\}$ and thus

$$\operatorname{Ind}(\bar{A}) \leq \operatorname{Ind}(\psi(\bar{A})) \leq k_0,$$

which contradicts (3-29). Therefore we have $b_j(a) \to +\infty$ as $j \to +\infty$. □

For any fixed $\mu \in (0, 1]$ and any $j \in \mathbb{N}^+$, by Lemmas 3.12 and 3.13, one can find a sequence $u_n \in \mathcal{S}_r(a)$ such that

$$I_\mu(u_n) \to c^j_\mu(a), \quad I_\mu|'_{\mathcal{S}(a)}(u_n) \to 0, \quad Q_\mu(u_n) = 0.$$

Then similar to Lemma 3.9, we have:

Lemma 3.14. *There exists a* $u_\mu^j \in \mathcal{X} \setminus \{0\}$ *and a* $\lambda_\mu^j \in \mathbb{R}$ *such that up to a subsequence,*

$$u_n^j \rightharpoonup u_\mu^j \quad \text{in } \mathcal{X},$$

$$I_\mu(u_\mu^j) = c_\mu^j(a) \quad \text{and} \quad I'_\mu(u_\mu^j) + \lambda_\mu^j u_\mu^j = 0.$$

Moreover, if $\lambda_\mu^j \neq 0$, *we have that*

$$u_n^j \to u_\mu^j \quad \text{in } \mathcal{X}.$$

Based on the above preliminary works, we conclude that:

Theorem 3.15. *For any fixed* $\mu \in (0, 1]$ *and any* $j \in \mathbb{N}^+$, *there exists a* $u_\mu^j \in \mathcal{X}_r \setminus \{0\}$ *and a* $\lambda_\mu^j \in \mathbb{R}$ *such that*

$$I'_\mu(u_\mu^j) + \lambda_\mu^j u_\mu^j = 0, \quad I_\mu(u_\mu^j) = c_\mu^j(a), \quad Q_\mu(u_\mu^j) = 0, \quad 0 < \|u_\mu^j\|_2^2 \leq a.$$

Moreover, if $\lambda_\mu^j \neq 0$, *we have that* $\|u_\mu^j\|_2^2 = a$, *i.e.,* $\{u_\mu^j : j \in \mathbb{N}^+\}$ *are infinitely many critical points of* $I_\mu|_{\mathcal{S}(a)}$ *with increasing energy.*

4. Convergence issues as $\mu \to 0^+$

In this section, letting $\mu \to 0^+$, we show that the sequences of critical points of $I_\mu|_{\mathcal{S}(a)}$ obtained in Section 3 converge to critical points of $I|_{\tilde{\mathcal{S}}(a)}$.

Theorem 4.1. *Let* $N \geq 2$. *Suppose that* $\mu_n \to 0^+$, $I'_{\mu_n}(u_{\mu_n}) + \lambda_{\mu_n} u_{\mu_n} = 0$ *with* $\lambda_{\mu_n} \geq 0$ *and* $I_{\mu_n}(u_{\mu_n}) \to c \in (0, +\infty)$ *for* $u_{\mu_n} \in \mathcal{S}_r(a_n)$ *with* $0 < a_n \leq a$. *Then there exists a subsequence* $u_{\mu_n} \rightharpoonup u$ *in* $W^{1,2}(\mathbb{R}^N)$ *with* $u \neq 0$, $u \in W^{1,2}_{rad}(\mathbb{R}^N) \cap L^\infty(\mathbb{R}^N)$ *and there exists a* $\lambda \in \mathbb{R}$ *such that*

$$I'(u) + \lambda u = 0, \quad I(u) = c \quad \text{and} \quad 0 < \|u\|_2^2 \leq a.$$

Moreover:

1. *If* $u_{\mu_n} \geq 0$ *for each* $n \in \mathbb{N}^+$, *then* $u \geq 0$,
2. *If* $\lambda \neq 0$, *we have that* $\|u\|_2^2 = \lim_{n\to\infty} a_n$.

Remark 4.2. We note that the condition $\lambda_{\mu_n} \geq 0$ is only used in the following Step 1 to realize the Morse iteration. If one can prove the conclusion in Step 1 without this condition, then the conclusion in Theorem 1.1 can be extended to $N = 3, 4$ with $4 + \frac{4}{N} < p < 22^*$.

Proof of Theorem 4.1. The proof is inspired by [27; 32]. First, by Lemma 2.1, $I'_{\mu_n}(u_{\mu_n}) + \lambda_{\mu_n} u_{\mu_n} = 0$ implies that

$$Q_{\mu_n}(u_{\mu_n}) = 0 \quad \text{for each } n \in \mathbb{N}^+.$$

Then from Lemma 3.3, we see that

$$\sup_{n\geq 1} \max\Big\{\mu_n\int_{\mathbb{R}^N}|\nabla u_n|^\theta,\ \int_{\mathbb{R}^N}|u_n|^2|\nabla u_n|^2,\ \int_{\mathbb{R}^N}|\nabla u_n|^2\Big\} < +\infty, \tag{4-1}$$

and hence u_{μ_n} is bounded in $W^{1,2}(\mathbb{R}^N)$. We claim that $\liminf_{n\to\infty} a_n > 0$ and hence $\lambda_{\mu_n} = \frac{1}{a_n} I'_{\mu_n}(u_{\mu_n})[u_{\mu_n}]$ is also bounded in $\mathbb{R}$. Indeed, if $a_n \to 0$, then $\|u_{\mu_n}\|_p \to 0$, and it follows from $\mathcal{Q}_{\mu_n}(u_n) = 0$ that $I_{\mu_n}(u_{\mu_n}) \to 0$ which contradicts $c > 0$. Thus, up to a subsequence, $\lambda_{\mu_n} \to \lambda$ in $\mathbb{R}$, $u_{\mu_n} \rightharpoonup u$ in $W^{1,2}_{\text{rad}}(\mathbb{R}^N)$, $u_{\mu_n} \to u$ in $L^q(\mathbb{R}^N)$ for $2 < q < 22^*$, and $u_{\mu_n} \to u$ a.e. on $\mathbb{R}^N$. So if $u_{\mu_n} \geq 0$ for each $n \in \mathbb{N}^+$, we have that $u \geq 0$. Moreover, a similar argument as in Lemma A.2 tells that $u_n\nabla u_n \to u\nabla u$ in $(L^2_{\text{loc}}(\mathbb{R}^N))^N$ and $\nabla u_{\mu_n} \to \nabla u$ a.e. on $\mathbb{R}^N$. Now we prove the conclusion in several steps.

Step 1: We prove that $\|u_{\mu_n}\|_\infty \leq C$ and $\|u\|_\infty \leq C$ for some positive constant C.

We just prove the case $N \geq 3$; the case $N = 2$ can be obtained similarly. Set $T > 2$, $r > 0$ and

$$v_n = \begin{cases} T, & u_n \geq T, \\ u_n, & |u_n| \leq T, \\ -T, & u_n \leq -T. \end{cases}$$

Let $\phi = u_{\mu_n}|v_n|^{2r}$, then $\phi \in \mathcal{X}$. From $I'_{\mu_n}(u_{\mu_n}) + \lambda_{\mu_n}u_{\mu_n} = 0$ and $\lambda_{\mu_n} \geq 0$,we obtain

$$\begin{aligned}\int_{\mathbb{R}^N}|u_{\mu_n}|^{p-2}u_{\mu_n}\phi &= \mu_{\mu_n}\int_{\mathbb{R}^N}|\nabla u_{\mu_n}|^{\theta-2}\nabla u_{\mu_n}\cdot\nabla\phi + \int_{\mathbb{R}^N}\nabla u_{\mu_n}\cdot\nabla\phi \\ &\qquad + 2\int_{\mathbb{R}^N}(u_{\mu_n}\phi|\nabla u_{\mu_n}|^2 + |u_{\mu_n}|^2\nabla u_{\mu_n}\cdot\nabla\phi) + \lambda_{\mu_n}\int_{\mathbb{R}^N}u_{\mu_n}\phi \\ &\geq 2\int_{\mathbb{R}^N}|u_{\mu_n}|^2\nabla u_{\mu_n}\cdot\nabla\phi \\ &= 2\int_{\mathbb{R}^N}|u_{\mu_n}|^2|\nabla u_{\mu_n}|^2|v_n|^{2r} + |u_{\mu_n}|^2 2r|v_n|^{2r-2}u_{\mu_n}v_n\nabla u_{\mu_n}\cdot\nabla v_n \\ &= \frac{1}{2}\int_{\mathbb{R}^N}|v_n|^r|\nabla u^2_{\mu_n}|^2 + \frac{4}{r}\int_{\mathbb{R}^N}\big|u^2_{\mu_n}\nabla|v_n|^r\big|^2 \\ &\geq \frac{1}{r+4}\int_{\mathbb{R}^N}\big|\nabla(u^2_{\mu_n}|v_n|^2)\big|^2 \geq \frac{C}{(r+2)^2}\Big(\int_{\mathbb{R}^N}\big|u^2_{\mu_n}|v_n|^2\big|^{2^*}\Big)^{\frac{2}{2^*}}.\end{aligned}$$

On the other hand, by the interpolation inequality, we have

$$\begin{aligned}\int_{\mathbb{R}^N}|u_{\mu_n}|^{p-2}u_{\mu_n}\phi &= \int_{\mathbb{R}^N}|u_{\mu_n}|^p|v_n|^{2r} \\ &\leq \Big(\int_{\mathbb{R}^N}|u_{\mu_n}|^{22^*}\Big)^{\frac{p-4}{22^*}}\Big(\int_{\mathbb{R}^N}(|v_n|^r|u_{\mu_n}|^2)^{\frac{42^*}{22^*-p+4}}\Big)^{\frac{22^*-p+4}{22^*}} \\ &\leq C\Big(\int_{\mathbb{R}^N}(|v_n|^r|u_{\mu_n}|^2)^{\frac{42^*}{22^*-p+4}}\Big)^{\frac{22^*-p+4}{22^*}}.\end{aligned} \tag{4-2}$$

Combining these inequalities, one has

$$(4\text{-}3)\qquad \left(\int_{\mathbb{R}^N} |u_{\mu_n}^2 |v_n|^2|^{2^*}\right)^{\frac{2}{2^*}} \le C(r+2)^2\left(\int_{\mathbb{R}^N} (|v_n|^r |u_{\mu_n}|^2)^{\frac{42^*}{22^*-p+4}}\right)^{\frac{22^*-p+4}{22^*}}.$$

Let $r_0 : (r_0+2)\,q = 22^*$ and $d = \frac{2^*}{q} > 1$ where $q = \frac{42^*}{22^*-p+4}$. Taking $r = r_0$ in (4-3), and letting $T \to +\infty$, we obtain

$$(4\text{-}4)\qquad \|u_{\mu_n}\|_{(2+r_0)qd} \le (C(r_0+2))^{\frac{1}{r_0+2}} \|u_{\mu_n}\|_{(2+r_0)q}.$$

Set $2 + r_{i+1} = (2 + r_i)\, d$ for $i \in \mathbb{N}$. Then inductively, we have

$$(4\text{-}5)\qquad \|u_{\mu_n}\|_{(2+r_0)qd^{i+1}} \le \prod_{k=0}^{i} (C(r_k+2))^{\frac{1}{r_k+2}} \|u_{\mu_n}\|_{(2+r_0)q} \le C_\infty \|u_{\mu_n}\|_{(2+r_0)q},$$

where C_∞ is a positive constant. Taking $i \to \infty$ in (4-5), we get

$$\|u_{\mu_n}\|_\infty \le C \quad \text{and} \quad \|u\|_\infty \le C.$$

Step 2: We prove that $I'(u) + \lambda u = 0$.

Take $\phi = \psi e^{-u_{\mu_n}}$ with $\psi \in C_0^\infty(\mathbb{R}^N)$, $\psi \ge 0$. We have

$$\begin{aligned}
0 &= (I'_{\mu_n}(u_{\mu_n}) + \lambda_{\mu_n} u_{\mu_n})[\phi]\\
&= \mu_n \int_{\mathbb{R}^N} |\nabla u_{\mu_n}|^{\theta-2} \nabla u_{\mu_n} (\nabla\psi e^{-u_{\mu_n}} - \psi e^{-u_{\mu_n}} \nabla u_{\mu_n})\\
&\qquad + \int_{\mathbb{R}^N} \nabla u_{\mu_n} (\nabla\psi e^{-u_{\mu_n}} - \psi e^{-u_{\mu_n}} \nabla u_{\mu_n})\\
&\qquad + 2\int_{\mathbb{R}^N} |u_{\mu_n}|^2 \nabla u_{\mu_n} (\nabla\psi e^{-u_{\mu_n}} - \psi e^{-u_{\mu_n}} \nabla u_{\mu_n}) + 2\int_{\mathbb{R}^N} u_{\mu_n} \psi e^{-u_{\mu_n}} |\nabla u_{\mu_n}|^2\\
&\qquad + \lambda_{\mu_n} \int_{\mathbb{R}^N} u_{\mu_n} \psi e^{-u_{\mu_n}} - \int_{\mathbb{R}^N} |u_{\mu_n}|^{p-2} u_{\mu_n} \psi e^{-u_{\mu_n}}\\
&\le \mu_n \int_{\mathbb{R}^N} |\nabla u_{\mu_n}|^{\theta-2} \nabla u_{\mu_n} \nabla\psi e^{-u_{\mu_n}} + \int_{\mathbb{R}^N} (1 + 2u_{\mu_n}^2) \nabla u_{\mu_n} \nabla\psi e^{-u_{\mu_n}}\\
&\qquad - \int_{\mathbb{R}^N} (1 + 2u_{\mu_n}^2 - 2u_{\mu_n}) \psi e^{-u_{\mu_n}} |\nabla u_{\mu_n}|^2\\
&\qquad + \lambda_{\mu_n} \int_{\mathbb{R}^N} u_{\mu_n} \psi e^{-u_{\mu_n}} - \int_{\mathbb{R}^N} |u_{\mu_n}|^{p-2} u_{\mu_n} \psi e^{-u_{\mu_n}}.
\end{aligned}$$

Since $\mu_n \to 0^+$ and $\|u_{\mu_n}\|_\infty \le C$, equation (4-1) implies

$$\mu_n \int_{\mathbb{R}^N} |\nabla u_{\mu_n}|^{\theta-2} \nabla u_{\mu_n} \nabla\psi e^{-u_{\mu_n}} \to 0.$$

By the weak convergence of u_{μ_n}, the Hölder inequality and by the Lebesgue's dominated convergence theorem we know that

$$\int_{\mathbb{R}^N} (1 + 2u_{\mu_n}^2) \nabla u_{\mu_n} \nabla\psi e^{-u_{\mu_n}} \to \int_{\mathbb{R}^N} (1 + 2u^2) \nabla u \nabla\psi e^{-u},$$

$$\lambda_{\mu_n} \int_{\mathbb{R}^N} u_{\mu_n} \psi e^{-u_{\mu_n}} \to \lambda \int_{\mathbb{R}^N} u\psi e^{-u},$$

and

$$\int_{\mathbb{R}^N} |u_{\mu_n}|^{p-2} u_{\mu_n} \psi e^{-u_{\mu_n}} \to \int_{\mathbb{R}^N} |u|^{p-2} u \psi e^{-u}.$$

Moreover, by Fatou's lemma, there holds

$$\liminf_{n\to\infty} \int_{\mathbb{R}^N} (1+2u_{\mu_n}^2 - 2u_{\mu_n}) \psi e^{-u_{\mu_n}} |\nabla u_{\mu_n}|^2 \geq \int_{\mathbb{R}^N} (1+2u^2-2u) \psi e^{-u} |\nabla u|^2.$$

Consequently, one has

$$\begin{aligned} 0 \leq \int_{\mathbb{R}^N} \nabla u (\nabla \psi e^{-u} - \psi e^{-u} \nabla u) + 2\int_{\mathbb{R}^N} |u|^2 \nabla u (\nabla \psi e^{-u} - \psi e^{-u} \nabla u) \\ + 2\int_{\mathbb{R}^N} u \psi e^{-u} |\nabla u|^2 + \lambda_{\mu_n} \int_{\mathbb{R}^N} u \psi e^{-u} - \int_{\mathbb{R}^N} |u|^{p-2} u \psi e^{-u}. \end{aligned} \tag{4-6}$$

For any $\varphi \in \mathcal{C}_0^\infty(\mathbb{R}^N)$ with $\varphi \geq 0$, choose a sequence of nonnegative functions $\psi_n \in \mathcal{C}_0^\infty(\mathbb{R}^N)$ such that $\psi_n \to \varphi e^u$ in $W^{1,2}(\mathbb{R}^N)$, $\psi_n \to \varphi e^u$ a.e. in $\mathbb{R}^N$, and that ψ_n is uniformly bounded in $L^\infty(\mathbb{R}^N)$. Then we obtain from (4-6) that

$$0 \leq \int_{\mathbb{R}^N} \nabla u \cdot \nabla \varphi + 2\int_{\mathbb{R}^N} (|u|^2 \nabla u \cdot \nabla \varphi + u\varphi |\nabla u|^2) + \lambda \int_{\mathbb{R}^N} u\varphi - \int_{\mathbb{R}^N} |u|^{p-2} u\varphi. \tag{4-7}$$

Similarly by choosing $\phi = \psi e^{u_{\mu_n}}$, we get an opposite inequality. Notice $\varphi = \varphi^+ - \varphi^-$ for any $\varphi \in \mathcal{C}_0^\infty(\mathbb{R}^N)$, we get $I'(u) + \lambda u = 0$.

Step 3: Here we complete the proof.

Similar to Lemma 2.1, we get from $I'(u) + \lambda u = 0$ that

$$Q(u) := Q_0(u) = 0.$$

It follows that

$$Q_{\mu_n}(u_{\mu_n}) + \gamma_p \int_{\mathbb{R}^N} |u_{\mu_n}|^p \to Q(u) + \gamma_p \int_{\mathbb{R}^N} |u|^p.$$

Then using the weak lower semicontinuous property, there must be

$$\begin{gathered} \mu_n \int_{\mathbb{R}^N} |\nabla u_{\mu_n}|^\theta \to 0, \quad \int_{\mathbb{R}^N} |\nabla u_{\mu_n}|^2 \to \int_{\mathbb{R}^N} |\nabla u|^2, \\ \int_{\mathbb{R}^N} |u_{\mu_n}|^2 |\nabla u_{\mu_n}|^2 \to \int_{\mathbb{R}^N} |u|^2 |\nabla u|^2. \end{gathered} \tag{4-8}$$

That gives $I(u) = \lim_{n\to\infty} I_\mu(u_{\mu_n}) = c$. Moreover, from (4-8), we obtain

$$I'_{\mu_n}(u_{\mu_n})[u_{\mu_n}] \to I'(u)[u]. \tag{4-9}$$

Thus there holds $\lambda \|u_{\mu_n}\|_2^2 \to \lambda \|u\|_2^2$. So if $\lambda \neq 0$, we have $\|u\|_2^2 = \lim_{n\to\infty} a_n$. □

Now we are able to complete the proof of Theorems 1.1 and 1.2.

Proof of Theorem 1.1 for $N \geq 2$. From Remarks 3.4 and 3.7, we see that

$$d^*(a) := \lim_{\mu\to 0^+} m_\mu(a) \in (0, +\infty).$$

By Theorem 3.10, we can take

$$\mu_n \to 0^+, \quad I'_{\mu_n}(u_{\mu_n}) + \lambda_{\mu_n} u_{\mu_n} = 0, \quad I_{\mu_n}(u_{\mu_n}) \to d^*(a)$$

for $u_{\mu_n} \in \mathcal{S}_r(a_n)$ with $0 < a_n \le a$ and $u_{\mu_n} \ge 0$. Then Lemma 2.2 implies that $\lambda_{\mu_n} > 0$. Now Theorem 4.1 gives that there exist $v \neq 0,\ v \ge 0,\ v \in W^{1,2}_{\text{rad}}(\mathbb{R}^N) \cap L^\infty(\mathbb{R}^N)$ and $\lambda_0 \in \mathbb{R}$ such that

$$I'(v) + \lambda_0 v = 0, \quad I(v) = d^*(a) \quad \text{and} \quad 0 < \|v\|_2^2 \le a.$$

Thus by Lemma 2.2, there is $\lambda_0 > 0$. Since $\lambda_{\mu_n} \to \lambda_0$, we may say that $\lambda_{\mu_n} \neq 0$ for n large. Then $a_n = a$ and $\|v\|_2^2 = a$. That is, v is a nontrivial nonnegative solution of (1-7). To consider the ground state normalized solution, we define

$$d(a) := \inf\{I(v) : v \in \tilde{\mathcal{S}}(a),\, I|'_{\tilde{\mathcal{S}}(a)}(v) = 0,\, v \neq 0\}.$$

Then $d(a) \le I(v) = d^*(a)$. Further, a similar approach to Lemma 3.3 tells that $d(a) > 0$. We take a sequence $v_n \in \tilde{\mathcal{S}}(a),\ I|'_{\tilde{\mathcal{S}}(a)}(v_n) = 0,\ v_n \neq 0$ and $v_n \ge 0$ such that $I(v_n) \to d(a)$. We can show that (the proof is similar to that of Theorem 4.1, so we omit it), up to a subsequence, there exist $u \neq 0,\ u \ge 0,\ u \in W^{1,2}_{\text{rad}}(\mathbb{R}^N) \cap L^\infty(\mathbb{R}^N)$ and $\lambda \in \mathbb{R}$ such that

$$I'(u) + \lambda u = 0 \quad \text{and} \quad I(u) = d(a).$$

Again by Lemma 2.2, there is $\lambda \neq 0$, and hence $\|u\|_2^2 = a$. That is, u is a minimizer of $d(a)$. Finally, by [41, Lemma 2.6], u is classical and strictly positive since $u \in L^\infty(\mathbb{R}^N)$. □

Proof of Theorem 1.2. From Lemma 3.13, we see that

$$b_j(a) = \lim_{\mu \to 0^+} c^j_\mu(a) \in (0, +\infty) \quad \text{and} \quad b_j(a) \to +\infty.$$

By Theorem 3.15, for each $j \in \mathbb{N}^+$ we can take

$$\mu^j_n \to 0^+, \quad I'_{\mu^j_n}(u^j_{\mu^j_n}) + \lambda^j_{\mu^j_n} u^j_{\mu^j_n} = 0, \quad I_{\mu^j_n}(u^j_{\mu^j_n}) \to b_j(a)$$

for $u_{\mu^j_n} \in \mathcal{S}_r(a^j_n)$ with $0 < a^j_n \le a$. And Lemma 2.2 implies that $\lambda^j_{\mu^j_n} > 0$. Now Theorem 4.1 gives that there exist

$$u^j \neq 0, \quad u^j \in W^{1,2}_{\text{rad}}(\mathbb{R}^N) \cap L^\infty(\mathbb{R}^N) \quad \text{and} \quad \lambda^j \in \mathbb{R}$$

such that

$$I'(u^j) + \lambda^j u^j = 0, \quad I(u^j) = b_j(a) \quad \text{and} \quad 0 < \|u^j\|_2^2 \le a.$$

Thus by Lemma 2.2, there is $\lambda^j > 0$. Going back since $\lambda^j_{\mu^j_n} \to \lambda^j$, we may say that $\lambda^j_{\mu^j_n} \neq 0$ for n large. Then $a^j_n = a$ and $\|u^j\|_2^2 = a$. That is, $\{u^j : j \in \mathbb{N}^+\}$ is a sequence of normalized solutions of (1-7). Moreover, $I(u^j) = b_j \to +\infty$. □

5. The mass critical case $p = 4 + \frac{4}{N}$

In this section we denote $p_* = 4 + \frac{4}{N}$ and assume that $p = p_*$. We still consider I_μ, but on an open subset of $\mathcal{X}$. Let

$$\mathcal{O} := \left\{ u \in \mathcal{X} : \int_{\mathbb{R}^N} u^2 |\nabla u|^2 < \frac{N}{4(N+1)} \int_{\mathbb{R}^N} |u|^{p_*} \right\} \tag{5-1}$$

and for simplicity, we still denote

$$\begin{aligned} \mathcal{S}(a) &:= \left\{ u \in \mathcal{O} : \int_{\mathbb{R}^N} u^2 = a \right\}, & \mathcal{Q}_\mu(a) &:= \{u \in \mathcal{S}(a) : Q_\mu(u) = 0\}, \\ \mathcal{S}_r(a) &:= \mathcal{S}(a) \cap \mathcal{X}_r, & \mathcal{Q}_\mu^r(a) &:= \mathcal{Q}_\mu(a) \cap \mathcal{X}_r. \end{aligned}$$

Lemma 5.1. *$\mathcal{S}(a)$ is nonempty when $a > a^*$.*

Proof. Let $u = Q_{p_*}^{\frac{1}{2}}$, then from (1-13), we have

$$\int_{\mathbb{R}^N} |u|^{p_*} = \frac{4(N+1)}{N} \int_{\mathbb{R}^N} u^2 |\nabla u|^2. \tag{5-2}$$

Let $w_a = \left(\frac{a}{a_*}\right)^{\frac{1}{2}} u$, then $\|w_a\|_2^2 = a$ and (5-2) implies that

$$\int_{\mathbb{R}^N} w_a^2 |\nabla w_a|^2 = \frac{N}{4(N+1)} \left(\frac{a}{a_*}\right)^{-\frac{2}{N}} \int_{\mathbb{R}^N} |w_a|^{p_*} < \frac{N}{4(N+1)} \int_{\mathbb{R}^N} |w_a|^{p_*}, \tag{5-3}$$

that is, $w_a \in \mathcal{S}(a)$. ☐

So from now on, we assume $a > a^*$. Then noting that when $p = p_*$, there is $p_* \gamma_{p_*} > \theta + \theta \gamma_\theta$ and $p_* \gamma_{p_*} = 2 + N$, we still have:

Lemma 5.2. *Let $0 < \mu \le 1$, then $\mathcal{Q}_\mu(a)$ is a $\mathcal{C}^1$-submanifold of codimension 1 in $\mathcal{S}(a)$, and hence a $\mathcal{C}^1$-submanifold of codimension 2 in $\mathcal{X}$.*

Lemma 5.3. *For any $0 < \mu \le 1$ and $u \in \mathcal{O} \setminus \{0\}$, the following statements hold.*

(1) *There exists a unique number $s_\mu(u) \in \mathbb{R}$ such that $Q_\mu(s_\mu(u) \star u) = 0$.*

(2) *$I_\mu(s \star u)$ is strictly increasing in $s \in (-\infty, s_\mu(u))$ and is strictly decreasing in $s \in (s_\mu(u), +\infty)$, and*

$$\lim_{s \to -\infty} I_\mu(s \star u) = 0^+, \qquad \lim_{s \to +\infty} I_\mu(s \star u) = -\infty, \qquad I_\mu(s_\mu(u) \star u) > 0.$$

(3) *$s_\mu(u) < 0$ if and only if $Q_\mu(u) < 0$.*

(4) *The map $u \in \mathcal{X} \setminus \{0\} \mapsto s_\mu(u) \in \mathbb{R}$ is of class $\mathcal{C}^1$.*

(5) *$s_\mu(u)$ is an even function with respect to $u \in \mathcal{X} \setminus \{0\}$.*

Similar to Lemma 3.3, there also holds:

Lemma 5.4. (1) *$\mathcal{D}(a) := \inf_{0 < \mu \le 1, u \in \mathcal{Q}_\mu(a)} \int_{\mathbb{R}^N} |u|^2 |\nabla u|^2 > 0$ is independent of μ.*

(2) *If* $\sup_{n\geq 1} I_\mu(u_n) < +\infty$ *for* $u_n \in \mathcal{Q}_\mu(a)$, *then*

$$\sup_{n\geq 1} \max\Big\{\mu\int_{\mathbb{R}^N}|\nabla u_n|^\theta,\ \int_{\mathbb{R}^N}|u_n|^2|\nabla u_n|^2,\ \int_{\mathbb{R}^N}|\nabla u_n|^2\Big\} < +\infty.$$

Proof. The proof is different from the one of Lemma 3.3.

(1) For any $u \in \mathcal{Q}_\mu(a)$, using the equality $Q_\mu(u) = 0$ and (1-16) we obtain

$$\int_{\mathbb{R}^N}|\nabla u|^2 \leq (N+2)\Big[\Big(\frac{a}{a_*}\Big)^{\frac{2}{N}} - 1\Big]\int_{\mathbb{R}^N}u^2|\nabla u|^2. \tag{5-4}$$

On the one hand, when $N \leq 3$, there holds $p_* < 2^*$. Therefore, the classical Gagliardo–Nirenberg inequality [42] tells that

$$\int_{\mathbb{R}^N}|\nabla u|^2 \leq \gamma_{p_*}\int_{\mathbb{R}^N}|u|^{p_*} \leq C(N)\, a^{1+\frac{2}{N}-\frac{N}{2}}\Big(\int_{\mathbb{R}^N}|\nabla u|^2\Big)^{\frac{N+2}{2}}, \tag{5-5}$$

following which there is

$$\int_{\mathbb{R}^N}|\nabla u|^2 \geq \frac{C(N)}{a^{\frac{4}{N^2}+\frac{2}{N}-1}}.$$

Combining with (5-4), one obtains

$$\inf_{0<\mu\leq 1, u\in\mathcal{Q}_\mu(a)} \int_{\mathbb{R}^N}|u|^2|\nabla u|^2 > 0.$$

On the other hand, when $N \geq 4$, there is $p_* > 2^*$. But using interpolation inequality and Young's inequality we have

$$\begin{aligned}(N+2)&\int_{\mathbb{R}^N}u^2|\nabla u|^2 + \int_{\mathbb{R}^N}|\nabla u|^2 \\ &\leq \gamma_{p_*}\int_{\mathbb{R}^N}|u|^{p_*} \leq \Big(\int_{\mathbb{R}^N}|u|^{2^*}\Big)^{\frac{22^*-p_*}{2^*}}\Big(\int_{\mathbb{R}^N}|u|^{22^*}\Big)^{\frac{p_*-2^*}{2^*}} \\ &\leq C(N)\Big(\int_{\mathbb{R}^N}|\nabla u|^2\Big)^{\frac{22^*-p_*}{2}}\Big(\int_{\mathbb{R}^N}u^2|\nabla u|^2\Big)^{\frac{p_*-2^*}{2}} \\ &\leq (N+2)\int_{\mathbb{R}^N}u^2|\nabla u|^2 + C(N)\Big(\int_{\mathbb{R}^N}|\nabla u|^2\Big)^{\frac{22^*-p_*}{2^*+2-p_*}},\end{aligned} \tag{5-6}$$

which gives that $\int_{\mathbb{R}^N}|\nabla u|^2 \geq C(N)$ and again

$$\inf_{0<\mu\leq 1, u\in\mathcal{Q}_\mu(a)} \int_{\mathbb{R}^N}|u|^2|\nabla u|^2 > 0.$$

(2) Since $p_*\gamma_{p_*} = 2 + N$, we see from (3-10) that

$$\sup_{n\geq 1} \max\Big\{\mu\int_{\mathbb{R}^N}|\nabla u_n|^\theta,\ \int_{\mathbb{R}^N}|\nabla u_n|^2\Big\} < +\infty.$$

On the one hand, when $N \leq 3$, we obtain from (5-5) that

$$\sup_{n\geq 1}\int_{\mathbb{R}^N}|u_n|^{p_*} \leq C\sup_{n\geq 1}\Big(\int_{\mathbb{R}^N}|\nabla u_n|^2\Big)^{\frac{N+2}{2}} < +\infty,$$

which in turn combining with $\mathcal{Q}_\mu(u_n)=0$ implies $\sup_{n\geq 1}\int_{\mathbb{R}^N}u_n^2|\nabla u_n|^2<+\infty$. On the other hand, when $N\geq 4$, for any $n\geq 1$ we obtain from (5-6) that

$$(N+2)\int_{\mathbb{R}^N}u_n^2|\nabla u_n|^2\leq\int_{\mathbb{R}^N}|u_n|^{p_*}\leq C\Big(\int_{\mathbb{R}^N}u_n^2|\nabla u_n|^2\Big)^{\frac{p_*-2^*}{2}},$$

which gives $\sup_{n\geq 1}\int_{\mathbb{R}^N}u_n^2|\nabla u_n|^2<+\infty$ since $0<p_*-2^*<2$ for $N\geq 4$. □

First, we will consider a minimization problem:

$$m_\mu(a):=\inf_{u\in\mathcal{Q}_\mu(a)}I_\mu(u). \tag{5-7}$$

Remark 5.5. It is easy to see from Lemma 5.4 and (3-10) that

$$\inf_{0\leq\mu\leq 1}m_\mu(a)\geq\frac{N}{2(2+N)}\inf_{0\leq\mu\leq 1,u\in\mathcal{Q}_\mu(a)}\int_{\mathbb{R}^N}|\nabla u|^2>0. \tag{5-8}$$

On the other hand, to use the convergence Theorem 4.1, we need to give an uniform upper bound of $m_\mu(a)$. Indeed for any fixed $a>a^*$, recalling the function

$$w_a=\Big(\frac{a}{a_*}\Big)^{\frac{1}{2}}Q_{p_*}^{\frac{1}{2}}\in\mathcal{S}(a)$$

in Lemma 5.1, and letting $s_\mu:=s_\mu(w_a)$, from $Q_\mu(s_\mu\star w_a)=0$ we obtain

$$\begin{aligned}(1+\gamma_\theta)\mu e^{-(2+N-\theta-\theta\gamma_\theta)s_\mu}\Big(\frac{a}{a_*}\Big)^{\frac{\theta}{2}}\int_{\mathbb{R}^N}|\nabla Q_{p_*}^{\frac{1}{2}}|^\theta+e^{-Ns_\mu}\Big(\frac{a}{a_*}\Big)\int_{\mathbb{R}^N}|\nabla Q_{p_*}^{\frac{1}{2}}|^2\\ =(1+\gamma_\theta)\mu e^{-(2+N-\theta-\theta\gamma_\theta)s_\mu}\int_{\mathbb{R}^N}|\nabla w_a|^\theta+e^{-Ns_\mu}\int_{\mathbb{R}^N}|\nabla w_a|^2\\ =\gamma_{p_*}\int_{\mathbb{R}^N}|w_a|^{p_*}-(2+N)\int_{\mathbb{R}^N}|w_a|^2|\nabla w_a|^2\\ =\frac{N(2+N)}{4(N+1)}\Big(1-\Big(\frac{a}{a_*}\Big)^{-\frac{2}{N}}\Big)\Big(\frac{a}{a_*}\Big)^{2+\frac{2}{N}}\|Q_{p_*}^{\frac{1}{2}}\|_1>0,\end{aligned} \tag{5-9}$$

it follows that $\sup_{0\leq\mu\leq 1}s_\mu<+\infty$. Therefore,

$$\begin{aligned}\sup_{0\leq\mu\leq 1}m_\mu(a)\leq\sup_{0\leq\mu\leq 1}I_\mu(s_\mu\star w_a)=\sup_{0\leq\mu\leq 1}I_\mu(s_\mu\star w_a)-Q_\mu(s_\mu\star w_a)\\ =\sup_{0\leq\mu\leq 1}\frac{2+N-\theta-\theta\gamma_\theta}{\theta(2+N)}\mu e^{\theta(1+\gamma_\theta)s_\mu}\int_{\mathbb{R}^N}|\nabla Q_{p_*}^{\frac{1}{2}}|^\theta\\ +\frac{N}{2(2+N)}e^{2s_\mu}\int_{\mathbb{R}^N}|\nabla Q_{p_*}^{\frac{1}{2}}|^2\\ <+\infty.\end{aligned} \tag{5-10}$$

Now we construct a special Palais–Smale sequence of $I_\mu|_{\mathcal{S}(a)}$ at level $m_\mu(a)$. But different from the one in Section 3B, in mass-critical case there is no result as Lemma 3.5, and hence there is no mountain-pass-type result as Lemma 3.6. So we will not consider I_μ directly. Instead, we study the auxiliary functional $K_\mu(u)$

defined by (3-28) and we point out that our approach is inspired by [6] (see also [12]). Similar to [6, Lemma 3.7], we have:

Lemma 5.6. *Let a sequence* $u_n \in \mathcal{S}(a)$ *with* $u_n \to u$ *in* $\mathcal{X}$ *as* $n \to \infty$. *Then if* $u \in \partial\mathcal{O}$, *we have* $K_\mu(u_n) \to \infty$ *as* $n \to \infty$.

Proof. If $u_n \to u$ in $\mathcal{X}$, then there are

$$\int_{\mathbb{R}^N} |\nabla u_n|^\theta \to \int_{\mathbb{R}^N} |\nabla u|^\theta > 0, \qquad \int_{\mathbb{R}^N} |\nabla u_n|^2 \to \int_{\mathbb{R}^N} |\nabla u|^2 > 0,$$
$$\int_{\mathbb{R}^N} |u_n|^2 |\nabla u_n|^2 \to \int_{\mathbb{R}^N} |u|^2 |\nabla u|^2 > 0, \qquad \int_{\mathbb{R}^N} |u_n|^{p_*} \to \int_{\mathbb{R}^N} |u|^{p_*} > 0.$$

Let $s_n = s_\mu(u_n)$. Since $Q_\mu(s_n \star u_n) = 0$, we obtain

$$\begin{aligned}(1+\gamma_\theta)\mu e^{-(2+N-\theta-\theta\gamma_\theta)s_n} \int_{\mathbb{R}^N} |\nabla u_n|^\theta + e^{-Ns_n} \int_{\mathbb{R}^N} |\nabla u_n|^2 \\ = \gamma_{p_*} \int_{\mathbb{R}^N} |u_n|^{p_*} - (2+N) \int_{\mathbb{R}^N} |u_n|^2 |\nabla u_n|^2 \\ \to \gamma_{p_*} \int_{\mathbb{R}^N} |u|^{p_*} - (2+N) \int_{\mathbb{R}^N} |u|^2 |\nabla u|^2 = 0,\end{aligned} \tag{5-11}$$

where the last equality comes from $u \in \partial\mathcal{O}$. It follows that $s_n \to +\infty$. So

$$\begin{aligned}K_\mu(u_n) &= I_\mu(s_n \star u_n) = I_\mu(s_n \star u_n) - Q_\mu(s_n \star u_n) \\ &= \frac{2+N-\theta-\theta\gamma_\theta}{\theta(2+N)} \mu e^{\theta(1+\gamma_\theta)s_n} \int_{\mathbb{R}^N} |\nabla u_n|^\theta + \frac{N}{2(2+N)} e^{2s_n} \int_{\mathbb{R}^N} |\nabla u_n|^2 \\ &\to +\infty.\end{aligned}$$ □

Recalling Definition A, we give directly the following results without a proof, since the proof is very similar to the one of [6, Proposition 3.9] (see also [12]).

Lemma 5.7. *Let* $\mathcal{G}$ *be a homotopy stable family of compact subsets of* $Y = \mathcal{S}_r(a)$ *with boundary* $B = \varnothing$, *and set*

$$d := \inf_{A \in \mathcal{G}} \max_{u \in A} K_\mu(u). \tag{5-12}$$

If $d > 0$, *then there exists a sequence* $u_n \in \mathcal{S}_r(a)$ *such that as* $n \to \infty$,

$$I_\mu(u_n) \to d, \quad I_\mu|'_{\mathcal{S}(a)}(u_n) \to 0, \quad Q_\mu(u_n) = 0.$$

Moreover, if one can find a minimizing sequence A_n *for* d *with the property that* $u \ge 0$ *a.e. for any* $u \in A_n$, *then one can find the sequence* u_n *satisfying the additional condition*

$$u_n^- \to 0, \quad \text{a.e. in } \mathbb{R}^N.$$

Remark 5.8. As pointed out in [6], the set $\mathcal{O}$ is neither complete nor connected, and hence in principle the assumptions of the minimax theorem (such as [19, Theorem 3.2]) are not satisfied. However, the connectedness assumption can be avoided considering the restriction of K_μ on the connected component of $\mathcal{O}$

(if $B \neq \varnothing$, we need to assume that B is contained in a connected component of $\mathcal{Q}_\mu(a)$). Regarding the completeness, what is really used in the deformation lemma [19, Lemma 3.7] is that the sublevel sets $K_\mu^c := \{u \in \mathcal{S}(a) : K_\mu(u) \leq c\}$ are complete for every $c \in \mathbb{R}$. This follows by Lemma 5.6. Hence the minimax theorem [19, Theorem 3.2] can be used to obtain the Palais–Smale sequence. The rest of the process is similar to Lemma 3.12.

Lemma 5.9. *For any fixed* $\mu \in (0, 1]$, *there exists a sequence* $u_n \in \mathcal{S}_r(a)$ *such that*

$$I_\mu(u_n) \to m_\mu(a), \quad I_\mu|'_{\mathcal{S}(a)}(u_n) \to 0, \quad \mathcal{Q}_\mu(u_n) = 0 \quad \textit{and} \quad u_n^- \to 0 \textit{ a.e. in } \mathbb{R}^N.$$

Proof. We use Lemma 5.7 by taking the set $\mathcal{G}$ of all singletons belonging to $\mathcal{S}_r(a)$. It is clearly a homotopy stable family of compact subsets of $\mathcal{S}_r(a)$ with boundary $B = \varnothing$. Observe that

$$\alpha_\mu(a) = \inf_{A \in \mathcal{G}} \max_{u \in A} K_\mu(u) = \inf_{u \in \mathcal{S}_r(a)} \max_{s \in \mathbb{R}} I_\mu(s \star u).$$

We claim that

$$\alpha_\mu(a) = m_\mu(a).$$

Indeed, on one hand, for any $u \in \mathcal{S}_r(a)$ there exists a $s_\mu(u)$ such that

$$s_\mu(u) \star u \in \mathcal{Q}_\mu(a) \quad \text{and} \quad I_\mu(s_\mu(u) \star u) = \max_{s \in \mathbb{R}} I_\mu(s \star u).$$

This implies that

$$\alpha_\mu(a) = \inf_{u \in \mathcal{S}_r(a)} \max_{s \in \mathbb{R}} I_\mu(s \star u) \geq \inf_{u \in \mathcal{Q}_\mu(a)} I_\mu(u) = m_\mu(a).$$

On the other hand, for any $u \in \mathcal{Q}_\mu^r(a)$, $I_\mu(u) = \max_{s \in \mathbb{R}} I_\mu(s \star u)$, so

$$m_\mu^r(a) := \inf_{u \in \mathcal{Q}_\mu^r(a)} I_\mu(u) \geq \inf_{u \in \mathcal{S}_r(a)} \max_{s \in \mathbb{R}} I_\mu(s \star u) = \alpha_\mu(a).$$

Finally, the inequality $m_\mu(a) \geq m_\mu^r(a)$ can be obtained easily by the symmetric decreasing rearrangement. So, the conclusion follows directly from Lemma 5.7. ☐

Then as in Section 3B, we have:

Theorem 5.10. *Let* $p = p_*$. *For any fixed* $\mu \in (0, 1]$, *there exists a* $u_\mu \in \mathcal{X}_r \setminus \{0\}$ *and a* $\lambda_\mu \in \mathbb{R}$ *such that*

$$I'_\mu(u_\mu) + \lambda_\mu u_\mu = 0,$$
$$I_\mu(u_\mu) = m_\mu(a), \quad \mathcal{Q}_\mu(u_\mu) = 0, \qquad 0 < \|u_\mu\|_2^2 \leq a, \quad u_\mu \geq 0.$$

Moreover, if $\lambda_\mu \neq 0$, *we have that* $\|u_\mu\|_2^2 = a$, *i.e.*, $m_\mu(a)$ *is achieved, and* u_μ *is a ground state critical point of* $I_\mu|_{\mathcal{S}(a)}$.

Proof of Theorem 1.4. The proof is exactly the same as the one of Theorem 1.1, so we omit the details. ☐

Remark 5.11. We are not able to obtain multiple solutions as in Section 3C. Indeed, if we consider an open subset $\mathcal{O}$ and follow the strategy in Section 3C, we need to prove a result like Lemma 3.13. However, for any finite dimensional subspace W_j of $\mathcal{X}$, using the equivalence of norms in finite dimensional spaces, we can only obtain that for any $j > 0$, there exists a $a(j) > 0$ large enough such that

$$\{u \in W_j : \|u\|_2^2 = a\} \subset \mathcal{O} \quad \text{when } a > a(j),$$

which is necessary to prove the nonemptiness of the sets of type $\mathcal{A}_j$. And another difficulty is that as $\mu \to 0^+$, we are unable to distinguish the energy

$$b_j(a) := \lim_{\mu\to 0^+} c_\mu^j(a) \quad \text{and} \quad b_k(a) := \lim_{\mu\to 0^+} c_\mu^k(a)$$

for $j \neq k$. As a result, we cannot distinguish the solutions related to $b_j(a)$ and $b_k(a)$.

Recalling Proposition 1.6, we prove the concentration theorem.

Proof of Theorem 1.8. Let u_n be a radially symmetric positive solution of (1-7) for $a = a_n$ with $a_n > a_*$ and $a_n \to a_*$. From Lemma 5.4, we see that

$$\int_{\mathbb{R}^N} u_n^2 |\nabla u_n|^2 \geq \frac{C}{\left(\frac{a_n}{a_*}\right)^{2/N} - 1} \to +\infty, \tag{5-13}$$

$$\frac{\int_{\mathbb{R}^N} |\nabla u_n|^2}{\int_{\mathbb{R}^N} u_n^2 |\nabla u_n|^2} \leq C\left(\left(\frac{a_n}{a_*}\right)^{2/N} - 1\right) \to 0. \tag{5-14}$$

Since $Q_\mu(u_n) = 0$, we know that

$$\frac{\int_{\mathbb{R}^N} |u_n|^{p_*}}{\int_{\mathbb{R}^N} u_n^2 |\nabla u_n|^2} \to \frac{4(N+1)}{N}. \tag{5-15}$$

Let $v_n(x) := \varepsilon_n^{N/2} u_n(\varepsilon_n x)$ with

$$\varepsilon_n = \left(\int_{\mathbb{R}^N} u_n^2 |\nabla u_n|^2\right)^{-\frac{1}{2+N}} \to 0^+.$$

Direct calculations show that

$$\|v_n\|_2^2 = a_n \to a_*, \quad \int_{\mathbb{R}^N} v_n^2 |\nabla v_n|^2 = 1, \quad \|v_n\|_{p_*}^{p_*} \to \frac{4(N+1)}{N} \quad \text{and} \quad \varepsilon_n^N \|\nabla v_n\|_2^2 \to 0.$$

Then v_n^2 is bounded in $\mathcal{E}^{p_*}$. Moreover, using [34, Lemma I.1], we deduce that there exist $\delta > 0$ and a sequence $y_n \in \mathbb{R}^N$ such that for some $R > 0$,

$$\int_{B_R(y_n)} v_n^2 \geq \delta.$$

Observing that $\mathcal{E}^q$ is a reflexive Banach space when $1 < q < \infty$, we know that there exists a nonnegative radially symmetric function $v \neq 0$ with $v^2 \in \mathcal{E}^{p_*} \cap L^2(\mathbb{R}^N)$

such that

$$\begin{aligned} &v_n^2(\cdot + y_n) \rightharpoonup v^2 && \text{in } \mathcal{E}^{p_*}, \\ &v_n(\cdot + y_n) \rightharpoonup v && \text{in } L^2(\mathbb{R}^N), \\ &v_n^2(\cdot + y_n) \to v^2 && \text{in } L^q(\mathbb{R}^N) \text{ for } 1 < q < 2^*, \\ &v_n(\cdot + y_n) \to v && \text{a.e. in } \mathbb{R}^N. \end{aligned}$$

Since u_n solves

$$-\Delta u_n - u_n \Delta u_n^2 + \lambda_n u_n = u_n^{p_*-1},$$

where the Lagrange multiplier is given by

$$\lambda_n = \frac{1}{a_n}\Big(\int_{\mathbb{R}^N} |u_n|^{p_*} - \int_{\mathbb{R}^N} |\nabla u_n|^2 - \int_{\mathbb{R}^N} u_n^2 |\nabla u_n|^2\Big),$$

v_n satisfies

$$-\varepsilon_n^N \Delta v_n - v_n \Delta v_n^2 + \varepsilon_n^{2+N} \lambda_n v_n = v_n^{p_*-1}.$$

Combining (5-14) and (5-15), we deduce that $\varepsilon_n^{2+N}\lambda_n \to \frac{4}{Na^*}$. Then a similar approach as Lemma A.2 tells that

$$-v\Delta v^2 + \varepsilon_n^{2+N} \lambda_n v = v^{p_*-1}. \tag{5-16}$$

Now setting

$$\begin{aligned} w_n(x) &:= \Big(\frac{Na^*}{4}\Big)^{\frac{N}{2+N}} v_n^2\Big(\Big(\frac{Na^*}{4}\Big)^{\frac{1}{2+N}} x + y_n\Big) \\ &= \Big[\Big(\frac{Na^*}{4}\Big)^{\frac{1}{2+N}} \varepsilon_n\Big]^N u_n^2\Big(\Big(\frac{Na^*}{4}\Big)^{\frac{1}{2+N}} \varepsilon_n x + \varepsilon_n y_n\Big), \end{aligned} \tag{5-17}$$

$$w(x) := \Big(\frac{Na^*}{4}\Big)^{\frac{N}{2+N}} v^2\Big(\Big(\frac{Na^*}{4}\Big)^{\frac{1}{2+N}} x\Big), \tag{5-18}$$

it is easily seen that $w_n \rightharpoonup w$ in $\mathcal{E}^{p_*}$ and $\|w_n\|_1 = \|v_n\|_2^2 = a_n$. Moreover, it follows from (5-16) that w is a solution of (1-14). Thus $w = Q_{p_*}$, and hence $\|w\|_1 = \|v\|_2^2 = a_*$. So we have $v_n \to v$ in $L^2(\mathbb{R}^N)$, which finishes the proof. □

Appendix

Lemma A.1. *In the setting of Section 2A*, $V(u) \in \mathcal{C}^1(\mathcal{X})$.

Proof. The proof is elementary. When $N = 2$, since $W^{1,\theta}(\mathbb{R}^2) \hookrightarrow \mathcal{C}^{0,\alpha}(\mathbb{R}^2)$, it is easy to check that $V(u) \in \mathcal{C}^1(\mathcal{X})$. Now we set $N \geq 3$. For any $u, \phi \in \mathcal{X}$,

$$\frac{V(u+t\phi)-V(u)}{t} = At + Bt^2 + Ct^3 + 2\int_{\mathbb{R}^N} u\phi|\nabla u|^2 + u^2 \nabla u \cdot \nabla \phi, \tag{A-1}$$

where

$$A=\int_{\mathbb{R}^N} u^2|\nabla\phi|^2+\phi^2|\nabla u|^2+4u\phi\nabla u\cdot\nabla\phi,$$

$$B=\int_{\mathbb{R}^N}\phi^2\nabla u\cdot\nabla\phi+u\phi|\nabla\phi|^2 \quad\text{and}\quad C=\int_{\mathbb{R}^N}\phi^2|\nabla\phi|^2.$$

We need to prove that A, B, C are finite numbers. Indeed, since $\frac{4N}{N+2}<\theta<\frac{4N+4}{N+2}<4$, there is $\theta<\frac{2\theta}{\theta-2}<\frac{\theta N}{N-\theta}$ and hence

$$\text{(A-2)}\qquad \begin{aligned}\int_{\mathbb{R}^N} u^2|\nabla\phi|^2 &\le \Big(\int_{\mathbb{R}^N}|u|^{2\theta/(\theta-2)}\Big)^{(\theta-2)/\theta}\Big(\int_{\mathbb{R}^N}|\nabla\phi|^\theta\Big)^{2/\theta}\\ &\le C\|u\|^{2/\theta}_{W^{1,\theta}(\mathbb{R}^N)}\|\phi\|^{2/\theta}_{W^{1,\theta}(\mathbb{R}^N)}<\infty.\end{aligned}$$

We can handle other terms in a similar way, so A, B, C are finite numbers. Now by letting $t\to 0$ in (A-1), we immediately get the Frèchet derivative as

$$DV(u)[\phi]=2\int_{\mathbb{R}^N}u\phi|\nabla u|^2+u^2\nabla u\cdot\nabla\phi.$$

Then in a similarly way to (A-2), one can prove that $DV(u)$ is continuous for $u\in\mathcal{X}$, so $V(u)\in\mathcal{C}^1(\mathcal{X})$ and $V'(u)=DV(u)$. □

Lemma A.2. *Assume that $I'_\mu(u_n)+\lambda u_n\to 0$ for some $\lambda\in\mathbb{R}$ with $u_n\in\mathcal{X}$, and that $u_n\rightharpoonup u$ in $\mathcal{X}$. Then up to a subsequence,*

1. *$u_n\to u$ in $\mathcal{X}_{\text{loc}}:=W^{1,\theta}_{\text{loc}}(\mathbb{R}^N)\cap W^{1,2}_{\text{loc}}(\mathbb{R}^N)$,*
2. *$u_n\nabla u_n\to u\nabla u$ in $(L^2_{\text{loc}}(\mathbb{R}^N))^N$,*
3. *$I'_\mu(u)+\lambda u=0$.*

Proof. The proof is inspired by [29, Lemma 14.3]. Since $u_{\mu_n}\rightharpoonup u$ in $\mathcal{X}$, we have $\|u_n\|_{\mathcal{X}}\le C_0$ for any $n\ge 1$. For any $R>1$, we set $\phi\in\mathcal{C}_0^\infty(\mathbb{R}^N)$ satisfying

$$0\le\phi\le 1,\quad \phi(x)=\begin{cases}1, & |x|\le R,\\ 0, & |x|\ge 2R,\end{cases}\quad\text{and}\quad |\nabla\phi|\le 2.$$

Then for any $n,m\in\mathbb{N}$,

$$\text{(A-3)}\quad \begin{aligned} o(1)_n+o(1)_m &= (I'_\mu(u_n)+\lambda u_n)[(u_n-u_m)\phi]-(I'_\mu(u_m)+\lambda u_m)[(u_n-u_m)\phi]\\ &=\mu\int_{\mathbb{R}^N}(|\nabla u_n|^{\theta-2}\nabla u_n-|\nabla u_m|^{\theta-2}\nabla u_m)\cdot\nabla((u_n-u_m)\phi)\\ &\qquad+\int_{\mathbb{R}^N}(\nabla u_n-\nabla u_m)\cdot\nabla((u_n-u_m)\phi)\\ &\qquad+2\int_{\mathbb{R}^N}(u_n|\nabla u_n|^2-u_m|\nabla u_m|^2)(u_n-u_m)\phi\\ &\qquad+2\int_{\mathbb{R}^N}(u_n^2\nabla u_n-u_m^2\nabla u_m)\cdot\nabla((u_n-u_m)\phi)\\ &\qquad-\int_{\mathbb{R}^N}(|u_n|^{p-2}u_n-|u_m|^{p-2}u_m)(u_n-u_m)\phi\\ &=: K_1+K_2+K_3+K_4+K_5.\end{aligned}$$

Next we estimate K_i for $i = 1, 2, 3, 4, 5$:

$$\begin{aligned}K_1 &= \mu\int_{B_R}(|\nabla u_n|^{\theta-2}\nabla u_n - |\nabla u_m|^{\theta-2}\nabla u_m)\cdot\nabla(u_n-u_m)\\&\qquad + \mu\int_{B_{2R}\setminus B_R}(|\nabla u_n|^{\theta-2}\nabla u_n - |\nabla u_m|^{\theta-2}\nabla u_m)\cdot\nabla(u_n-u_m)\phi\\&\qquad + \mu\int_{B_{2R}\setminus B_R}(|\nabla u_n|^{\theta-2}\nabla u_n - |\nabla u_m|^{\theta-2}\nabla u_m)\cdot\nabla\phi(u_n-u_m)\\&\geq C\mu\int_{B_R}|\nabla u_n-\nabla u_m|^\theta + C\mu\int_{B_{2R}\setminus B_R}|\nabla u_n-\nabla u_m|^\theta\phi\\&\qquad - C(\|u_n\|_\theta^{\theta-1}+\|u_m\|_\theta^{\theta-1})\|u_n-u_m\|_{L^\theta(B_{2R})}\\&\geq C\mu\|\nabla u_n-\nabla u_m\|^\theta_{L^\theta(B_R)} - C\|u_n-u_m\|_{L^\theta(B_{2R})},\end{aligned}$$

and similarly

$$K_2 \geq C\|\nabla u_n-\nabla u_m\|^2_{L^2(B_R)} - C\|u_n-u_m\|_{L^2(B_{2R})}, \qquad K_3 \geq -C\|u_n-u_m\|_{L^\theta(B_{2R})},$$

$$K_4 \geq 2\|u_n\nabla u_n-u_m\nabla u_m\|^2_{L^2(B_R)} - C\|u_n-u_m\|_{L^\theta(B_{2R})}, \quad K_5 \geq -C\|u_n-u_m\|_{L^p(B_{2R})}.$$

Substituting these estimates into (A-3), we obtain

$$\begin{aligned}&\mu\|\nabla u_n-\nabla u_m\|^\theta_{L^\theta(B_R)} + \|\nabla u_n-\nabla u_m\|^2_{L^2(B_R)} + \|u_n\nabla u_n-u_m\nabla u_m\|^2_{L^2(B_R)}\\&\quad\leq C\|u_n-u_m\|_{L^\theta(B_{2R})} + C\|u_n-u_m\|_{L^2(B_{2R})} + C\|u_n-u_m\|_{L^\theta(B_{2R})} + o(1)_n + o(1)_m\\&\quad\to 0, \quad \text{as } n\to\infty,\ m\to\infty,\end{aligned}$$

where in the last estimate we use the compact embedding theorem in bounded domains. Thus for any $R > 1$, u_n is a Cauchy sequence in $W^{1,\theta}(B_R)\cap W^{1,2}(B_R)$, and $u_n\nabla u_n$ is also a Cauchy sequence in $(L^2(B_R))^N$. So up to a subsequence $u_n \to u$ in $\mathcal{X}_{\text{loc}}$ and $u_n\nabla u_n \to u\nabla u$ in $(L^2_{\text{loc}}(\mathbb{R}^N))^N$. Finally, we need to prove that for any $\varphi\in\mathcal{X}$, there holds $(I'_\mu(u)+\lambda u)[\varphi] = 0$. Since $u_n\nabla u_n \to u\nabla u$ a.e. in $\mathbb{R}^N$ and u_n is bounded in $\mathcal{X}$, we obtain that

$$\begin{aligned}|\nabla u_n|^{\theta-2}\nabla u_n &\rightharpoonup |\nabla u|^{\theta-2}\nabla u && \text{in } L^{\frac{\theta}{\theta-1}}(\mathbb{R}^N),\\ u_n|\nabla u_n|^2 &\rightharpoonup u|\nabla u|^2 && \text{in } L^{\frac{4}{3}}(\mathbb{R}^N),\\ u_n^2\nabla u_n &\rightharpoonup u^2\nabla u && \text{in } (L^{\frac{4}{3}}(\mathbb{R}^N))^N,\end{aligned}$$

it follows that

$$(I'_\mu(u)+\lambda u)[\varphi] = \lim_{n\to\infty}(I'_\mu(u_n)+\lambda u_n)[\varphi] = 0. \qquad \square$$

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HOUWANG LI
DEPARTMENT OF MATHEMATICAL SCIENCES
TSINGHUA UNIVERSITY
BEIJING
CHINA

li-hw17@mails.tsinghua.edu.cn

WENMING ZOU
DEPARTMENT OF MATHEMATICAL SCIENCES
TSINGHUA UNIVERSITY
BEIJING
CHINA

zou-wm@mail.tsinghua.edu.cn

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THOMAE'S FUNCTION ON A LIE GROUP

MARK REEDER

Let $\mathfrak{g}$ be a simple complex Lie algebra of finite dimension. This paper gives an inequality relating the order of an automorphism of $\mathfrak{g}$ to the dimension of its fixed-point subalgebra and characterizes those automorphisms of $\mathfrak{g}$ for which equality occurs. This amounts to an inequality/equality for Thomae's function on the automorphism group of $\mathfrak{g}$. The result has applications to characters of zero-weight spaces, graded Lie algebras, and inequalities for adjoint Swan conductors.

1. Introduction

Thomae's function $\tau : \mathbb{R} \to \mathbb{R}$ is discontinuous precisely on the rational numbers. It is traditionally defined as $\tau(x) = \frac{1}{m}$ if $x = \frac{n}{m}$ is rational in lowest terms with $m > 0$, and $\tau(x) = 0$ if x is irrational. So $\tau(n) = 1$ for every integer n, and on each open interval $(n, n+1)$ the maximum value of τ is $\frac{1}{2}$, taken just at the midpoint of the interval. More succinctly, $\tau(x)$ is the reciprocal of the order of x in the group $\mathbb{R}/\mathbb{Z}$, with the convention that $\frac{1}{\infty} = 0$.

Every group G has an analogous function $\tau_G : G \to \mathbb{R}$, whose value at $g \in G$ is equal to the reciprocal of the order of g.

Consider the group $G = \mathrm{SO}_3$ of rotations about a fixed point O in three-dimensional Euclidean space. Here, $\tau_G(g) = \frac{1}{m}$ if g rotates by a rational multiple $\frac{n}{m}$ (in lowest terms) of a full circle, and $\tau_G(g) = 0$ otherwise. So $\tau_G(g) = 1$ if g is the identity rotation, and elsewhere τ_G has maximum value $\frac{1}{2}$ taken just on the conjugacy class of half-turns. Since every element of G is conjugate to a rotation

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about a fixed axis through O, this example is essentially the same as Thomae's original one, but now we observe that $\frac{1}{2} = \frac{1}{h}$, where h is the Coxeter number of G.

Suppose G is either a compact Lie group or a complex algebraic group. For such groups the function τ_G is discontinuous precisely on the set of torsion elements in G. The proof is the same as for $\tau = \tau_{\mathbb{R}/\mathbb{Z}}$, using the facts: (1) torsion elements can be approximated by elements of infinite order, (2) for every $\epsilon > 0$, there are only finitely many conjugacy classes in G whose elements have order $\leq \frac{1}{\epsilon}$, and (3) the conjugacy class of any torsion element is closed in G.

If G is connected and simple as an abstract group, then on the regular elements of G we have $\tau_G(g) \leq \frac{1}{h}$, where h is the Coxeter number of G. Equality holds on just the conjugacy class of *principal elements*. These are the analogues of the half-turns in SO_3 and were studied be Kostant [1959].

The aim of this paper is to extend this inequality/equality for Thomae's function to singular elements in the group $G = \mathrm{Aut}(\mathfrak{g})$ of automorphisms of a simple complex Lie algebra $\mathfrak{g}$ of finite dimension. We also indicate some applications of the result.

We will measure the singularity of an element $\theta \in G$ by the dimension of the fixed-point subalgebra $\mathfrak{g}^\theta$. We will give an upper bound for $\tau_G(\theta)$ in terms of $\dim \mathfrak{g}^\theta$, along with precise conditions for equality.

To explain these conditions, we need some preparation. We say that an element $\theta \in G$ is *ell-reg* if θ normalizes a Cartan subalgebra $\mathfrak{t} \subset \mathfrak{g}$ such that (i) $\mathfrak{t}^\theta = 0$ and (ii) the cyclic group generated by θ permutes the roots of $\mathfrak{t}$ in $\mathfrak{g}$ freely.

The set of ell-reg automorphisms in G is partitioned into finitely many conjugacy classes. Each ell-reg automorphism has finite order. In fact, for each integer $m > 1$, there is at most one ell-reg conjugacy class whose elements have order m. The classification of ell-reg automorphisms was given in [Reeder et al. 2012] and is recalled in the Appendix. A uniform set of representatives for each ell-reg class is given in [Reeder et al. 2012, Proposition 12], see Section 2.1 below for the inner case.[1]

For ell-reg automorphisms it is known that the automorphism of $\mathfrak{t}$ given by $\theta|_{\mathfrak{t}}$, as in (i) and (ii), has the same order as θ. It follows that if $\theta \in G$ is ell-reg, then

$$\tau_G(\theta) = \frac{\dim \mathfrak{g}^\theta}{\dim(\mathfrak{g}/\mathfrak{t})}, \tag{1}$$

where $\mathfrak{t}$ is any Cartan subalgebra of $\mathfrak{g}$.

Fix a connected component Γ of G, and let $e \in \{1, 2, 3\}$ be the order of Γ in the group $\mathrm{Out}(\mathfrak{g})$ of connected components of G. If $\theta \in \Gamma$, the rank of $\mathfrak{g}^\theta$ depends only on e; we write

$$n_e = \mathrm{rank}(\mathfrak{g}^\theta).$$

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[1] *Ell-reg* automorphisms are called *$\mathbb{Z}$-regular* in [Reeder et al. 2012], in deference to [Springer 1974]. Except for the classes P_Γ described below, ell-reg automorphisms of $\mathfrak{g}$ are not regular elements of G. The point of "ell-reg", besides brevity, is to avoid conflict between these two meanings of the word "regular".

In Γ there is a unique conjugacy class P_Γ of elements θ of minimal order for which $\mathfrak{g}^\theta$ is a Cartan subalgebra of $\mathfrak{g}^\theta$. This order, denoted h_e, is the *twisted Coxeter number* of the coset Γ [Reeder 2010]. The elements of P_Γ are ell-reg, and it is known that

$$\frac{1}{h_e} = \frac{n_e}{\dim(\mathfrak{g}/\mathfrak{t})}. \tag{2}$$

It follows that if $\theta \in \Gamma$ has order $m \geq h_e$, then

$$\tau_G(\theta) = \frac{1}{m} \leq \frac{\dim \mathfrak{g}^\theta}{\dim(\mathfrak{g}/\mathfrak{t})}, \tag{3}$$

with equality only if $\theta \in P_\Gamma$, where τ_G is Thomae's function for the group $G = \mathrm{Aut}(\mathfrak{g})$. In this paper, we extend (3) to all $\theta \in \mathrm{Aut}(\mathfrak{g})$ as follows:

Theorem 1. *Let $\mathfrak{g}$ be a simple complex Lie algebra of finite dimension, and let τ_G be Thomae's function for the group $G = \mathrm{Aut}(\mathfrak{g})$. Then for all $\theta \in G$, we have*

$$\tau_G(\theta) \leq \frac{\dim \mathfrak{g}^\theta}{\dim(\mathfrak{g}/\mathfrak{t})}. \tag{4}$$

Equality holds in (4) if and only if θ is ell-reg.

From (2), we have equality in (4) if $\theta \in P_\Gamma$. Also (4) holds trivially, and is a strict inequality, if the order of θ is larger than h_e, by (3). Equality in (4) holds for ell-reg elements, by (1). Therefore, the content of Theorem 1 is (i) the inequality (4) for all $\theta \in G$ whose order m lies in the range $1 < m < h_e$, and (ii) the assertion that only ell-reg automorphisms attain equality.

The proof of Theorem 1 consists of computations with Kac diagrams. It is given in Section 3.

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2. Applications

First we give some applications of Theorem 1 and connections to other results.

2.1. ***Characters of zero-weight spaces.*** The original motivation for Theorem 1 was to compute characters of zero weight spaces in [Reeder 2022].[2]

Let G be a connected and simply connected complex Lie group. Fix a maximal torus T in G, with Lie algebra $\mathfrak{t}$, normalizer N, and Weyl group $W = N/T$. In every finite-dimensional irreducible representation V of G, the zero-weight space V^T is a representation of W. The problem is to compute the W-character afforded by V^T, as a function of the highest weight of V.

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[2] The first version of this paper was an appendix to an earlier version of [Reeder 2022].

For example, Kostant [1976] used his results on principal elements to calculate the trace $\operatorname{tr}(\mathsf{cox}, V^T)$ of a Coxeter element $\mathsf{cox} \in W$. He showed that $\operatorname{tr}(\mathsf{cox}, V^T)$ is 0 or ± 1 and gave an explicit formula for this trace in terms of the highest weight of V.

In [Prasad 2016], Kostant's proof was reformulated in terms of the dual group $\hat{G}$ of G. Since G is simply connected, $\hat{G}$ is the group of inner automorphisms of the Lie algebra $\hat{\mathfrak{g}}$ whose root system is dual to that of $\mathfrak{g}$. In [Reeder 2022], Theorem 1 is applied to both $\operatorname{Ad}(G)$ and $\hat{G}$ to compute traces of other Weyl group elements on V^T. A brief description of this result, indicating the role of Theorem 1, is as follows:

We call an element $w \in W$ *ell-reg* if (i) $\mathfrak{t}^w = 0$ and (ii) the group $\langle w \rangle$ generated by w acts freely on the roots of $\mathfrak{t}$ in $\mathfrak{g}$. It is easy to see that w satisfies condition (i) if and only if all lifts of w in N are T-conjugate. By [Reeder et al. 2012, Proposition 1], condition (ii) is equivalent to Springer's notion of regularity of Weyl group elements in [Springer 1974]. Springer [1974, Theorem 4.2] showed that if two regular elements of W have the same order, then they are conjugate. Finally, if w is ell-reg, it follows from [Reeder et al. 2012, Proposition 12] that if n is a lift of w to N, then w and $\operatorname{Ad}(n)$ have the same order. From these facts it follows that the set $\mathcal{E}_m(N) = \{n \in N : nT \text{ is ell-reg in } W \text{ of order } m\}$, if nonempty, is a single conjugacy class in N whose elements have order m in $\operatorname{Ad}(N)$. Hence, there is an order-preserving bijection between the set of W-conjugacy classes of ell-reg elements in W and the set of G-conjugacy classes of ell-reg elements in $\operatorname{Ad}(G)$. The classification of these classes (in W and $\operatorname{Ad}(G)$) is given in the Appendix.

Let P and Q be the weight- and root-lattices of T. Let $R^+ \subset Q$ be a system of positive roots for T in G, and let $\rho \in P$ be the half-sum of the roots in R^+. We may regard P as the group of one-parameter subgroups of a dual maximal torus $\hat{T}$ of $\hat{G}$. Assuming $\mathcal{E}_m(N)$ is nonempty, we set $\zeta_m = e^{2\pi i/m}$. From [Reeder et al. 2012, Proposition 12], we have that $\rho(\zeta_m)$ has order m and is ell-reg in $\hat{G} \subset \operatorname{Aut}(\hat{\mathfrak{g}})$.

Now let $\lambda \in P$ be the highest weight of V (with respect to R^+), and let $\theta_\lambda \in \hat{T}$ be the value at ζ_m of the one-parameter subgroup $\lambda + \rho$. Let $n \in \mathcal{E}_m(N)$, and let $w = nT \in W$. Applying Theorem 1 to both $\operatorname{Ad}(n) \in \operatorname{Ad}(G)$ and $\theta_\lambda \in \hat{G}$, one obtains an inequality of centralizers

$$\dim C_G(n) \le \dim C_{\hat{G}}(\theta_\lambda), \tag{5}$$

with equality if and only if $(\lambda + \rho) + mQ$ is conjugate to $\rho + mQ$ under the natural W-action on P/mQ, see [Reeder 2022, Section 3.1] for the proof. From the inequality (5) and the theory of W-harmonic polynomials, one can show that $\operatorname{tr}(w, V^T) = 0$ unless there exists $v \in W$ such that $v(\lambda+\rho) \in \rho + mQ$, in which case

$$\operatorname{tr}(w, V^T) = \operatorname{sgn}(v) \prod_{\check{\alpha} \in \check{R}_m^+} \frac{\langle v(\lambda+\rho), \check{\alpha} \rangle}{\langle \rho, \check{\alpha} \rangle},$$

where the product is over the positive coroots $\check{\alpha}$ of G for which $\langle\rho,\check{\alpha}\rangle\in m\mathbb{Z}$, see [Reeder 2022, Theorem 3.4]. If $m=h$ is the Coxeter number then $\check{R}_m^+$ is empty, the product is 1, and we recover Kostant's result for $\operatorname{tr}(\mathsf{cox}, V^T)$. If $m<h$, then R_m^+ is nonempty.

2.2. *Graded Lie algebras.* Let $\theta\in\operatorname{Aut}(\mathfrak{g})$ have order m, and let $\zeta=e^{2\pi i/m}$. Then θ determines a $\mathbb{Z}/m\mathbb{Z}$ grading

$$\mathfrak{g}=\bigoplus_{k\in\mathbb{Z}/m\mathbb{Z}}\mathfrak{g}_k\,, \tag{6}$$

where $\mathfrak{g}_k=\{x\in\mathfrak{g}:\ \theta(x)=\zeta^k x\}$. Note that $\mathfrak{g}_0=\mathfrak{g}^\theta$.

From [Reeder et al. 2012, Corollary 14], it is known that the following are equivalent:

(i) There exists a semisimple element $x\in\mathfrak{g}_1$ for which $\operatorname{ad}(x):\mathfrak{g}_0\to\mathfrak{g}_1$ is injective.

(ii) θ is ell-reg.

Therefore, we can also use (i) as the condition for equality in Theorem 1.

Theorem 1 makes no *a priori* assumptions on the kinds of elements contained in $\mathfrak{g}_1$. But let us now assume that $\mathfrak{g}_1$ contains nonzero semisimple elements. Such gradings are said to have *positive rank*. Their classification is contained in [Vinberg 1976; Levy 2009; Reeder et al. 2012].

In the case of positive rank gradings, Theorem 1 complements results of Panyushev. Assume $x\in\mathfrak{g}_1$ is semisimple. According to [Panyushev 2005, Proposition 2.1], we have

$$\dim[\mathfrak{g}_0,x]=\frac{\dim[\mathfrak{g},x]}{m}. \tag{7}$$

Since $\dim[\mathfrak{g}_0,x]\le\dim\mathfrak{g}_0$ with equality exactly when (i) holds for x, and since $\dim[\mathfrak{g},x]\le\dim(\mathfrak{g}/\mathfrak{t})$ with equality exactly when x is a regular element of $\mathfrak{g}$, Theorem 1 combines with (7) to interpose $\dim(\mathfrak{g}/\mathfrak{t})/m$ in $\dim[\mathfrak{g}_0,x]\le\dim\mathfrak{g}_0$. That is, we have:

Corollary 2. *Assume $x\in\mathfrak{g}_1$ is semisimple. Then we have two inequalities*

$$\dim[\mathfrak{g}_0,x]\overset{(1)}{\le}\frac{\dim(\mathfrak{g}/\mathfrak{t})}{m}\overset{(2)}{\le}\dim\mathfrak{g}_0.$$

Here, inequality (1) *is equality if and only if x is regular* (*semisimple*), *and inequality* (2) *is equality if and only if θ is ell-reg.*

Under the additional assumption that $\mathfrak{g}_1$ contains a regular semisimple element, Panyushev [2005, Theorem 4.2] also showed that

$$\dim\mathfrak{g}_0=\frac{\dim[\mathfrak{g}/\mathfrak{t}]}{m}+k_0,$$

where $k_0 \geq 0$ is an integer depending only on the orders m and e of θ in $\mathrm{Aut}(\mathfrak{g})$ and $\mathrm{Out}(\mathfrak{g})$. For example, if $e = 1$, then k_0 is the number of exponents of $\mathfrak{g}$ divisible by m. This is a sharper form of Corollary 2 in the case that $\mathfrak{g}_1$ contains a regular semisimple element.

2.3. ***Adjoint Swan conductors.*** In the setting of Section 2.1, sending a representation V to its highest weight λ is a simple case of the much broader and still mostly conjectural local Langlands correspondence (LLC). In Section 2.1, we saw that the inequalities/equalities of Theorem 1 appear on the dual side of this LLC.

They also appear on the dual side of the LLC for reductive p-adic groups, now as measures of ramification.

We use notation parallel to that of Section 2.1. Let k be a p-adic field, and let G be the group of k-rational points in a connected and simply connected almost simple k-group $\boldsymbol{G}$.

Let $\hat{\mathfrak{g}}$ be a simple complex Lie algebra whose root system is dual to that of $\boldsymbol{G}$.

The LLC predicts the existence of a partition

$$\mathrm{Irr}^2(G) = \bigsqcup_{\varphi} \Pi_{\varphi}$$

of the set $\mathrm{Irr}^2(G)$ of irreducible discrete series representations of G (up to equivalence) into finite sets Π_{φ}, where φ ranges over certain representations

$$\varphi : \mathcal{W}_k \times \mathrm{SL}_2(\mathbb{C}) \to \mathrm{Aut}(\hat{\mathfrak{g}})$$

of the Weil group of k. For simplicity, we assume φ is trivial on $\mathrm{SL}_2(\mathbb{C})$. (See [Gross and Reeder 2010] for more background on the LLC.) It is of interest to find invariants relating the discrete series representation π of G to the parameter φ for which $\pi \in \Pi_{\varphi}$.

One invariant of φ is its *adjoint Swan conductor* $\mathsf{sw}(\varphi, \mathfrak{g})$. This is an integer depending only on the image $I = \varphi(\mathcal{I})$ of the inertia subgroup $\mathcal{I} \subset \mathcal{W}_k$. There is a factorization $I = S \ltimes P$, where P is a p-group and S is a cyclic group of order prime to p. We have $\mathsf{sw}(\varphi, \mathfrak{g}) \geq 0$, with equality if and only if P is trivial.

Expected properties of the LLC imply certain inequalities for $\mathsf{sw}(\varphi, \mathfrak{g})$ which have been found to hold unconditionally. For example, if φ is totally ramified (that is, if $\mathfrak{g}^I = 0$), then the LLC predicts that

$$\dim \mathfrak{g}^{\theta} \leq \mathsf{sw}(\varphi, \mathfrak{g}), \tag{8}$$

where θ is a generator of S. This inequality has been proved in [Reeder 2018] and [Bushnell and Henniart 2020].

Assume now that p does not divide the order of W. By a result of Borel and Serre [1953], this ensures that P is contained in a maximal torus of $\mathrm{Aut}(\hat{\mathfrak{g}})$, which we may choose to be normalized by θ.

Let m be the order of θ. Combining (8) with Theorem 1 gives the inequality

$$\frac{\dim(\mathfrak{g}/\mathfrak{t})}{m} \leq \mathsf{sw}(\varphi, \mathfrak{g}), \tag{9}$$

which is weaker than (8), but which depends only on the order m of S, not on S itself. Moreover, the two inequalities (8) and (9) coincide if and only if θ is ell-reg.

3. Proof of Theorem 1

The torsion automorphisms of $\mathfrak{g}$ are classified by Kac diagrams. We start with a summary of Kac diagrams so that the reader can follow the computations. For more background, see [Kac 1995; Reeder 2010].

3.1. ***Kac diagrams.*** Fix a divisor $e \in \{1, 2, 3\}$ of the order of the component group $\mathrm{Out}(\mathfrak{g})$ of $\mathrm{Aut}(\mathfrak{g})$. Let $\mathrm{Aut}(\mathfrak{g}, e)$ be the set of elements in $\mathrm{Aut}(\mathfrak{g})$ whose image in $\mathrm{Out}(\mathfrak{g})$ has order e. Then $\mathrm{Aut}(\mathfrak{g}, e)$ has one or two connected components, the latter only when $\mathfrak{g} = \mathfrak{so}_8$ and $e = 3$.

For any torsion automorphism $\theta \in \mathrm{Aut}(\mathfrak{g}, e)$, the rank of the fixed point subalgebra $\mathfrak{g}^\theta$ depends only on e; we denote this rank by n_e. If $e = 1$, then $G_1 := \mathrm{Aut}(\mathfrak{g}, 1)$ is the identity component of $\mathrm{Aut}(\mathfrak{g})$ and n_1 is the rank of $\mathfrak{g}$.

To the pair $(\mathfrak{g}, e)$ one associates an affine Dynkin diagram $\mathcal{D}(\mathfrak{g}, e)$. As we vary over all pairs $(\mathfrak{g}, e)$, the diagrams $\mathcal{D}(\mathfrak{g}, e)$ range exactly over the affine Coxeter diagrams together with all possible orientations on the multiple edges. If $e = 1$, then $\mathcal{D}(\mathfrak{g}, 1)$ is the usual affine Dynkin diagram of $\mathfrak{g}$.

The vertices in $\mathcal{D}(\mathfrak{g}, e)$ are indexed by a set I whose cardinality is $n_e + 1$, and these vertices are labeled by certain positive integers $\{c_i : i \in I\}$, where $1 \leq c_i \leq 6$.

The automorphism group $\mathrm{Aut}(\mathcal{D}(\mathfrak{g}, e))$ of the oriented and labeled diagram $\mathcal{D}(\mathfrak{g}, e)$ contains a (very small) subgroup Ω with the following property: If $e > 1$, then $\Omega = \mathrm{Aut}(\mathcal{D}(\mathfrak{g}, e))$. If $e = 1$, then $\Omega \simeq \pi_1(G_1)$.

We fix a connected component Γ of $\mathrm{Aut}(\mathfrak{g}, e)$. For any positive integer m, let Γ_m be the set of elements of Γ having order m. Then Γ_m is nonempty only if e divides m. The G_1-conjugacy classes in Γ_m are parametrized as follows: Let S_m be the set of I-tuples $s = (s_i : i \in I)$ consisting of integers $s_i \geq 0$ such that $\gcd\{s_i : i \in I\} = 1$ and

$$m = e \cdot \sum_{i \in I} c_i s_i .$$

There is a surjective mapping from S_m to the set of G_1-conjugacy classes in Γ_m (Kac coordinates). The *Kac-diagram* of the conjugacy class corresponding to s consists of the diagram $\mathcal{D}(\mathfrak{g}, e)$ with each node i replaced by s_i. Two elements s and $s' \in S_m$ map to the same conjugacy class in Γ_m if and only if their Kac diagrams are conjugate under the group Ω.

For example, in Γ there is a unique conjugacy class of automorphisms of minimal order having abelian fixed-point subalgebras. Such automorphisms are called *principal*. They are ell-reg and have Kac coordinates $s = (s_i)$, where $s_i = 1$ for all i. The order of a principal automorphism in Γ, namely

$$h_e := e \cdot \sum_{i \in I} c_i,$$

is the Coxeter number of $\mathrm{Aut}(\mathfrak{g}, e)$. It is known from [Reeder 2010] that equality holds in Theorem 1 for principal elements, namely, we have

$$\frac{1}{h_e} = \frac{n_e}{[\mathfrak{g} : \mathfrak{t}]}. \tag{10}$$

The Kac diagrams of all ell-reg automorphisms of $\mathfrak{g}$ were tabulated in [Reeder et al. 2012, Section 7] and are recalled in the Appendix. These diagrams have all Kac-coordinates $s_i \in \{0, 1\}$ and are determined by the subset $J = \{j \in I : s_j = 0\} \subsetneq I$.

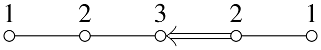
For any subset $J \subsetneq I$, we set

$$c_J = \sum_{j \in J} c_j \quad \text{and} \quad c^J = \sum_{i \notin J} c_i.$$

The subgraph of $\mathcal{D}(\mathfrak{g}, e)$ supported on J is the finite Dynkin graph of a reductive subalgebra $\mathfrak{g}_J$ of $\mathfrak{g}$. Let $|R_J|$ be the number of roots of $\mathfrak{g}_J$.

Let $\theta \in \Gamma$ be a torsion automorphism with Kac-coordinates $s = (s_i)$, and let $J = \{j \in I : s_j = 0\}$. Then $J \neq I$, and we have $\mathfrak{g}^\theta \simeq \mathfrak{g}_J$.

Example. Consider $\mathfrak{g}$ of type E_6. The labeled diagram $\mathcal{D}(\mathfrak{g}, 2)$ for all outer automorphisms of $\mathfrak{g}$ is



The Kac diagram

$$1 \text{———} 1 \text{———} 0 \Longleftarrow 0 \text{———} 1$$

represents the conjugacy class of an outer automorphism $\theta \in \mathrm{Aut}(\mathfrak{g})$ having order

$$m = 2 \cdot (1 \cdot 1 + 2 \cdot 1 + 3 \cdot 0 + 2 \cdot 0 + 1 \cdot 1) = 8.$$

We have $c_J = 3 + 2 = 5$, $c^J = 1 + 2 + 1 = 4$, and $\mathfrak{g}^\theta \simeq \mathfrak{so}_5$. This automorphism has minimal order among those with fixed-point subalgebra $\mathfrak{so}_5$.

Lemma 3. *The inequality in Theorem 1 for all torsion automorphisms in a component $\Gamma \subset \mathrm{Aut}(\mathfrak{g}, e)$ is equivalent to the inequality*

$$n_e \cdot c_J \leq c^J \cdot |R_J| \tag{11}$$

for every subset $J \subsetneq I$.

Proof. Let $\theta \in \Gamma_m$ have Kac coordinates (s_i), and let

$$J = \{j \in I : s_j = 0\}.$$

Then $m \geq e \cdot c^J$ with equality if and only if $s_i = 1$ for all $i \in I - J$. Since

$$\dim \mathfrak{g}^\theta = \dim \mathfrak{g}_J = n_e + |R_J| \quad \text{and} \quad \dim(\mathfrak{g}/\mathfrak{t}) = h_e n_e = e \cdot c_I \cdot n_e,$$

it follows that

$$\frac{1}{m} \leq \frac{1}{e \cdot c^J} \quad \text{and} \quad \frac{\dim \mathfrak{g}^\theta}{\dim(\mathfrak{g}/\mathfrak{t})} = \frac{n_e + |R_J|}{e \cdot c_I \cdot n_e}.$$

So, for every θ, the inequality in Theorem 1 is equivalent to having

$$e \cdot c_I \cdot n_e \leq (n_e + |R_J|) \cdot e \cdot c^J$$

for every J. Since $c_I = c^J + c_J$, the result follows. □

If J is empty then both sides of (11) are zero. We may assume from now on that J is nonempty and that $s_i = 1$ for all $i \in I - J$. Thus J is identified with a Kac diagram with labels in $\{0, 1\}$, where the nodes in J are labeled 0 and the nodes in $I - J$ are labeled 1.

We will show that the integer $f(\mathfrak{g}, e, J)$ defined by

$$f(\mathfrak{g}, e, J) = c^J |R_J| - n_e c_J$$

satisfies $f(\mathfrak{g}, e, J) \geq 0$. Our analysis will also find those J for which $f(\mathfrak{g}, e, J) = 0$. It turns out that the Kac diagrams of ell-reg automorphisms are exactly those for which $f(\mathfrak{g}, e, J) = 0$.

3.2. ***Type A_n.*** The case $\mathfrak{g} = \mathfrak{sl}_{n+1}$ and $e = 1$ is very simple but different from the other cases, so we treat it separately here. Fix a nonempty subset $J \subsetneq I$. The root system R_J has type

$$\prod_{i=1}^{a} A_{q_i}$$

for some positive integers $q_1, \ldots, q_a$. Let $q = \sum q_i$. Since all $c_i = 1$, we have $c_J = q$ and $c^J = n + 1 - q \geq a$. Now,

$$\begin{aligned} f(\mathfrak{g}, 1, J) &= c^J \sum_{i=1}^{a} q_i(q_i + 1) - (c^J + q - 1)q \\ &= c^J \sum_{i=1}^{a} q_i^2 - q^2 + q \geq a \sum_{i=1}^{a} q_i^2 - q^2 + q \geq q, \end{aligned}$$

where the arithmetic-geometric inequality is used in the last step. Since $J \neq \varnothing$, we have $f(\mathfrak{g}, 1, J) \geq q > 0$.

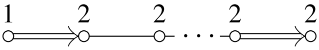
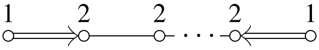
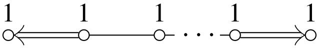
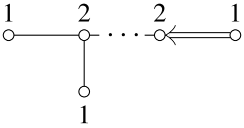
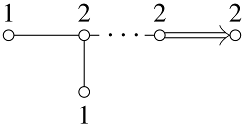
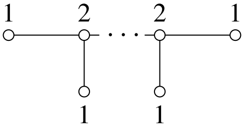
$(\mathfrak{g}, e)$	$\mathcal{D}(\mathfrak{g}, e)$	$h = e \cdot c_I$
${}^2A_{2n},\ n \geq 2$		$2(2n+1)$
$C_n,\ n \geq 2$		$2n$
${}^2D_{n+1},\ n \geq 2$		$2(n+1)$
${}^2A_{2n-1},\ n \geq 3$		$2(2n-1)$
$B_n,\ n \geq 3$		$2n$
$D_n,\ n \geq 4$		$2n-2$

Table 1. The relevant diagrams $\mathcal{D}(\mathfrak{g}, e)$ for $n \geq 2$.

3.3. ***The remaining classical Lie algebras.*** In this section, $(\mathfrak{g}, e)$ is of classical type not equal to $(\mathfrak{sl}_n, 1)$. We will write

$$n = n_e \quad \text{and} \quad h = h_e.$$

Since the criteria in Lemma 3 are easy to check for outer automorphisms of $\mathfrak{sl}_3$, we may assume $n \geq 2$.

The relevant diagrams $\mathcal{D}(\mathfrak{g}, e)$, for $n \geq 2$, are listed in Table 1. Each diagram has $n+1$ nodes. They are grouped according to their underlying Coxeter diagram. Note that ${}^2A_3 = {}^2D_3$ and $B_2 = C_2$.

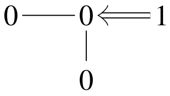
3.3.1. *Small rank.* For the reduction arguments to come, it is necessary to directly verify Theorem 1 for classical $\mathfrak{g}$ of minimal rank in Table 1. (One can shorten the task by using the first parts of Sections 3.4.1 and 3.4.2 below.) For $J \neq \varnothing$, we obtain the following:

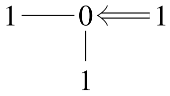
For $(\mathfrak{g}, e)$ of types ${}^2A_4$, C_2, and ${}^2D_3$, we have $f(\mathfrak{g}, e, J) \geq 0$ with equality just for the Kac diagrams:

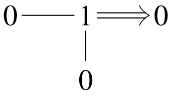
$$1 \Longrightarrow 0 \Longrightarrow 0 \qquad\qquad 1 \Longrightarrow 0 \Longleftarrow 1 \qquad\qquad 0 \Longleftarrow 1 \Longrightarrow 0$$

respectively. These diagrams represent the nonprincipal ell-reg automorphisms of $\mathfrak{sl}_5$, $\mathfrak{sp}_4$, and $\mathfrak{so}_6$; each is an involution. See Sections A.1, A.4, and A.5.

For $(\mathfrak{g}, e)$ of types ${}^2A_5$ and B_3, we have $f(\mathfrak{g}, e, J) \geq 0$, with equality just for the Kac diagrams:

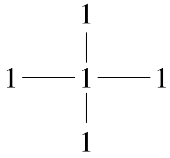


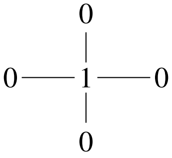


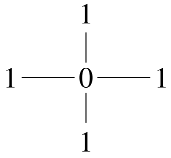


These are the nonprincipal ell-reg automorphisms of $\mathfrak{sl}_6$ and $\mathfrak{so}_7$; see Sections A.2 and A.3.

Finally consider $(\mathfrak{g}, e)$ of type D_4. We write $I = \{0, 1, 2, 3, 4\}$, where 0 is the degree-four vertex in $\mathcal{D}(\mathfrak{so}_8, 1)$. Let q be the number of degree-one vertices in J. One easily computes the following: If $s_0 = 1$, then $f(\mathfrak{so}_8, 1, J) = 2q(4-q)$. If $s_0 = 0$, then $f(\mathfrak{so}_8, 1, J) \geq 0$, with equality just for $q = 0$. Hence the inequality of Theorem 1 holds, with equality just for the Kac diagrams:







These are the Kac diagrams for the ell-reg inner automorphisms of $\mathfrak{so}_8$; see Section A.5.

3.4. ***Refinements.*** Let $\mathcal{X}$ be the set of all triples $(\mathfrak{g}, e, J)$, where $(\mathfrak{g}, e)$ is one of the above classical types for $n \geq 2$ and J is a nonempty proper subset of the set I of vertices of $\mathcal{D}(\mathfrak{g}, e)$. For any subset $\mathcal{Y} \subset \mathcal{X}$, let $\mathcal{Y}_0 = \{(\mathfrak{g}, e, J) \in \mathcal{Y} : f(\mathfrak{g}, e, J) = 0\}$. We must prove that $f \geq 0$ on $\mathcal{X}$ and that $\mathcal{X}_0$ consists precisely of the diagrams listed in the Appendix for classical $(\mathfrak{g}, e)$.

Definition. If $\mathcal{Y}' \subset \mathcal{Y}$ are subsets of $\mathcal{X}$, we say $\mathcal{Y}'$ is a *refinement* of $\mathcal{Y}$ if for every $(\mathfrak{g}, e, J) \in \mathcal{Y} - \mathcal{Y}'$, we have either:

(i) $f(\mathfrak{g}, e, J) > 0$ or

(ii) there exists $(\mathfrak{g}', e', J') \in \mathcal{Y}'$ and a positive integer c such that

$$c \cdot f(\mathfrak{g}, e, J) > f(\mathfrak{g}', e', J').$$

We note the following:

(i) Refinement is transitive: if $\mathcal{Y}''$ is a refinement of $\mathcal{Y}'$ and $\mathcal{Y}'$ is a refinement of $\mathcal{Y}$, then $\mathcal{Y}''$ is a refinement of $\mathcal{Y}$.

(ii) If $\mathcal{Y}$ is a refinement of $\mathcal{X}$ and $f \geq 0$ on $\mathcal{Y}$, then $f > 0$ on $\mathcal{X} - \mathcal{Y}$ and $\mathcal{X}_0 = \mathcal{Y}_0$.

From (ii), it suffices to find a refinement $\mathcal{Y}$ of $\mathcal{X}$ such that $f \geq 0$ on $\mathcal{Y}$ and $\mathcal{Y}_0$ consists precisely of the ell-reg triples listed in the Appendix.

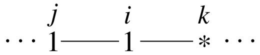
This classification guides our refinements. Ignoring the principal automorphisms as we may, we observe that in classical ell-reg Kac diagrams the vertices in $I-J$ are: (i) never adjacent and (ii) tend to be equally spaced from each other.

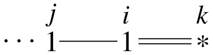
We say that a vertex $i \in I$ is *interior* if i is adjacent to at least two other vertices in $\mathcal{D}(\mathfrak{g}, e)$. If i is adjacent to just one other vertex in $\mathcal{D}(\mathfrak{g}, e)$, we say i is a *boundary vertex*. Since $n \geq 3$, every pair of adjacent vertices has at least one interior vertex. Table 1 shows that all interior i have the same value c of c_i ($c = 1$ in type ${}^2D_{n+1}$ and $c = 2$ in the other classical diagrams), and $c \geq c_i$ for all $i \in I$.

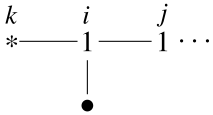
Lemma 4. *Let $\mathcal{Y}$ be the set of $(\mathfrak{g}, e, J) \in \mathcal{X}$ for which no two interior vertices of $I-J$ are adjacent in $\mathcal{D}(\mathfrak{g}, e)$. Then $\mathcal{Y}$ is a refinement of $\mathcal{X}$.*

Proof. Consider a triple $(\mathfrak{g}, e, J) \in \mathcal{X}$, and let $i, j \in I-J$ be adjacent interior vertices in $\mathcal{D}(\mathfrak{g}, e)$.

Let k be another vertex adjacent to i. The possible configurations of i, j, k in the Kac diagram are:







where the double bond has either orientation and $*, \bullet \in \{0, 1\}$ are arbitrary.

Removing i and joining j to k with a bond of the same type as the bond previously joining i to k, we obtain a diagram $\mathcal{D}(\mathfrak{g}', e)$ of the same type as $\mathcal{D}(\mathfrak{g}, e)$. The vertices of $\mathcal{D}(\mathfrak{g}', e)$ are indexed by $I' = I - \{i\}$, and we have $J \subset I'$. In this way, the diagram $\mathcal{D}(\mathfrak{g}, e, J)$ contracts by one vertex to the diagram $\mathcal{D}(\mathfrak{g}', e, J)$. The root system R'_J of $\mathfrak{g}'_J$ is isomorphic to R_J, we have $\sum_{i' \in I'-J} c_{i'} = c^J - c$, and c_J is unchanged. It follows that

$$f(\mathfrak{g}, e, J) - f(\mathfrak{g}', e, J) = c^J|R_J| - nc_J - (c^J - c)|R_J| + (n-1)c_J = c|R_J| - c_J.$$

Since $|R_J| \geq 2|J|$ and $c_J \leq c|J|$, we have

$$f(\mathfrak{g}, e, J) - f(\mathfrak{g}', e, J) \geq c|J| > 0. \tag{12}$$

Since $|I' - J| = |I - J| - 1$, repeating this procedure will eventually produce a diagram $\mathcal{D}(\mathfrak{g}'', e, J) \in \mathcal{Y}$, and we will have $f(\mathfrak{g}, e, J) > f(\mathfrak{g}'', e, J)$. ☐

Our next refinement heads toward equilibrium for the interior components of R_J.

Given a diagram $\mathcal{D}(\mathfrak{g}, e, J) \in \mathcal{X}$, let J° be the set of interior vertices in J. We have a decomposition of root systems

$$R_J = R_J^\circ \sqcup R_{\partial J},$$

where R_J° (respectively, $R_{\partial J}$) is the union of those irreducible components of R_J whose bases are (respectively, are not) contained in J°. Let $R_1, R_2, \ldots, R_a$ be the components of R_J°. Each R_i has type A_{q_i} for some integer $q_i \geq 1$. Let

$$d(J) = \max\{|q_i - q_j| : \ 1 \leq i \leq j \leq a\}.$$

Lemma 5. *Let $\mathcal{Y}$ be as in Lemma 4, and let $\mathcal{Y}'$ be the set of $(\mathfrak{g}, e, J) \in \mathcal{Y}$ for which $d(J) \leq 1$. Then $\mathcal{Y}'$ is a refinement of $\mathcal{Y}$.*

Proof. The value of $f(\mathfrak{g}, e, J)$ is unchanged by permuting the components $R_1, \ldots, R_a$. If $d(J) \geq 2$, then we may choose such a permutation to arrange that $q_1 - q_2 \geq 2$, and there are three interior vertices $\{i, j, k\}$ such that $j \in R_1$, $i \in I - J$, $k \in R_2$, as shown:

$$\cdots \overset{j}{0} \text{——} \overset{i}{1} \text{——} \overset{k}{0} \cdots$$

Now switch s_i and s_j to obtain a diagram

$$\mathcal{D}(\mathfrak{g}, e, J') \quad = \quad \cdots \overset{j}{1} \text{——} \overset{i}{0} \text{——} \overset{k}{0} \cdots$$

Note that $\mathcal{D}(\mathfrak{g}, e, J') \in \mathcal{Y}$, since $q_1 \geq 2$. The values n, c_J, and c^J are unchanged, and one checks that

$$f(\mathfrak{g}, e, J) - f(\mathfrak{g}, e, J') = 2c^J(q_1 - q_2 - 1) > 0.$$

Repeating this process, we eventually find a subset $J'' \subset I$ with $f(\mathfrak{g}, e, J) > f(\mathfrak{g}, e, J'')$ and $d(J'') \leq 1$. $\square$

We next strengthen the refinement of Lemma 4 to include boundary vertices.

Lemma 6. *Let $\mathcal{Y}'$ be as in Lemma 5, and let $\mathcal{Z}$ be the set of $(\mathfrak{g}, e, J) \in \mathcal{Y}'$ for which no two vertices of $I - J$ are adjacent in $\mathcal{D}(\mathfrak{g}, e)$. Then $\mathcal{Z}$ is a refinement of $\mathcal{Y}'$.*

Proof. Assume $(\mathfrak{g}, e, J) \in \mathcal{Y}'$ and that i and j are adjacent vertices in $\mathcal{D}(\mathfrak{g}, e, J)$. Since $\mathcal{Y}' \subset \mathcal{Y}$, we may assume that i is an interior vertex and j is a boundary vertex. Lemma 6 has been proved for the minimal cases in Section 3.3.1, so we may also assume there is another interior vertex k adjacent to i. Near i, the possibilities for $\mathcal{D}(\mathfrak{g}, e, J)$ are as shown:

$$(13) \quad \text{(i)}\ \overset{j}{1} \Longrightarrow \overset{i}{1} \text{——} \overset{k}{0} \cdots \qquad \text{(ii)}\ \overset{j}{1} \Longleftarrow \overset{i}{1} \text{——} \overset{k}{0} \cdots \qquad \text{(iii)}\ \overset{j}{1} \text{——} \underset{\underset{s}{|}}{\overset{i}{1}} \text{——} \overset{k}{0} \cdots$$

where $s \in \{0, 1\}$.

In cases (i) and (ii), we proceed as in Lemma 4 by removing i and joining jk by the bond ji to obtain $\mathcal{D}(\mathfrak{g}', e, J)$. The same calculation as Lemma 4 shows that $f(\mathfrak{g}, e, J) > f(\mathfrak{g}', e, J)$.

Now for case (iii), let R_K be the component of R_J containing k, where $k \in K \subset J$, and let $q = |K| \geq 1$.

Suppose $R_K \subset R_{\partial J}$. Then R_K and the right-hand boundary of $\mathcal{D}(\mathfrak{g}, e, J)$ have one of these types (where $* \in \{0, 1\}$):

$$\begin{array}{l} k \\ 0 \ \cdots \ 0 \Longrightarrow 0 \end{array} \qquad\qquad \begin{array}{l} k \\ 0 \ \cdots \ 0 \Longleftarrow 0 \end{array} \qquad\qquad \begin{array}{ccccc} k & & & & \\ 0 & \cdots & 0 & \text{———} & 0 \\ & & | & & \\ & & * & & \end{array}$$

In view of (13), the diagram $\mathcal{D}(\mathfrak{g}, e, J)$ is specific enough to compute $f(\mathfrak{g}, e, J) > 0$ in each of these cases.

From now on, we may assume that R_K is an interior component of R_J, hence of type A_q, where $q \geq 1$. As in Lemma 5, after permuting components of R_J°, we may also assume that $R_J^\circ = xA_{q-1} + yA_q$ for integers x, y with $y > 0$. An expanded view of the neighborhood of i containing R_K, with single bonds omitted, is

$$\mathcal{D}(\mathfrak{g}, e, J) \quad = \quad \begin{array}{cccc} j & i & k & \\ 1 & 1 & 0 & \overbrace{0 \ \ 0 \cdots 0}^{q-1 \text{ vertices}} \\ & \mathrm{s} & & \end{array}$$

with $s \in \{0, 1\}$. Switch s_i and s_k to obtain

$$\mathcal{D}(\mathfrak{g}, e, J') \quad = \quad \begin{array}{ccccc} j & i & k & & \\ 1 & 0 & 1 & \overbrace{0 \ \ 0 \cdots 0}^{q-1 \text{ vertices}} & \cdots \\ & \mathrm{s} & & & \end{array} \tag{14}$$

Since $c^{J'} = c^J$, $n' = n$, and $c_{J'} = c_J$, we find that

$$f(\mathfrak{g}, e, J) - f(\mathfrak{g}, e, J') = 2(q + s - 2)c^J.$$

If $q + s > 2$, then $f(\mathfrak{g}, e, J) > f(\mathfrak{g}, e, J')$, so we may assume $q + s \leq 2$.

Assume that $q+s = 1$. Then $q = 1$ and $s = 0$, so $R_J^\circ = yA_1$. Since cases (i) and (ii) of (13) have been eliminated, we may assume $\mathcal{D}(\mathfrak{g}, e, J)$ has one of the forms below, where each diagram has y copies of 0 1 in the top row and single bonds are omitted:

$$\begin{array}{cccccccc} 1 & 1 & 0 & 1 & 0 & 1 \cdots 0 & 1 & \overbrace{0 \ 0 \cdots \Rightarrow 0}^{B_r} \\ & 0 & & & & & & \end{array} \qquad \begin{array}{cccccccc} 1 & 1 & 0 & 1 & 0 & 1 \cdots 0 & 1 & \overbrace{0 \ 0 \cdots \Leftarrow 0}^{C_r} \\ & 0 & & & & & & \end{array} \quad (r \geq 1)$$

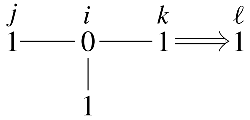
$$\begin{array}{cccccc} 1 & 1 & 0 & 1 \cdots 0 & 1 & 0 \Rightarrow 1 \\ & 0 & & & & \end{array} \qquad \begin{array}{cccccc} 1 & 1 & 0 & 1 \cdots 0 & 1 & 0 \Leftarrow 1 \\ & 0 & & & & \end{array}$$

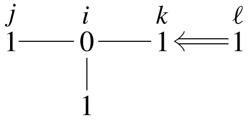
$$\begin{array}{cccccc} 1 & 1 & 0 & 1 \cdots 0 & 1 & \overbrace{0 \cdots 0 \ \ 0}^{D_r} \\ & 0 & & & & \quad\ \ 0 \ \ \ \end{array} \qquad \begin{array}{cccccc} 1 & 1 & 0 & 1 \cdots 0 & 1 & \overbrace{0 \cdots 0 \ \ 0}^{A_r} \\ & 0 & & & & \quad\ \ 1 \ \ \ \end{array} \quad (r \geq 2)$$

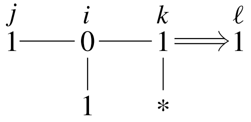
$$\begin{array}{ccccc} 1 & 1 & 0 & 1 \cdots 0 & 1 \\ & 0 & & 1 \quad & \end{array} \qquad \begin{array}{cccccc} 1 & 1 & 0 & 1 \cdots 0 & 1 & 1 \\ & 0 & & & 1 & \end{array}$$

In each of the above cases, it is straightforward to calculate that $f(\mathfrak{g}, e, J) = y\beta(r) + \gamma(r)$, where β and γ are polynomials (of degree at most two) which are positive for all integer values of r.

Assume $q = s = 1$. Then we have $f(\mathfrak{g}, e, J) = f(\mathfrak{g}, e, J')$, with J' as in (14). Since k is interior, there is a boundary vertex ℓ adjacent to k, with $s_\ell = 1$. Then $\mathcal{D}(\mathfrak{g}, e, J')$ has one of the forms:







with $* \in \{0, 1\}$. Again, one easily checks that $f(\mathfrak{g}, e, J) > 0$.

For the remaining case $q = 2$ and $s = 0$, we have $f(\mathfrak{g}, e, J) = f(\mathfrak{g}, e, J')$ and

$$\mathcal{D}(\mathfrak{g}, e, J') = \begin{array}{ccccc} j & i & k & & \\ 1 & 0 & 1 & 0 & \cdots \\ & 0 & & & \end{array} \tag{15}$$

where single bonds have been omitted. Here, $R_{J'}$ has no adjacent vertices, except possibly at the other end of $\mathcal{D}(\mathfrak{g}, e, J')$, where one of the configurations of (13) could be mirrored. In that case, starting with (15), we repeat the above steps at the other end of $\mathcal{D}(\mathfrak{g}, e, J')$ to produce a triple $(\mathfrak{g}', e, J'') \in \mathcal{Z}$ such that $f(\mathfrak{g}, e, J) \geq f(\mathfrak{g}', e, J'')$. These steps only affect vertices to the right of k, so the A_2 boundary component of i in (15) persists in $R_{J''}$. In Sections 3.4.2 and 3.4.3, we will find by direct computation that $f > 0$ on every triple in $\mathcal{Z}$ having a boundary component of type A_n, for $n \geq 2$. This completes the proof of Lemma 6. □

To prove Theorem 1, it now suffices to calculate f on the set $\mathcal{Z}$ from Lemma 6. Recall that $\mathcal{Z}$ consists of those triples $(\mathfrak{g}, e, J)$ for which no two vertices in $I - J$ are adjacent and whose components of R_J° have at most two types A_{q-1} and A_q, occurring x and y times, respectively.

The refinement calculations made above were (mostly) local, using only data near the modification of the Kac diagram $\mathcal{D}(\mathfrak{g}, e, J)$ to estimate $f(\mathfrak{g}, e, J)$ from below. To actually calculate $f(\mathfrak{g}, e, J)$ requires the entire Kac diagram $\mathcal{D}(\mathfrak{g}, e, J)$, including the boundary. From here on we must proceed in cases, according to the various labeled boundaries of the graphs $\mathcal{D}(\mathfrak{g}, e)$.

Recall that $R_{\partial J}$ is the union of the components of R_J not in R_J°. Let ∂J be the subset of J supporting $R_{\partial J}$. Then $R_{\partial J}$ is a product of two classical root systems whose ranks (possibly zero) we will denote by p and r. We have

$$|R_J| = |R_{\partial J}| + q(q-1)x + q(q+1)y \quad \text{and} \quad c_J = c_{\partial J} + c(q-1)x + cqy,$$

where

$$c_{\partial J} = \sum_{j \in \partial J} c_j.$$

Define integers a and b by

$$c^J = a + cx + cy \quad \text{and} \quad n = b + qx + (q+1)y,$$

where c is the common value of c_i on the interior vertices of I. A straightforward computation gives the following:

Lemma 7. *For* $(\mathfrak{g}, e, J) \in \mathcal{Z}$, *the integer* $f(\mathfrak{g}, e, J) = |R_J|c^J - nc_J$ *has the form*

$$f(\mathfrak{g}, e, J) = cxy + \alpha x + \beta y + \gamma,$$

where α, β, *and* γ *are polynomial expressions in* p, q, *and* r *given by*:

$$\begin{aligned} \alpha &= \big(c|R_{\partial J}| + aq(q-1)\big) - \big(bc(q-1) + qc_{\partial J}\big), \\ \beta &= \big(c|R_{\partial J}| + aq(q+1)\big) - \big(bcq + (q+1)c_{\partial J}\big), \\ \gamma &= a|R_{\partial J}| - bc_{\partial J}. \end{aligned} \tag{16}$$

We will show that $\alpha, \gamma \geq 0$. Since β is obtained from α upon replacing q by $q+1$, then also $\beta \geq 0$, so this will imply that

$$f(\mathfrak{g}, e, J) \geq 0,$$

with equality if and only if $0 = xy = \alpha = \gamma$. Without loss of generality, we may then assume $y = 0$. Theorem 1 will then follow by comparison with the tables of ell-reg automorphisms in the Appendix.

3.4.1. *Types* ${}^2A_{2n}$*,* C_n*, and* ${}^2D_{n+1}$. The underlying Coxeter diagram with indexing set $I = \{0, 1, \dots, n\}$ is

$$0 \Longleftrightarrow 1 \text{---} 2 \text{---} \cdots \text{---} (n-1) \Longleftrightarrow n$$

The three types differ only in the labels c_i, which do not affect $|R_J|$. Let $(\mathfrak{g}, e)$ and $(\mathfrak{g}', e')$ be two of ${}^2A_{2n}$, C_n, and ${}^2D_{n+1}$, with corresponding labellings c_i and c_i'. For each subset $A \subset I$, we set

$$c_A = \sum_{i \in A} c_i \quad \text{and} \quad c_A' = \sum_{i \in A} c_i'.$$

We set $K = I - J$.

One more local calculation will reduce the number of cases further. Set:

$$f = f(\mathfrak{g}, e, J) = |R_J|c_K - nc_J \quad \text{and} \quad f' = f(\mathfrak{g}', e', J) = |R_J|c_K' - nc_J'.$$

Suppose $(\mathfrak{g}, e) = {}^2A_{2n}$ and $(\mathfrak{g}', e') = C_n$. If $n \in K$, then $c_K = c_K' + 1$ and $c_J = c_J'$, so $f > f'$. If $n \in J$, then $c_K = c_K'$ and $c_J = c_J' + 1$, so $f < f'$.

Suppose $(\mathfrak{g}, e) = {}^2A_{2n}$ and $(\mathfrak{g}', e') = {}^2D_{n+1}$. If $0 \in K$, then $1 + c_K = 2c_K'$ and $c_J = 2c_J'$, so $2f' > f$. If $0 \in J$, then $1 + c_J = 2c_J'$ and $c_K = 2c_K'$, so $f > 2f'$.

Suppose $(\mathfrak{g}, e) = C_n$ and $(\mathfrak{g}', e') = {}^2D_{n+1}$. If $\{0, n\} \in J$, then $2c'_K = c_K$ and $2c'_J = c_J + 2$, so $f = 2f' + 2n > 2f'$. If $0 \in J$ and $n \in K$, then $c_K + 1 = 2c'_K$ and $c_J + 1 = 2c'_J$, so $2f' = f + |R_J| - n$. Since no two vertices in K are adjacent, it follows that $|R_J| > n$, so $2f' > f$.

This discussion shows that we need only consider the following three cases:

(1) $(\mathfrak{g}, e) = {}^2A_{2n}$, with $0 \in K$ and $n \in J$,

(2) $(\mathfrak{g}, e) = C_n$, with $\{0, n\} \in K$,

(3) $(\mathfrak{g}, e) = {}^2D_{n+1}$, with $\{0, n\} \subset J$.

Indeed, if $f(\mathfrak{g}, e, J) \geq 0$ in Cases 1–3, then $f(\mathfrak{g}, e, J) \geq 0$ in all cases and $f(\mathfrak{g}, e, J) = 0$ can only occur in Cases 1–3.

Case 1. Assume $(\mathfrak{g}, e) = {}^2A_{2n}$ and $R_J = B_r + xA_{q-1} + yA_q$, with $r \geq 1$. Then:

$$\begin{aligned} |R_J| &= 2r^2 + q(q-1)x + q(q+1)y, & c_K &= 1 + 2x + 2y, \\ n &= r + xq + y(q+1), & c_J &= 2r + 2(q-1)x + 2qy, \\ \gamma &= 0, & \alpha &= (q-2r)(q-2r-1). \end{aligned}$$

Thus we have $f(\mathfrak{g}, e, J) \geq 0$, with equality if and only if $q = 2r$ or $2r + 1$. These cases are the last two rows in the table in Section A.1 for $n \geq 2$.

Case 2. Assume $(\mathfrak{g}, e) = C_n$ and $R_J = xA_{q-1} + yA_q$. Then:

$$\begin{aligned} |R_J| &= q(q-1)x + q(q+1)y, & c_K &= 2x + 2y, \\ n &= qx + (q+1)y, & c_J &= 2(q-1)x + 2qy, \\ \gamma &= 0, & \alpha &= 0. \end{aligned}$$

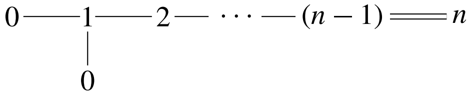
Thus we have $f(\mathfrak{g}, e, J) \geq 0$, with equality if and only if $xy = 0$. These are the cases with $k = q$ in the table in Section A.4.

Case 3. Assume $(\mathfrak{g}, e) = {}^2D_{n+1}$ and $R_J = B_p + xA_{q-1} + yA_q + B_r$, with $p, r > 0$ and $q > 1$. Then:

$$\begin{aligned} |R_J| &= 2p^2+2r^2+q(q-1)x+q(q+1)y, & c_K &= 1+x+y, \\ n &= p+r+qx+(q+1)y, & c_J &= p+r+(q-1)x+qy, \\ \gamma &= (p-r)^2, & \alpha &= (p-r)^2+(p+r-q)(p+r-q+1). \end{aligned}$$

Thus we have $f(\mathfrak{g}, e, J) \geq 0$, with equality if and only if $xy = 0$, $p = r$ and $q = 2p$ or $q = 2p + 1$. These are the cases in the last two rows of the table in Section A.6.

3.4.2. *Types* $^2A_{2n-1}$ *and* B_n. The underlying Coxeter diagram with indexing set $I=\{0,1,\dots,n\}$ is



The two types differ only in the label $c_n=1$ for $^2A_{2n-1}$ and $c_n=2$ for B_n. Comparing, as in the previous section, we may assume $n\in K$ for $^2A_{2n-1}$ and $n\in J$ for B_n.

*Case A*1. Assume $n\in K$, $\{0,1\}\subset J$, $R_J=D_p+xA_{q-1}+yA_q$, with $p\geq 2$. Then:

$$\begin{aligned} |R_J|&=2p(p-1)+q(q-1)x+q(q+1)y, & c_K&=1+2x+2y,\\ n&=p+qx+(q+1)y, & c_J&=2(p-1)+2(q-1)x+2qy,\\ \gamma&=0, & \alpha&=(2p-q)(2p-q-1). \end{aligned}$$

In this case, we have $f(\mathfrak{g},e,J)\geq 0$, with equality if and only if $xy=0$ and $q=2p$ or $q=2p-1$. These are the cases with $d=1$ or $k=p$ in Section A.2.

*Case A*2. Assume $\{0,n\}\subset K$, $1\in J$, and $R_J=A_p+xA_{q-1}+yA_q$. Then:

$$\begin{aligned} |R_J|&=p(p+1)+q(q-1)x+q(q+1)y, & c_K&=2+2x+2y,\\ n&=1+p+qx+(q+1)y, & c_J&=2p-1+2(q-1)x+2qy,\\ \gamma&=p+1, & \alpha&=2(p-q+1)^2+q. \end{aligned}$$

In this case, we have $f(\mathfrak{g},e,J)>0$.

*Case A*3. Assume $\{0,1,n\}\subset K$ and $R_J=xA_{q-1}+yA_q$, where $q\geq 2$. Then:

$$\begin{aligned} |R_J|&=q(q-1)x+q(q+1)y, & c_K&=1+2x+2y,\\ n&=1+qx+(q+1)y, & c_J&=2(q-1)x+2qy,\\ \gamma&=0, & \alpha&=(q-1)(q-2). \end{aligned}$$

In this case, we have $f(\mathfrak{g},e,J)\geq 0$, with equality if and only if $q=2$. This is the case $d=n$ in Section A.2.

*Case B*1. Assume $\{0,1,n\}\subset J$ and $R_J=D_p+xA_{q-1}+yA_q+B_r$. Then:

$$\begin{aligned} |R_J|&=2p(p-1)+2r^2+q(q-1)x+q(q+1)y, & c_K&=2(1+x+y),\\ n&=p+r+qx+(q+1)y, & c_J&=2(p+r-1)+2(q-1)x+2qy,\\ \gamma&=2(p-r)(p-r-1), & \alpha&=2(p-r)(p-r-1)+2(p+r-q)^2. \end{aligned}$$

In this case, we have $f(\mathfrak{g},e,J)\geq 0$, with equality if and only if $p=r$ and $q=2r$, or $p=r+1$ and $q=2r+1$. these are the cases in the last two rows of the table in Section A.3 with $k=q$.

*Case B*2. Assume $\{1, n\} \subset J$, $0 \in K$, and $R_J = A_p + xA_{q-1} + yA_q + B_r$, where $p, r \geq 1$. Then:

$$\begin{aligned} |R_J| &= p(p+1)+2r^2+q(q-1)x+q(q+1)y, & c_K &= 3+2x+2y, \\ n &= p+r+1+qx+(q+1)y, & c_J &= 2p+2r-1+2(q-1)x+2qy, \\ \gamma &= (2r-p-1)^2+3r, & \alpha &= 2(p-q+1)^2+(q-2r)^2+2r. \end{aligned}$$

In this case, we have $f(\mathfrak{g}, e, J) > 0$.

*Case B*3. Assume $n \in J$, $\{0, 1\} \subset K$, and $R_J = xA_{q-1} + yA_q + B_r$, where $r \geq 1$. Then:

$$\begin{aligned} |R_J| &= 2r^2 + q(q-1)x + q(q+1)y, & c_K &= 2 + 2x + 2y, \\ n &= r + 1 + qx + (q+1)y, & c_J &= 2r + 2(q-1)x + 2qy, \\ \gamma &= 2r(r-1), & \alpha &= 2(q-r-1)^2 + 2r(r-1). \end{aligned}$$

In this case, we have $f(\mathfrak{g}, e, J) \geq 0$, with equality if and only if $r = 1$ and $q = 2$. This is the case $k = 2$ in Section A.3

3.4.3. *Type D_n.* Since the case $n = 4$ was covered in Section 3.3.1, we assume $n \geq 5$. Choose the indexing set $I = \{0, 1, \ldots, n\}$ as in [Bourbaki 2002], so that $\{i \in I : c_i = 1\} = \{0, 1, n-1, n\}$. Up to automorphisms of $\mathcal{D}(\mathfrak{so}_{2n}, 1)$, there are six cases for $J \cap \{0, 1, n-1, n\}$.

Case 1. Assume $\{0, 1, n-1, n\} \subset J$ and $R_J = D_p \times xA_{q-1} \times yA_q \times D_r$, where $p, q, r \geq 2$. Then:

$$\begin{aligned} |R_J| &= 2p(p-1)+2r(r-1)+q(q-1)x & c_K &= 2+2x+2y, \\ &\qquad +q(q+1)y, \\ n &= p+r+qx+(q+1)y, & c_J &= 2\big(p+r-2+(q-1)x+qy\big), \\ \gamma &= 2(p-r)^2, & \alpha &= 2(p-r)^2+2(p-q+r)(p-q+r-1). \end{aligned}$$

In this case, we have $f(\mathfrak{g}, e, J) \geq 0$, with equality if and only if $p = r$ and $q = 2p$ or $q = 2p - 1$. These are the cases $2 < k = q$ in Section A.5

Case 2. Assume $\{0, 1, n-1\} \subset J$, where $n \in K$, and $R_J = D_p \times xA_{q-1} \times yA_q \times A_r$, where $p, q, r \geq 2$. Then:

$$\begin{aligned} |R_J| &= 2p(p-1)+r(r+1)+q(q-1)x & c_K &= 3+2x+2y, \\ &\qquad +q(q+1)y, \\ n &= 1+p+r+qx+(q+1)y, & c_J &= 2p+2r-3+2(q-1)x+2qy, \\ \gamma &= (2p-r-1)(2p-r-2)+p+r+1, & \alpha &= (2p-q-1)^2+2(q-r-1)^2+2p-1. \end{aligned}$$

In this case, $f(\mathfrak{g}, e, J) > 0$.

Case 3. Assume $\{0, n\} \subset J$, $\{1, n-1\} \subset K$, and $R_J = A_{p-1} + xA_{q-1} + yA_q + A_{r-1}$, where $p, q, r \geq 2$. Then:

$$\begin{aligned} |R_J| &= p(p-1)+r(r-1)+q(q-1)x+q(q+1)y, & c_K &= 4+2x+2y, \\ n &= p+r+qx+(q+1)y, & c_J &= 2\big(p+r-3+(q-1)x+qy\big), \\ \gamma &= 2(p-r)^2+2(p+r), & \alpha &= 2(p-q)^2+2(q-r)^2+2q. \end{aligned}$$

In this case, $f(\mathfrak{g}, e, J) > 0$.

Case 4. Assume $\{0, 1\} \subset J$, $\{n-1, n\} \subset K$, and $R_J = D_p + xA_{q-1} + yA_q$, where $p \geq 2$. Then:

$$\begin{aligned} |R_J| &= 2p(p-1)+q(q-1)x+q(q+1)y, & c_K &= 2(1+x+y), \\ n &= 1+p+qx+(q+1)y, & c_J &= 2\big(p-1+(q-1)x+qy\big), \\ \gamma &= 2(p-1)^2, & \alpha &= 2(p-q+1)^2+2(p-2)(p-1) \\ & & &\qquad +2(q-2). \end{aligned}$$

In this case, $f(\mathfrak{g}, e, J) > 0$.

Case 5. Assume $0 \in J$, $\{1, n-1, n\} \subset K$, and $R_J = A_{p-1} + xA_{q-1} + yA_q$. Then:

$$\begin{aligned} |R_J| &= p(p-1) + q(q-1)x + q(q+1)y, & c_K &= 3 + 2x + 2y, \\ n &= 1 + p + qx + (q+1)y, & c_J &= 2p - 3 + 2(q-1)x + 2qy, \\ \gamma &= (p-1)^2 + 2, & \alpha &= 2(p-q)^2 + (q-1)^2 + 1. \end{aligned}$$

In this case, $f(\mathfrak{g}, e, J) > 0$.

Case 6. Assume $\{0, 1, n-1, n\} \subset K$ and $R_J = xA_{q-1} + yA_q$, where $q \geq 2$. Then:

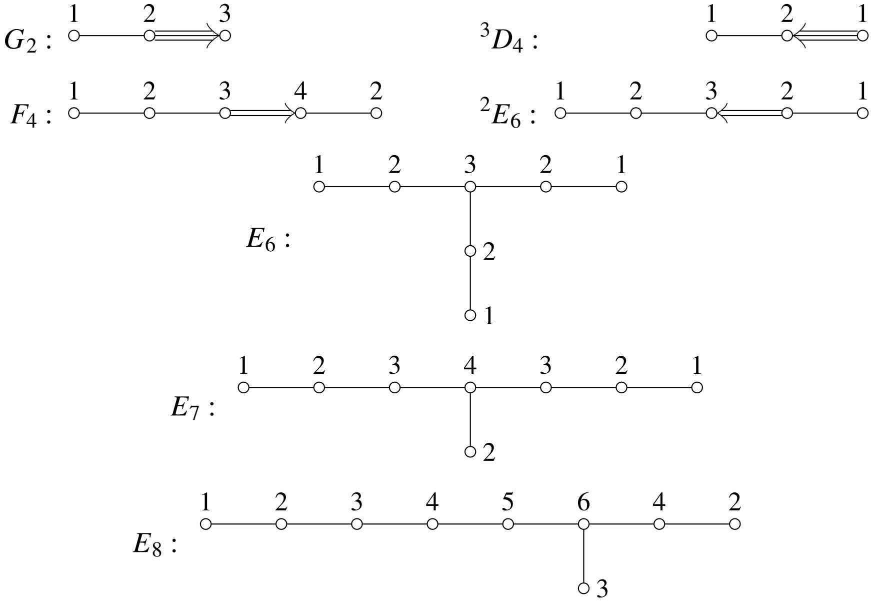
$$\begin{aligned} |R_J| &= q(q-1)x + q(q+1)y, & c_K &= 2 + 2x + 2y, \\ n &= 2 + qx + (q+1)y, & c_J &= 2(q-1)x + 2qy, \\ \gamma &= 0, & \alpha &= 2(q-1)(q-2). \end{aligned}$$

In this case, $f(\mathfrak{g}, e, J) \geq 0$, with equality if and only if $q = 2$. This is the case $k = 2$ in Section A.5.

4. Exceptional Lie algebras

On a computer one can verify Theorem 1 for the exceptional Lie algebras and ${}^3D_4$ by checking the theorem for each subset $J \subset I$. (See [Reeder 2010, (2.6)] for $\mathfrak{g} = E_8$.) The aim of this section is to make this verification somewhat more transparent.

Assume the diagram $\mathcal{D}(\mathfrak{g}, e)$, with labels c_i has one of the following types:

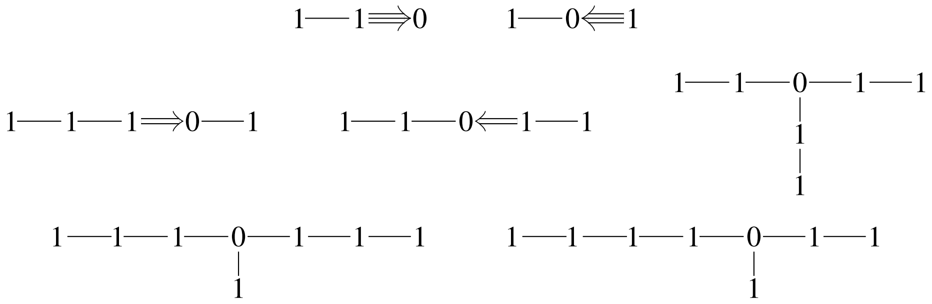


4.1. ***Small J.*** We begin with cases where $|R_J| \leq 8$.

When $R_J = A_1$, Theorem 1 follows from an observation which applies uniformly to all exceptional cases. Namely, each coefficient c_i is at most twice the average of the remaining coefficients, with equality just for the unique largest coefficient $c_{i_0} = c$; the vertex i_0 is the target of the arrow or is the branch node. Equivalently, we have

$$2c_I = (n+2)c. \tag{17}$$

On the other hand, the Kac diagrams:



are those of the ell-reg automorphisms of order $h - ec$.

Now suppose $R_J = 2A_1$. Then $J = \{i, j\}$, where i, j are not adjacent in $\mathcal{D}(\mathfrak{g}, e)$. The maximum value of $c_i + c_j$ is $2c - 2$, with c as above. From (17), we obtain

$$|R_J| c^J - nc_J \geq 2(n - 2c + 4).$$

We check that the latter is ≥ 0, with equality only in G_2, F_4, and E_8. On the other hand, the Kac diagrams:

$$\begin{tikzcd} 0 \arrow[r, dash] & 1 \arrow[r, Rrightarrow] & 0 \end{tikzcd} \qquad \begin{tikzcd} 1 \arrow[r, dash] & 0 \arrow[r, dash] & 1 \arrow[r, Rightarrow] & 0 \arrow[r, dash] & 1 \end{tikzcd} \qquad \begin{tikzcd} 1 \arrow[r, dash] & 1 \arrow[r, dash] & 1 \arrow[r, dash] & 0 \arrow[r, dash] & 1 \arrow[r, dash] & 0 \arrow[r, dash] \arrow[d, dash] & 1 \arrow[r, dash] & 1 \\ & & & & & 1 & & \end{tikzcd}$$

are those of ell-reg automorphisms of order $h - 2c + 2$.

If $R_J = A_2$, one finds similarly that

$$|R_J|c^J - nc_J = 6c_I - (n+6)(c_i + c_j) \geq 0,$$

with equality only in ${}^3D_4$. The Kac diagram

$$\begin{tikzcd} 0 \arrow[r, dash] & 0 \arrow[r, Leftarrow] & 1 \end{tikzcd}$$

is the ell-reg outer automorphism $\mathfrak{so}_8$ of order $e = 3$.

If $R_J = B_2$ or G_2, one finds that $|R_J|c^J - nc_J > 0$.

At this point, the theorem is proved for G_2 and ${}^3D_4$, and we may assume R_J has rank at least three in the remaining cases.

Assume that $R_J = 3A_1$. Then $f(\mathfrak{g}, e, J) = 6c_I - (n+6)c_J$. The Kac diagrams with maximal c_J are:

$$\begin{tikzcd} 0 \arrow[r, dash] & 1 \arrow[r, dash] & 0 \arrow[r, Rightarrow] & 1 \arrow[r, dash] & 0 \end{tikzcd} \qquad \begin{tikzcd} 0 \arrow[r, dash] & 1 \arrow[r, dash] & 0 \arrow[r, Leftarrow] & 1 \arrow[r, dash] & 0 \end{tikzcd} \qquad \begin{tikzcd} 1 \arrow[r, dash] & 0 \arrow[r, dash] & 1 \arrow[r, dash] \arrow[d, dash] & 0 \arrow[r, dash] & 1 \\ & & 0 \arrow[d, dash] & & \\ & & 1 & & \end{tikzcd}$$

$$\begin{tikzcd} 1 \arrow[r, dash] & 0 \arrow[r, dash] & 1 \arrow[r, dash] & 0 \arrow[r, dash] \arrow[d, dash] & 1 \arrow[r, dash] & 0 \arrow[r, dash] & 1 \\ & & & 1 & & & \end{tikzcd} \qquad \begin{tikzcd} 1 \arrow[r, dash] & 1 \arrow[r, dash] & 0 \arrow[r, dash] & 1 \arrow[r, dash] \arrow[d, dash] & 0 \arrow[r, dash] & 1 \arrow[r, dash] & 1 \\ & & & 0 & & & \end{tikzcd}$$

$$\begin{tikzcd} 1 \arrow[r, dash] & 0 \arrow[r, dash] & 1 \arrow[r, dash] & 0 \arrow[r, dash] & 1 \arrow[r, dash] & 0 \arrow[r, dash] \arrow[d, dash] & 1 \arrow[r, dash] & 1 \\ & & & & & 1 & & \end{tikzcd} \qquad \begin{tikzcd} 1 \arrow[r, dash] & 1 \arrow[r, dash] & 0 \arrow[r, dash] & 1 \arrow[r, dash] & 0 \arrow[r, dash] & 1 \arrow[r, dash] \arrow[d, dash] & 0 \arrow[r, dash] & 1 \\ & & & & & 1 & & \end{tikzcd}$$

$$\begin{tikzcd} 1 \arrow[r, dash] & 1 \arrow[r, dash] & 1 \arrow[r, dash] & 0 \arrow[r, dash] & 1 \arrow[r, dash] & 0 \arrow[r, dash] \arrow[d, dash] & 1 \arrow[r, dash] & 0 \\ & & & & & 1 & & \end{tikzcd} \qquad \begin{tikzcd} 1 \arrow[r, dash] & 1 \arrow[r, dash] & 1 \arrow[r, dash] & 1 \arrow[r, dash] & 0 \arrow[r, dash] & 1 \arrow[r, dash] \arrow[d, dash] & 0 \arrow[r, dash] & 1 \\ & & & & & 0 & & \end{tikzcd}$$

These all have $f(\mathfrak{g}, e, J) \geq 0$, with equality just in the E_6 case, where we find the Kac diagram of the ell-reg inner automorphism of $\mathfrak{g} = E_6$ of order six.

Assume that $R_J = A_1 + A_2$. In the same manner we find $f(\mathfrak{g}, e, J) \geq 0$, with equality only in the cases

$$\begin{tikzcd} 1 \arrow[r, dash] & 0 \arrow[r, dash] & 1 \arrow[r, Rightarrow] & 0 \arrow[r, dash] & 0 \end{tikzcd} \quad \text{and} \quad \begin{tikzcd} 1 \arrow[r, dash] & 0 \arrow[r, dash] & 0 \arrow[r, Leftarrow] & 1 \arrow[r, dash] & 0 \end{tikzcd}$$

which are the Kac diagrams for the ell-reg automorphisms of F_4 of order four and the outer ell-reg automorphism of E_6 of order six.

Assume that $R_J = 4A_1$. This only exists in type E. We find $f(\mathfrak{g}, e, J) \geq 0$, with equality only in the case

$$\begin{tikzcd}[column sep=small, row sep=small]
1 \arrow[r, dash] & 1 \arrow[r, dash] & 0 \arrow[r, dash] & 1 \arrow[r, dash] & 0 \arrow[r, dash] & 1 \arrow[r, dash] \arrow[d, dash] & 0 \arrow[r, dash] & 1 \\
 & & & & & 0 & &
\end{tikzcd}$$

This is the ell-reg automorphism of E_8 of order 15.

4.2. ***Types F_4 and $^2E_6$.*** We now complete the proof of Theorem 1 for $(\mathfrak{g}, e)$ of types F_4 and $^2E_6$, for which $\mathcal{D}(\mathfrak{g}, e)$ has the same underlying Coxeter diagram. By the previous section, we may assume $|R_J| > 8$. Arguing as in Section 3.4.1, we need only consider cases of the form:

$$* - * - * \Rightarrow 0 - 0 \qquad * - * - * \Leftarrow 1 - 1$$

$$* - * - * \Leftarrow 1 - 0 \qquad * - * - * \Leftarrow 0 - 1$$

The Kac diagrams of these types, with $|R_J| > 8$ are tabulated as follows (the first four rows are for F_4 and the last six for $^2E_6$):

J	$R_J \cdot c^J$	$4 \cdot c_J$
$1 - 0 - 0 \Rightarrow 0 - 0$	$48 \cdot 1$	$4 \cdot 11$
$0 - 1 - 0 \Rightarrow 0 - 0$	$20 \cdot 2$	$4 \cdot 10$ ←
$0 - 0 - 1 \Rightarrow 0 - 0$	$12 \cdot 3$	$4 \cdot 9$ ←
$1 - 1 - 0 \Rightarrow 0 - 0$	$18 \cdot 3$	$4 \cdot 9$
$0 - 0 - 0 \Leftarrow 1 - 1$	$12 \cdot 3$	$4 \cdot 6$
$0 - 0 - 0 \Leftarrow 1 - 0$	$14 \cdot 2$	$4 \cdot 7$ ←
$0 - 0 - 0 \Leftarrow 0 - 1$	$32 \cdot 1$	$4 \cdot 8$ ←
$1 - 0 - 0 \Leftarrow 0 - 1$	$18 \cdot 2$	$4 \cdot 7$
$0 - 1 - 0 \Leftarrow 0 - 1$	$10 \cdot 3$	$4 \cdot 6$

We have $f(\mathfrak{g}, e, J) \geq 0$ with equality in the cases marked by ←. These are the ell-reg automorphisms of orders 2 and 3 for F_4 and outer ell-reg automorphisms of E_6 of orders 4 and 2. This completes the proof of Theorem 1 in the cases F_4 and $^2E_6$.

4.3. ***Types E_6, E_7, and E_8.*** Here, $e = 1$. We consider the ends of the interval $1 < m < h$ in two steps:

Step 1. For each $1 < m < n$, we compute the minimum

$$r(m) = \min\{|R_J| : \ c^J = m\}.$$

In the tables below, we check that

$$r(m) \geq \frac{|R|}{m} - n \tag{18}$$

for each $m < n$, and we verify that equality holds in (18) for at most one J with $c^J = m$. This will prove Theorem 1 when $m < n$.

Next we will consider $|R_J|$, where $c^J \geq n$. If $|R_J| > h - n$, then

$$c^J |R_J| - nc_J > c^J (h - n) - nc_J = c^J h - n(c^J + c_J) = (c^J - n)h \geq 0,$$

so $f(\mathfrak{g}, 1, J) > 0$. Hence, we may also assume $|R_J| \leq h - n$. Since we have already proved Theorem 1 for $|R_J| \leq 8$, we may in fact assume that

$$10 \leq |R_J| \leq h - n.$$

Step 2. For each even integer $r \leq h - n$, we compute the minimum

$$m(r) = \min\{c^J : |R_J| = r\}.$$

In the tables below, we check that

$$r \geq \frac{|R|}{m(r)} - n, \tag{19}$$

and we verify that equality holds in (19) for at most one J with $|R_J| = r$. This will complete the proof of Theorem 1.

4.3.1. *Type* E_6. In Step 1 for E_6, we take $1 < m < 6$ and compute $r(m)$ in the following table. The types of R_J for which $c^J = m$ are shown; those for which $|R_J| = r(m)$ are in bold. We write the irreducible components of R_J multiplicatively. The rightmost column indicates the unique J for which $r(m) = (|R|/m) - n$, if it exists. The tabulations of Step 1 are as follows, with single bonds omitted:

m	types of R_J with $c^J = m$	$r(m)$	$(\|R\|/m) - 6$	J
2	$\boldsymbol{A_1A_5}$, D_5	32	30	none
3	$\boldsymbol{A_2^3}$, A_1A_4, D_4, A_5	18	18	$\begin{matrix} 0\ 0\ 1\ 0\ 0 \\ 0 \\ 0 \end{matrix}$
4	$\boldsymbol{A_1A_2^2}$, $\boldsymbol{A_1A_3}$, $A_1^2A_3$, A_4	14	12	none
5	$\boldsymbol{A_1^2A_2}$, $A_1A_2^2$, A_1A_3, A_3	10	$\frac{42}{5}$	none

Since $h - n = 12 - 6 < 8$, the proof of Theorem 1 for E_6 is completed by Step 1 alone.

4.3.2. *Type* E_7. In Step 1 for E_7, we take $1 < m < 7$ and compute $r(m)$ in the following table, using the same notational conventions as for E_6 above, with single bonds omitted:

m	types of R_J with $c^J = m$	$r(m)$	$(\lvert R\rvert/m)-7$	J
2	$\boldsymbol{A_7}$, A_1D_6, E_6	56	56	0 0 0 0 0 0 0 1
3	$\boldsymbol{A_2A_5}$, A_1D_5, A_6, D_6	36	35	none
4	$\boldsymbol{A_1A_3^2}$, $\boldsymbol{A_2A_4}$, $A_1^2D_4$, A_5, A_1A_5, D_5	26	$\frac{49}{2}$	none
5	$\boldsymbol{A_1A_2A_3}$, A_1A_4, A_2A_4, A_1D_4, A_5, A_1A_5	20	$\frac{91}{5}$	none
6	$\boldsymbol{A_1A_2^2}$, $A_1^2A_3$, A_2A_3, A_2^3, $A_1^3A_3$, A_4, A_1A_4, A_3^2, D_4, A_5	14	14	1 0 0 1 0 0 1 0

For Step 2, we need only consider $r = 10$. The only simply laced root systems with 10 roots are A_1^5 and $A_1^2A_2$. All occurrences of these as R_J in E_7 have $c^J \geq 8$. Since

$$\frac{|R|}{8} - 7 = \frac{35}{4} < 10,$$

Theorem 1 is now proved for E_7.

4.3.3. *Type* E_8. In Step 1 for E_8, we take $1 < m < 8$ and compute $r(m)$ in the following table, using the same notational conventions as for E_6 and E_7 above, with single bonds omitted:

m	types of R_J with $c^J = m$	$r(m)$	$(240/m) - 8$	J
2	$\boldsymbol{D_8}$, A_1E_7	112	112	0 0 0 0 0 0 0 1 0
3	$\boldsymbol{A_8}$, A_2E_6, D_7, E_7	72	72	0 0 0 0 0 0 0 0 1
4	$\boldsymbol{A_3D_5}$, A_7, A_1A_7, A_1D_6, A_1E_6	52	52	0 0 0 1 0 0 0 0 0
5	$\boldsymbol{A_4^2}$, A_1A_6, A_2D_5, A_7, D_6, A_1E_6	40	40	0 0 0 0 1 0 0 0 0
6	$\boldsymbol{A_3A_4}$, $A_1^2A_5$, A_3D_4, A_2A_5, $A_1A_2A_5$, A_1D_5, A_6, $A_1^2D_5$, A_7, E_6	32	32	1 0 0 0 1 0 0 0 0
7	$\boldsymbol{A_1A_2A_4}$, A_2D_4, A_3A_4, A_1A_5 A_1D_5, A_6, A_1A_6, A_2D_5	28	$\frac{184}{7}$	none

For Step 2, we take $r = 10, 12, \ldots, 22$ and compute $m(r)$ in the following table. The types of R_J for which $|R_J| = r$ are shown; those for which $c^J = m(r)$ are in bold; and that J for which $|R_J| = (240/c^J) - n$, if it exists, is shown in the right column (single bonds have been omitted).

r	types of R_J with $\lvert R_J\rvert = r$	$m(r)$	$[240/m(r)] - 8$	J
10	$\boldsymbol{A_1^5}$, $\boldsymbol{A_1^2A_2}$	14	$\frac{64}{7}$	none
12	$\boldsymbol{A_1^3A_2}$, A_2^2, A_3	12	12	1 0 1 0 0 1 0 1 0
14	$\boldsymbol{A_1^4A_2}$, $\boldsymbol{A_1A_2^2}$, $\boldsymbol{A_1A_3}$	12	12	none
16	$\boldsymbol{A_1^2A_2^2}$, $A_1^2A_3$	10	16	1 0 1 0 0 1 0 0 0
18	$\boldsymbol{A_2A_3}$, $\boldsymbol{A_1^3A_3}$, A_2^3	10	16	none
20	$\boldsymbol{A_1A_2A_3}$, $\boldsymbol{A_1A_2^3}$, A_4	9	$\frac{56}{3}$	none
22	$\boldsymbol{A_1^2A_2A_3}$, A_1A_4	8	22	0 1 0 0 0 1 0 0 0

In each case, we have

$$r \geq \left[\frac{240}{m(r)}\right] - 8,$$

and equality is achieved by at most one J, as indicated in the rightmost column.

The proof of Theorem 1 for E_8 is now complete.

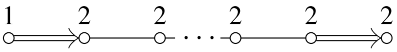
Appendix: The classification of ell-reg automorphisms

For reference in the proofs above, we recall the classification of ell-reg automorphisms given in [Reeder et al. 2012]. There is only one inner ell-reg automorphism of $\mathfrak{sl}_n$, namely the principal one, so we ignore this case. Recall that m denotes the order of an ell-reg automorphism of $\mathfrak{g}$.

A.1. ***Type*** $\boldsymbol{{}^2A_{2n}}$**.** The ell-reg outer automorphisms of $\mathfrak{sl}_{2n+1}$ correspond to odd quotients d of $2n$ and $2n+1$. The graphs $\mathcal{D}(\mathfrak{sl}_{2n+1}, 2)$ are as shown:

$n \geq 1 :$

$n > 1 :$



The ell-reg outer automorphisms of $\mathfrak{sl}_{2n+1}$ correspond to odd quotients d of $2n+1$ and $2n$. We write these quotients as

$$d = \frac{2n+1}{2k+1} \quad \text{and} \quad d = \frac{n}{k},$$

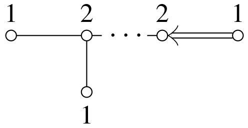
respectively. The cases overlap only when $d = 1$. The corresponding ell-reg automorphism has order $m = 2d$ in both cases:

$d = m/2$	s
3	$1 \Rrightarrow 1$
2	$1 \Rrightarrow 0$

$d = m/2$	s
$2n+1$	$1 \Longrightarrow 1 - 1 - \cdots - 1 - 1 \Longrightarrow 1$
1	$1 \Longrightarrow 0 - 0 - \cdots - 0 - 0 \Longrightarrow 0$
$\frac{2n+1}{2k+1}$	$1 \Longrightarrow \overbrace{0 \cdots 0}^{A_{2k}} - 1 - \overbrace{0 \cdots 0}^{A_{2k}} - 1 \cdots 1 - \overbrace{0 \cdots 0 \Longrightarrow 0}^{B_k}$
$\frac{n}{k}$	$1 \Longrightarrow \overbrace{0 \cdots 0}^{A_{2k-1}} - 1 - \overbrace{0 \cdots 0}^{A_{2k-1}} - 1 \cdots 1 - \overbrace{0 \cdots 0 \Longrightarrow 0}^{B_k}$

In the two last rows we have $0 < k < n$ such that d is odd and the number of type-A factors is $(d-1)/2$. The next-to-last row corrects an error in [Reeder et al. 2012].

A.2. ***Type*** $^2A_{2n-1}$**.** The graph $\mathcal{D}(\mathfrak{sl}_{2n}, 2)$, with $n \geq 3$ and labels $c_0, c_1, \ldots, c_n$, is shown here, with $c_0 = c_n = 1$:



The ell-reg outer automorphisms of $\mathfrak{sl}_{2n}$ correspond to odd quotients d of $2n-1$ and $2n$. We write these quotients as

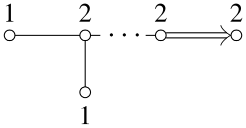
$$d = \frac{2n-1}{2k-1} \quad \text{and} \quad d = \frac{n}{k},$$

respectively. The cases overlap only when $d = 1$. The corresponding ell-reg automorphism has order $m = 2d$ in both cases.

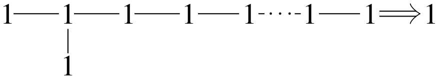
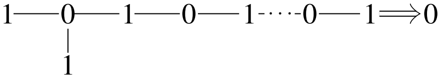
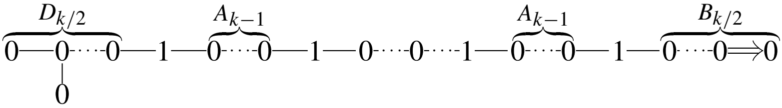
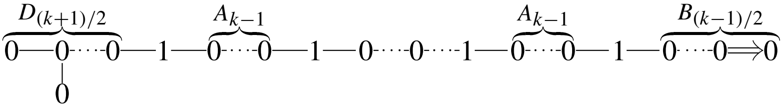
$d = m/2$	s
$2n-1$	$1 - \underset{\substack{\vert \\ 1}}{1} - 1 - 1 \cdots 1 - 1 \Longleftarrow 1$
1	$0 - \underset{\substack{\vert \\ 0}}{0} - 0 - 0 \cdots 0 - 0 \Longleftarrow 1$
n, n odd	$1 - \underset{\substack{\vert \\ 1}}{0} - 1 - 0 - 1 \cdots 1 - 0 \Longleftarrow 1$
$\frac{2n-1}{2k-1}$	$\overbrace{0 - \underset{\substack{\vert \\ 0}}{0} \cdots 0}^{D_k} - 1 - \overbrace{0 \cdots 0}^{A_{2k-2}} - 1 \cdots 1 - \overbrace{0 \cdots 0}^{A_{2k-2}} \Longleftarrow 1$
$\frac{n}{k}$	$\overbrace{0 - \underset{\substack{\vert \\ 0}}{0} \cdots 0}^{D_k} - 1 - \overbrace{0 \cdots 0}^{A_{2k-1}} - 1 \cdots 1 - \overbrace{0 \cdots 0}^{A_{2k-1}} \Longleftarrow 1$

In the last two rows we have $1 < k < n$ such that d is odd and there are $(d-1)/2$ components of type A.

A.3. ***Type B_n.*** The graph $\mathcal{D}(\mathfrak{so}_{2n+1}, 1)$ with labels $c_0, c_1, \dots, c_n$ is shown here, with $c_0 = c_n = 1$:

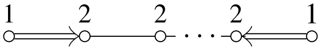


The ell-reg automorphisms of $\mathfrak{so}_{2n+1}$ are of the form π^k, where π is a principal automorphism and k is a divisor of n. The order m of π^k is $m = 2n/k$, and the Kac coordinates of π^k are given in the table below. We replace each node i by the Kac coordinate $s_i \in \{0, 1\}$, and also omit the single bonds in the graph. Recall that $J = \{i \in I : s_i = 0\}$.

$k \mid n$	m	$s = (s_0, s_1, \dots, s_n)$
1	$2n$	
2	n	
$k > 2$, k even	$\frac{2n}{k}$	
$k > 1$, k odd	$\frac{2n}{k}$	

The second line, where $m = n$, only occurs if n is even. In the last two lines there are $(n/k) - 1$ factors of type A_{k-1}.

A.4. ***Type C_n.*** The graph $\mathcal{D}(\mathfrak{sp}_{2n}, 1)$ with labels $c_0, c_1, \dots, c_n$ is shown here, with $c_0 = c_n = 1$:



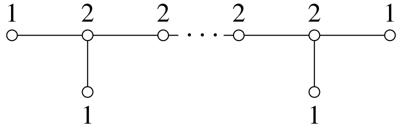
The Coxeter number is $2n$. As with $\mathfrak{so}_{2n+1}$, the ell-reg automorphisms of $\mathfrak{sp}_{2n}$ are powers π^k of a principal automorphism π, where k is a divisor of n. The order m

of π^k is $m = 2n/k$, and the Kac coordinates of π^k are these:

$k \mid n$	m	$s = (s_0, s_1, \dots, s_n)$
1	$2n$	$1 \Rightarrow 1 - 1 - 1 - 1 \cdots 1 - 1 \Leftarrow 1$
$k > 1$	$\frac{2n}{k}$	$0 \Rightarrow \overbrace{0 \cdots 0}^{A_{k-1}} - 1 - \overbrace{0 \cdots 0}^{A_{k-1}} - 1 \cdots 1 - \overbrace{0 \cdots 0}^{A_{k-1}} \Leftarrow 1$

In the last line, for $k > 1$, there are n/k factors of type A_{k-1}.

A.5. ***Type D_n.*** The graph $\mathcal{D}(\mathfrak{so}_{2n}, 1)$ with labels $c_0, c_1, \dots, c_n$ is shown here, with $c_0 = c_1 = c_{n-1} = c_n = 1$:



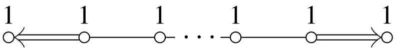
The ell-reg conjugacy classes in $\mathrm{Aut}(\mathfrak{so}_{2n}, 1)$ correspond to even divisors k of n, where $m = 2n/k$, and odd divisors k of $n - 1$, where $m = (2n - 2)/k$, as shown in the table below:

k	m	$s = (s_i)$
1	$2n-2$	$1 - \underset{\overset{\vert}{1}}{1} - 1 \cdots 1 - \underset{\overset{\vert}{1}}{1} - 1$
2	n, n even	$1 - \underset{\overset{\vert}{1}}{0} - 1 - 0 - 1 \cdots 1 - 0 - 1 - \underset{\overset{\vert}{1}}{0} - 1$
n, n even	2	$\overbrace{0 - \underset{\overset{\vert}{0}}{0} \cdots 0}^{D_{n/2}} - 1 - \overbrace{0 \cdots \underset{\overset{\vert}{0}}{0} - 0}^{D_{n/2}}$
k even, $k \mid n$, $2 < k < n$	$\frac{2n}{k}$	$\overbrace{0 - \underset{\overset{\vert}{0}}{0} \cdots 0}^{D_{k/2}} - 1 - \overbrace{0 \cdots 0}^{A_{k-1}} - 1 - 0 \cdots 0 - 1 - \overbrace{0 \cdots 0}^{A_{k-1}} - 1 - \overbrace{0 \cdots \underset{\overset{\vert}{0}}{0} - 0}^{D_{k/2}}$
k odd, $k \mid n-1$, $1 < k < n-1$	$\frac{2n-2}{k}$	$\overbrace{0 - \underset{\overset{\vert}{0}}{0} \cdots 0}^{D_{(k+1)/2}} - 1 - \overbrace{0 \cdots 0}^{A_{k-1}} - 1 - 0 \cdots 0 - 1 - \overbrace{0 \cdots 0}^{A_{k-1}} - 1 - \overbrace{0 \cdots \underset{\overset{\vert}{0}}{0} - 0}^{D_{(k+1)/2}}$

In the last two rows, the number of type-A factors is one less than n/k and $(n - 1)/k$, respectively.

A.6. ***Type ${}^2D_{n+1}$.*** The graph $\mathcal{D}(\mathfrak{so}_{2n+2}, 2)$, with $n \geq 2$ and $c_0 = c_1 = \cdots = c_n = 1$:

${}^2D_{n+1}$:



The ell-reg classes in $\mathrm{Aut}(\mathfrak{so}_{2n+2}, 2)$ correspond to even divisors k of n with order $m = 2n/k$ and odd divisors k of $n+1$ with order $m = 2(n+1)/k$.

k	m	$s = (s_0, s_1, \dots, s_n)$
1	$2n+2$	$1 \Longleftarrow 1 - 1 \cdots 1 - 1 \Longrightarrow 1$
2	n, n even	$0 \Longleftarrow 1 - 0 - 1 - 0 \cdots 0 - 1 - 0 - 1 \Longrightarrow 0$
k even, $k \mid n$, $2 < k$	$\frac{2n}{k}$	$\overbrace{0 \Leftarrow 0 \cdots 0}^{B_{k/2}} - 1 - \overbrace{0 \cdots 0}^{A_{k-1}} - 1 \cdots 1 - \overbrace{0 \cdots 0}^{A_{k-1}} - 1 - \overbrace{0 \cdots 0 \Rightarrow 1}^{B_{k/2}}$
k odd, $k \mid n+1$, $1 < k$	$\frac{2n+2}{k}$	$\overbrace{0 \Leftarrow 0 \cdots 0}^{B_{(k-1)/2}} - 1 - \overbrace{0 \cdots 0}^{A_{k-1}} - 1 \cdots 1 - \overbrace{0 \cdots 0}^{A_{k-1}} - 1 - \overbrace{0 \cdots 0 \Rightarrow 0}^{B_{(k-1)/2}}$

In the last two rows, the number of type A factors is one less than n/k and $(n+1)/k$, respectively.

A.7. *Exceptional Lie algebras.* When only single bonds are present, they have been omitted.

E_6

m	s
12	1 1 1 1 1 1 1
9	1 1 0 1 1 1 1
6	1 0 1 0 1 0 1
3	0 0 1 0 0 0 0

${}^2E_6$

m	s
18	$1 - 1 - 1 \Leftarrow 1 - 1$
12	$1 - 1 - 0 \Leftarrow 1 - 1$
6	$1 - 0 - 0 \Leftarrow 1 - 0$
4	$0 - 0 - 0 \Leftarrow 1 - 0$
2	$0 - 0 - 0 \Leftarrow 0 - 1$

E_7

m	s
18	1 1 1 1 1 1 1 1
14	1 1 1 0 1 1 1 1
6	1 0 0 1 0 0 1 0
2	0 0 0 0 0 0 0 1

E_8

m	s
30	1 1 1 1 1 1 1 1 1
24	1 1 1 1 1 0 1 1 1
20	1 1 1 0 1 0 1 1 1
15	1 1 0 1 0 1 0 1 0
12	1 0 1 0 0 1 0 1 0
10	1 0 1 0 0 1 0 0 0
8	0 1 0 0 0 1 0 0 0
6	1 0 0 0 1 0 0 0 0
5	0 0 0 0 1 0 0 0 0
4	0 0 0 1 0 0 0 0 0
3	0 0 0 0 0 0 0 0 1
2	0 0 0 0 0 0 0 1 0

G_2

m	s
6	$1 - 1 \Rrightarrow 1$
3	$1 - 1 \Rrightarrow 0$
2	$0 - 1 \Rrightarrow 0$

F_4

m	s
12	$1 - 1 - 1 \Rightarrow 1 - 1$
8	$1 - 1 - 1 \Rightarrow 0 - 1$
6	$1 - 0 - 1 \Rightarrow 0 - 0$
4	$1 - 0 - 1 \Rightarrow 0 - 0$
3	$0 - 0 - 1 \Rightarrow 0 - 0$
2	$0 - 1 - 0 \Rightarrow 0 - 0$

${}^3D_4$

m	s
12	$1 - 1 \Lleftarrow 1$
6	$1 - 0 \Lleftarrow 1$
3	$0 - 0 \Lleftarrow 1$

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MARK REEDER
DEPARTMENT OF MATHEMATICS
BOSTON COLLEGE
CHESTNUT HILL, MA
UNITED STATES

reederma@bc.edu

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ON THE POTENTIAL FUNCTION OF THE COLORED JONES POLYNOMIAL WITH ARBITRARY COLORS

SHUN SAWABE

We consider the potential function of the colored Jones polynomial for a link with arbitrary colors and obtain the cone-manifold structure for the link complement. In addition, we establish a relationship between a saddle point equation and hyperbolicity of the link complement. This provides evidence for the Chen–Yang conjecture on the link complement.

1. Introduction

The volume conjecture is one of the most important problems in low-dimensional topology. Kashaev [1997] discovered that a certain limit of the Kashaev invariant of specific hyperbolic knots such as the figure-eight knot is equal to the hyperbolic volume of their complements. Murakami and Murakami [2001] proved that the Kashaev invariant is a specialization of the colored Jones polynomial and conjectured that a similar limit of the colored Jones polynomial for an arbitrary knot is equal to the simplicial volume of its complement. In addition, Chen and Yang [2018] considered the volume conjectures for 3-manifold invariants such as the Reshetikhin–Turaev invariant and the Turaev–Viro invariant, and provided numerical evidence for them for specific 3-manifolds. Detcherry, Kalfagianni, and Yang [Detcherry et al. 2018] showed the relationship between the colored Jones polynomial for a link and the Turaev–Viro invariant of its complement. By using this relation, they mathematically verified the Chen–Yang conjecture for complements of the figure-eight knot and Borromean rings. In addition, Belletti, Detcherry, Kalfagianni, and Yang verified the Chen–Yang conjecture for fundamental shadow links in [Belletti et al. 2022].

Meanwhile, theoretical evidence of the original volume conjecture has been considered. Kashaev and Tirkkonen [2000] proved the volume conjecture for torus knots. On the other hand, Yokota [2000] found a correspondence between quantum factorials in the Kashaev invariant and an ideal triangulation of a hyperbolic knot complement. He showed that a saddle point equation for the potential function (see Section 3 for the definition) of the invariant is equivalent to a hyperbolicity equation.

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Also, the potential function of the colored Jones polynomial $J_N(K; e^{2\pi\sqrt{-1}/N})$ for a hyperbolic knot K is considered in [Cho 2016a; 2016b; Cho and Murakami 2013].

In this study, we consider the potential function of the colored Jones polynomial for a link L with arbitrary colors. We establish a relationship between a saddle point equation and a hyperbolicity equation of the link complement. More precisely, for a fixed diagram D of the link L, we introduce a potential function $\Phi_D(a_1, \dots, a_n, w_1, \dots, w_\nu)$ of the colored Jones polynomial $J_{\boldsymbol{a}(N)}(L; e^{2\pi\sqrt{-1}/N})$ with new parameters corresponding to the colors $\boldsymbol{a}(N)$ of link components. When we fix the new parameters $\boldsymbol{a} = (a_1, \dots, a_n)$, the saddle point $(\sigma_1(\boldsymbol{a}), \dots, \sigma_\nu(\boldsymbol{a}))$ of $\Phi_D(\boldsymbol{a}, -)$ gives a noncomplete hyperbolic structure to the link complement. In fact, the manifold $M_{a_1,\dots,a_n}$ with the hyperbolic structure is a cone-manifold. Specifically, we prove the following statement:

Theorem 4.1. *The hyperbolic volume of the cone-manifold $M_{a_1,\dots,a_n}$ is equal to the imaginary part of*

$$\tilde{\Phi}_D = \Phi_D - \sum_{j=1}^{\nu} w_j \frac{\partial \Phi_D}{\partial w_j} \log w_j$$

evaluated at $w_j = \sigma_j(\boldsymbol{a})$ for $j = 1, \dots, \nu$.

Here, the function $\Phi_D(\boldsymbol{a}, \sigma_1(\boldsymbol{a}), \dots, \sigma_\nu(\boldsymbol{a}))$ determines the Neumann–Zagier potential function [Neumann and Zagier 1985]. Furthermore, we prove that the derivatives of the potential function with respect to the new parameters correspond to the completeness of the hyperbolic structure of the link complement. Note that similar arguments for the Kashaev invariant of the 5_2 knot are indicated in [Yokota 2003]. As an application, we prove the following theorem:

Theorem 5.3. *Let D be a diagram of a hyperbolic link with n components, and let $\mathbf{1}$ be $(1, \dots, 1) \in \mathbb{Z}^n$. The point $(\mathbf{1}, \sigma_1(\mathbf{1}), \dots, \sigma_\nu(\mathbf{1}))$ is a saddle point of the function $\Phi_D(a_1, \dots, a_n, w_1, \dots, w_\nu)$ and gives a complete hyperbolic structure to the link complement.*

The paper is organized as follows: In Section 2, we recall the facts on the colored Jones polynomial and the Turaev–Viro invariant. In Section 3, we give the potential function of the colored Jones polynomial. In Section 4, we consider the case where the new parameters are fixed and prove Theorem 4.1. In Section 5, we regard the new parameters as variables and prove Theorem 5.3. In Section 6, we briefly mention the Witten–Reshetikhin–Turaev invariant.

2. Preliminaries

In this section, we review some facts on the invariants for a link and a 3-manifold.

The colored Jones polynomial and the Turaev–Viro invariant. Let L be an oriented n-component link, let $\boldsymbol{i}$ be a multiinteger, and let t be an indeterminate. The colored Jones polynomial $J_{\boldsymbol{i}}(L; t)$ is defined skein-theoretically by using the Kauffman bracket, which is a map $\langle \cdot \rangle$ from the set of all unoriented diagrams of links to the ring of Laurent polynomials $\mathbb{Z}[A, A^{-1}]$ in an indeterminate A given by the following axioms:

(1) For the trivial diagram $\bigcirc$,

$$\langle \bigcirc \rangle = 1.$$

(2) For an unoriented diagram D with the trivial component added,

$$\langle D \sqcup \bigcirc \rangle = (-A^2 - A^{-2})\langle D \rangle.$$

(3) For each crossing,

$$\langle \times \rangle = A\langle)\,(\rangle + A^{-1}\langle \asymp \rangle$$

Let D_0 be an unoriented diagram of the link L. The colored Jones polynomial $J_{\boldsymbol{i}}(L; t)$ for the link L is a certain normalization of the Kauffman bracket of the parallelized diagram of D_0 in which the Jones–Wenzl idempotent is inserted, where $t = A^{-4}$ [Detcherry et al. 2018].

Remark 2.1. In this paper, we normalize the colored Jones polynomial so that the one for the trivial knot is equal to 1.

From the perspective of skein theory, we can define the 3-manifold invariants such as the Reshetikhin–Turaev invariant or the Turaev–Viro invariant. Detcherry, Kalfagianni, and Yang [Detcherry et al. 2018] presented the relationship between the Turaev–Viro invariant for the link complement and the colored Jones polynomial.

Theorem 2.2 [Detcherry et al. 2018]. *Let $L \subset S^3$ be a link with n components and $\bar{t} = q^2$. Namely, $\bar{t} = q^2 = A^4$.*

(1) *For an integer $r \geq 3$ and a primitive $4r$-th root of unity A,*

$$TV_r(S^3 \setminus L, q) = \eta_r^2 \sum_{1 \leq \boldsymbol{i} \leq r-1} |J_{\boldsymbol{i}}'(L; \bar{t})|^2.$$

(2) *For an odd integer $r = 2m+1 \geq 3$ and a primitive $2r$-th root of unity A,*

$$TV_r(S^3 \setminus L, q) = 2^{n-1}(\eta_r')^2 \sum_{1 \leq \boldsymbol{i} \leq m} |J_{\boldsymbol{i}}'(L; \bar{t})|^2.$$

Here, η_r and η_r' are

$$\eta_r = \frac{A^2 - A^{-2}}{\sqrt{-2r}} \quad \textit{and} \quad \eta_r' = \frac{A^2 - A^{-2}}{\sqrt{-r}}.$$

In addition, for a multiinteger $\boldsymbol{i} = (i_1, \dots, i_n)$, we let $1 \leq \boldsymbol{i} \leq m$ denote that $1 \leq i_k \leq m$ for all integers $k = 1, \dots, n$.

Remark 2.3. In [Detcherry et al. 2018], the normalization of the colored Jones polynomial and conventions on parameters are slightly different from the ones in this paper. Therefore, we use the notation $J'_i(L;\bar{t})$ in Theorem 2.2.

These invariants are conjectured to relate to the geometry of the 3-manifold. Murakami and Murakami [2001] conjectured that a certain limit of the colored Jones polynomial for a knot is equal to the volume of the complement of the knot.

Conjecture 2.4 (volume conjecture [Murakami and Murakami 2001]). *For any knot K,*

$$2\pi \lim_{N\to\infty} \frac{\log|J_N(K; t=e^{2\pi\sqrt{-1}/N})|}{N} = v_3\|K\|,$$

where v_3 is the volume of the ideal regular tetrahedron in the three-dimensional hyperbolic space and $\|\cdot\|$ is the simplicial volume for the complement of K.

This conjecture was generalized to the one for 3-manifold invariants.

Conjecture 2.5 (Chen–Yang conjecture [2018]). *For any 3-manifold M with a complete hyperbolic structure of the finite volume,*

$$2\pi \lim_{r\to\infty} \frac{\log TV_r(M, q=e^{2\pi\sqrt{-1}/r})}{r} = \mathrm{Vol}(M),$$

where r runs over all odd integers, $TV(M)$ is a Turaev–Viro invariant of M and $\mathrm{Vol}(M)$ is a hyperbolic volume of M.

Moreover, Detcherry, Kalfagianni, and Yang proved the following theorem by using Theorem 2.2:

Theorem 2.6 [Detcherry et al. 2018]. *Let L be either the figure-eight knot or the Borromean rings, and let M be the complement of L in S^3. Then,*

$$2\pi \lim_{r\to\infty} \frac{\log TV_r(M, q=e^{2\pi\sqrt{-1}/r})}{r} = 4\pi \lim_{m\to\infty} \frac{\log\bigl|J'_m(L;\bar{t}=e^{4\pi\sqrt{-1}/(2m+1)})\bigr|}{2m+1} = \mathrm{Vol}(M),$$

where $r=2m+1$ runs over all odd integers.

Remark 2.7. If t is a root of unity, $\bar{t}$ is the complex conjugate of t. Therefore,

$$\lim_{m\to\infty} \frac{\log\bigl|J'_m(L;\bar{t}=e^{4\pi\sqrt{-1}/(2m+1)})\bigr|}{2m+1} = \lim_{m\to\infty} \frac{\log\bigl|J_m(L;t=e^{4\pi\sqrt{-1}/(2m+1)})\bigr|}{2m+1}.$$

Meanwhile, the evidence of the volume conjecture was established in [Yokota 2000]. What is important is that a saddle point equation of a potential function of the colored Jones polynomial for a knot coincides with a gluing condition of the ideal triangulation of the knot complement. This and Theorem 2.2 indicate that if we can establish a similar relationship between a hyperbolicity equation and a potential function of the colored Jones polynomial with arbitrary colors, the relationship is evidence of the Chen–Yang conjecture for a link complement.

The R-matrix of the colored Jones polynomial. In this subsection, we give the R-matrix of the colored Jones polynomial by following [Kirby and Melvin 1991]. For an integer $r > 1$, let $\mathcal{A}_r$ be the algebra generated by X, Y, K, and $\overline{K}$ with the following relations:

$$\overline{K} = K^{-1}, \qquad KX = sXK, \qquad KY = s^{-1}YK,$$
$$XY - YX = \frac{K^2 - \overline{K}^2}{s - s^{-1}}, \qquad X^r = Y^r = 0, \qquad K^{4r} = 1,$$

where $s = e^{\pi\sqrt{-1}/r}$. Namely, $\mathcal{A}_r$ is $\mathcal{U}_q(\mathrm{sl}_2)$ with the last 3 relations. The universal R-matrix $\mathcal{R} \in \mathcal{A}_r \otimes \mathcal{A}_r$ is given by

$$\mathcal{R} = \frac{1}{4r} \sum_{\substack{0 \le k < r \\ 0 \le a, b < 4r}} \frac{(s - s^{-1})^k}{[k]_s!} s^{-(ab+(b-a)k+k)/2} X^k K^a \otimes Y^k K^b.$$

Here, we put

$$[k]_s = \frac{s^k - s^{-k}}{s - s^{-1}}, \quad [k]_s! = [k]_s \cdots [1]_s, \quad [0]_s! = 1.$$

Let N be a positive integer and m be the half-integer satisfying $N = 2m + 1$. We define the action of $\mathcal{A}_r$ on an N-dimensional complex vector space V with a basis $\{e_{-m}, e_{-m+1}, \dots, e_m\}$ by

$$Xe_i = [m - i + 1]_s e_{i-1}, \quad Ye_i = [m + i + 1]_s e_{i+1}, \quad Ke_i = s^{-i} e_i.$$

Here, e_i in this paper corresponds to e_{-i} in [Kirby and Melvin 1991]. Let V' be an $(N' = 2m' + 1)$-dimensional complex vector space with basis $\{e'_{-m'}, \dots, e'_{m'}\}$. Then, the quantum R-matrix $R_{VV'} : V \otimes V' \to V' \otimes V$ is given by

$$\begin{aligned} &R_{VV'}(e_i \otimes e'_j) \\ &\quad = \sum_{k=0}^{\min\{m+i, m'-j\}} \frac{\{m - i + k\}_s! \, \{m' + j + k\}_s!}{\{k\}_s! \, \{m - i\}_s! \, \{m' + j\}_s!} s^{2ij+k(i-j)-k(k+1)/2} e'_{j+k} \otimes e_{i-k}, \end{aligned}$$

where $\{k\}_s = s^k - s^{-k}$, $\{k\}_s! = \{k\}_s \cdots \{1\}_s$, and $\{0\}_s! = 1$.

Also, its inverse is

$$\begin{aligned} &R^{-1}_{VV'}(e'_i \otimes e_j) \\ &= \sum_{k=0}^{\min\{m-i, m'+j\}} (-1)^k \frac{\{m - j + k\}_s! \, \{m' + i + k\}_s!}{\{k\}_s! \, \{m - j\}_s! \, \{m' + i\}_s!} s^{-2ij+k(i-j)/2+k(k+1)/2} e_{j-k} \otimes e'_{i+k}. \end{aligned}$$

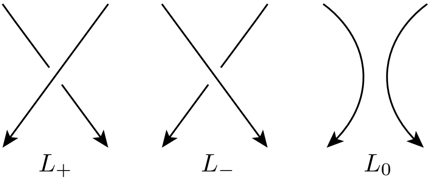

Figure 2.1. The links that are identical except for these regions.

These matrices and the isomorphism $\mu : V \to V$, where

$$\mu(e_i) = s^{-2i} e_i, \quad i = -m, \dots, m,$$

defines a link invariant $\tilde{J}$. If $V = V'$ and $\dim V = 2$, then

$$R_{VV} = \begin{pmatrix} s^{1/2} & 0 & 0 & 0 \\ 0 & 0 & s^{-1/2} & 0 \\ 0 & s^{-1/2} & s^{1/2} - s^{-3/2} & 0 \\ 0 & 0 & 0 & s^{1/2} \end{pmatrix}$$

and satisfies

$$s^{1/2} R_{VV} - s^{-1/2} R_{VV}^{-1} = (s - s^{-1}) I_4,$$

where I_4 is the 4×4 identity matrix. Considering the writhes, this implies

$$s^2 \tilde{J}(L_+) - s^{-2} \tilde{J}(L_-) = (s - s^{-1}) \tilde{J}(L_0), \tag{2.1}$$

where L_+, L_-, and L_0 are the links in Figure 2.1.

Under the substitution $s = -t^{-1/2}$, the relation (2.1) coincides with the skein relation of the Jones polynomial. Therefore, under this substitution the R-matrix of the colored Jones polynomial $J_{\boldsymbol{i}}(L; t)$ for L with colors $\boldsymbol{i} = (i_1, \dots, i_n) \in \mathbb{Z}^n_{>0}$, where i_j, with $j = 1, \dots, n$, is the dimension of the assigned representation, is

$$R_{VV'}(e_i \otimes e'_j) = \sum_{k=0}^{\min\{m+i, m'-j\}} (-1)^{k+k(m+m')+2ij} \frac{\{m-i+k\}!\,\{m'+j+k\}!}{\{k\}!\,\{m-i\}!\,\{m'+j\}!} \times t^{-ij-k(i-j)/2+k(k+1)/4} e'_{j+k} \otimes e_{i-k}, \tag{2.2}$$

and its inverse is

$$R^{-1}_{VV'}(e'_i \otimes e_j) = \sum_{k=0}^{\min\{m-i, m'+j\}} (-1)^{-k(m+m')-2ij} \frac{\{m-j+k\}!\,\{m'+i+k\}!}{\{k\}!\,\{m-j\}!\,\{m'+i\}!} \times t^{ij-k(i-j)/2-k(k+1)/4} e_{j-k} \otimes e'_{i+k},$$

where

$$\{k\} = t^{k/2} - t^{-k/2}, \quad \{k\}! = \{k\}\{k-1\} \cdots \{1\}, \quad \{0\}! = 1.$$

3. Potential function

Let $L = L_1 \cup \cdots \cup L_n$ be an oriented n-component link. We deform L so that L is a closure of a braid. Let D be its oriented diagram, and $\xi_N = e^{2\pi\sqrt{-1}/N}$ be the primitive N-th root of unity. For each link component L_i, with $i = 1, \dots, n$, we assign its color $a_i(N) \in \mathbb{Z}_{>0}$. We put $\boldsymbol{a}(N) = (a_1(N), \dots, a_n(N))$. In this section, we determine a potential function of the colored Jones polynomial $J_{\boldsymbol{a}(N)}(L; \xi_N^p)$ for L, where p is a nonzero integer. See [Cho 2016b] for details.

Definition 3.1. Suppose that the asymptotic behavior of a certain quantity Q_N for a sufficiently large N is

$$Q_N \sim \int \cdots \int_\Omega P_N e^{N/(2\pi\sqrt{-1})\Phi(z_1,\dots,z_\nu)}\, dz_1 \cdots dz_\nu,$$

where P_N grows at most polynomially and Ω is a region in $\mathbb{C}^\nu$. We call this function $\Phi(z_1, \dots, z_\nu)$ a potential function of Q_N.

We can easily verify that

$$\{k\}! = (-1)^k t^{-k(k+1)/4} (t)_k, \tag{3.1}$$

where $(t)_k = (1-t)(1-t^2)\cdots(1-t^k)$. Thus, we approximate $(\xi_N^p)_k$ by continuous functions.

Proposition 3.2. *For a sufficiently large integer N,*

$$\log(\xi_N^p)_k = \frac{N}{2p\pi\sqrt{-1}}\Bigl(-\operatorname{Li}_2(\xi_N^{pk}) + \frac{\pi^2}{6} + o(1)\Bigr),$$

where Li_2 *is a dilogarithm function*

$$\operatorname{Li}_2(z) = -\int_0^z \frac{\log(1-x)}{x}\, dx.$$

Remark 3.3. The dilogarithm function satisfies

$$\operatorname{Li}_2(z) = \sum_{k=1}^{\infty} \frac{z^2}{k^2}, \quad \text{for } |z| < 1, \qquad \text{and} \qquad \operatorname{Li}_2(1) = \sum_{k=1}^{\infty} \frac{1}{k^2} = \frac{\pi^2}{6}.$$

Proof. By the direct calculation, we have

$$\begin{aligned}\log(\xi_N^p)_k = \sum_{j=1}^{k} \log(1-e^{2p\pi j\sqrt{-1}/N}) &= N\Bigl(\int_0^{k/N} \log\bigl(1-e^{2p\pi\sqrt{-1}\theta}\bigr)\, d\theta + o(1)\Bigr)\\ &= \frac{N}{2p\pi\sqrt{-1}}\Bigl(\int_1^{\xi_N^{pk}} \frac{\log(1-x)}{x}\, dx + o(1)\Bigr)\\ &= \frac{N}{2p\pi\sqrt{-1}}\Bigl(-\operatorname{Li}_2(\xi_N^{pk}) + \frac{\pi^2}{6} + o(1)\Bigr). \qquad \square\end{aligned}$$

First, we consider the case where the strings at a crossing are in the different components. Let $\{a(N)\}_{N=1,2,\dots}$ and $\{b(N)\}_{N=1,2,\dots}$ be sequences of natural numbers. We can approximate the R-matrix by Proposition 3.2. For a positive crossing of the link diagram, the R-matrix $R_{VV'}$ of (2.2) is labeled. For convenience, we recall the summand of the R-matrix:

$$(-1)^{k+k(m_N+m'_N)+2ij}t^{-ij-k(i-j)/2+k(k+1)/4}\frac{\{m_N-i+k\}!\,\{m'_N+j+k\}!}{\{k\}!\,\{m_N-i\}!\,\{m'_N+j\}!}.$$

Here, m_N and m'_N are the half-integers satisfying $a(N)=2m_N+1$ and $b(N)=2m'_N+1$. If we assume that $a(N)$ and $b(N)$ are odd numbers, indices i and j are integers. Moreover, by adding 2 to $a(N)$ or $b(N)$ if necessary, we can assume that $m_N+m'_N$ is an even integer without changing the values of the limit $a(N)/N$ and $b(N)/N$. Therefore, under these assumptions the summand is

$$(-1)^{k}t^{-ij-k(i-j)/2+k(k+1)/4}\frac{\{m_N-i+k\}!\,\{m'_N+j+k\}!}{\{k\}!\,\{m_N-i\}!\,\{m'_N+j\}!}.$$

From (3.1), we have

$$t^{-ij-((m_N+m'_N)/2)k}\frac{(t)_{m_N-i+k}(t)_{m'_N+j+k}}{(t)_k(t)_{m_N-i}(t)_{m'_N+j}}.$$

Under substitution $x=\xi_N^i$, $y=\xi_N^j$, and $z=\xi_N^k$, the potential function for a positive crossing is

$$\frac{1}{p}\biggl\{-\pi\sqrt{-1}p\frac{a+b}{2}\log(z^p)-\log(x^p)\log(y^p)-\frac{\pi^2}{6}\\ -\mathrm{Li}_2\Bigl(e_a^p\frac{z^p}{x^p}\Bigr)-\mathrm{Li}_2(e_b^p y^p z^p)+\mathrm{Li}_2\Bigl(\frac{e_a^p}{x^p}\Bigr)+\mathrm{Li}_2(e_b^p y^p)+\mathrm{Li}_2(z^p)\biggr\},$$

where $a(N)/N\to a$, $b(N)/b\to b$, and $e_a=e^{\pi\sqrt{-1}a}$. Note that the indices of the summand are labeled to the edges of the link diagram. We change these indices to the ones corresponding to regions of the link diagram as shown in Figure 3.1.

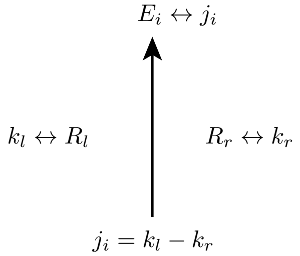

Figure 3.1. Indices corresponding to an edge E_i and regions R_l and R_r.

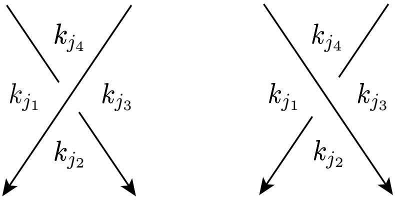

Figure 3.2. Indices corresponding to regions around a crossing.

If $k_{j_1}, \dots, k_{j_4}$ are indices around a crossing as shown in Figure 3.2, we have

$$i = k_{j_2} - k_{j_1}, \quad j = k_{j_3} - k_{j_2}, \quad j + k = k_{j_4} - k_{j_1}, \quad i - k = k_{j_3} - k_{j_4}.$$

From the above equations, we have $k = k_{j_2} + k_{j_4} - k_{j_1} - k_{j_3}$. Therefore, by putting $w_{j_i} = \xi_N^{k_{j_i}}$ and substituting

$$x = \frac{w_{j_2}}{w_{j_1}}, \quad y = \frac{w_{j_3}}{w_{j_2}}, \quad z = \frac{w_{j_2} w_{j_4}}{w_{j_1} w_{j_3}},$$

the potential function for a positive crossing c is

$$\begin{aligned}\Phi^+_{c,p} = \frac{1}{p}\Biggl\{ \pi\sqrt{-1}p^2 \frac{a+b}{2} \log \frac{w_{j_1} w_{j_3}}{w_{j_2} w_{j_4}} - p^2 \log \frac{w_{j_2}}{w_{j_1}} \log \frac{w_{j_3}}{w_{j_2}} \\ - \mathrm{Li}_2\left(e_a^p \frac{w_{j_4}^p}{w_{j_3}^p}\right) - \mathrm{Li}_2\left(e_b^p \frac{w_{j_4}^p}{w_{j_1}^p}\right) + \mathrm{Li}_2\left(\frac{w_{j_2}^p w_{j_4}^p}{w_{j_1}^p w_{j_3}^p}\right) \\ + \mathrm{Li}_2\left(e_a^p \frac{w_{j_1}^p}{w_{j_2}^p}\right) + \mathrm{Li}_2\left(e_b^p \frac{w_{j_3}^p}{w_{j_2}^p}\right) - \frac{\pi^2}{6} \Biggr\}.\end{aligned}$$

If the strings at a crossing are in the same component, we have to consider the modification on the Reidemeister move I. The Reidemeister move I on the component with a color $a(N)$ leads to the multiplication by $s^{2m_N^2 + 2m_N} = (-1)^{2m_N^2+2m_N} t^{-m_N^2 - m_N}$. Therefore, we have to multiply $(-1)^{-2m_N^2-2m_N} t^{m_N^2 + m_N}$ to cancel it. Under the assumption that $a(N)$ is an odd integer, this corresponds to the addition of the function $(\pi\sqrt{-1}pa)^2/p$. Therefore, the potential function is

$$\begin{aligned}\Phi^+_{c,p} = \frac{1}{p}\Biggl\{ (\pi\sqrt{-1}pa)^2 + \pi\sqrt{-1}p^2 a \log \frac{w_{j_1} w_{j_3}}{w_{j_2} w_{j_4}} - p^2 \log \frac{w_{j_2}}{w_{j_1}} \log \frac{w_{j_3}}{w_{j_2}} - \frac{\pi^2}{6} \\ - \mathrm{Li}_2\left(e_a^p \frac{w_{j_4}^p}{w_{j_3}^p}\right) - \mathrm{Li}_2\left(e_a^p \frac{w_{j_4}^p}{w_{j_1}^p}\right) + \mathrm{Li}_2\left(\frac{w_{j_2}^p w_{j_4}^p}{w_{j_1}^p w_{j_3}^p}\right) + \mathrm{Li}_2\left(e_a^p \frac{w_{j_1}^p}{w_{j_2}^p}\right) + \mathrm{Li}_2\left(e_a^p \frac{w_{j_3}^p}{w_{j_2}^p}\right) \Biggr\}.\end{aligned}$$

Similarly, we obtain

$$\begin{aligned}\Phi^{-}_{c,p} = \frac{1}{p}\biggl\{&-\pi\sqrt{-1}p^2\frac{a+b}{2}\log\frac{w_{j_1}w_{j_3}}{w_{j_2}w_{j_4}} + p^2\log\frac{w_{j_3}}{w_{j_4}}\log\frac{w_{j_4}}{w_{j_1}} \\ &-\mathrm{Li}_2\biggl(e_a^p\frac{w_{j_1}^p}{w_{j_4}^p}\biggr)-\mathrm{Li}_2\biggl(e_b^p\frac{w_{j_3}^p}{w_{j_4}^p}\biggr)-\mathrm{Li}_2\biggl(\frac{w_{j_2}^p w_{j_4}^p}{w_{j_1}^p w_{j_3}^p}\biggr) \\ &+\mathrm{Li}_2\biggl(e_a^p\frac{w_{j_2}^p}{w_{j_3}^p}\biggr)+\mathrm{Li}_2\biggl(e_b^p\frac{w_{j_2}^p}{w_{j_1}^p}\biggr)+\frac{\pi^2}{6}\biggr\}\end{aligned}$$

for a negative crossing c between different components, and

$$\begin{aligned}\Phi^{-}_{c,p} = \frac{1}{p}\biggl\{&-(\pi\sqrt{-1}pa)^2-\pi\sqrt{-1}p^2a\log\frac{w_{j_1}w_{j_3}}{w_{j_2}w_{j_4}}+p^2\log\frac{w_{j_3}}{w_{j_4}}\log\frac{w_{j_4}}{w_{j_1}}+\frac{\pi^2}{6} \\ &-\mathrm{Li}_2\biggl(e_a^p\frac{w_{j_1}^p}{w_{j_4}^p}\biggr)-\mathrm{Li}_2\biggl(e_a^p\frac{w_{j_3}^p}{w_{j_4}^p}\biggr)-\mathrm{Li}_2\biggl(\frac{w_{j_2}^p w_{j_4}^p}{w_{j_1}^p w_{j_3}^p}\biggr)+\mathrm{Li}_2\biggl(e_a^p\frac{w_{j_2}^p}{w_{j_3}^p}\biggr)+\mathrm{Li}_2\biggl(e_a^p\frac{w_{j_2}^p}{w_{j_1}^p}\biggr)\biggr\}\end{aligned}$$

for a negative crossing c between the same component. The potential function $\Phi_{D,p}$ of $J_{\boldsymbol{a}(N)}(L,\xi_N^p)$ is a summation of these potential functions with respect to all crossings of D. That is,

$$\Phi_{D,p}(\boldsymbol{a}, w_1, \dots, w_\nu) = \sum_{c\text{ is a crossing}} \Phi_{c,p}^{\mathrm{sgn}(c)},$$

where

$$\boldsymbol{a} = (a_1, \dots, a_n), \quad a_i = \lim_{N\to\infty}\frac{a_i(N)}{N}$$

and $\mathrm{sgn}(c)$ is a signature of a crossing c. This potential function essentially coincides with Yoon's generalized potential function [Yoon 2021]. We can easily verify the following property by the definition of $\Phi_{D,p}$:

Proposition 3.4. $\Phi_{D,p}(\boldsymbol{a}, w_1, \dots, w_\nu)$ *satisfies*

$$\Phi_{D,p}(\boldsymbol{a}, w_1, \dots, w_\nu) = \frac{1}{p}\Phi_{D,1}(p\boldsymbol{a}, w_1^p, \dots, w_\nu^p).$$

Therefore, We mainly consider the case where $p = 1$ and write $\Phi_D = \Phi_{D,1}$.

4. A noncomplete hyperbolic structure

In this section, we provide geometric meanings of the potential function. In the rest of this paper, we assume that L is a hyperbolic link with n components. In this section, we also assume that $a_i \in [1-\varepsilon, 1]$ for all $i = 1, \dots, n$, where ε is a sufficiently small positive real number. First, we consider derivatives of the potential functions with respect to the parameters corresponding to the regions of the link diagram [Cho and Murakami 2013]. For a positive crossing c between different components, we have:

$$\begin{aligned}
w_{j_1}\frac{\partial\Phi_c^+}{\partial w_{j_1}} &= \pi\sqrt{-1}\,\frac{a-b}{2}+\log\left(1-e_a\frac{w_{j_1}}{w_{j_2}}\right)^{-1}\left(1-e_b^{-1}\frac{w_{j_1}}{w_{j_4}}\right)^{-1}\left(1-\frac{w_{j_1}w_{j_3}}{w_{j_2}w_{j_4}}\right),\\
w_{j_2}\frac{\partial\Phi_c^+}{\partial w_{j_2}} &= \pi\sqrt{-1}\,\frac{a+b}{2}+\log\left(1-e_a^{-1}\frac{w_{j_2}}{w_{j_1}}\right)\left(1-e_b^{-1}\frac{w_{j_2}}{w_{j_3}}\right)\left(1-\frac{w_{j_2}w_{j_4}}{w_{j_1}w_{j_3}}\right)^{-1},\\
w_{j_3}\frac{\partial\Phi_c^+}{\partial w_{j_3}} &= \pi\sqrt{-1}\,\frac{-a+b}{2}+\log\left(1-e_a^{-1}\frac{w_{j_3}}{w_{j_4}}\right)^{-1}\left(1-e_b\frac{w_{j_3}}{w_{j_2}}\right)^{-1}\left(1-\frac{w_{j_1}w_{j_3}}{w_{j_2}w_{j_4}}\right),\\
w_{j_4}\frac{\partial\Phi_c^+}{\partial w_{j_4}} &= -\pi\sqrt{-1}\,\frac{a+b}{2}+\log\left(1-e_a\frac{w_{j_4}}{w_{j_3}}\right)\left(1-e_b\frac{w_{j_4}}{w_{j_1}}\right)\left(1-\frac{w_{j_2}w_{j_4}}{w_{j_1}w_{j_3}}\right)^{-1}.
\end{aligned}\tag{4.1}$$

Similarly, for a negative crossing c between different components, we have

$$\begin{aligned}
w_{j_1}\frac{\partial\Phi_c^-}{\partial w_{j_1}} &= \pi\sqrt{-1}\,\frac{-a+b}{2}+\log\left(1-e_a\frac{w_{j_1}}{w_{j_4}}\right)\left(1-e_b^{-1}\frac{w_{j_1}}{w_{j_2}}\right)\left(1-\frac{w_{j_1}w_{j_3}}{w_{j_2}w_{j_4}}\right)^{-1},\\
w_{j_2}\frac{\partial\Phi_c^-}{\partial w_{j_2}} &= \pi\sqrt{-1}\,\frac{a+b}{2}+\log\left(1-e_a\frac{w_{j_2}}{w_{j_3}}\right)^{-1}\left(1-e_b\frac{w_{j_2}}{w_{j_1}}\right)^{-1}\left(1-\frac{w_{j_2}w_{j_4}}{w_{j_1}w_{j_3}}\right),\\
w_{j_3}\frac{\partial\Phi_c^-}{\partial w_{j_3}} &= \pi\sqrt{-1}\,\frac{a-b}{2}+\log\left(1-e_a^{-1}\frac{w_{j_3}}{w_{j_2}}\right)\left(1-e_b\frac{w_{j_3}}{w_{j_4}}\right)\left(1-\frac{w_{j_1}w_{j_3}}{w_{j_2}w_{j_4}}\right)^{-1},\\
w_{j_4}\frac{\partial\Phi_c^-}{\partial w_{j_4}} &= -\pi\sqrt{-1}\,\frac{a+b}{2}+\log\left(1-e_a^{-1}\frac{w_{j_4}}{w_{j_1}}\right)^{-1}\left(1-e_b^{-1}\frac{w_{j_4}}{w_{j_3}}\right)^{-1}\left(1-\frac{w_{j_2}w_{j_4}}{w_{j_1}w_{j_3}}\right).
\end{aligned}\tag{4.2}$$

If a crossing is between the same component, the derivatives are (4.1) and (4.2) with $a = b$. These correspond to Thurston's triangulation [1999] of the link complement (see Figure 4.1).

Here, we put

$$\begin{aligned}
&u_1 = e_a\frac{w_{j_1}}{w_{j_2}}, && u_2 = e_a^{-1}\frac{w_{j_3}}{w_{j_4}}, && u_3 = \frac{w_{j_2}w_{j_4}}{w_{j_1}w_{j_3}}, && u_4 = e_b^{-1}\frac{w_{j_1}}{w_{j_4}}, && u_5 = e_b\frac{w_{j_3}}{w_{j_2}},\\
&v_1 = e_a^{-1}\frac{w_{j_4}}{w_{j_1}}, && v_2 = e_a\frac{w_{j_2}}{w_{j_3}}, && v_3 = \frac{w_{j_1}w_{j_3}}{w_{j_2}w_{j_4}}, && v_4 = e_b\frac{w_{j_2}}{w_{j_1}}, && v_5 = e_b^{-1}\frac{w_{j_4}}{w_{j_3}}
\end{aligned}$$

in Figure 4.1. Furthermore, for a complex number z, denote

$$z' = \frac{1}{1-z} \quad\text{and}\quad z'' = 1-\frac{1}{z}.$$

Note that if there exists a nonalternating part, the ideal tetrahedron abuts the one with the inverse complex number labeled. Thus we can ignore the contribution of such a part. Let G_i be a product of the parameters of ideal tetrahedra around the

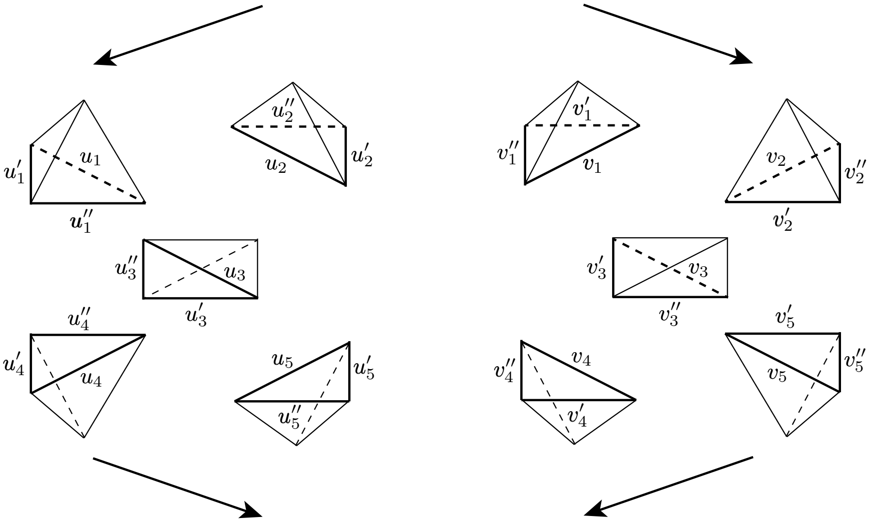

Figure 4.1. Ideal tetrahedra on a positive crossing (left), and ideal tetrahedra on a negative crossing (right).

region R_i corresponding to the parameter w_i. Then, we have

$$w_i \frac{\partial \Phi_D}{\partial w_i} = \frac{\pi\sqrt{-1}}{2} r(a_1, \dots, a_n) + \log G_i,$$

where $\pi\sqrt{-1}r(a_1, \dots, a_n)/2$ is the summation of first terms of $w_i \partial\Phi_c^{\pm}/\partial w_i$ with c running over all crossings around R_i. However, this is equal to 0 because the contribution of each parameter a to $r(a_1, \dots, a_n)$ is canceled as in Figure 4.2.

Therefore, the equations

$$\exp\left(w_i \frac{\partial \Phi_D}{\partial w_i}\right) = 1, \quad i = 1, 2, \dots, \nu, \tag{4.3}$$

coincide with the gluing condition of the ideal tetrahedra. Hence, we can obtain a hyperbolic structure from a saddle point $(\sigma_1(\boldsymbol{a}), \dots, \sigma_\nu(\boldsymbol{a}))$ of $\Phi_D(\boldsymbol{a}, -)$,

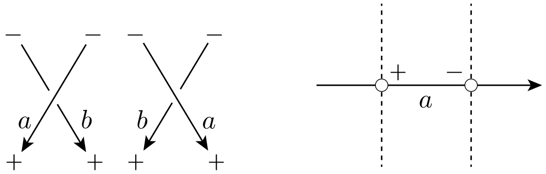

Figure 4.2. Signatures of parameters corresponding to edges (left). Note that the pattern of signatures is independent of the signature of a crossing. Contributions of each parameter (right). White circles represent either positive or negative crossings.

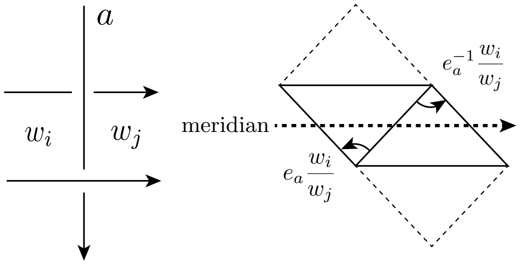

Figure 4.3. The dilation component of the meridian of the link component with the parameter a.

where $\boldsymbol{a} = (a_1, \dots, a_n)$. In addition, this hyperbolic structure is not complete in general because the dilation component of the meridian of the link component with the color a is equal to e_a^{-2} (see Figure 4.3).

Note that $\boldsymbol{a} = (1, \dots, 1)$ is the case of the original volume conjecture. So we suppose that $(\sigma_1(\boldsymbol{a}), \dots, \sigma_\nu(\boldsymbol{a}))$ gives $S^3 \setminus L$ the hyperbolic structure with the finite volume $\mathrm{Vol}(S^3 \setminus L)$ when $\boldsymbol{a} = (1, \dots, 1)$ [Cho 2016a]. Let $M_{a_1,\dots,a_n}$ be a manifold with the hyperbolic structure given by $(\sigma_1(\boldsymbol{a}), \dots, \sigma_\nu(\boldsymbol{a}))$. We will determine the detail of this noncomplete hyperbolic manifold $M_{a_1,\dots,a_n}$. Let a be a real number slightly less than 1. Note that the action derived from each meridian does not change a length because $|e_a^{-2}| = 1$. Therefore, the action derived from each longitude changes a length, since otherwise, both meridians and longitudes do not change a length and this results in the complete hyperbolic structure [Benedetti and Petronio 1992]. Therefore, the developing image in the upper half-space $\mathbb{H}^3$ of the link complement around the edge corresponding to parameter a should be as shown in Figure 4.4. If we glue faces by the action of meridians in Figure 4.4, each face is glued with the face rotated $2\pi(1-a)$ around the singular set. Therefore, $M_{a_1,\dots,a_n}$ is a cone-manifold of L with cone-angle $2\pi(1-a_i)$ around the component corresponding to a_i. Specifically, we can prove the following proposition:

Theorem 4.1. *The hyperbolic volume of the cone-manifold $M_{a_1,\dots,a_n}$ is equal to the imaginary part of the value*[1] *of a function*

$$\tilde{\Phi}_D = \Phi_D - \sum_{j=1}^{\nu} w_j \frac{\partial \Phi_D}{\partial w_j} \log w_j$$

evaluated at $w_j = \sigma_j(\boldsymbol{a})$, with $j = 1, \dots, \nu$.

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[1] In [Murakami 2000], this value is called the optimistic limit.

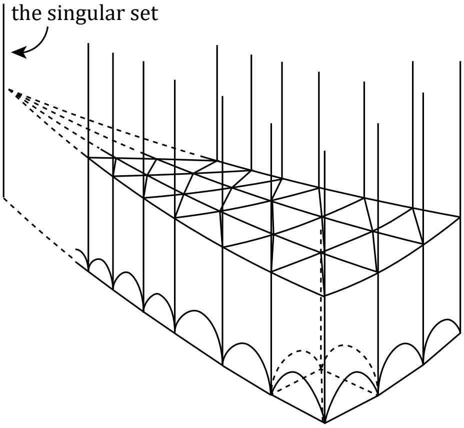

Figure 4.4. The developing image of the link complement with the noncomplete hyperbolic structure.

Proof. The hyperbolic volume $V(z)$ of the ideal tetrahedron with modulus z is given by the Bloch–Wigner function [Zagier 2007]

$$V(z) = \operatorname{Im} \operatorname{Li}_2(z) + \log|z| \arg(1-z). \tag{4.4}$$

We only consider the case where a crossing is between different components. Let $V_c^{\pm}(a,b)$ be the sum of hyperbolic volumes of five ideal tetrahedra at a positive or negative crossing c, respectively. By using (4.4), we can show that

$$\operatorname{Im}\Phi_c^+ - V_c^+(a,b) = A_{j_1}^+ \log|w_{j_1}| + A_{j_2}^+ \log|w_{j_2}| + A_{j_3}^+ \log|w_{j_3}| + A_{j_4}^+ \log|w_{j_4}|,$$

where $A_{j_i}^+$, with $i = 1, 2, 3, 4$, are:

$$A_{j_1}^+ = \frac{\pi}{2}(a-b) + \arg\left(1 - e_a \frac{w_{j_1}}{w_{j_2}}\right)^{-1}\left(1 - e_b^{-1}\frac{w_{j_1}}{w_{j_4}}\right)^{-1}\left(1 - \frac{w_{j_1}w_{j_3}}{w_{j_2}w_{j_4}}\right),$$

$$A_{j_2}^+ = \frac{\pi}{2}(a+b) + \arg\left(1 - e_a^{-1} \frac{w_{j_2}}{w_{j_1}}\right)\left(1 - e_b^{-1}\frac{w_{j_2}}{w_{j_3}}\right)\left(1 - \frac{w_{j_2}w_{j_4}}{w_{j_1}w_{j_3}}\right)^{-1},$$

$$A_{j_3}^+ = \frac{\pi}{2}(-a+b) + \arg\left(1 - e_a^{-1} \frac{w_{j_3}}{w_{j_4}}\right)^{-1}\left(1 - e_b\frac{w_{j_3}}{w_{j_2}}\right)^{-1}\left(1 - \frac{w_{j_1}w_{j_3}}{w_{j_2}w_{j_4}}\right),$$

$$A_{j_4}^+ = -\frac{\pi}{2}(a+b) + \arg\left(1 - e_a \frac{w_{j_4}}{w_{j_3}}\right)\left(1 - e_b\frac{w_{j_4}}{w_{j_1}}\right)\left(1 - \frac{w_{j_2}w_{j_4}}{w_{j_1}w_{j_3}}\right)^{-1}.$$

Similarly, we can show that

$$\operatorname{Im}\Phi_c^- - V_c^-(a,b) = A_{j_1}^- \log|w_{j_1}| + A_{j_2}^- \log|w_{j_2}| + A_{j_3}^- \log|w_{j_3}| + A_{j_4}^- \log|w_{j_4}|,$$

where $A^-_{j_i}$, with $i = 1, 2, 3, 4$, are:

$$\begin{aligned}
A^-_{j_1} &= \frac{\pi}{2}(-a+b) + \arg\left(1 - e_a \frac{w_{j_1}}{w_{j_4}}\right)\left(1 - e_b^{-1} \frac{w_{j_1}}{w_{j_2}}\right)\left(1 - \frac{w_{j_1} w_{j_3}}{w_{j_2} w_{j_4}}\right)^{-1}, \\
A^-_{j_2} &= \frac{\pi}{2}(a+b) + \arg\left(1 - e_a \frac{w_{j_2}}{w_{j_3}}\right)^{-1}\left(1 - e_b \frac{w_{j_2}}{w_{j_1}}\right)^{-1}\left(1 - \frac{w_{j_2} w_{j_4}}{w_{j_1} w_{j_3}}\right), \\
A^-_{j_3} &= \frac{\pi}{2}(a-b) + \arg\left(1 - e_a^{-1} \frac{w_{j_3}}{w_{j_2}}\right)\left(1 - e_b \frac{w_{j_3}}{w_{j_4}}\right)\left(1 - \frac{w_{j_1} w_{j_3}}{w_{j_2} w_{j_4}}\right)^{-1}, \\
A^-_{j_4} &= -\frac{\pi}{2}(a+b) + \arg\left(1 - e_a^{-1} \frac{w_{j_4}}{w_{j_1}}\right)^{-1}\left(1 - e_b^{-1} \frac{w_{j_4}}{w_{j_3}}\right)^{-1}\left(1 - \frac{w_{j_2} w_{j_4}}{w_{j_1} w_{j_3}}\right).
\end{aligned}$$

By summing up over all crossings, we verify the proposition. □

Example 4.2 (figure-eight knot). Let θ be a real number in $\left[0, \frac{\pi}{3}\right]$. The volume $V(\theta)$ of the cone-manifold of the figure-eight knot with a cone-angle θ is given by the formula [Mednykh 2003; Mednykh and Rasskazov 2006]

$$V(\theta) = \int_\theta^{2\pi/3} \operatorname{arccosh}(1 + \cos\theta - \cos 2\theta)\, d\theta.$$

In this case, the cone-manifold admits a hyperbolic structure. On the other hand, the colored Jones polynomial for the figure-eight knot is given by Habiro and Le's formula [Habiro 2000]

$$J_N(4_1; t) = \frac{1}{\{N\}} \sum_{p=0}^{N-1} \frac{\{N+p\}!}{\{N-p-1\}!}.$$

We assume that a is in $\left(\frac{5}{6}, 1\right)$ so that $0 < 2\pi(1-a) < \frac{\pi}{3}$. The potential function of $J_{a(N)}(4_1, \xi_N)$ is

$$\Phi(a, x) = -2\pi\sqrt{-1}\, a \log x - \mathrm{Li}_2(e_a^2 x) + \mathrm{Li}_2(e_a^2 x^{-1}),$$

and the derivative of this function with respect to x is

$$\frac{\partial \Phi}{\partial x} = \frac{1}{x} \log(-x + e_a^2 + e_a^{-2} - x^{-1}).$$

As a solution of the equation $\partial\Phi/\partial x = 0$, we obtain

$$x_0(a) = \left(\cos 2\pi a - \tfrac{1}{2}\right) - \sqrt{\left(\cos 2\pi a - \tfrac{3}{2}\right)\left(\cos 2\pi a + \tfrac{1}{2}\right)}.$$

Since $\frac{5}{6} < a < 1$, the absolute value of $x_0(a)$ is equal to 1. So we put $x_0(a) = e^{\sqrt{-1}\varphi(a)}$, where $\varphi(a) \in (-\pi, \pi]$. Then, the imaginary part of $\Phi(a, x_0(a))$ is

$$\operatorname{Im} \Phi(a, x_0(a)) = -2\Lambda\left(\pi a + \frac{\varphi(a)}{2}\right) + 2\Lambda\left(\pi a - \frac{\varphi(a)}{2}\right).$$

We will show that $\operatorname{Im}\Phi(a, x_0(a)) = V(2\pi(1-a))$ as a function on the closed interval $\left[\frac{2}{3}, 1\right]$. If $a = \frac{2}{3}$, they are both 0. The derivative with respect to a is

$$\begin{aligned}\frac{d\Phi(a, x_0(a))}{da} &= \frac{\partial\Phi}{\partial a}(a, x_0(a)) + \frac{\partial\Phi}{\partial x}(a, x_0(a))\frac{dx_0(a)}{da}\\ &= 2\pi\sqrt{-1}\log\frac{1-e_a^2x_0(a)}{x_0(a)-e_a^2}\\ &= -2\pi^2 + 2\pi\sqrt{-1}\log\left(\frac{e_a^2x_0(a)-1}{e_a^{-2}x_0(a)-1}e_a^{-2}\right).\end{aligned}$$

Since $e^{\sqrt{-1}\theta} - 1 = 2\sin(\theta/2)e^{\sqrt{-1}(\pi+\theta)/2}$, we obtain

$$\frac{d\Phi(a, x_0(a))}{da} = -2\pi^2 + 2\pi\sqrt{-1}\log\frac{\sin\bigl((\varphi(a)+2\pi a)/2\bigr)}{\sin\bigl((\varphi(a)-2\pi a)/2\bigr)}.$$

Let $f(a)$ be the function inside the log, then

$$\cosh\log f(a) = \frac{\sin^2\bigl((\varphi(a)+2\pi a)/2\bigr)+\sin^2\bigl((\varphi(a)-2\pi a)/2\bigr)}{2\sin\bigl((\varphi(a)+2\pi a)/2\bigr)\sin\bigl((\varphi(a)-2\pi a)/2\bigr)}.$$

Note that the denominator of the right-hand side is $\cos(2\pi a) - \cos\varphi(a) = \frac{1}{2}$. Then,

$$\begin{aligned}\cosh\log f(a) &= 2\left(\sin^2\frac{\varphi(a)+2\pi a}{2} + \sin^2\frac{\varphi(a)-2\pi a}{2}\right)\\ &= 2-\cos(\varphi(a)+2\pi a)-\cos(\varphi(a)-2\pi a)\\ &= 2-2\cos\varphi(a)\cos 2\pi a\\ &= 1+\cos 2\pi a-\cos 4\pi a.\end{aligned}$$

Therefore, we obtain

$$\frac{d\Phi(a, x_0(a))}{da} = -2\pi^2 + 2\pi\sqrt{-1}\operatorname{arccosh}(1+\cos 2\pi a-\cos 4\pi a).$$

Clearly, the imaginary part of this function is $2\pi\operatorname{arccosh}(1+\cos 2\pi a-\cos 4\pi a)$ which is equal to $dV(2\pi(1-a))/da$. This shows that $V(2\pi(1-a)) = \operatorname{Im}\Phi(a, x_0(a))$.

Remark 4.3. We can show the following statement by the same procedure that appeared in [Murakami 2004][2]: Let $a \in \left(\frac{5}{12}, \frac{1}{2}\right)$ be the limit of $a(N)/N$, where $N \to \infty$. Then, the limit

$$4\pi\lim_{N\to\infty}\frac{\log|J_{a(N)}(4_1;\xi_N^2)|}{N}$$

is equal to the volume of the cone-manifold of the figure-eight knot with a cone-angle $2\pi - 4\pi a$, where N runs over all odd integers.

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[2] In [Murakami 2004], the value substituted for t is slightly changed from the N-th root of unity.

Example 4.4 (Borromean rings). Let K_B be the Borromean rings, $K_B(\alpha, \beta, \gamma)$ be the cone manifold of K_B with cone-angles α, β, γ, and $\Delta(\alpha, \theta) = \Lambda(\alpha+\theta) - \Lambda(\alpha-\theta)$, where $\Lambda(x)$ is the Lobachevsky function. If $0 < \alpha, \beta, \gamma < \pi$, then $K_B(\alpha, \beta, \gamma)$ admits a hyperbolic structure, and its volume is given by

$$\operatorname{Vol} K_B(\alpha, \beta, \gamma) = 2\Big(\Delta\Big(\frac{\alpha}{2}, \theta\Big) + \Delta\Big(\frac{\beta}{2}, \theta\Big) + \Delta\Big(\frac{\gamma}{2}, \theta\Big) - 2\Delta\Big(\frac{\pi}{2}, \theta\Big) - \Delta(0, \theta)\Big),$$

where $\theta \in \big(0, \frac{\pi}{2}\big)$ is defined by the following conditions [Mednykh 2003]:

$$T = \tan\theta, \quad L = \tan\frac{\alpha}{2}, \quad M = \tan\frac{\beta}{2}, \quad N = \tan\frac{\gamma}{2},$$
$$T^4 - (L^2 + M^2 + N^2 + 1)T^2 - L^2M^2N^2 = 0.$$

We define the function $\tilde{\Delta}(x, y, z, \theta)$ by

$$\tilde{\Delta}(x, y, z, \theta) = 2\Big(\Delta(x, \theta) + \Delta(y, \theta) + \Delta(z, \theta) - 2\Delta\Big(\frac{\pi}{2}, \theta\Big) - \Delta(0, \theta)\Big)$$

for convenience. On the other hand, the colored Jones polynomial for K_B is given by [Habiro 2000]

$$J_{(l,m,n)}(K_B; t) = \sum_{i=1}^{\min(l,m,n)-1} \frac{\{l+i\}!\,\{m+i\}!\,\{n+i\}!\,(\{i\}!)^2}{\{1\}\{l-i-1\}!\,\{m-i-1\}!\,\{n-i-1\}!\,(\{2i+1\}!)^2}.$$

Let a, b, and c be the limit of l/N, m/N, and n/N, respectively. The potential function $\Phi_{K_B}(x)$ of $J_{(l,m,n)}(K_B; \xi_N)$ is

$$\begin{aligned}\Phi_{K_B}(a, b, c, x) = -2\pi\sqrt{-1}(a+b+c)\log x + \frac{3}{2}(\log x)^2 \\ - \operatorname{Li}_2(e_a^2 x) - \operatorname{Li}_2(e_b^2 x) - \operatorname{Li}_2(e_c^2 x) - 2\operatorname{Li}_2(x) \\ + \operatorname{Li}_2\Big(\frac{e_a^2}{x}\Big) + \operatorname{Li}_2\Big(\frac{e_b^2}{x}\Big) + \operatorname{Li}_2\Big(\frac{e_c^2}{x}\Big) + 2\operatorname{Li}_2(x^2).\end{aligned}$$

The derivative of $\Phi_{K_B}(x)$ with respect to x is

$$x\frac{\partial\Phi_{K_B}}{\partial x} = \log\Big(e_a^{-2}e_b^{-2}e_c^{-2}F(a, x)F(b, x)F(c, x)\frac{x^3(1-x)^2}{(1-x^2)^4}\Big),$$

where $F(a, x) = (1-e_a^2 x)(1-e_a^2/x)$. Under the substitution $x = e^{2\pi\sqrt{-1}\zeta}$, we obtain

$$\begin{aligned}&\frac{1}{2\pi\sqrt{-1}}\frac{\partial\Phi_{K_B}}{\partial\zeta} \\ &\quad= \log\frac{\sin\pi(\zeta+a)\sin\pi(\zeta-a)\sin\pi(\zeta+b)\sin\pi(\zeta-b)\sin\pi(\zeta+c)\sin\pi(\zeta-c)}{\sin^2\pi\zeta\cos^4\pi\zeta} \\ &\quad= \log\frac{\tan^2\pi\zeta - A^2}{1+A^2}\frac{\tan^2\pi\zeta - B^2}{1+B^2}\frac{\tan^2\pi\zeta - C^2}{1+C^2}\frac{1}{\tan^2\pi\zeta},\end{aligned}$$

where $A = \tan \pi(1-a)$, $B = \tan \pi(1-b)$, and $C = \tan \pi(1-c)$. Therefore, if $\pm \tan \pi \zeta$ are solutions of the equation

$$\frac{t^2-A^2}{1+A^2}\frac{t^2-B^2}{1+B^2}\frac{t^2-C^2}{1+C^2}\frac{1}{t^2} = 1,$$

which is equivalent to the equation

$$(t^2+1)(t^4-(A^2+B^2+C^2+1)t^2-A^2B^2C^2) = 0,$$

then $x = e^{2\pi\sqrt{-1}\zeta}$ is a saddle point of $\Phi_{K_B}(a,b,c,x)$. By using the properties of the Lobachevsky function, such as

$$\begin{aligned} \mathrm{Li}_2(e^{2\sqrt{-1}\theta}) &= \frac{\pi^2}{6} - \theta(\pi-\theta) + 2\sqrt{-1}\Lambda(\theta), \\ \Lambda(2\theta) &= 2\Lambda(\theta) + 2\Lambda\Big(\theta + \frac{\pi}{2}\Big), \end{aligned}$$

we obtain

$$\begin{aligned} \operatorname{Im} \Phi_{K_B}(a,b,c,e^{2\pi\sqrt{-1}\zeta}) &= \tilde{\Delta}\big(\pi(1-a), \pi(1-b), \pi(1-c), \pi(1-\zeta)\big) \\ &= \operatorname{Vol} K_B\big(2\pi(1-a), 2\pi(1-b), 2\pi(1-c)\big). \end{aligned}$$

5. The completeness condition

In the previous section, we fixed $a_1, \ldots, a_n$. In this section, we regard them as variables and find a geometric meaning. First, we consider the case where a crossing is between different components. The derivatives of the potential function with respect to the parameters corresponding to the colors are:

$$\begin{aligned} \frac{\partial \Phi_c^+}{\partial a} &= \frac{\pi\sqrt{-1}}{2} \log\Big(1 - e_a\frac{w_{j_4}}{w_{j_3}}\Big)\Big(1 - e_a\frac{w_{j_1}}{w_{j_2}}\Big)^{-1}\Big(1 - e_a^{-1}\frac{w_{j_3}}{w_{j_4}}\Big)\Big(1 - e_a^{-1}\frac{w_{j_2}}{w_{j_1}}\Big)^{-1}, \\ \frac{\partial \Phi_c^+}{\partial b} &= \frac{\pi\sqrt{-1}}{2} \log\Big(1 - e_b\frac{w_{j_4}}{w_{j_1}}\Big)\Big(1 - e_b\frac{w_{j_3}}{w_{j_2}}\Big)^{-1}\Big(1 - e_b^{-1}\frac{w_{j_1}}{w_{j_4}}\Big)\Big(1 - e_b^{-1}\frac{w_{j_2}}{w_{j_3}}\Big)^{-1}, \\ \frac{\partial \Phi_c^-}{\partial a} &= \frac{\pi\sqrt{-1}}{2} \log\Big(1 - e_a\frac{w_{j_1}}{w_{j_4}}\Big)\Big(1 - e_a\frac{w_{j_2}}{w_{j_3}}\Big)^{-1}\Big(1 - e_a^{-1}\frac{w_{j_4}}{w_{j_1}}\Big)\Big(1 - e_a^{-1}\frac{w_{j_3}}{w_{j_2}}\Big)^{-1}, \\ \frac{\partial \Phi_c^-}{\partial b} &= \frac{\pi\sqrt{-1}}{2} \log\Big(1 - e_b\frac{w_{j_3}}{w_{j_4}}\Big)\Big(1 - e_b\frac{w_{j_2}}{w_{j_1}}\Big)^{-1}\Big(1 - e_b^{-1}\frac{w_{j_4}}{w_{j_3}}\Big)\Big(1 - e_b^{-1}\frac{w_{j_1}}{w_{j_2}}\Big)^{-1}. \end{aligned}$$

We can observe the correspondence between these derivatives and dilation components by cusp diagrams (Figure 5.1). In Figure 5.1, $\partial\Phi_c^+/\partial a$ corresponds to the upper side of a positive crossing (top left), $\partial\Phi_c^+/\partial b$ to the lower side of a positive crossing (top right), $\partial\Phi_c^-/\partial a$ to the upper side of a negative crossing (bottom left), and $\partial\Phi_c^-/\partial b$ to the upper side of a negative crossing (bottom right). A similar correspondence holds in the case where a crossing is between the same component.

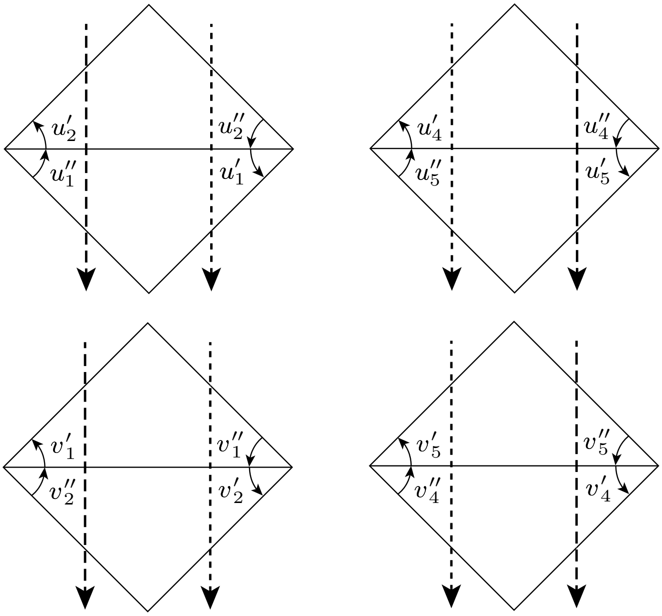

Figure 5.1. Cusp diagrams: upper side of a positive crossing (top left), lower side of a positive crossing (top right), upper side of a negative crossing (bottom left), and lower side of a negative crossing (bottom right).

Let l_i be the longitude that is parallel to the component L_i, and let $\tilde{l}_i$ be the longitude of the component L_i with $\mathrm{lk}(\tilde{l}_i, L_i) = 0$. For a curve γ on the cusp diagram, we define $\delta(\gamma)$ as the dilation component of γ. Then, by the above observation

$$\exp\left(\frac{1}{\pi\sqrt{-1}}\frac{\partial \Phi_D'}{\partial a_i}\right) = \exp\left(\frac{1}{2}\log \delta(l_i)^2\right) = \delta(l_i),$$

where Φ_D' is a potential function of the colored Jones polynomial without the modification for the Reidemeister move I. Next, we consider the contribution of the modification. For a positive crossing between the same component with a parameter a, the modification corresponds to the addition of $(\pi\sqrt{-1}\,a)^2$, and its derivative is

$$\frac{1}{\pi\sqrt{-1}}\frac{d}{da}(\pi\sqrt{-1}\,a)^2 = 2\pi\sqrt{-1}\,a = \log e_a^2.$$

Here, e_a^2 is equal to the dilation component of the meridian with the inverse orientation. Similarly, for a negative crossing, the derivative of $-(\pi\sqrt{-1}\,a)^2$ corresponds to the dilation component of the meridian. Therefore,

$$\exp\left(\frac{1}{\pi\sqrt{-1}}\frac{\partial \Phi_D}{\partial a_i}\right) = \delta(\tilde{l}_i). \tag{5.1}$$

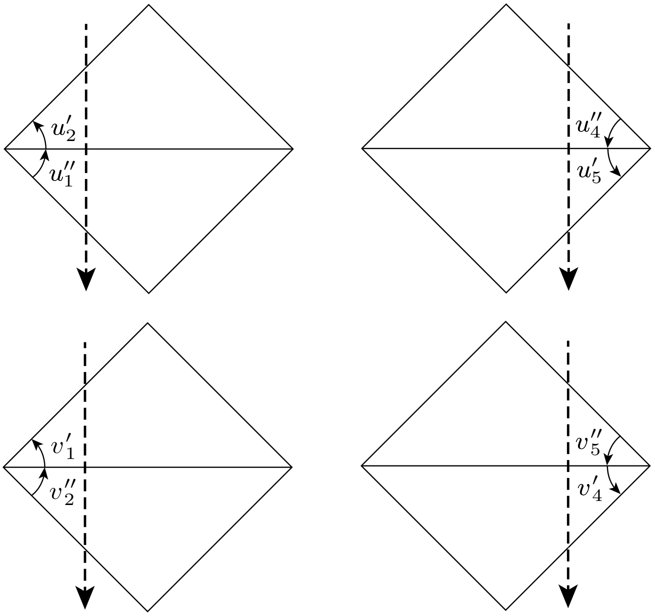

Figure 5.2. Cusp diagrams of a knot complement: upper side of a positive crossing (top left), lower side of a positive crossing (top right), upper side of a negative crossing (bottom left), lower side of a negative crossing (bottom right).

Remark 5.1. If K is a knot, we have a more simple correspondence. The derivatives of $\Phi_c^{\pm}$ with respect to a are:

$$\begin{aligned}(5.2)\quad &\frac{1}{\pi\sqrt{-1}}\frac{\partial\Phi_c^{+}}{\partial a}\\ &\quad=\log e_a^2+\log\left(1-e_a^{-1}\frac{w_{j_3}}{w_{j_4}}\right)\left(1-e_a\frac{w_{j_4}}{w_{j_1}}\right)\left(1-e_a^{-1}\frac{w_{j_2}}{w_{j_1}}\right)^{-1}\left(1-e_a\frac{w_{j_3}}{w_{j_2}}\right)^{-1},\end{aligned}$$

$$\begin{aligned}(5.3)\quad &\frac{1}{\pi\sqrt{-1}}\frac{\partial\Phi_c^{-}}{\partial a}\\ &\quad=\log e_a^{-2}+\log\left(1-e_a^{-1}\frac{w_{j_4}}{w_{j_1}}\right)\left(1-e_a\frac{w_{j_3}}{w_{j_4}}\right)\left(1-e_a^{-1}\frac{w_{j_3}}{w_{j_2}}\right)^{-1}\left(1-e_a\frac{w_{j_2}}{w_{j_1}}\right)^{-1}.\end{aligned}$$

The second term of (5.2) corresponds to the upper side and the lower side of a positive crossing (Figure 5.2, top left and right), and the second term of (5.3) corresponds to the upper side and the lower side of a negative crossing (Figure 5.2, bottom left and right)

Remark 5.2. Changing the variable a_i to $u_i = 2\pi\sqrt{-1}\,a_i$, we have

$$2\frac{\partial\Phi_D}{\partial u_i}=\frac{1}{\pi\sqrt{-1}}\frac{\partial\Phi_D}{\partial a_i}.$$

Then,

$$\Psi(\boldsymbol{u}) = 4\big(\Phi_D\big(\boldsymbol{u}, \sigma_1(\boldsymbol{u}), \dots, \sigma_\nu(\boldsymbol{u})\big) - \Phi_D\big(\boldsymbol{0}, \sigma_1(\boldsymbol{0}), \dots, \sigma_\nu(\boldsymbol{0})\big)\big),$$

where $\boldsymbol{u} = (u_1, \dots, u_n)$ and $\boldsymbol{0} = (0, \dots, 0)$ satisfy the conditions of the Neumann–Zagier potential function [1985]. Namely, Ψ satisfies $\Psi(\boldsymbol{0}) = 0$ and

$$\frac{1}{2}\frac{\partial \Psi}{\partial u_i} = \log \delta(\tilde{l}_i).$$

If $a_i = 1$, with $i = 1, \dots, n$, all the dilation components of meridians are 1. Furthermore, the contributions of parts, as shown in Figure 4.3, to the dilation component of the longitude is 1, hence $\delta(\tilde{l}_i) = 1,\ (1, \dots, n)$. Therefore, the point $(\boldsymbol{1}, \sigma_1(\boldsymbol{1}), \dots, \sigma_\nu(\boldsymbol{1}))$ gives a complete hyperbolic structure to the link complement [Benedetti and Petronio 1992], where $\boldsymbol{1} = (1, \dots, 1)$. Moreover, by (4.3) and (5.1) the point is a solution of the following system of equations:

$$\begin{cases} \exp\left(w_i \dfrac{\partial \Phi_D}{\partial w_i}\right) = 1, & i = 1, \dots, \nu, \\ \exp\left(\dfrac{1}{\pi\sqrt{-1}} \dfrac{\partial \Phi_D}{\partial a_j}\right) = 1, & j = 1, \dots, n. \end{cases}$$

Hence, we obtain the following theorem:

Theorem 5.3. *Let D be a diagram of a hyperbolic link with n components, and let $\boldsymbol{1}$ be $(1, \dots, 1) \in \mathbb{Z}^n$. The point $(\boldsymbol{1}, \sigma_1(\boldsymbol{1}), \dots, \sigma_\nu(\boldsymbol{1}))$ is a saddle point of the function $\Phi_D(a_1, \dots, a_n, w_1, \dots, w_\nu)$ and gives a complete hyperbolic structure to the link complement.*

6. The Witten–Reshetikhin–Turaev invariant

In [Kirby and Melvin 1991], the Witten–Reshetikhin–Turaev invariant for the manifold obtained by Dehn surgery on a link is stated. Furthermore, Murakami [2000] calculated the optimistic limit of the Witten–Reshetikhin–Turaev invariant for the manifold obtained by integer surgery on the figure-eight knot. By a similar argument as in Section 4, we would be able to explain the correspondence of the Witten–Reshetikhin–Turaev invariant and the geometry of the manifold obtained by Dehn surgery on a link. The procedure might be as follows: The Witten–Reshetikhin–Turaev invariant for the manifold $M_{f_1,\dots,f_n}$ obtained by Dehn surgery on a link $L = L_1 \cup \dots \cup L_n$ with a framing f_i on L_i, where $i = 1, \dots, n$, can be written as a summation of the colored Jones polynomial $J_{\boldsymbol{k}}(L; \xi_N)$ multiplied by $t^{-(1/4)\sum f_j k_j^2}$, where $\boldsymbol{k} = (k_1, \dots, k_n)$ are colors of L. See [Kirby and Melvin 1991] for details, but note that t in [Kirby and Melvin 1991] and t in this paper are different. We suppose that $M_{f_1,\dots,f_n}$ admits a hyperbolic structure. Let α_i be $e^{\pi\sqrt{-1}a_i}$ and regard

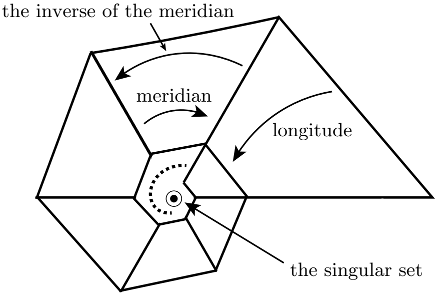

Figure 6.1. The schematic diagram of the developing image in the case of $f_i = 6$.

it as a complex parameter that is not necessarily in the unit circle. Then, we have

$$\frac{1}{\pi\sqrt{-1}}\frac{\partial\Phi}{\partial a_i} = \alpha_i\frac{\partial\Phi}{\partial\alpha_i}.$$

Multiplying $t^{-(1/4)\sum f_j k_j^2}$ leads to the addition of $-\sum f_j(\log\alpha_j)^2$ to the potential function. The derivative of it with respect to α_i is

$$\alpha_i\frac{\partial}{\partial\alpha_i}\left(-\sum_{j=1}^{n} f_j(\log\alpha_j)^2\right) = -2f_i\log\alpha_i = \log\alpha_i^{-2f_i}.$$

Then, the saddle point equation is equivalent to the system of equations consisting of the gluing condition and

$$\delta(\tilde{l}_i) = \alpha_i^{2f_i}, \quad i = 1, \dots, n.$$

Recall that the dilation component of the meridian m_i of L_i is α_i^{-2}, which implies that $\delta(m_i)^{-f_i} = \delta(\tilde{l}_i)$. If we suppose that $|\alpha_i|$ is less than 1 and f_i is a positive integer, the developing image would be as shown in Figure 6.1. By filling in the singular set, the developing image becomes complete.

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SHUN SAWABE
DEPARTMENT OF PURE AND APPLIED MATHEMATICS
SCHOOL OF FUNDAMENTAL SCIENCE AND ENGINEERING
WASEDA UNIVERSITY
TOKYO
JAPAN
sa-shun.1729ttw@asagi.waseda.jp

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PUSHFORWARD AND SMOOTH VECTOR PSEUDO-BUNDLES

ENXIN WU

We study a new operation named pushforward on diffeological vector pseudo-bundles, which is left adjoint to the pullback. We show how to pushforward projective diffeological vector pseudo-bundles to get projective diffeological vector spaces, producing many concrete new examples, together with applications to smooth splittings of some projective diffeological vector spaces related to geometry. This brings new objects to diffeology from classical vector bundle theory.

1. Introduction

Diffeological spaces are elegant generalisations of smooth manifolds, including many infinite-dimensional spaces, like mapping spaces and diffeomorphism groups, and singular spaces, e.g., smooth manifolds with boundary or corners, orbifolds and irrational tori.

On diffeological spaces, one can still do some differential geometry and topology, such as differential forms and tangent bundles. These tangent bundles are, in general, no longer locally trivial. Instead, they are diffeological vector pseudo-bundles. We studied these objects and operations on them in [Christensen and Wu 2022], on which the current paper is based.

On the other hand, the theory of diffeological vector spaces and their homological algebra is intimately related to analysis and geometry; see [Wu 2015; Christensen and Wu 2016; 2021]. The projective objects there deserve special attention. However, in general, neither is it easy to test whether a given diffeological vector space is projective or not, nor is it straightforward to construct many concrete projective objects.

In this paper, we propose a way to use diffeological vector pseudo-bundles to study diffeological vector spaces. We generalise some results of projective objects for diffeological vector spaces to such bundles. In particular, we show that every classical vector bundle is such a projective object. We introduce a left adjoint called pushforward to the pullback on diffeological vector pseudo-bundles, we show that

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the free diffeological vector space generated by a diffeological space has a canonical bundle-theoretical explanation, and we show that pushforward preserves projectives. In this way, we construct many concrete projective diffeological vector spaces from classical vector bundle theory, together with applications of classical vector bundle theory to smooth splittings of some projective diffeological vector spaces.

Here is the structure of the paper. In Section 2, we briefly review some necessary background. In Section 3, we introduce pushforward on diffeological vector pseudo-bundles. Section 4 contains three parts, including necessary and sufficient conditions of smooth splittings of short exact sequences of diffeological vector pseudo-bundles, examples and properties of the projective objects, and preservation of projectives by pushforward. In particular, we get many new examples of projective diffeological vector spaces from classical vector bundles. In Section 5, we apply the established theory to smooth splittings of projective diffeological vector spaces. Readers interested in concrete examples are suggested to take a look at the last part of this section first.

2. Background

In this section, we give a very brief review, together with many related references.

Definition 2.1. A *diffeological space* is a set X together with a collection of maps $U \to X$ (called *plots*) from open subsets U of Euclidean spaces, such that:

(1) Every constant map is a plot.

(2) The composite $V \to U \to X$ is a plot if the first map is smooth between open subsets of Euclidean spaces and the second one is a plot.

(3) The map $U \to X$ is a plot if there is an open cover of U such that each restriction is a plot.

A *smooth map* $X \to Y$ between diffeological spaces is a map which sends plots of X to plots of Y. Diffeological spaces with smooth maps form a category denoted by Diff.

The idea of a diffeological space was introduced in [Souriau 1980], and [Iglesias-Zemmour 2013] is currently the standard reference for the subject. Also see [Christensen et al. 2014, Section 2] for a concise summary for the basics of diffeological spaces.

The category Diff has excellent properties. It contains the category of smooth manifolds as a full subcategory, and it is complete, cocomplete and cartesian closed. In particular, we have subspaces, quotient spaces and mapping spaces for diffeological spaces. Like charts for manifolds, we have various generating sets of plots for a diffeological space. Every diffeological space has a canonical topology called the D-topology; see [Iglesias-Zemmour 1985; Christensen et al. 2014]. Every diffeological space has a tangent bundle; see [Hector 1995; Christensen and Wu 2016; 2017]. Diffeological vector spaces are the vector space objects in Diff. Every vector space can be equipped with a smallest diffeology called the fine diffeology, making it a diffeological vector space; see [Iglesias-Zemmour 2007]. There are many other kinds of diffeological vector spaces in practice. Hierarchies of diffeological vector spaces were studied in [Christensen and Wu 2019], and homological algebra of diffeological vector spaces was developed in [Wu 2015]. The following two types of diffeological vector spaces will be needed:

Definition 2.2. A diffeological vector space V is called *projective* if for any linear subduction[1] $f : V_1 \to V_2$ and any smooth linear map $g : V \to V_2$, there exists a smooth linear map $h : V \to V_1$ such that $g = f \circ h$.

Proposition 2.3 [Wu 2015, Proposition 3.5]. *Given any diffeological space X, there exist a diffeological vector space V and a smooth map $i : X \to V$ satisfying the following universal property: for any diffeological vector space W and any smooth map $f : X \to W$, there exists a unique smooth linear map $g : V \to W$ such that $f = g \circ i$.*

The diffeological vector space V in the above proposition is unique up to isomorphism. We call it the *free diffeological vector space generated by X*, and we write $i_X : X \to F(X)$ for $i : X \to V$. As a model, $F(X) = \oplus_{x \in X}\mathbb{R}$ as a vector space, a plot $U \to F(X)$ locally factors via a smooth map through some $\mathbb{R} \times U_1 \times \cdots \times \mathbb{R} \times U_k \to F(X)$ with $(r_1, u_1, \dots, r_k, u_k) \mapsto \sum_i r_i[p_i(u_i)]$ for some $k \in \mathbb{Z}^{>0}$ and plots $p_i : U_i \to X$, and $i_X(x) = [x]$, the element 1 in the copy of $\mathbb{R}$ corresponding to $x \in X$.

We recall the following concepts from [Christensen and Wu 2022]:

Definition 2.4. A *diffeological vector pseudo-bundle* over a diffeological space B is a smooth map $\pi : E \to B$ between diffeological spaces such that the following conditions hold:

(1) For each $b \in B$, $\pi^{-1}(b) =: E_b$ is a vector space.

(2) The fibrewise addition $E \times_B E \to E$ and the fibrewise scalar multiplication $\mathbb{R} \times E \to E$ are smooth.

(3) The zero section $\sigma : B \to E$ is smooth.

Definition 2.5. Given a diffeological space B, a *bundle map over B* is a commutative triangle

$$\begin{tikzcd} E_1 \arrow[rr, "f"] \arrow[dr, "\pi_1"'] & & E_2 \arrow[dl, "\pi_2"] \\ & B & \end{tikzcd}$$

---

[1] A *subduction* is a smooth map that is isomorphic to a quotient map in Diff.

where π_1, π_2 are diffeological vector pseudo-bundles over B, f is smooth and for each $b \in B$, the restriction $f|_{E_{1,b}} : E_{1,b} \to E_{2,b}$ is linear.

Such f is called a *bundle subduction* (respectively, *bundle induction*) *over* B if it is both a bundle map over B and a subduction (respectively, an induction[2]).

For a fixed diffeological space B, all diffeological vector pseudo-bundles over B and bundle maps over B form a category, denoted by DVPB_B. An isomorphism in DVPB_B is called a *bundle isomorphism over* B. A bundle map over B is a bundle isomorphism if and only if it is both a bundle induction and a bundle subduction over B.

Definition 2.6. A commutative square

$$\begin{tikzcd} E \arrow[r, "g"] \arrow[d, "\pi"'] & E' \arrow[d, "\pi'"] \\ B \arrow[r, "f"'] & B' \end{tikzcd}$$

in Diff, with π and π' being diffeological vector pseudo-bundles, is called a *bundle map*, if for each $b \in B$, the map $g|_{E_b} : E_b \to E'_{f(b)}$ is linear.

A bundle map (g, f), as above, is called a *bundle subduction* if both g and f are subductions.

All diffeological vector pseudo-bundles and bundle maps form a category denoted by DVPB.

Note that diffeological vector pseudo-bundles are neither diffeological fibre bundles in [Iglesias-Zemmour 1985; 2013], nor diffeological fibrations in [Christensen and Wu 2014]. They were introduced to encode tangent bundles of diffeological spaces [Christensen and Wu 2016]. Many operations on DVPB_B and DVPB were studied in [Christensen and Wu 2022], such as direct product, direct sum, free diffeological vector pseudo-bundle induced by a smooth map, tensor product, and exterior product. We will use the following construction later:

Proposition 2.7 [Christensen and Wu 2022, Proposition 3.3]. *Let $\pi : E \to B$ be a smooth map between diffeological spaces such that each fibre is a vector space. Then there is a smallest diffeology on E which contains the given diffeology and which makes π into a diffeological vector pseudo-bundle over B.*

We call the original $\pi : E \to B$ a *diffeological vector prebundle* , and the procedure in this proposition is called *dvsification*. More precisely, every plot in the new diffeology of the total space is locally of the following form: Given a plot $q : U \to B$, some $k \in \mathbb{N}$, plots $q_1, \dots, q_k : U \to E$ such that $\pi \circ q_i = q$ for all i, and plots $r_1, \dots, r_k : U \to \mathbb{R}$, the linear combination $U \to E$ with $u \mapsto \sum_i r_i(u) q_i(u) \in E_{q(u)}$

---

[2] An *induction* is a smooth map that is isomorphic to an inclusion of a subspace in Diff.

is a plot in the new diffeology. Note that when $k = 0$, this is $\sigma \circ q$ for the zero section $\sigma : B \to E$.

3. Pushforward

Recall from [Christensen and Wu 2022, Section 3.1] that one can pullback diffeological vector pseudo-bundles via smooth maps, i.e., a smooth map $f : B \to B'$ induces a functor $f^* : \mathrm{DVPB}_{B'} \to \mathrm{DVPB}_B$ by pullback. Now we define a related operation as follows:

Given a smooth map $f : B \to B'$ and a diffeological vector pseudo-bundle $\pi : E \to B$, we define

$$E' = \coprod_{b' \in B'} \Big(\bigoplus_{b \in f^{-1}(b')} E_b \Big). \tag{1}$$

Note that when $f^{-1}(b') = \varnothing$, the term in the above parentheses is $\mathbb{R}^0$. There are canonical maps $\pi_f : E' \to B'$ sending the fibre above b' to b', and $\alpha_f : E \to E'$ with $E_b \hookrightarrow \bigoplus_{\tilde{b} \in f^{-1}(f(b))} E_{\tilde{b}}$. We then have a natural commutative square

$$\begin{tikzcd} E \arrow[r, "\alpha_f"] \arrow[d, "\pi"'] & E' \arrow[d, "\pi_f"] \\ B \arrow[r, "f"'] & B' \end{tikzcd}$$

Hence, we can equip E' with the dvsification of the diffeology generated by the upper horizontal map α_f of the above square, making the right vertical map π_f a diffeological vector pseudo-bundle over B', and hence the above square becomes a bundle map from π to π_f. (As a *warning*, each fibre of E' may not be the direct sum of those of E as diffeological vector spaces; see Proposition 3.5. Also notice that the notation α_f will be used later in the paper.) More precisely, we have the following explicit description of a generating set of plots on E':

Lemma 3.1. *A plot on E' is locally of one of the following forms*:

(1) *$U \to E'$ defined by a finite sum $\sum_i \alpha_f \circ p_i$, where $p_i : U \to E$ are plots on E such that all $f \circ \pi \circ p_i$'s match*;

(2) *the composite of a plot of B' followed by the zero section $B' \to E'$.*

Proof. This is straightforward from the description of dvsification as recalled in the paragraph right after Proposition 2.7. □

It is straightforward to check that we get a functor $f_* : \mathrm{DVPB}_B \to \mathrm{DVPB}_{B'}$, called the *pushforward of f*, and we write E' above as $f_*(E)$. Moreover, from the above lemma, we have:

(1) $f'_* \circ f_* = (f' \circ f)_*$ for any smooth maps $f : B \to B'$ and $f' : B' \to B''$;

(2) $(1_B)_* =$ the identity on DVPB_B.

Example 3.2. Pushforward has been used implicitly in [Christensen and Wu 2022, Section 5]. For example, E_1 and E_2 in [Christensen and Wu 2022, Proposition 5.1] are the pushforward of the tangent bundle $\mathbb{R}^2 \cong T\mathbb{R} \to \mathbb{R}$ along the inclusions $\mathbb{R} \to X_g$ to the x-axis and the y-axis, respectively.

Here is the key result for pushforward:

Theorem 3.3. *Given a smooth map $f : B \to B'$, we have an adjoint pair of functors*

$$f_* : \mathrm{DVPB}_B \rightleftharpoons \mathrm{DVPB}_{B'} : f^*.$$

Proof. We show that there is a natural bijection

$$\mathrm{DVPB}_B(E, f^*(E')) \cong \mathrm{DVPB}_{B'}(f_*(E), E').$$

Given a bundle map $E \to f^*(E')$ over B, we have $E_b \to E'_{f(b)}$ for each $b \in B$, which induce $\bigoplus_{b \in f^{-1}(b')} E_b \to E'_{b'}$, and hence a map $f_*(E) \to E'$. This is clearly a bundle map over B'. Conversely, given a bundle map $f_*(E) \to E'$ over B', we have a map $\bigoplus_{b \in f^{-1}(b')} E_b \to E'_{b'}$ for each $b' \in \mathrm{Im}(f)$. It then induces a map $E_b \to E'_{f(b)}$, which together give a map $E \to f^*(E')$. It is straightforward to check that this is a bundle map over B. These procedures are inverses to each other, and therefore we proved the desired result. □

We have the following bundle-theoretical explanation of a free diffeological vector space:

Proposition 3.4. *For any diffeological space B, the total space of the pushforward of the trivial bundle $B \times \mathbb{R} \to B$ along the map $B \to \mathbb{R}^0$ is the free diffeological vector space $F(B)$.*

Proof. This follows directly from the diffeology of the total space of the pushforward (see Lemma 3.1) and the diffeology on free diffeological vector space, as recalled in the paragraph right after Proposition 2.3. □

From [Christensen and Wu 2022, Section 3], we know that the usual operations on diffeological vector pseudo-bundles have the obvious diffeology on each fibre indicated by the operation. But pushforward is an exception, although it is expected to be so.

Proposition 3.5. *Let $f : B \to B'$ be a smooth map, and let $E \to B$ be a diffeological vector pseudo-bundle. Then the diffeology on the fibre at b' of the pushforward $f_*(E)$ has the direct sum diffeology of the diffeological vector spaces E_b with $f(b) = b'$ if and only if $f^{-1}(b')$ as a subspace of B has the discrete diffeology.*

Proof. This follows directly from Lemma 3.1. □

Here is the universal property for pushforward:

Proposition 3.6. *Given a bundle map*

$$\begin{tikzcd} E \arrow[r, "f"] \arrow[d, "\pi"'] & E' \arrow[d, "\pi'"] \\ B \arrow[r, "g"'] & B' \end{tikzcd}$$

there exists a unique bundle map $\beta : g_*(E) \to E'$ *over* B' *such that* $f = \beta \circ \alpha_g$.

Proof. This is clear by the construction of pushforward, or from the adjoint (Theorem 3.3). □

Pushforward can send nonisomorphic bundles to isomorphic ones:

Example 3.7. Write B for the cross with the gluing diffeology, and write B' for the cross with the subset diffeology of $\mathbb{R}^2$. Then $B \to B'$ defined as the identity underlying set map is smooth, but its inverse is not; see [Christensen and Wu 2016, Example 3.19]. We show below that the induced map $F(B) \to F(B')$ between the free diffeological vector spaces, which is the identity for the underlying vector spaces, is indeed an isomorphism of diffeological vector spaces. This means that the pushforward of the two trivial bundles $B \times \mathbb{R} \to B$ and $B' \times \mathbb{R} \to B'$ along the maps $B \to \mathbb{R}^0$ and $B' \to \mathbb{R}^0$ are isomorphic, but clearly the two bundles are not.

By definition of a free diffeological vector space, every plot $p : U \to F(B')$ can be locally written as a finite sum $p(u) = \sum_i r_i(u)(p_{1i}(u), p_{2i}(u))$ for smooth maps r_i, p_{1i}, p_{2i} with codomain $\mathbb{R}$ satisfying $p_{1i}(u)p_{2i}(u) = 0$ for all u. It is enough to show that p can be viewed as a plot of $F(B)$. This is the case since $(p_{1i}(u), p_{2i}(u))$ can be written as $(p_{1i}(u), 0) + (0, p_{2i}(u)) - (0, 0)$, with each term viewed as a plot of B.

As a consequence of the above example, the canonical map $i_X : X \to F(X)$ from a diffeological space to the free diffeological vector space generated by it is *not* necessarily an induction.

On the other hand, we have:

Proposition 3.8. *The canonical map* $i_X : X \to F(X)$ *is an induction if and only if there exists a family of diffeological vector spaces* $\{V_i\}_{i \in I}$ *such that the diffeology on* X *is determined by the union of all* $C^\infty(X, V_i)$, *in the sense that* $U \to X$ *is a plot if and only if the composite* $U \to X \to V_i$ *is smooth for every smooth map* $X \to V_i$.

In particular, for every Frölicher space X (i.e., the diffeology on X is determined by $C^\infty(X, \mathbb{R})$), the canonical map $X \to F(X)$ is an induction. This applies to B' in Example 3.7.

Proof. This follows immediately from the universal property of the free diffeological vector space generated by a diffeological space. □

4. Projective diffeological vector pseudo-bundles

4A. *Enough projectives.* In this subsection, we will work in the category DVPB_B for a fixed diffeological space B. So we will omit the phrase "over B" in many places, as long as no confusion shall occur. Note that when we take $B = \mathbb{R}^0$, we recover the corresponding results for the category of diffeological vector spaces.

We first study smooth splittings of diffeological vector pseudo-bundles, which will be used later in the paper.

Definition 4.1. A diagram of morphisms

$$\begin{tikzcd} E_1 \arrow[r, "f"] & E_2 \arrow[r, "g"] & E_3 \end{tikzcd}$$

in DVPB_B is called a *short exact sequence* if f is a bundle induction, g is a bundle subduction and

$$\begin{tikzcd} E_{1,b} \arrow[r, "f_b"] & E_{2,b} \arrow[r, "g_b"] & E_{3,b} \end{tikzcd}$$

is exact (i.e., $\ker(g_b) = \mathrm{Im}(f_b)$) for every $b \in B$.

As a direct consequence of the above definition, we have:

Corollary 4.2. *Given a short exact sequence*

$$\begin{tikzcd} E_1 \arrow[r] & E_2 \arrow[r] & E_3 \end{tikzcd}$$

of diffeological vector pseudo-bundles over B, *we have a bundle isomorphism* $E_2/E_1 \cong E_3$ *over* B.

The splitting of a short exact sequence goes as usual:

Theorem 4.3. *Assume that*

$$\begin{tikzcd} E_1 \arrow[r, "f"] & E_2 \arrow[r, "g"] & E_3 \end{tikzcd}$$

is a short exact sequence of diffeological vector pseudo-bundles over B. *Then the following are equivalent*:

(1) *There exists a bundle map* $g' : E_3 \to E_2$ *over* B *such that* $g \circ g' = 1_{E_3}$.

(2) *There exists a bundle map* $f' : E_2 \to E_1$ *over* B *such that* $f' \circ f = 1_{E_1}$.

(3) *There exists a bundle isomorphism* $E_2 \to E_1 \oplus E_3$ *over* B *making the following diagram commutative*:

$$\begin{tikzcd} E_1 \arrow[r, "f"] \arrow[d, "="'] & E_2 \arrow[r, "g"] \arrow[d] & E_3 \arrow[d, "="] \\ E_1 \arrow[r, "i_1"'] & E_1 \oplus E_3 \arrow[r, "p_2"'] & E_3 \end{tikzcd}$$

If any one of the conditions holds in the theorem, we say that the short exact sequence *splits smoothly*, and that E_1 (respectively, E_3) is a *smooth direct summand* of E_2. Although every short exact sequence of vector spaces splits, it is not the case in DVPB_B, even when $B = \mathbb{R}^0$; see [Wu 2015, Example 4.3] or [Christensen and Wu 2019, Example 4.1].

Proof. We show below that (1) $\Longleftrightarrow$ (3), and (2) $\Longleftrightarrow$ (3) can be proved similarly.

(1) $\Longrightarrow$ (3): Since we have bundle maps $f : E_1 \to E_2$ and $g' : E_3 \to E_2$, we define the map $E_1 \oplus E_3 \to E_2$ by $(x_1, x_3) \mapsto f(x_1) + g'(x_3)$ for any $x_1 \in E_{1,b}$, $x_3 \in E_{3,b}$ and $b \in B$. This is clearly a bundle map over B. Its inverse is given by $x \mapsto (f^{-1}(x - g' \circ g(x)), g(x))$. It is straightforward to check that this is well defined, and it is smooth since f is an induction.

(3) $\Longrightarrow$ (1): The map g' is defined by the composite $E_3 \xrightarrow{i_2} E_1 \oplus E_3 \xrightarrow{\cong} E_2$. The rest are straightforward to check. □

Now we can define projective diffeological vector pseudo-bundles and show that there are *enough* such objects.

Definition 4.4. A diffeological vector pseudo-bundle $E \to B$ is called *projective* if for any bundle subduction $f : E_1 \to E_2$ over B and any bundle map $g : E \to E_2$ over B, there exists a bundle map $h : E \to E_1$ over B making the triangle commutative:

$$\begin{tikzcd}
& E \arrow[dl, dotted, "h"'] \arrow[d, "g"] \\
E_1 \arrow[r, "f"'] & E_2
\end{tikzcd}$$

Formally, we have the following basic properties:

Proposition 4.5. (1) *Let $\{E_i \to B\}$ be a family of diffeological vector pseudo-bundles. Then the direct sum $\bigoplus_i E_i \to B$ is projective if and only if each $E_i \to B$ is.*

(2) *The projectiveness of diffeological vector pseudo-bundles is inherited by taking retracts.*

(3) *Any bundle subduction to a projective diffeological vector pseudo-bundle splits smoothly.*

Recall from [Christensen and Wu 2022, Section 3.2.5] that given a smooth map $f : X \to B$, we get a diffeological vector pseudo-bundle $\pi : F_B(X) \to B$. More precisely, it is constructed as follows: For each $b \in B$, write X_b for $f^{-1}(b)$ with the subset diffeology of X. As a set $F_B(X) = \coprod_{b \in B} F(X_b)$, the disjoint union of the free diffeological vector spaces generated by these X_b and $\pi : F_B(X) \to B$ is the canonical projection. So we have the commutative triangle

$$\begin{tikzcd} X \arrow[r, "i"] \arrow[dr, "f"'] & F_B(X) \arrow[d, "\pi"] \\ & B \end{tikzcd}$$

where the horizontal map is given by $x \in X_b \mapsto [x] \in F(X_b)$. The dvsification of i makes $\pi : F_B(X) \to B$ into a diffeological vector pseudo-bundle[3]. Then we have the following universal property for $\pi : F_B(X) \to B$: Given any diffeological vector pseudo-bundle $E \to B$ and any smooth map $h : X \to E$ over B, there is a unique bundle map $g : F_B(X) \to E$ over B such that $h = g \circ i$.

Lemma 4.6. *Let $f : X \to B$ be a smooth map. The corresponding diffeological vector pseudo-bundle $\pi : F_B(X) \to B$ is projective if and only if for any bundle subduction $\alpha : E_1 \to E_2$ over B and any smooth map $\beta : X \to E_2$ over B, there exists a smooth map $\gamma : X \to E_1$ over B such that $\beta = \alpha \circ \gamma$.*

Proof. As usual, this follows from the universal property of $\pi : F_B(X) \to B$. □

Proposition 4.7. *Every plot $U \to B$ induces a projective diffeological vector pseudo-bundle $F_B(U) \to B$.*

Proof. Given any bundle subduction $f : E_1 \to E_2$ over B and any smooth map $g : U \to E_2$ over B, we have smooth local liftings h_i of g to E_1. Let $\{\lambda_i\}$ be a smooth partition of unity subordinate to the corresponding open cover $\{U_i\}$ of U. Then $\sum_i \lambda_i \cdot h_i : U \to E_1$ is a global smooth lifting of g over B, where each $\lambda_i \cdot h_i : U \to E_1$ is defined as

$$(\lambda_i \cdot h_i)(u) = \begin{cases} \lambda_i(u) h_i(u), & \text{if } u \in U_i, \\ \sigma_1 \circ \pi_2 \circ g(u), & \text{else,} \end{cases}$$

with $\sigma_1 : B \to E_1$ denoting the zero section and $\pi_2 : E_2 \to B$ denoting the given diffeological vector pseudo-bundle. The result then follows from Lemma 4.6. □

As a direct consequence of the above proof, we have:

Corollary 4.8. *For every bundle subduction, a plot of the total space of the codomain **globally** lifts to a plot of the total space of the domain.*

Theorem 4.9. *For every diffeological space B, the category* DVPB_B *has enough projectives, i.e., given any diffeological vector pseudo-bundle $E \to B$, there exists a projective diffeological vector pseudo-bundle $E' \to B$ together with a bundle subduction $E' \to E$ over B.*

---

[3] More precisely, the map i transfers the diffeology of X to the set $F_B(X)$, which makes $\pi : F_B(X) \to B$ into a diffeological vector prebundle because of the above commutative triangle. The dvsification is then applied to this prebundle.

Proof. We take $E' \to B$ to be the direct sum in DVPB_B of all $F_B(U) \to B$ indexed over all plots $U \to E$. By Proposition 4.7, each $F_B(U) \to B$ is projective, and hence by Proposition 4.5 (1), $E' \to B$ is projective. By the universal property of $F_B(U) \to B$, we get a bundle map $F_B(U) \to E$ over B, and hence a bundle map $E' \to E$ over B. By construction, this map is a subduction. □

In summary, for a fixed diffeological space B, the pair of projective diffeological vector pseudo-bundles over B and the bundle subductions over B forms a projective class.

4B. ***Examples and properties of projectives.*** We first give some examples of projective diffeological vector pseudo-bundles related to classical vector bundle theory. To do so, we need:

Lemma 4.10. *For a smooth map $f : B \to B'$, the pullback f^* sends a bundle subduction over B' to a bundle subduction over B, and hence it preserves short exact sequences.*

Proof. Let $g : E'_1 \to E'_2$ be a bundle subduction over B'. Then $f^*(E'_1) \to f^*(E'_2)$ is given by sending (b, x) to $(b, g(x))$. Every plot $p : U \to f^*(E'_2)$ gives rise to smooth maps $p_1 : U \to B$ and $p_2 : U \to E'_2$ via composition with the two projections. Since g is a bundle subduction, p_2 locally lifts as a smooth map to E'_1, which together with p_1 induces a local lifting of p to $f^*(E'_1)$, showing the first claim.

Since f^* is a right adjoint by Theorem 3.3, it preserves bundle inductions, which together with the first claim proves the second one. □

Remark 4.11. The above lemma also follows from the fact that the pullback $f^* : \mathrm{DVPB}_{B'} \to \mathrm{DVPB}_B$ has a right adjoint $f_!$. Given a diffeological vector pseudo-bundle $\pi : E \to B$, the bundle $f_!(E) \to B'$ is constructed as

$$f_!(E) = \coprod_{b' \in B'} \Gamma(\pi|_{f^{-1}(b')}).$$

When $f^{-1}(b') = \varnothing$, $\Gamma(\pi|_{f^{-1}(b')})$ is $\mathbb{R}^0$. A map $p : U \to f_!(E)$ is a plot if:

(1) The composite $U \xrightarrow{p} f_!(E) \xrightarrow{\tilde{\pi}} B'$ is a plot of B', where $\tilde{\pi}$ sends $\Gamma(\pi|_{f^{-1}(b')})$ to b'.

(2) For any smooth map $g : V \to U$ and any plot $h : V \to B$ such that the following diagram commutes:

$$\begin{tikzcd} V \arrow[r, "g"] \arrow[d, "h"'] & U \arrow[r, "p"] & f_!(E) \arrow[d, "\tilde{\pi}"] \\ B \arrow[rr, "f"'] & & B' \end{tikzcd}$$

the map $V \to E$ defined by $v \mapsto (p(g(v)))(h(v))$ is a plot of E.

It is straightforward to check that $\tilde{\pi}$ is a smooth map between diffeological spaces such that each fibre is a vector space. After dvsification, we get the desired diffeology on the total space $f_!(E)$. One can check that $f_!$ is a functor which is right adjoint to the pullback f^*. Moreover, each fibre of $f_!(E) \to B'$ has the diffeology of the section space; see [Christensen and Wu 2022, Section 3.1]. (I would like to thank J. Daniel Christensen for the suggestion of the set-theoretical construction of $f_!(E)$ in this remark from a type theory point of view.)

Projectiveness is local in the following sense:

Proposition 4.12. *Let $\pi : E \to B$ be a diffeological vector pseudo-bundle. Assume that there exists a D-open cover $\{B_j\}$ of B such that $i_j^*(E) \to B_j$ is projective in* DVPB_{B_j} *for each j, where $i_j : B_j \to B$ denotes the inclusion, together with a smooth partition of unity $\{\lambda_j : B \to \mathbb{R}\}$ subordinate to this cover. Then π is projective in* DVPB_B.

Proof. For any bundle subduction $f : E_1 \to E_2$ over B and any bundle map $g : E \to E_2$ over B, we get a diagram over B_j for each j:

$$\begin{tikzcd}
 & i_j^*(E) \arrow[d, "i_j^*(g)"] \\
i_j^*(E_1) \arrow[r, "i_j^*(f)"'] & i_j^*(E_2)
\end{tikzcd}$$

Lemma 4.10 shows that the horizontal arrow is a bundle subduction over B_j. By assumption, we have a smooth lifting $h_j : i_j^*(E) \to i_j^*(E_1)$ over B_j. Then $\sum_j \lambda_j \cdot h_j : E \to E_1$ is a bundle map over B, as we desired. □

We also have the following expected result:

Proposition 4.13. *Let V be a projective diffeological vector space, and let B be a smooth manifold. Then the trivial bundle $B \times V \to B$ is projective.*

Surprisingly, note that the result can fail if B is an arbitrary diffeological space; see Example 4.27.

Proof. We first reduce the above statement to a special case. By Proposition 4.12, it is enough to prove this for the case when B is an open subset of a Euclidean space. Recall that every projective diffeological vector space is a smooth direct summand of direct sums of $F(U)$ for open subsets U of Euclidean spaces [Wu 2015, Corollary 6.15]. By Proposition 4.5 (1) and (2), it is enough to show this for the case when $V = F(U)$ for an open subset U of a Euclidean space.

Now we prove the statement for the special case when $V = F(U)$ and both B and U are Euclidean open subsets. As diffeological vector pseudo-bundles over B, we have isomorphisms $F_B(B \times U) \cong B \times F(U)$ of total spaces. The result then follows directly from Proposition 4.7. ☐

Combining the above two propositions together with the fact that every fine diffeological vector space is projective, we get:

Corollary 4.14. *Vector bundles in classical differential geometry are projective.*

However, a projective diffeological vector pseudo-bundle does not need to be locally trivial, even when the base space is Euclidean:

Example 4.15. Let $f : \mathbb{R} \to \mathbb{R}$ be the square function $x \mapsto x^2$. By Proposition 4.7, $F_{\mathbb{R}}(\mathbb{R}) \to \mathbb{R}$ is projective. Clearly, the fibre is $\mathbb{R}^0$ for $b < 0$, $\mathbb{R}$ for $b = 0$ and $\mathbb{R}^2$ for $b > 0$. Therefore, a projective diffeological vector pseudo-bundle does not need to be locally trivial.

Now we discuss some properties of projective diffeological vector pseudo-bundles.

Proposition 4.16. *Every projective diffeological vector pseudo-bundle $E \to B$ is a smooth direct summand of direct sum in* DVPB_B *of $F_B(U) \to B$ induced by some plots $U \to B$.*

Proof. By the proof of Theorem 4.9, we get a bundle subduction $E' \to E$ over B, with E' a direct sum in DVPB_B of $F_B(U) \to B$ induced by the plots $U \to E$ (and hence some plots $U \to B$, where repetition is allowed). Since $E \to B$ is projective, the result then follows from Proposition 4.5 (3). ☐

We are going to use the following notation from [Christensen and Wu 2019]: Let V be a diffeological vector space, and let X be a diffeological space.

(1) We say that all smooth linear functionals $V \to \mathbb{R}$ separate points of V, if for any $v \in V \setminus \{0\}$, there exists a smooth linear map $f : V \to \mathbb{R}$ such that $f(v) \neq 0$. Write $\mathcal{SV}$ for the family of all such diffeological vector spaces.

(2) We say that all smooth functions $X \to \mathbb{R}$ separate points of X, if for any $x, x' \in X$ with $x \neq x'$, there exists a smooth function $f : X \to \mathbb{R}$ such that $f(x) \neq f(x')$. Write $\mathcal{SD}'$ for the family of all such diffeological spaces.

Corollary 4.17. *Let $E \to B$ be a projective diffeological vector pseudo-bundle. Then $E_b \in \mathcal{SV}$ for every $b \in B$, i.e., the smooth linear functionals on E_b separate points.*

Proof. By Proposition 4.16, we know that E is a smooth direct summand of direct sums in DVPB_B of $F_B(U) \to B$ induced by some plots $U \to B$. As $\mathcal{SV}$ is closed under taking both smooth direct summands and direct sums [Christensen and Wu 2019, Proposition 3.11], it is enough to show the claim for the special case $F_B(U) \to B$ which is induced by a plot $p : U \to B$. In this case, the fibre at $b \in B$ is the free diffeological vector space generated by $p^{-1}(b)$ [Christensen and Wu 2022, Section 3.2.5], which is a subset of a Euclidean space, and hence $p^{-1}(b) \in \mathcal{SD}'$, i.e., the smooth functions on $p^{-1}(b)$ separate points. The result then follows from [Christensen and Wu 2019, Proposition 3.13]. ☐

One would expect that each fibre of a projective diffeological vector pseudo-bundle is a projective diffeological vector space. This is equivalent to the statement that the free diffeological vector space generated by *any* subset with the subset diffeology of a Euclidean space is projective, by a similar argument as above. But I don't know whether this is true or not. Nevertheless, we have:

Proposition 4.18. *Let B be a diffeological space. Then every fibre of a projective diffeological vector pseudo-bundle $E \to B$ is a projective diffeological vector space if and only if for every plot $p : U \to B$ and every $b \in B$, the free diffeological vector space generated by $p^{-1}(b)$ is projective.*

Proof. (⇒): This follows directly from Proposition 4.7.

(⇐): The proof follows from a similar argument as the one in the proof of the above corollary. ☐

Proposition 4.19. *Let B be a discrete diffeological space*, i.e., *every plot is locally constant. Then a diffeological vector pseudo-bundle over B is projective if and only if each fibre is a projective diffeological vector space.*

Proof. (⇒): This follows from the definition of a discrete diffeological space, together with Proposition 4.18 and [Wu 2015, Corollary 6.4].

(⇐): This follows from the fact that every diffeological vector pseudo-bundle over a discrete diffeological space is a coproduct in DVPB of diffeological vector spaces over a point. ☐

Also, we have the following results:

Proposition 4.20. *Let $\pi : E \to B$ be a projective diffeological vector pseudo-bundle, and let $\pi_1 \to \pi_2 \to \pi_3$ be a short exact sequence in DVPB_B, with $\pi_i : E_i \to B$. Then $\mathrm{Hom}_B(\pi, \pi_1) \to \mathrm{Hom}_B(\pi, \pi_2) \to \mathrm{Hom}_B(\pi, \pi_3)$ is also a short exact sequence in DVPB_B.*

Proof. By Proposition 4.16, we know that π is a smooth direct summand of direct sums of $F_B(U) \to B$ indexed by some plots $U \to B$. It is straightforward to check that both direct summand and direct product preserve short exact sequences in DVPB_B. For the direct product case, one needs Corollary 4.8 for the subduction part. By the universal property of a free bundle induced by a smooth map (see [Christensen and Wu 2022, Section 3.2.5] or the paragraph above Lemma 4.6), one has a bundle isomorphism over B from $\mathrm{Hom}_B(F_B(U), E_i)$ to the set $\mathrm{Hom}_B(U, E_i)$ of all smooth maps $U \to E_i$ preserving B, equipped with the subset diffeology of $C^\infty(U, E_i)$. Again by Corollary 4.8, it is direct to check that the functor $\mathrm{Hom}_B(U, -)$ preserves short exact sequences in DVPB_B. The result then follows by the above observations together with the first isomorphism in [Christensen and Wu 2022, Proposition 3.13] □

Remark 4.21. The converse of Proposition 4.20 is false. This is due to the fact that $\mathrm{Hom}_B(\pi, -)$ always preserves short exact sequences in DVPB_B for the trivial bundle $\pi : B \times \mathbb{R} \to B$, as it is naturally isomorphic to the identity functor. But the trivial bundle may not be projective; see Example 4.27.

As a consequence of Proposition 4.20 and [Christensen and Wu 2022, Proposition 3.12], we have:

Corollary 4.22. *If $E_1 \to B$ and $E_2 \to B$ are projective diffeological vector pseudo-bundles, then so is their tensor product $E_1 \otimes E_2 \to B$.*

Since $\bigwedge^k E$ is a smooth direct summand of $E^{\otimes k}$ (as a result of [Pervova 2019, Lemma 2.11] and Theorem 4.3), by the above corollary and Proposition 4.5 (2), we have:

Corollary 4.23. *If $E \to B$ is a projective diffeological vector pseudo-bundle, then so is each exterior product $\bigwedge^k E \to B$ for $k \geq 1$.*

4C. *Base change.*

Theorem 4.24. *The pushforward $f_* : \mathrm{DVPB}_B \to \mathrm{DVPB}_{B'}$ sends projectives in the domain to the projectives in the codomain.*

Proof. By the adjunction of Theorem 3.3, the following lifting problems are equivalent:

$$\begin{tikzcd} & f_*(E) \arrow[dl, dotted] \arrow[d] \\ E'_1 \arrow[r] & E'_2 \end{tikzcd} \iff \begin{tikzcd} & E \arrow[dl, dotted] \arrow[d] \\ f^*(E'_1) \arrow[r] & f^*(E'_2) \end{tikzcd}$$

where $E'_1 \to E'_2$ is a bundle subduction over B'. By Lemma 4.10 and Definition 4.4, we know that the lifting problem on the right has a solution, and hence so is the one on the left. □

This theorem has several applications. We first give another class of examples of projective diffeological vector pseudo-bundles from tangent bundles of diffeological spaces. To do so, we need the following result:

Note that projective diffeological vector pseudo-bundles are defined in DVPB_B, but they have a similar property in DVPB as follows:

Proposition 4.25. *Given a bundle subduction $f : E_1' \to E_2'$ over B' and a bundle map*

$$\begin{tikzcd} E \arrow[r, "g"] \arrow[d, "\pi"'] & E_2' \arrow[d] \\ B \arrow[r, "l"'] & B' \end{tikzcd}$$

with π projective, there exists a bundle map $h : E \to E_1'$ such that $g = f \circ h$.

Proof. By the universal property of pushforward (Proposition 3.6), we can write g as a bundle map $\tilde{g} : l_*(E) \to E_2'$ over B' followed by the bundle map $\alpha_l : E \to l_*(E)$. By Theorem 4.24, the assumption that π is projective over B implies that $\pi_l : l_*(E) \to B'$ is projective over B'. Therefore, we have a bundle map $\tilde{h} : l_*(E) \to E_1'$ over B' such that $\tilde{g} = f \circ \tilde{h}$. Then the composite $\tilde{h} \circ \alpha_l$ is the bundle map h we are looking for. ☐

Let B be an arbitrary diffeological space, and let $b \in B$. The local structure of B at b is encoded by the pointed plot category whose objects are the pointed plots $(U, 0) \to (B, b)$ for open subsets U of some Euclidean spaces containing the origin 0, and whose morphisms are the obvious commutative triangles preserving the base points. The (internal) tangent space $T_b(B)$ is defined to be the colimit of the functor from the pointed plot category to the category of vector spaces by sending $p : (U, 0) \to (B, b)$ to $T_0(U)$. As a set, the total space TB of the (internal) tangent bundle of B is the disjoint union of all these $T_b(B)$, and $TB \to B$ is the obvious projection. Every plot $p : U \to B$ gives rise to a natural commutative square

$$\begin{tikzcd} TU \arrow[r, "Tp"] \arrow[d] & TB \arrow[d] \\ U \arrow[r, "p"'] & B \end{tikzcd}$$

Hector [1995] defined a diffeology on the set TB as the smallest one containing all such Tp, and we denote this diffeological space as $T^H B$. In this way, $T^H B \to B$ is in general a diffeological vector prebundle, but not necessarily a diffeological vector pseudo-bundle. Its dvsification is denoted by $T^{\text{dvs}} B \to B$.

Equivalently, [Christensen and Wu 2016, Theorem 4.17] claims that every tangent bundle $T^{\text{dvs}} B \to B$ of a diffeological space B is a colimit in DVPB of the tangent bundles $TU \to U$ indexed by the plots $U \to B$. Each $TU \to U$ is projective by Corollary 4.14. It is possible that some tangent bundles are projective. (But this is not always the case; see Example 4.27.) We show this by an example:

Example 4.26. Write B for the cross with the gluing diffeology. We show below that the tangent bundle $T^{\text{dvs}} B \to B$ is projective.

Note that B is the pushout of

$$\begin{tikzcd} \mathbb{R} & \mathbb{R}^0 \arrow[l, "0"'] \arrow[r, "0"] & \mathbb{R} \end{tikzcd}$$

in Diff. It is straightforward to check that the tangent bundle $T^{\mathrm{dvs}}B \to B$ is the colimit of

$$\begin{tikzcd}
T\mathbb{R} \arrow[d] & T\mathbb{R}^0 \arrow[l, "T0"'] \arrow[r, "T0"] \arrow[d] & T\mathbb{R} \arrow[d] \\
\mathbb{R} & \mathbb{R}^0 \arrow[l, "0"] \arrow[r, "0"'] & \mathbb{R}
\end{tikzcd}$$

in DVPB. Write $Tx : T\mathbb{R} \to T^{\mathrm{dvs}}B$ and $Ty : T\mathbb{R} \to T^{\mathrm{dvs}}B$ for the two structural maps. Given a bundle subduction $f : E_1 \to E_2$ over B and a bundle map $g : T^{\mathrm{dvs}}B \to E_2$, since $T\mathbb{R} \to \mathbb{R}$ is projective, by Proposition 4.25 we have bundle maps $hx, hy : T\mathbb{R} \to E_1$ such that $g \circ Tx = f \circ hx$ and $g \circ Ty = f \circ hy$. By the universal property of pushout, we get a desired bundle map $h : T^{\mathrm{dvs}}B \to E_1$ over B with the required property.

As another consequence of Theorem 4.24, we have the following example which gives counterexamples to several arguments:

Example 4.27. If the free diffeological vector space $F(B)$ is not projective, then the trivial bundle $B \times \mathbb{R} \to B$ is not projective. This happens when the D-topology on B is not Hausdorff [Christensen and Wu 2019, Corollary 3.17]. The proof of the statement follows from Proposition 3.4 and Theorem 4.24.

This example shows that not every trivial bundle is projective, even when the fibre is a projective (or fine) diffeological vector space. It also shows that the pullback functor does *not* preserve projectives, since the trivial bundle $B \times \mathbb{R} \to B$ is the pullback of $\mathbb{R} \to \mathbb{R}^0$ along the map $B \to \mathbb{R}^0$. Furthermore, it shows that not every tangent bundle is projective. For example, $TB \to B$ is not projective when B is an irrational torus, since in this case $TB = B \times \mathbb{R}$ [Christensen and Wu 2016, combining Examples 3.23 and 4.19 (3) with Theorem 4.15] and the D-topology on B is not Hausdorff.

Moreover, via Theorem 4.24 and Section 4B, we get many examples of projective diffeological vector spaces from classical differential geometry!

5. Applications to smooth splittings of projective diffeological vector spaces

By [Christensen and Wu 2019, Proposition 3.14 and Theorem 4.2], we know that every finite-dimensional linear subspace of a projective diffeological vector space is a smooth direct summand; or in other words, the only indecomposable projective diffeological vector space is $\mathbb{R}$. In this section, we use classical smooth bundle theory, and the theory established so far, to get some general criteria and interesting examples of smooth splittings of projective diffeological vector spaces.

To simplify notation, we write V_π (or V_E when the bundle is understood) for the diffeological vector space obtained from the pushforward of the diffeological vector pseudo-bundle $\pi : E \to B$ along the map $B \to \mathbb{R}^0$.

5A. ***General theory.*** Here is the general setup. Given a classical fibre (respectively, principal) bundle $E \to B$, we get a linear subduction $F(E) \to F(B)$ of diffeological vector spaces which splits smoothly since $F(B)$ is projective. We aim to give a bundle-theoretical explanation of its kernel. In fact, we will prove more general results as follows:

Given a bundle map

$$\begin{tikzcd} E_1 \arrow[r, "g"] \arrow[d, "\pi_1"'] & E_2 \arrow[d, "\pi_2"] \\ B_1 \arrow[r, "f"'] & B_2 \end{tikzcd}$$

from a diffeological vector pseudo-bundle π_1 to another π_2, by Proposition 3.6, we get a bundle map $h : f_*(E_1) \to E_2$ over B_2 so that $g = h \circ \alpha_f$, where $\alpha_f : E_1 \to f_*(E_1)$ is the structural map introduced at the beginning of Section 3. Write $\pi : E \to B_2$ for the kernel of h.

Here is the key result:

Theorem 5.1. *Let* $(g, f) : \pi_1 \to \pi_2$ *be a bundle map as above, with* E_1 *locally Euclidean, and* B_2 *Hausdorff and filtered*[4]. *Then we have a smooth linear map* $g_* : V_{\pi_1} \to V_{\pi_2}$ *between diffeological vector spaces, whose kernel is isomorphic to* V_π, *with* $\pi : E \to B_2$ *defined above.*

Proof. By Proposition 3.6, we get a smooth linear map $g_* : V_{\pi_1} \to V_{\pi_2}$. Write K for its kernel. It consists of elements of finite sum $\sum_i e_i$ in V_{π_1}, with $e_i \in E_1$, such that for each $b_2 \in B_2$, the subsum $\sum_{i:\pi_2 \circ g(e_i)=b_2} g(e_i) = 0$. So there is a canonical isomorphism $\alpha : V_\pi \to K$ as vector spaces, which is smooth by Lemma 3.1.

Now we use all the extra assumptions to show that the inverse map α^{-1} is smooth. Take a plot $p : U \to K$ and fix $u_0 \in U$. Since the composite $U \to K \hookrightarrow V_{\pi_1}$ is smooth, by Lemma 3.1, there exist finitely many plots $p_i : U \to E_1$, by shrinking U around u_0 if necessary, such that $p(u) = \sum_i p_i(u)$ which satisfies that for each $b_2 \in B_2$, the subsum $\sum_{i:f\circ\pi_1\circ p_i(u)=b_2} g(p_i(u)) = 0$ for every $u \in U$. Fix $b_2^0 \in B_2$. Since B_2 is Hausdorff, we may assume that the image of the composites $f \circ \pi_1 \circ p_i$ do not intersect if their value at u_0 are distinct. Now take all the index i so that $f \circ \pi_1 \circ p_i(u_0) = b_2^0$, and denote this index subset by I_{u_0,b_2^0}. Since E_1 is locally

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[4] A diffeological space X is *filtered*, if for every $x \in X$, the germ category of X at x is filtered, i.e., every finite diagram in the germ category has a cocone. Here, the germ category is like the pointed plot category, with morphisms changed to be smooth germs at the base points instead of genuine pointed maps. See [Christensen and Wu 2017; 2022] for more details.

Euclidean and B_2 is filtered, there exist a pointed plot $q : (V, 0) \to (B_2, b_2^0)$ and smooth pointed germs $h_i : (E_1, p_i(u_0)) \to (V, 0)$, so that $q \circ h_i = f \circ \pi_1$ and $h_i \circ p_i$ is independent of i, for all $i \in I_{u_0, b_2^0}$. This then implies that $f \circ \pi_1 \circ p_i = q \circ h_i \circ p_i$ are independent of i for all $i \in I_{u_0, b_2^0}$, and hence follows the smoothness of α^{-1}. ☐

Proposition 5.2. *If* $(g, f) : \pi_1 \to \pi_2$ *is a bundle subduction, then we get a linear subduction* $g_* : V_{\pi_1} \to V_{\pi_2}$ *of diffeological vector spaces.*

Proof. This follows directly from Proposition 3.6 and Lemma 3.1. ☐

As a consequence of the above results, we have:

Corollary 5.3. *Let* $(g, f) : \pi_1 \to \pi_2$ *be a bundle subduction so that* E_1 *is locally Euclidean, and* B_2 *is Hausdorff and filtered. Then we have a short exact sequence of diffeological vector spaces*

$$0 \to V_\pi \to V_{\pi_1} \to V_{\pi_2} \to 0.$$

Now we discuss a special case:

$$\begin{tikzcd} Y \times \mathbb{R} \arrow[r, "f \times 1_{\mathbb{R}}"] \arrow[d, "\mathrm{Pr}_1"'] & B \times \mathbb{R} \arrow[d, "\mathrm{Pr}_1"] \\ Y \arrow[r, "f"'] & B \end{tikzcd} \tag{2}$$

where f is an arbitrary smooth map.

Observe that:

Proposition 5.4. *The pushforward of* $\mathrm{Pr}_1 : Y \times \mathbb{R} \to Y$ *along* $f : Y \to B$ *is exactly the free bundle* $F_B(Y) \to B$.

Proof. This follows directly from the definition of the free bundle (see [Christensen and Wu 2022, Section 3.2.5] or the paragraph right after Proposition 4.5) and the definition of pushforward of a diffeological vector pseudo-bundle from Section 3. ☐

Note that the bundle map $F_B(Y) \to B \times \mathbb{R}$ over B is given by $\sum_i r_i [y_i] \mapsto \big(b, \sum_i r_i\big)$, where $f(y_i) = b$ for all i. We write $\bar{f}_* : \bar{F}_B(Y) \to B$ for its kernel.

Remark 5.5. (1) This proposition generalises Proposition 3.4 by taking $B = \mathbb{R}^0$.

(2) From above, we know that $F(Y)$ always has a smooth direct summand $\mathbb{R}$ (i.e., $F(Y) \cong \mathbb{R} \oplus \bar{F}(Y)$), since $\mathbb{R}$ is a projective diffeological vector space. This can be viewed as a property of the free diffeological vector space, and not every diffeological vector space is free over some diffeological space.

On the contrary, not every trivial line bundle $B \times \mathbb{R} \to B$ is projective when $B \neq \mathbb{R}^0$ (see Example 4.27), so the free bundle $F_B(Y) \to B$ may not have a smooth direct summand $B \times \mathbb{R} \to B$.

In the current special case, we have:

Corollary 5.6. *Let $f : Y \to B$ be a smooth map, with Y locally Euclidean and B Hausdorff and filtered.*

(1) *The kernel of $f_* : F(Y) \to F(B)$ is isomorphic to $V_{\bar{f}_*}$ with $\bar{f}_* : \bar{F}_B(Y) \to B$ as defined above.*

(2) *If f is a subduction, then we get a short exact sequence of diffeological vector spaces*

$$0 \to V_{\bar{f}_*} \to F(Y) \to F(B) \to 0.$$

(3) *The pushforward of the free bundle $F_B(Y) \to B$ along $B \to \mathbb{R}^0$ is isomorphic to the free diffeological vector space $F(Y)$.*

Remark 5.7. To make $f_* : F(Y) \to F(B)$ a linear subduction, it is not necessary to require $f : Y \to B$ to be a subduction; see Example 3.7.

Now we discuss a more special case, which occurs often in practice: In the diagram (2), we further assume that f is a principal G-bundle[5] for some diffeological group G. We give an alternative description of the bundle $V_{\bar{f}_*}$ as follows.

As a setup, assume that G acts smoothly on Y on the right. Note that G acts smoothly on $F(G)$ on the left by $G \times F(G) \to F(G)$, given by $g \cdot \sum_i r_i[g_i] = \sum_i r_i[gg_i]$, and it passes to a smooth left action of G on $\bar{F}(G)$, where $\bar{F}(G)$ is the linear subspace of $F(G)$ consisting of elements of finite sum $\sum_i r_i[g_i]$ with $\sum_i r_i = 0$. So we get a commutative square in Diff:

$$\begin{tikzcd} Y \times \bar{F}(G) \arrow[r] \arrow[d] & \tilde{E} \arrow[d, "\tilde{\pi}"] \\ Y \arrow[r, "f"'] & B \end{tikzcd} \tag{3}$$

where $\tilde{E}$ is the quotient of $Y \times \bar{F}(G)$ with $(y, v) \sim (y \cdot g, g^{-1} \cdot v)$ for $y \in Y$, $g \in G$ and $v \in \bar{F}(G)$, and $\tilde{\pi}[y, v] = f(y)$.

Lemma 5.8. *With the above notations, $\tilde{\pi}$ is a vector bundle over B with fibre $\bar{F}(G)$.*

Proof. Let $p : U \to B$ be a plot. Since $f : Y \to B$ is a principal G-bundle, we may shrink U so that we have a pullback diagram:

$$\begin{tikzcd} U \times G \arrow[r, "\phi"] \arrow[d] & Y \arrow[d, "f"] \\ U \arrow[r, "p"'] & B \end{tikzcd}$$

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[5] Principal bundle here is in the sense of [Iglesias-Zemmour 1985], i.e., pullback along every plot of the base space is locally trivial. The same applies to all principal (respectively, vector, fibre) bundles and coverings discussed afterwards.

We are left to show that there is an isomorphism $\alpha : P \to U \times \overline{F}(G)$ as diffeological vector pseudo-bundles over U, where P is the pullback of

$$\begin{tikzcd} U \arrow[r, "p"] & B & \tilde{E}. \arrow[l, "\tilde{\pi}"'] \end{tikzcd}$$

We define $\alpha(u, [y, v]) = (u, \theta(u, y) \cdot v)$, where $y = \phi(u, e) \cdot \theta(u, y)$ since $f(y) = p(u) = f(\phi(u, e))$, and e is the identity element in the group G. It is clear that α is smooth and fibrewise isomorphic as vector spaces. And α^{-1} is given by $(u, v) \mapsto (u, [\phi(u, e), v])$, which is obviously smooth. □

It is straightforward to check that the above square (3) is a bundle map.

Proposition 5.9. *Recall that the kernel of the bundle map $F_B(Y) \to B \times \mathbb{R}$ over B is denoted by $\bar{f}_* : \overline{F}_B(Y) \to B$. It is isomorphic to $\tilde{\pi} : \tilde{E} \to B$ as vector bundles over B.*

Proof. The isomorphism as vector bundles over B is given by $\tilde{E} \to \overline{F}_B(Y)$ with $\left[y, \sum_i r_i[g_i]\right] \mapsto \sum_i r_i[y \cdot g_i]$, and it is easy to check all the required conditions. □

As a consequence of the above results, we have:

Corollary 5.10. *Let $f : Y \to B$ be a principal G-bundle with Y being locally Euclidean, and B being Hausdorff and filtered. Then we have a short exact sequence of diffeological vector spaces*

$$0 \to V_{\tilde{\pi}} \to F(Y) \to F(B) \to 0.$$

Note that when $f : Y \to B$ is a classical fibre (respectively, principal) bundle, the conditions (f being a subduction, Y being locally Euclidean, and B being Hausdorff and filtered) are satisfied.

Proposition 5.11. *Let $\pi : E \to Y$ be a vector bundle of fibre type a diffeological vector space V, and let $f : Y \to B$ be a fibre bundle of fibre type a diffeological space X.*

1. *If X is finite discrete*[6]*, then the pushforward $f_*(E) \to B$ is a vector bundle with fibre type $F(X) \otimes V$.*
2. *Assume that both π and f are locally trivial, and there exists a D-open covering $\{B_i\}_i$ of B which trivialises f and simultaneously the D-open covering $\{f^{-1}(B_i)\}_i$ trivialises π. Then the pushforward $f_*(E) \to B$ is also a locally trivial vector bundle of fibre type $F(X) \otimes V$.*
3. *If π is trivial, then $f_*(E) \to B$ is a vector bundle of fibre type $F(X) \otimes V$.*

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[6] When the fibre of a fibre bundle $f : Y \to B$ is discrete, f is also called a covering.

Proof. (1): Let $p : U \to B$ be a plot. Since $f : Y \to B$ is a covering with fibre type X, we may shrink U to get a pullback diagram:

$$\begin{tikzcd}
U \times X \arrow[r, "\phi"] \arrow[d] & Y \arrow[d, "f"] \\
U \arrow[r, "p"'] & B
\end{tikzcd}$$

Since $\pi : E \to Y$ is a vector bundle of fibre type V, for each $x \in X$, we may further shrink U to get a pullback diagram:

$$\begin{tikzcd}
U \times \{x\} \times V \arrow[r, "\psi_x"] \arrow[d] & E \arrow[d, "\pi"] \\
U \times \{x\} \arrow[r, "\phi|_{U \times \{x\}}"'] & Y
\end{tikzcd}$$

As X is finite discrete, we gather these together and get a pullback diagram:

$$\begin{tikzcd}
U \times X \times V \arrow[r, "\psi"] \arrow[d] & E \arrow[d, "\pi"] \\
U \times X \arrow[r, "\phi"'] & Y
\end{tikzcd}$$

Write P for the pullback of $U \xrightarrow{p} B \leftarrow f_*(E)$. Then P consists of elements of the form $\big(u, \sum_i e_{y_i}\big)$, with $p(u) = f(y_i)$ for all i. Define $U \times (F(X) \otimes V) \to P$ by linear expansion of $(u, [x] \otimes v) \mapsto (u, \psi(u, x, v))$. It is straightforward to check that this map is smooth and an isomorphism of vector spaces, and its inverse is also smooth.

(2) and (3) can be proved in a similar way. ☐

Corollary 5.12. *If $f : Y \to B$ is a (locally trivial) fibre bundle of fibre type a diffeological space X, then $F_B(Y) \to B$ is a (locally trivial) vector bundle of fibre type $F(X)$.*

Proof. This follows immediately from Propositions 5.4 and 5.11. ☐

5B. *Examples.* Now we deal with the case of a principal bundle whose group G is discrete. In this case, $F(G)$ is a fine diffeological vector space whose dimension matches the cardinality of G, and $\bar{F}(G)$ is a codimension-one linear subspace of $F(G)$, and hence also a fine diffeological vector space.

Example 5.13. For the principal $\mathbb{Z}/2\mathbb{Z}$-bundle $S^n \to \mathbb{R}P^n$, $F(\mathbb{Z}/2\mathbb{Z}) \cong \mathbb{R}^2$ and $\bar{F}(\mathbb{Z}/2\mathbb{Z}) \cong \mathbb{R}$. And therefore, the bundle $\tilde{\pi}$ in the commutative square (3) in the previous subsection can be viewed as the quotient of $S^n \times \mathbb{R}$ with the equivalence relation given by $(z, x) \sim (-z, -x)$, which is the tautological line bundle γ_n^1 on $\mathbb{R}P^n$. So we have an isomorphism

$$F(S^n) \cong F(\mathbb{R}P^n) \oplus V_{\gamma_n^1}. \tag{4}$$

Taking $n = 1$, γ_1^1 is the Möbius band. Moreover, since $\mathbb{R}P^1$ is diffeomorphic to S^1, we get

$$F(S^1) \cong F(S^1) \oplus V_{\gamma_1^1} \cong \cdots \cong F(S^1) \oplus (V_{\gamma_1^1})^m \tag{5}$$

for any $m \in \mathbb{N}$.

By some results from [Milnor and Stasheff 1974], we have:

Example 5.14. (1) Since the tangent bundle $TS^n \to S^n$ direct sum the normal bundle (which is the trivial line bundle) of S^n in $\mathbb{R}^{n+1}$ is a trivial bundle over S^n of rank $n + 1$, we get

$$F(S^n)^{n+1} \cong F(S^n) \oplus V_{TS^n}.$$

Moreover, by [Adams 1962], V_{TS^n} has a smooth direct summand $F(S^n)^{\rho(n+1)-1}$, where $\rho(n + 1) = 2^c + 8d$ with $n + 1 = 2^b(2a + 1)$, $b = c + 4d$ and $0 \leq c \leq 3$.

(2) Since the tangent bundle $T\mathbb{R}P^n \to \mathbb{R}P^n$ direct sum the trivial line bundle over $\mathbb{R}P^n$ is isomorphic to the direct sum of $n + 1$ copies of the tautological line bundle $\gamma_n^1 \to \mathbb{R}P^n$, we get

$$(V_{\gamma_n^1})^{n+1} \cong F(\mathbb{R}P^n) \oplus V_{T\mathbb{R}P^n}.$$

(3) The total space of the tangent bundle $TS^n \to S^n$ can be viewed as a submanifold of $\mathbb{R}^{n+1} \times \mathbb{R}^{n+1}$, with the first component for the base and the second one for the tangent part. If we identify (x, v) with $(-x, -v)$ in TS^n, we get the total space of the tangent bundle $T\mathbb{R}P^n \to \mathbb{R}P^n$; if we identify (x, v) with $(-x, v)$ in TS^n, we get another locally trivial vector bundle $\pi : E \to \mathbb{R}P^n$ of rank n. (In the case $n = 1$, π is exactly the Möbius band over $\mathbb{R}P^1$; notice the difference from Example 5.13, based on the different meaning of the coordinates!) Write $f : S^n \to \mathbb{R}P^n$ for the quotient map. Note that $E \to f_*(TS^n)$ given by $[x, v] \mapsto (x, v) + (-x, v)$ is a bundle map over $\mathbb{R}P^n$, using Proposition 5.11 (1), which is the kernel of the canonical bundle map $f_*(TS^n) \to T\mathbb{R}P^n$. Hence, we have an isomorphism

$$V_{TS^n} \cong V_{T\mathbb{R}P^n} \oplus V_\pi,$$

which also recovers the first isomorphism in (5) in Example 5.13.

Therefore, if we combine the three isomorphisms in this example, we get

$$F(\mathbb{R}P^n) \oplus F(S^n)^{n+1} \cong F(S^n) \oplus V_\pi \oplus (V_{\gamma_n^1})^{n+1}.$$

By taking $n = 1$, we obtain

$$F(S^1)^3 \cong F(S^1) \oplus (V_{\gamma_1^1})^3 \cong F(S^1).$$

Remark 5.15. (1) The isomorphism $F(S^1)^3 \cong F(S^1)$ implies that pushforward can take nonisomorphic bundles over the same base space into isomorphic diffeological vector spaces.

(2) The isomorphism $F(S^1)^3 \cong F(S^1)$ can also be derived directly by considering the covering map $S^1 \to S^1$ with $z \mapsto z^3$.

(3) I don't know if $F(S^1)^2$ is isomorphic to $F(S^1)$ as diffeological vector spaces. If it is not, then there seems to be some connection with Bott periodicity in the complex case.

(4) I wonder if the approach here can lead to an alternative proof of the maximal number of linearly independent vector fields on spheres.

Finally, we show by the following example that the extra condition of filteredness added to the results in the previous subsection is necessary:

Example 5.16. Let $\mathbb{Z}/2\mathbb{Z}$ act on $\mathbb{R}$ by $\pm 1 \cdot x = \pm x$, and write B for the quotient space. Then B is weakly filtered but not filtered [Christensen and Wu 2017, Example 4.7], and B with the D-topology is homeomorphic to the subspace $[0, \infty)$ of $\mathbb{R}$ (hence is Hausdorff). Write $f : \mathbb{R} \to B$ for the quotient map, and write K for the kernel of $F(\mathbb{R}) \to F(B)$. It consists of elements of the form of a finite sum $\sum_i r_i[x_i]$ with $r_i, x_i \in \mathbb{R}$ such that for every fixed $x \in X$, the subsum $\sum_{i:x_i=\pm x} r_i = 0$. So, $p : \mathbb{R} \to K$ defined by $t \mapsto [t] - [-t]$ is a plot of K. On the other hand, the map $f_* : F_B(\mathbb{R}) \to B$ has fibre $\mathbb{R}$ over $[0] \in B$ and fibre $\mathbb{R}^2$ over $[b] \in B$ for $b \neq 0$. Hence, $\bar{f}_* : \bar{F}_B(\mathbb{R}) \to B$ has fibre $\mathbb{R}^0$ over $[0] \in B$ and fibre $\mathbb{R}$ over $[b] \in B$ for $b \neq 0$. The canonical smooth linear bijection $\alpha : V_{\bar{f}_*} \to K$ is not an isomorphism of diffeological vector spaces since $\alpha^{-1} \circ p$ is not a plot of $V_{\bar{f}_*}$. If it were, then by iterated use of Lemma 3.1, there exist finitely many smooth germs $(p^1_{i,j}, p^2_{i,j}) : \mathbb{R} \to \mathbb{R}_{(\text{base})} \times \mathbb{R}_{(\text{fibre})}$ at $0 \in \mathbb{R}$ such that

$$p(t) = \alpha\Big(\sum_{i,j} \alpha_g\big(\alpha_f(p^1_{i,j}(t), p^2_{i,j}(t))\big)\Big),$$

where $g : B \to \mathbb{R}^0$, both α_f and α_g are structural maps from Section 3, the range of j depends on i, $f \circ p^1_{i,j}$ is independent of j for any fixed i, $p^2_{i,j}(t) = 0$ whenever $p^1_{i,j}(t) = 0$ (by the description of $V_{\bar{f}_*}$), which causes the contradiction as follows: By evaluating at $t = 0$, we know that

$$\sum_{i,j:p^1_{i,j}(0)=x} p^2_{i,j}(0) = 0$$

for any fixed $x \in \mathbb{R} \setminus \{0\}$. By continuity of the $p^2_{i,j}$, we know that

$$\sum_{i,j:p^1_{i,j}(t)=t} p^2_{i,j}(t) \neq 1$$

for $t \neq 0$ but sufficiently close to 0, which implies that $\alpha^{-1} \circ p$ cannot be a plot.

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ENXIN WU
DEPARTMENT OF MATHEMATICS
SHANTOU UNIVERSITY
GUANGDONG
CHINA
exwu@stu.edu.cn

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