A GEOMETRIC APPROACH TO THE EMBEDDING CALCULUS KNOT INVARIANTS

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Summary

In this thesis we consider two homotopy theoretic approaches to the study of spaces of knots: the theory of *finite type invariants* of Vassiliev and the *embedding calculus* of Goodwillie and Weiss, and address connections between them.

Our results confirm that the knot invariants ev_n produced by the embedding calculus for (long) knots in a 3-manifold M are *surjective* for all $n \geq 1$. On one hand, this solves certain remaining open cases of the connectivity estimates of Goodwillie and Klein, and on the other hand, confirms a part of the conjecture by Budney, Conant, Scannell and Sinha that for the case $M = I^3$ of classical knots ev_n are universal additive Vassiliev invariants over $\mathbb{Z}$.

There are two crucial ingredients for this result.

Firstly, we study the so-called Taylor tower of the embedding calculus more generally for long knots in any manifold with $\dim(M) \geq 3$ and develop a geometric understanding of its layers (fibres between two consecutive spaces in the tower). In particular, we describe their first non-vanishing homotopy groups in terms of groups of decorated trees.

Secondly, we give an explicit interpretation of ev_n when $\dim(M) = 3$ using *capped grope cobordisms.* These objects were introduced by Conant and Teichner in a geometric approach to the finite type theory, but turn out to exactly describe certain points in the layers.

Our main theorem then states that *the first possibly non-vanishing embedding calculus invariant of a knot which is grope cobordant to the unknot is precisely the equivalence class of the underlying decorated tree of the grope in the homotopy group of the layer.*

The surjectvity of ev_n onto the components of the Taylor tower follows from this immediately.

As another corollary we obtain a sufficient condition for the mentioned conjecture to hold over a certain coefficient group A. Namely, it is enough that the spectral sequence for the homotopy groups of the Taylor tower, tensored with A, collapses along the diagonal. In particular, such a collapse result is known for $A = \mathbb{Q}$, confirming that the embedding calculus invariants are universal rational additive Vassiliev invariants, and that they factor configuration space integrals through the Taylor tower. It also follows that they are universal over the p-adic integers in a range depending on the prime p, using recent results of Boavida de Brito and Horel.

Moreover, the surjectivity of ev_n implies that any two group structures on the path components of the tower, which are compatible with the connected sum of knots, must agree.

Finally, we also discuss the geometric approach to the finite type theory in terms of the Gusarov–Habiro filtration of the set of isotopy classes of knots in a 3-manifold. We extend some known techniques to prove that the associated graded quotients of this filtration are *abelian groups*, and study the map which relates these groups to certain graph complexes.

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Part I

Introduction

In contrast to the study of spaces of continuous maps $\mathrm{Map}(P, M)$ between two topological spaces which gave rise to numerous techniques of homotopy theory, the study of embedding spaces $\mathcal{E}\mathrm{mb}(P, M)$ between smooth manifolds seems less tractable from the *homotopy* viewpoint. Already at the level of components, which can be broadly understood as the field of knot theory, one often uses purely *geometric* arguments. In this thesis we isolate two attempts to reconcile these viewpoints, and study how they relate.

The first approach, *Vassiliev's theory of finite type knot invariants* [Vas90], starts from the observation that having understood the space of smooth maps, we can try to study its subspace of embeddings by studying homotopy types of the strata of the complement $\mathrm{Map}(\mathbb{S}^1, \mathbb{R}^3) \setminus \mathcal{E}\mathrm{mb}(\mathbb{S}^1, \mathbb{R}^3)$. The second approach, *the embedding calculus of Goodwillie and Weiss* [Wei99; GW99], builds on the idea (having its roots in the Hirsch–Smale immersion theory) that, since we understand embeddings of disjoint unions of disks, we could use them to approximate the space $\mathcal{E}\mathrm{mb}(P, M)$.

It was suggested early on by [GW99; GKW01] that these two theories should be closely related. The study was initiated in [BCSS05], where a conjecture about the exact relationship was stated (see Conjecture 1), and proven in the first non-trivial degree. The work of [Vol06; Tou07; Con08] then showed that, roughly speaking, graph complexes appearing in the two theories agree. More recently a part of the conjecture was proven in [BCKS17], confirming that the invariants coming from the embedding calculus are *additive finite type invariants*. According to the mentioned conjecture they are actually *universal* among such invariants.

One of our main results is the proof of the 'surjectivity part' of that conjecture, see Corollary 1.1. Starting from a geometric viewpoint, we use somewhat different techniques compared to the mentioned thread of work, namely – *gropes* for the finite type theory, and the *punctured knots model* for the embedding calculus. These tools already appeared in the literature, but perhaps have not been explored enough; we will study them in detail and assuming almost no background.

We actually study, more generally, spaces of *long knots* in a compact manifold M with boundary; that is, smoothly embedded arcs whose endpoints are fixed in the boundary of M, together with transverse tangent vectors at those points. On one hand, we develop the punctured knots model for any such manifold with $\dim(M) \geq 3$, and on the other hand, we formulate the results related to gropes for any $\dim(M) = 3$. The two pieces together enable us to prove a more general result which implies Corollary 1.1, namely we confirm Goodwillie–Klein 'connectivity estimates' for a class of the remaining open cases, see Theorem A.

Before turning to those more general results, let us give a brief survey of the two theories for the case of *classical long knots*. More precisely, this is the space

$$\mathcal{K}(I^3) := \mathcal{E}\mathrm{mb}_\partial(I, I^3) := \{ f : I \hookrightarrow I^3 \mid f \equiv \mathrm{U} \text{ near } \partial I \},$$

where $I = [0, 1]$ and $\mathrm{U} \colon I \hookrightarrow I^3, t \mapsto (t, \frac{1}{2}, \frac{1}{2})$ is the standard *unknot*. This is a homotopy-commutative H-space, with multiplication given by concatenation of cubes along the x-axis and rescaling back to the unit cube. Therefore, the isotopy classes $\mathbb{K}(I^3) := \pi_0\mathcal{K}(I^3)$ form an abelian monoid – which is isomorphic to the more commonly used $\pi_0\mathcal{E}\mathrm{mb}(\mathbb{S}^1, \mathbb{R}^3)$ of round knots.

The geometric calculus. Vassiliev's study of the strata of the discriminant $\mathrm{Map}_\partial(I, I^3) \setminus \mathcal{K}(I^3)$ gave rise to the filtration $\mathcal{V}_n^*(A)$ by type $n \geq 1$ of the set $H^0(\mathcal{K}(I^3); A)$ of knot invariants with values in an abelian group A, as formulated by [BL93]. A new, very active field emerged: it was shown that all quantum invariants (when suitably parametrised) are of finite type [Lin91]; that for $A = \mathbb{Q}$ there is a universal such invariant – the Kontsevich integral [Kon93; LM96]; a comprehensive treatment of its target, the rational Hopf algebra of chord diagrams, was given in [Bar95a].

A geometric approach to the field was introduced independently by Gusarov [Gus00] and Habiro [Hab00]. They defined a sequence of operations on knots called surgeries on *claspers* (or variations) of degree $n \geq 1$. This gives a sequence of equivalence relations $\sim_n$ on $\mathbb{K}(I^3)$ and a decreasing filtration $\mathbb{K}_n(I^3) := \{K \in \mathbb{K}(I^3) : K \sim_n \mathrm{U}\}$ by submonoids. The related work of Stanford [Sta98] exhibits a close connection of this filtration with the lower central series of the pure braid group.

Notably, these authors show that the map $\mathbb{K}(I^3) \to \mathbb{Z}[\mathbb{K}(I^3)] = H_0(\mathcal{K}(I^3); \mathbb{Z})$ defined by $K \mapsto K - \mathrm{U}$, takes $\mathbb{K}_n(I^3)$ into $\mathcal{V}_n(\mathbb{Z})$, the dual of the Vassiliev–Gusarov filtration for $A = \mathbb{Z}$. Hence, this indeed gives a geometric version of the theory (or its primitive/additive[1] part): one works with knots instead of their linear combinations or invariants; see Section 7.1 for a comparison.

By the work of Conant and Teichner [CT04b; CT04a] instead of claspers one can equivalently use *capped grope cobordisms in* I^3, and this is the approach we take. Gropes first appeared in the theory of topological 4-manifolds, and can be viewed as a tool for detecting 'embedded commutators'. See Section 7 for the background and Remark 8.3 for an advantage of using gropes.

Lastly, the quotient $\mathbb{K}(I^3)/\sim_n$ is actually *an abelian group* and the projection

$$\nu_n : \mathbb{K}(I^3) \twoheadrightarrow \mathbb{K}(I^3)/\sim_n$$

is a *universal additive invariant of type* $\leq n-1$ [Hab00, Thm. 6.17] – meaning that any additive invariant $v : \mathbb{K}(I^3) \to A$ of type $\leq n-1$ factors through ν_n. However, the target here is a mysterious group and one would ideally have something combinatorially defined instead, perhaps the primitive part of the mentioned algebra of diagrams (see Section 2.1.5).

The embedding calculus. The pioneering approach of Goodwillie and Weiss [Wei99; GW99] for studying embedding spaces[2] $\mathcal{E}\mathrm{mb}_\partial(P, M)$ produces a tower of spaces, called *the Taylor tower*,

$$\cdots \to \mathsf{T}_n\mathcal{E}\mathrm{mb}_\partial(P, M) \to \mathsf{T}_{n-1}\mathcal{E}\mathrm{mb}_\partial(P, M) \to \cdots \to \mathsf{T}_1\mathcal{E}\mathrm{mb}_\partial(P, M)$$

and the *evaluation maps* $\mathsf{ev}_n : \mathcal{E}\mathrm{mb}_\partial(P, M) \to \mathsf{T}_n\mathcal{E}\mathrm{mb}_\partial(P, M)$, starting from the space of immersions $\mathsf{T}_1\mathcal{E}\mathrm{mb}_\partial(P, M) \simeq \mathcal{I}\mathrm{mm}_\partial(P, M)$. Since the definition of these objects is homotopy theoretic – analogously to the description of immersions due to Hirsch and Smale – we obtain an inductive way for studying the homotopy type of $\mathcal{E}\mathrm{mb}_\partial(P, M)$, using a variety of tools.

Indeed, a fundamental result in the field is the theorem of Goodwillie and Klein [GK15] (announced in [GW99]) that for $\dim M - \dim P > 2$ the limit of the tower is equivalent to the space of embeddings, that is, the induced map $\mathsf{ev}_\infty : \mathcal{E}\mathrm{mb}_\partial(P, M) \to \lim_n \mathsf{T}_n\mathcal{E}\mathrm{mb}_\partial(P, M)$ is a weak homotopy equivalence (the tower is said to *converge to the embedding space*). To prove this they show that ev_n is $\big(3 - \dim M + (n+1)(\dim M - \dim P - 2)\big)$-connected[3], except when $\dim P = 1$ and $\dim M = 3$.

Taylor towers for various pairs (P, M) have been extensively studied in recent years. To mention just a few results, in [LTV10; AT14] the rational homology of spaces $\mathcal{E}\mathrm{mb}_\partial(\mathbb{D}^k, \mathbb{D}^{k+c})$ of disks of codimension $c > 2$ was expressed as the homology of certain graph complexes, and similarly for the

[1] An additive knot invariant is a monoid map $v : \mathbb{K}(I^3) \to A$ to an abelian group.
[2] We take compact manifolds with a fixed boundary condition for all embeddings, or closed manifolds.
[3] A map is k-connected if it induces an isomorphism on homotopy groups below degree k and a surjection on π_k.

rational homotopy groups [ALTV08; AT15; FTW17]. The spaces $\mathsf{T}_n\mathcal{E}\mathrm{mb}_\partial(\mathbb{D}^k, \mathbb{D}^{k+c})$ were shown to be iterated loop spaces in [DH12; Tur14; BW18]. A different model for $\mathsf{T}_n\mathcal{E}\mathrm{mb}_\partial(I, M)$ was constructed in [Sin09] and studied in [SS02] for $M = I^d$ with $d \geq 4$.

Note that the excluded case for the connectivity of ev_n is precisely the setting of knot theory. Actually, by an argument of Goodwillie, the tower for classical long knots $\mathcal{K}(I^3)$ does not converge (see Proposition 2.21). Nevertheless, it still remains a source of interesting knot invariants: taking path components gives a tower of sets to which the monoid $\mathbb{K}(I^3)$ maps.

Moreover, the delooping results of [Tur14; BW18] apply in this case as well: for $n \geq 2$ each $\mathsf{T}_n\mathcal{K}(I^3)$ is weakly equivalent to a double loop space, so each $\pi_0\mathsf{T}_n\mathcal{K}(I^3)$ is *an abelian group* (the trivial group for $n = 1$, since $\mathsf{T}_1\mathcal{K}(I^3) \simeq \Omega\mathbb{S}^2$). Moreover, [Gri19] showed that in the model from [BW18] $\mathsf{ev}_n^{BW} \colon \mathcal{K}(I^3) \to \mathsf{T}_n^{BW}(I^3)$ is a map of H-spaces. Hence, $\pi_0\mathsf{ev}_n^{BW}$ is a monoid map.

A different approach by [BCKS17] uses the model for $\mathsf{T}_n\mathcal{K}(I^3)$ from [Sin09] to equip $\pi_0\mathsf{T}_n\mathcal{K}(I^3)$ directly with an abelian group structure, so that the corresponding $\pi_0 ev_n$ is also a monoid map. To our knowledge, it has been an open problem whether the group structures of [BW18] and [BCKS17] on $\pi_0\mathsf{T}_n\mathcal{K}(I^3)$ agree. This is a corollary of our results, see Corollary 2.23.

The conjecture mentioned above, regarding a relation of the Taylor tower for $\mathcal{K}(I^3)$ to the finite type theory, predicts that the space $\mathsf{T}_n\mathcal{K}(I^3)$ precisely encodes the n-equivalence relation.

Conjecture 1 ([BCSS05])**.** *For each $n \geq 1$ the map $\pi_0\mathsf{ev}_n \colon \mathbb{K}(I^3) \to \pi_0\mathsf{T}_n\mathcal{K}(I^3)$ is a universal additive Vassiliev invariant of type $\leq n-1$ over $\mathbb{Z}$. In other words, it factors as*

$$\begin{tikzcd}
\mathbb{K}(I^3) \arrow[rr, "\pi_0\mathsf{ev}_n"] \arrow[dr, "\nu_n"'] & & \pi_0\mathsf{T}_n\mathcal{K}(I^3) \\
& \mathbb{K}(I^3)/{\sim_n} \arrow[ur, hook, two heads] &
\end{tikzcd}$$

and the induced map is an isomorphism of groups.

The existence of the factorisation (and additivity) was shown in [BCKS17] and means that $\pi_0\mathsf{ev}_n$ is an additive invariant of type $\leq n-1$. Our joint work [KST] reproves this, see also Theorem D.

1 Statements of the results

In this thesis we more generally study spaces of knotted arcs in a *connected compact smooth manifold M of dimension d and with non-empty boundary.* More precisely, we fix a neat[4] embedding $b \colon [0, \epsilon) \sqcup (1-\epsilon, 1] \hookrightarrow M$ and consider the space of smooth neat embeddings

$$\mathcal{K}(M) := \mathcal{E}\mathrm{mb}_\partial(I, M) := \{ f \colon I \hookrightarrow M \mid f \equiv b \text{ near } \partial I \}, \tag{1.1}$$

and the corresponding Taylor tower with evaluation maps $\mathsf{ev}_n \colon \mathcal{K}(M) \to \mathsf{T}_n\mathcal{K}(M)$.

Theorem A. *For $d = 3$ and $n \geq 1$ the map of sets $\pi_0\mathsf{ev}_n \colon \pi_0\mathcal{K}(M) \to \pi_0\mathsf{T}_n\mathcal{K}(M)$ is surjective.*

This was expected to hold by analogy to the mentioned Goodwillie–Klein connectivity formula: for $\dim P = 1$ and $\dim M = 3$ the formula predicts that ev_n is 0-connected, and for P connected this is precisely our Theorem A. In future work we will investigate if this also extends to disconnected cases. As a consequence of Theorem A we confirm a part of Conjecture 1.

Corollary 1.1. *For each $n \geq 1$ the homomorphism $\pi_0\mathsf{ev}_n \colon \mathbb{K}(I^3) \to \pi_0\mathsf{T}_n\mathcal{K}(I^3)$ is surjective.*

[4] An embedding $b \colon P \to M$ is neat if $b(P) \cap \partial M = b(\partial P)$.

In [Vol06] Volić asks 'Can one in general understand the geometry of finite type invariants using the evaluation map?', and we make a step forward in that direction. Namely, there is a graph complex computing the homotopy groups of $\mathsf{T}_n\mathcal{K}(I^3)$ and our main Theorem E implies that (Corollary 2.18)

the evaluation map detects the underlying tree of a grope (or clasper) in the graph complex.

Analogous results hold for universal rational Vassiliev knot invariants of Kontsevich [Kon93] and Bott–Taubes [BT94; AF97], as well as for similar invariants of families of diffeomorphisms of $\mathbb{S}^4$, shown by Watanabe [Wat18] to detect the underlying graph of a family constructed using analogous claspers. However, one important difference is that while all these invariants use integrals over configuration spaces – and so can provide results only in characteristic zero – the embedding calculus offers a tool for studying homotopy types in general.

Indeed, Theorem E can be used both to confirm Conjecture 1 rationally and show that Kontsevich and Bott–Taubes integrals factor through the tower (see Remark 2.19), and also more generally.

Corollary 1.2. *Let A be a torsion-free abelian group. If the homotopy spectral sequence $E^*_{-n,t}(I^3)\otimes A$ for the Taylor tower of $\mathcal{K}(I^3)$ collapses at the E^2-page along the diagonal, then the map $\pi_0\mathsf{ev}_n$ is a universal additive Vassiliev invariant of type $\leq n-1$ over A, meaning that*

$$\pi_0\mathsf{ev}_n\otimes A\colon \mathbb{K}(I^3)/\!\sim_n \otimes A \xrightarrow{\cong} \pi_0\mathsf{T}_n\mathcal{K}(I^3)\otimes A.$$

Here $E^*_{-n,t}(I^3)$ is the usual spectral sequence for the homotopy groups of the tower of fibrations $p_n\colon \mathsf{T}_n\mathcal{K}(I^3)\to\mathsf{T}_{n-1}\mathcal{K}(I^3)$ and can be related to graph complexes, see Section 2.3. The collapse condition is equivalent to the statement that *the canonical projection from the group $E^2_{-n,n}\cong\mathcal{A}^T_{n-1}$ of Jacobi trees (as identified by Conant [Con08]) to $E^\infty_{-n,n}=\ker(\pi_0 p_n)$ is an isomorphism over A.*

This has already been confirmed in certain cases.

Corollary 1.3.

(1) $\pi_0\mathsf{ev}_n$ is a universal additive Vassiliev invariant of type $\leq n-1$ over $\mathbb{Q}$.

(2) For any prime p, the evaluation map $\pi_0\mathsf{ev}_n$ is a universal additive Vassiliev invariant of type $\leq n-1$ over the p-adic integers $\mathbb{Z}_p$ if $n\leq p+2$.

(3) $\pi_0\mathsf{ev}_n$ is a universal additive Vassiliev invariant of type $\leq n-1$ over $\mathbb{Z}$ if $n\leq 7$.

Namely, it follows from [FTW17] or [BH20] that the spectral sequence $E^*_{-n,t}(I^3)\otimes\mathbb{Q}$ collapses at the whole E^2 page, implying the first statement. Furthermore, Boavida de Brito and Horel [BH20] study this spectral sequence also in positive characteristic and show the vanishing of certain differentials, which implies (2). The last result uses certain existing low-degree computations in the algebra of Jacobi diagrams. For the proofs of these corollaries and further details see Section 2.2.3.

In Section 2 we more generally discuss analogous statements in other settings. Firstly, in Section 2.1 we define similar groups $\mathcal{A}^T_n(M)$ for any d-manifolds M with $d\geq 3$, now consisting of trees which are decorated by fundamental group elements; in Section 2.2.1 we state our results which relate these decorated trees to gropes in dimension 3. Finally, in Section 2.3 we discuss how this should fit into a more general picture for manifolds of arbitrary dimensions.

In the rest of this introductory Section 1 we discuss in detail the central parts of this thesis.

We first introduce the necessary notation so that we can state Theorem B which implies Theorem A. We then state the crucial technical results Theorems C (in §1) and D (in §2), and finally our main results, Theorems E and F (in §3), which imply Theorem B and the corollaries explained above.

For M as in (1.1) we pick *an arbitrary knot* $\mathrm{U} \in \mathcal{K}(M)$ as our basepoint and call it *the unknot*. In Section 3 we will recall and extend the following notions and results.

– Let $\mathsf{P}_n(M)$ be *the punctured knots model* for $\mathsf{T}_n\mathcal{K}(M)$, defined as the homotopy limit of a certain punctured cubical diagram, and let $\mathsf{ev}_n \colon \mathcal{K}(M) \to \mathsf{P}_n(M)$ be the natural map. We choose $\mathsf{ev}_n(\mathrm{U})$ as the basepoint of $\mathsf{P}_n(M)$ and consider the *homotopy fibre*

$$\mathsf{H}_n(M) := \mathrm{hofib}_{\mathsf{ev}_n\mathrm{U}}(\mathsf{ev}_n) := \big\{ (K,\gamma) \in \mathcal{K}(M) \times \mathrm{Map}([0,1], \mathsf{P}_n(M)) \mid \gamma(0) = \mathsf{ev}_n(K), \gamma(1) = \mathsf{ev}_n(\mathrm{U}) \big\}.$$

– The natural projection $p_n \colon \mathsf{P}_n(M) \to \mathsf{P}_{n-1}(M)$ preserves basepoints since $p_n \circ \mathsf{ev}_n = \mathsf{ev}_{n-1}$. In Section 3.1 we prove p_n is a *surjective* fibration (surjectivity is new, see Corollary 3.10).

– Let $\mathsf{F}_n(M) := \mathrm{fib}_{\mathsf{ev}_{n-1}\mathrm{U}}(p_n)$ be its fibre, called *the layer of the Taylor tower*. There is a canonical inclusion $\iota \colon \mathsf{F}_n(M) \hookrightarrow \mathrm{hofib}_{\mathsf{ev}_{n-1}\mathrm{U}}(p_n)$ to the homotopy fibre (which is a homotopy equivalence).

– In Section 3.2 we construct a direct map $\mathsf{e}_n \colon \mathsf{H}_{n-1}(M) \to \mathsf{F}_n(M)$, such that the natural map $\mathsf{H}_{n-1}(M) \to \mathrm{hofib}_{\mathsf{ev}_{n-1}\mathrm{U}}(p_n)$, $(K,\gamma) \mapsto (\mathsf{ev}_n K, \gamma)$ induced from ev_n factors as $\iota \circ \mathsf{e}_n$.

We can summarise this in the commutative diagram whose columns are homotopy fibre sequences:

$$\begin{tikzcd}
\mathsf{H}_{n-1}(M) \arrow[r, "\mathsf{e}_n"] \arrow[d] & \mathsf{F}_n(M) \arrow[d, hook] \\
\mathcal{K}(M) \arrow[r, "\mathsf{ev}_n"] \arrow[d, "\mathsf{ev}_{n-1}"'] & \mathsf{P}_n(M) \arrow[d, two heads, "p_n"] \\
\mathsf{P}_{n-1}(M) \arrow[r, equal] & \mathsf{P}_{n-1}(M)
\end{tikzcd} \tag{1.2}$$

Theorem B. *For $d = 3$ and all $n \geq 2$ the map of sets $\pi_0\mathsf{e}_n \colon \pi_0\mathsf{H}_{n-1}(M) \to \pi_0\mathsf{F}_n(M)$ is surjective.*

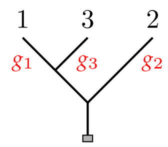
Proof of Theorem A assuming Theorem B. There is a homotopy equivalence $\mathsf{P}_1(M) \simeq \Omega(\mathbb{S}M)$ with the loop space on the unit tangent bundle $\mathbb{S}M$ of M, so its group of components is isomorphic to $\pi_1 M$. Since each class can be represented by an embedded loop, $\pi_0\mathsf{ev}_1$ is surjective. Assume by induction that $\pi_0\mathsf{ev}_{n-1}$ is surjective for some $n \geq 1$.

Let us pick $x \in \mathsf{P}_n(M)$ and show it is in the image of $\pi_0\mathsf{ev}_n$. Denote $y := p_n(x) \in \mathsf{P}_{n-1}(M)$ and the corresponding fibres $\mathsf{F}_n^y(M) := \mathrm{fib}_y(p_n)$ and $\mathsf{H}_{n-1}^y(M) := \mathrm{hofib}_y(\mathsf{ev}_{n-1})$. We also have $\mathsf{e}_n^y \colon \mathsf{H}_{n-1}^y(M) \to \mathsf{F}_n^y(M)$ and since by definition $x \in \mathsf{F}_n^y(M)$, it suffices to prove that $\pi_0\mathsf{e}_n^y$ is surjective.

However, it is instead enough to check that $\pi_0\mathsf{e}_n^{\mathsf{ev}_{n-1}K}$ is surjective, where $K \in \mathcal{K}(M)$ is any knot such that there is a path γ in $\mathsf{P}_{n-1}(M)$ from $\mathsf{ev}_{n-1}(K)$ to y (exists by the induction hypothesis). Indeed, e_n is equivalent to the map induced on the homotopy fibres, and changing the basepoint on both sides using γ induces homotopy equivalences which commute with e_n.

As our choice of U was arbitrary, we can take $\mathrm{U} := K$, so $\mathsf{e}_n^{\mathsf{ev}_{n-1}K} = \mathsf{e}_n$. Now apply Theorem B. □

There are two essential ingredients for the proof of Theorem B – a homotopy theoretic one about $\mathsf{F}_n(M)$, and a geometric one concerning $\mathsf{H}_{n-1}(M)$. Remarkably, they are both related to the set $\mathrm{Tree}_{\pi_1 M}(n-1)$ of $\pi_1 M$*-decorated trees*: rooted planar binary trees whose leaves are both bijectively labelled by the set $\underline{n-1} := \{1,\dots,n-1\}$ and also decorated by elements $g_i \in \pi_1(M)$. For example,

$\Gamma^{g_{\underline{3}}} :=$  $\in \mathrm{Tree}_{\pi_1 M}(3).$

On one hand, $\pi_0\mathsf{F}_n(M)$ is isomorphic via an explicit map to the group of Lie trees $\mathsf{Lie}_{\pi_1 M}(n-1)$, defined as the quotient of the $\mathbb{Z}$-span of $\mathsf{Tree}_{\pi_1 M}(\mathsf{n}-1)$ by the antisymmetry and Jacobi relations. See Section 2.1 for all definitions related to trees.

On the other hand, we use our understanding of knots which are $(n-1)$-equivalent in terms of grope cobordisms $\mathbf{G}$ to construct some concrete points $\psi(\mathbf{G}) \in \mathsf{H}_{n-1}(M)$. Crucially, the underlying combinatorics of a degree $(n-1)$ grope is also described by an element of $\mathsf{Tree}_{\pi_1 M}(n-1)$.

Finally, in Main Theorem E we merge the two ingredients by showing that $\mathsf{e}_n\colon \mathsf{H}_{n-1}(M) \to \mathsf{F}_n(M)$ takes $\psi(\mathbf{G})$ to the generator of $\pi_0\mathsf{F}_n(M)$ which precisely corresponds to the underlying tree of $\mathbf{G}$. In Theorem F we extend this to linear combinations of trees. Theorem B will immediately follow.

We now outline both parts in detail, as certain intermediate results can be of independent interest.

§1 A careful study of the Taylor tower layers

In the homotopy theoretic part, Part II, we study the space $\mathsf{F}_n(M)$ for $n \geq 1$ and M *any smooth manifold with non-empty boundary and* $\dim(M) = d \geq 3$. The upshot is the following theorem which will, in particular, give us explicit generators of $\pi_0\mathsf{F}_n(M)$ for $d = 3$.

THEOREM C. *For each $n \geq 2$ the space $\mathsf{F}_n(M)$ is $((n-1)(d-3)-1)$-connected and its first non-trivial homotopy group admits an (explicit) isomorphism*

$$\mathsf{Lie}_{\pi_1 M}(n-1) \xrightarrow[\cong]{W} \pi_{(n-1)(d-2)} \operatorname{tofib}\big(\Omega(M \vee \mathbb{S}_\bullet), \Omega\mathsf{col}\big) \xrightarrow[\cong]{(\mathsf{retr}\circ\mathscr{D}\circ\chi)_*^{-1}} \pi_{(n-1)(d-3)}\mathsf{F}_n(M).$$

Let us give more details. *Firstly,* $\mathsf{F}_n(M)$ in Section 3.2 is described as the total homotopy fibre

$$\mathsf{F}_n(M) = \operatorname*{tofib}_{S\subseteq \underline{n-1}}(\mathscr{F}^n_S, r)$$

of a cube[5] of spaces[6] $\mathscr{F}^n_S := \mathscr{E}\mathrm{mb}_\partial([0,1], M_{0S})$ where $M_{0S} \subseteq M$ is obtained by removing $|S|+1$ balls $\mathbb{B}^d$ from M, and r-maps induced by $\rho^k_S\colon M_{0S} \hookrightarrow M_{0Sk}$. *Secondly,* in Section 4 we show that this is an n-fold loop space, via an explicit homotopy equivalence, namely $\mathsf{F}_1(M) \simeq \Omega\mathbb{S}M$ and for $n \geq 2$:

$$\mathsf{F}_n(M) \xrightarrow[\sim]{\chi} \Omega^{n-1}\operatorname{tofib}\big(\mathscr{F}^n_\bullet, l\big) \xrightarrow[\sim]{\mathscr{D}} \Omega^{n-1}\operatorname{tofib}\big(\Omega M_\bullet, \Omega\lambda\big) \xrightarrow[\sim]{\mathsf{retr}} \Omega^{n-1}\operatorname{tofib}\Big(\Omega\big(M \vee \mathbb{S}_\bullet\big), \Omega\mathsf{col}\Big).$$

- The homotopy equivalence $\chi\colon \operatorname{tofib}(\mathscr{F}^n_\bullet, r) \to \Omega^{n-1}\operatorname{tofib}(\mathscr{F}^n_\bullet, l)$ and its inverse are constructed in Theorem 4.3, and maps l^k_S are defined using left homotopy inverses $\lambda^k_S\colon M_{0Sk} \to M_{0S}$ for ρ^k_S.
- In Theorem 4.11 taking unit derivatives is shown to give a homotopy equivalence of contravariant cubes $\mathscr{D}_\bullet\colon (\mathscr{F}^n_\bullet, l) \to (\Omega\mathbb{S}M_\bullet, \Omega\mathbb{S}\lambda)$, where $M_S \supseteq M_{0S}$ are obtained by gluing in a ball. In the total fibre of the latter cube the unit tangent data can be omitted.
- Finally, for $\mathbb{S}_S := \bigvee_{i\in S}\mathbb{S}^{d-1}_i$ there are deformation retractions $\mathsf{retr}_S\colon M_S \xrightarrow{\sim} M \vee \mathbb{S}_S$, such that λ^k_S commutes with the collapse map $\mathsf{col}^k_S\colon M \vee \mathbb{S}_S \to M \vee \mathbb{S}_{S\setminus k}$. Hence, retr gives an equivalence of (contravariant) cubes $\mathsf{retr}\colon (\Omega M_\bullet, \Omega\lambda) \to (\Omega\big(M \vee \mathbb{S}_\bullet\big), \Omega\mathsf{col})$.

Thirdly, in Section 5 we calculate the homotopy type of $\operatorname{tofib}\big(\Omega(M \vee \mathbb{S}_\bullet), \Omega\mathsf{col}\big)$ in terms of suspensions of iterated smashes of ΩM with itself. Indeed, it not hard to show (see (5.1)) that the map forg which forgets all homotopies gives an inclusion

$$\pi_*\operatorname{tofib}(M \vee \mathbb{S}_\bullet) \xhookrightarrow{\cong} \bigcap\nolimits_{1\leq k\leq n-1}\ker(\pi_*\mathsf{col}^k_{\underline{n-1}}) \subseteq \pi_*(M \vee \mathbb{S}_{\underline{n-1}}).$$

[5] An n-cube $X_\bullet$ consists of a space X_S for each $S \subseteq \underline{n}$ and a compatible collection of maps $x^k_S : X_S \to X_{Sk}$ for $k \notin S$. The total homotopy fibre $\operatorname{tofib}(X_\bullet, x)$ generalises the notion of a homotopy fibre of a 1-cube.
[6] Of course, $\mathscr{F}^n_S$ depends on M, but we omit it from the notation.

– Therefore, we can use a generalisation of the Hilton–Milnor theorem to find (Theorem 5.4)

$$\prod_{w\in \mathsf{N'B}(\underline{n-1})} \Omega\Sigma^{1+(d-2)l_w}(\Omega M)^{\wedge l'_w} \xrightarrow[\sim]{\mu\circ hm} \operatorname{tofib}\Big(\Omega(M\vee \mathbb{S}_\bullet), \Omega\mathsf{col}\Big). \tag{1.3}$$

Here $\mathsf{N'B}(\underline{n-1})$ consists of those words w in a Hall basis for the free Lie algebra on letters $x^i, x^{i'}, i \in \underline{n-1}$, in which for each $1 \le i \le n-1$ at least one of the letters x^i or $x^{i'}$ appears. The word length of w is denoted by l_w, while l'_w is the number of letters in w with a prime.

– In Section 5.1 we conclude that $\operatorname{tofib}(M\vee\mathbb{S}_\bullet)$ is $((n-1)(d-2)-1)$-connected and find an isomorphism W as in the theorem: it takes a decorated tree $\Gamma^{g_{\underline{n-1}}}$ to a certain Samelson product $\Gamma(x_i^{g_i})\colon \mathbb{S}^{(n-1)(d-2)} \to \Omega(M\vee\mathbb{S}_{\underline{n-1}})$, according to the word Γ and using classes $g_{\underline{n-1}} \in (\pi_1 M)^{n-1}$.

Thus, to find maps which generate $\pi_{(n-1)(d-3)}\mathsf{F}_n(M) \cong \mathsf{Lie}_{\pi_1 M}(n-1)$ we would need to invert the isomorphism $(\mathsf{retr}\mathcal{D}\chi)_*$. At least for retr there is an obvious map $m_i\colon \mathbb{S}^{d-2} \to \Omega(M\setminus\mathbb{B}^d_i) \to \Omega M_{\underline{n-1}}$ satisfying $\mathsf{retr}\circ m_i \simeq x_i$. It simply 'swings a lasso' around the missing d-ball, see Figure 11. In Section 5.2 we discuss the following corollary and Section 5.3 contains examples.

Corollary 1.4. *The group $\pi_{(n-1)(d-2)}\operatorname{tofib}(\Omega M_\bullet, \Omega\lambda)$ is generated by the canonical extensions to the total homotopy fibre of the Samelson products $\Gamma(m_i^{\varepsilon_i\gamma_i})\colon \mathbb{S}^{(n-1)(d-2)} \to \Omega M_{\underline{n-1}}$, for $\varepsilon_i \in \{\pm 1\}$, $\gamma_i \in \Omega M$, and*

$$m_i^{\varepsilon_i\gamma_i}\colon \mathbb{S}^{d-2} \to \Omega M_{\underline{n-1}}, \qquad \vec{t} \mapsto \gamma_i\cdot m_i(\vec{t})^{\varepsilon}\cdot\gamma_i^{-1}$$

Remark 1.5. *If M is simply connected, $\mathsf{Lie}_{\pi_1 M}(n-1)$ is isomorphic to the free abelian group $\mathsf{Lie}_d(n-1) \cong \mathbb{Z}^{(n-2)!}$, the arity $(n-1)$ of the Lie operad, but shifted to degree $(n-1)(d-2)$.*

Interestingly, in the Goodwillie calculus of functors the layer $D_n(F) = \operatorname{hofib}(P_n(F) \to P_{n-1}(F))$ for a functor $F\colon \mathsf{Top}_* \to \mathsf{Top}_*$ is given by $D_n(F) \simeq \Omega^\infty(\partial_n(F)\wedge(-)^{\wedge n})_{h\mathcal{S}_n}$. It turns out that $\partial_*(\mathrm{Id})$ is a an operad [Chi05], whose homology is precisely the Lie operad. See Section 2.1.

Remark 1.6. *When $M \simeq \Sigma Y$ is homotopy equivalent to a suspension, the homotopy type of $\mathsf{F}_n(M)$ was calculated in [GW99]; we recover their result using the James splitting $\Sigma\Omega\Sigma Y \simeq \bigvee_{i=1}^\infty \Sigma Y^{\wedge i}$. See also [Wei99; Göp18] for other descriptions of the layers, and [BCKS17] for $M = I^3$.*

However, in neither of those approaches could we understand the comparison maps, which are of crucial importance for the proof of Main Theorem E. Actually, we hope that our construction of such a map χ might be of independent interest.

Let us point out that we obtain our results from scratch, starting simply with the definition of the punctured knot model and assuming only the Hilton–Milnor–Gray–Spencer theorem (whose proof we briefly recall in Appendix A). In particular, independently of the rest of the literature on Goodwillie–Weiss calculus we reprove the following.

Corollary 1.7. *The Taylor tower for the space $\mathcal{K}(M)$ of knotted arcs in a d-manifold M converges if $d \ge 4$, meaning that the connectivity of $p_n\colon \mathsf{P}_n(M) \to \mathsf{P}_{n-1}(M)$ increases with $n \ge 1$.*

In order to reprove that for $d \ge 4$ the *tower converges precisely to* $\mathcal{K}(M)$ [GK15] we would need to show that the connectivity of $\mathsf{H}_n(M)$ increases with $n \ge 1$. Actually, $\mathsf{e}_n\colon \mathsf{H}_{n-1}(M) \to \mathsf{F}_n(M)$ is a $n(d-3)$-connected map for $d \ge 4$ (so ev_n is $n(d-3)$-connected), and our Theorem B proves this for $d = 3$. We do not pursue extending our proof for $d \ge 4$ here, but this might be possible using constructions of families of embeddings from generalised claspers [KT]. See Section 2.3.

Finally, the Taylor towers for embedding spaces are closely related to configuration spaces of manifolds $\mathsf{Conf}_S(M) := \mathcal{E}\mathrm{mb}(S, M)$, see [Sin09; BW18; FTW17] to mention just a few.

They are behind the scenes in our approach as well, and we can isolate related corollaries.

COROLLARY 1.8. *For a d-manifold M with non-empty boundary there is an additive isomorphism*

$$\pi_*\mathsf{Conf}_n(M) \cong (\pi_* M)^n \oplus \bigoplus_{i=0}^{n-1} \bigoplus_{w\in \mathsf{B}(\{1,\dots,i\}\sqcup\{1,\dots,i\}')} \pi_{*+1}\Big(\Sigma^{1+l_w(d-2)}(\Omega M)^{\wedge l'_w}\Big).$$

Proof. Since $\partial M \neq \emptyset$ there is an isomorphism $\pi_*\mathsf{Conf}_n(M) \cong \bigoplus_{i=0}^{n-1}\pi_*(M_{-i})$, where M_{-i} is the manifold M with i points removed [Lev95]. By Lemma 5.1 for a finite set $S \neq \emptyset$ there is a retraction $\mathsf{retr}\colon M\setminus S \xrightarrow{\sim} M\vee \mathbb{S}_S := M\vee\bigvee_S \mathbb{S}^{d-1}$, and in Section 5.1 we find $\Omega(M\vee\mathbb{S}_S)\simeq \Omega M\times Z_S$ and $Z_S \simeq \prod_{w\in\mathsf{B}(S\sqcup S')}\Omega\Sigma^{1+l_w(d-2)}(\Omega M)^{\wedge l'_w}$. □

COROLLARY 1.9. [7] *For M as before consider the contravariant n-cube $\big(\mathsf{Conf}_\bullet(M), \jmath\big)$ where for $k\in S\subseteq \underline{n}$ the map $\jmath^k_S\colon \mathsf{Conf}_S(M)\to\mathsf{Conf}_{S\setminus k}(M)$ forgets the k-th point in the configuration. Then*

$$\Omega\,\mathrm{tofib}\,\big(\mathsf{Conf}_\bullet(M),\jmath\big) \simeq \prod_{w\in\mathsf{N}'\mathsf{B}(\underline{n-1})} \Omega\Sigma^{1+(d-2)l_w}(\Omega M)^{\wedge l'_w}\,.$$

Hence, the first non-trivial homotopy group is $\pi_{(n-1)(d-2)+1}\,\mathrm{tofib}\,\big(\mathsf{Conf}_\bullet(M),\jmath\big)\cong \mathsf{Lie}_{\pi_1 M}(n-1)$.

Proof. Each map $\jmath^n_{S\cup n}$ for $S\subseteq \underline{n-1}$ is a fibre bundle [FN62] whose fibre is homeomorphic to $M\setminus S\simeq M\vee\mathbb{S}_S$. By taking fibres first in the direction of $\jmath^n$-maps, the total fibre of $\big(\Omega\mathsf{Conf}_\bullet(M),\Omega\jmath\big)$ is equivalent to $\mathrm{tofib}\,\big(\Omega(M\vee\mathbb{S}_\bullet),\Omega\mathsf{col}\big)$, and this was computed in (1.3). □

Sinha [Sin09] uses certain compactifications of configuration spaces to construct the mentioned model $AM_n(M)$ for $\mathsf{T}_n\mathcal{K}(M)$, then employed in [BCKS17]. See Remark 4.16 for a comparison to our approach. Configuration spaces were also used by Koschorke [Kos97] to construct invariants of link maps in arbitrary dimensions. His results are very similar in spirit to ours, showing that certain invariants related to Samelson products agree with Milnor invariants for classical links.

§2 Gropes give points in the Taylor tower layers

In Part III we specialise to $d=3$, but this restriction is not essential, see Remark 1.10. Namely, in our joint work [KST] we construct certain points in $\mathsf{H}_n(I^3)$ from the input data given by *(simple capped genus one) grope cobordisms* of degree n from [CT04b]. In this thesis we show that this result readily extends to any 3-manifold M.

Gropes. Grope cobordisms are certain geometric objects modelled on trees, that 'witness' n-equivalence of the two knots on 'the boundary of a cobordism'.

More precisely, one first defines an *abstract (capped) grope* G_Γ modelled on an undecorated tree $\Gamma\in\mathrm{Tree}(n)$ as a 2-complex with circle boundary built by inductively attaching surface stages according to Γ: each leaf contributes a disk (called a cap), and each trivalent vertex a torus with one boundary component. We also fix an oriented subarc $a_0\subseteq\partial G_\Gamma=\mathbb{S}^1$, as on the left[8] of Figure 1 (see Definition 7.9). Moreover, the tree is canonically embedded $\Gamma\hookrightarrow G_\Gamma$ into this 2-complex.

A *(capped) grope cobordism on a knot $K\in\mathcal{K}(M)$ modelled on* Γ is a map $\mathcal{G}\colon G_\Gamma\to M$ which embeds all stages mutually disjointly and disjointly from K except that $\mathcal{G}(a_0)\subseteq K$ and for $i\in\underline{n}$ the i-th cap intersects K transversely in a point p_i so that $\mathcal{G}(a_0)<p_1<\cdots<p_n$ in K (see Definition 7.10).

[7] That this cube is $\big((n-1)(d-2)+1\big)$-cartesian can also be calculated using the Blakers–Massey theorem, but we could not find a computation of the homotopy type in the literature.

[8] Although our pictures sometimes seem not smooth, the corners are present only for convenience.

The *degree of* $\mathcal{G}$ is the number n of leaves in the tree $\Gamma \in \mathrm{Tree}(n)$. A simple example of a grope cobordism of degree 2 is shown on the right of Figure 1. Note how the 'arms' could instead be twisted and tied into knots, producing non-isotopic grope cobordisms on K which are all modelled on the same tree Γ.

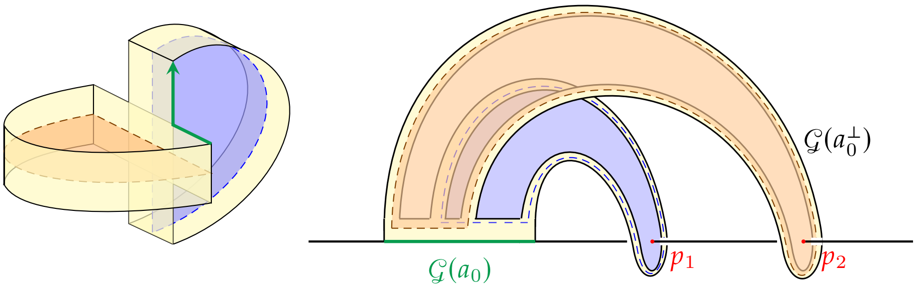


Figure 1. *Left*: The abstract capped grope G_Γ modelled on the tree $\Gamma =$ (2 1) is the union of the yellow torus and the two disks. *Right*: A capped grope cobordism $\mathcal{G} \colon G_\Gamma \to I^3$ on $K = \mathrm{U}$, the horizontal line. The knot $\partial^\perp \mathcal{G}$ is the union of $\mathrm{U} \setminus \mathcal{G}(a_0)$ and the long black arc $\mathcal{G}(a_0^\perp)$, and is isotopic to a trefoil.

Furthermore, for the relation of gropes to the Taylor tower it is convenient to consider thickenings (tubular neighbourhoods) of grope cobordisms which we call *thick gropes* (see Definition 7.13). They are given as embeddings

$$\mathbf{G} \colon \mathsf{B}_\Gamma \hookrightarrow M$$

of a certain model ball $\mathsf{B}_\Gamma \cong \mathbb{B}^3$ which contains G_Γ, so that $\mathbf{G}(G_\Gamma)$ is a grope cobordism on K. We denote $a_0^\perp := \partial G_\Gamma \setminus a_0$ and define the *output of* $\mathbf{G}$ as the knot

$$\partial^\perp \mathbf{G} := (K \setminus \mathbf{G}(a_0)) \cup \mathbf{G}(a_0^\perp).$$

Thus, a grope describes a modification of the knot K by replacing its arc $\mathbf{G}(a_0) \subseteq K$ by $\mathbf{G}(a_0^\perp)$. We say that K is n-equivalent to this modified knot $\partial^\perp \mathbf{G}$ and write $K \sim_n \partial^\perp \mathbf{G}$. More generally, two knots are n-equivalent if there is a sequence of thick gropes of degree n from one to another. This gives the variant due to [CT04b] of the filtration $\mathbb{K}_n(M; \mathrm{U}) := \{K \in \mathbb{K}(M) : K \sim_n \mathrm{U}\}$ of Gusarov and Habiro, mentioned above. We study it in the final Part IV.

Finally, we define a space $\mathsf{Grop}_n^1(M; K)$ of thick gropes of degree n in M on K (see Definition 7.15). Taking the output knot gives a continuous map $\partial^\perp \colon \mathsf{Grop}_n^1(M; K) \to \mathcal{K}(M)$.

Theorem D ([KST][9])**.** *If* $\mathbf{G}$ *be a thick grope of degree* $n \geq 1$ *in* M *on a knot* K*, then there is a path* $\Psi^{\mathbf{G}} \colon I \to \mathsf{P}_n(M)$ *from* $\mathsf{ev}_n(K)$ *to* $\mathsf{ev}_n(\partial^\perp \mathbf{G})$*. Moreover, for* $K = \mathrm{U}$ *this gives a continuous map*

$$\psi \colon \mathsf{Grop}_n^1(M; \mathrm{U}) \to \mathsf{H}_n(M), \quad \psi(\mathbf{G}) := (\partial^\perp \mathbf{G}, \Psi^{\mathbf{G}}).$$

We prove this in Section 8.1, using the crucial *isotopy between the two surgeries on a capped torus.* Combining such isotopies for each stage of an abstract grope G_Γ gives one $(n-1)$-parameter family of disks $\mathbb{D}_u$, all contained in the model ball B_Γ and with the boundary $\partial \mathbb{D}_u = \partial G_\Gamma$, and for which $\mathbf{G}(\mathbb{D}_u)$ intersects K only within certain subarcs of K. The combinatorics of these intersections is such that the homotopy of $\mathbf{G}(a_0)$ across each of those disks precisely defines a path in $\mathsf{P}_n(M)$.

The theorem immediately implies that there is a factorisation

$$\begin{tikzcd}
\mathbb{K}(M) \arrow[rr, "\pi_0 \mathsf{ev}_n"] \arrow[dr, "\nu_n"'] & & \pi_0 \mathsf{P}_n(M) \\
& \mathbb{K}(M)/{\sim_n} \arrow[ur] &
\end{tikzcd} \tag{1.4}$$

[9] The first statement was first proven in [Shi19] for $M = I^3$.

Indeed, if $K \sim_n K'$, then there is a sequence of thick gropes witnessing this, so concatenation of the corresponding paths in $\mathsf{P}_n(M)$ is a path from $\mathsf{ev}_n K$ to $\mathsf{ev}_n K'$. In particular, as mentioned in the discussion after Conjecture 1, for $M = I^3$ this is *equivalent* to the claim that $\pi_0\mathsf{ev}_n$ is a Vassiliev invariant of type $\leq n-1$, and this was first shown by [BCKS17].

This equivalence between the geometric and the classical approach to the Vassiliev theory is due to [Hab00] (see Corollary 7.5). In contrast, it is an open problem (Conjecture 7.8) if this holds for any 3-manifold M, so the factorisation (1.4) just says that $\pi_0\mathsf{ev}_n$ is an invariant of n-equivalence of knots in M. See also Section 7.1 for more on the relation between the two approaches.

There is one more important notion related to a thick grope $\mathbf{G}$ modelled on $\Gamma \in \mathrm{Tree}(n)$: it has a *signed decoration* $(\varepsilon_i, \gamma_i)_{i\in\underline{n}}$, where $\varepsilon_i \in \{\pm1\}$ is the sign of the intersection point $p_i \in K$ and $\gamma_i \in \Omega M$ is the loop which goes from $K(0)$ to p_0 along the unique path in the tree $\mathbf{G}(\Gamma)$ and then back along K (see Definition 7.12). Then we let $\varepsilon := \sqcap_i \varepsilon_i$ and $g_i = [\gamma_i] \in \pi_1 M$ and define a class

$$\mathcal{T}_n(\mathbf{G}) := \varepsilon\Gamma^{g_{\underline{n}}} \in \{\pm1\} \times \mathrm{Tree}_{\pi_1 M}(n).$$

Grope forests. Observe that each $\pm\Gamma^{g_{\underline{n}}} \in \mathbb{Z}[\mathrm{Tree}_{\pi_1 M}(n)]$ can be realised by many mutually non-isotopic gropes of degree n. However, we will also need to realise arbitrary linear combinations of decorated trees. The corresponding notion on the geometric side is a 'linear combination of thick gropes', which we call a *grope forest*. It is defined as an embedding

$$\mathbf{F}\colon \bigsqcup_{1\leq l\leq N} \mathsf{B}_{\Gamma_l} \hookrightarrow M$$

so that $\mathbf{F}|_{\mathsf{B}_{\Gamma_l}}$ for $1 \leq l \leq N$ are mutually disjoint thick gropes on K whose arcs $\mathbf{F}|_{\mathsf{B}_{\Gamma_l}}(a_0)$ appear in the order of their label l (Definition 7.14). We also define a space $\mathsf{Grop}_n(M;\mathrm{U}) := \bigsqcup_{N\geq1}\mathsf{Grop}_n^N(M;\mathrm{U})$ of grope forests of any cardinality, with the space of thick gropes given as the component $N = 1$.

Taking decorated trees of thick gropes in a grope forest we get the *underlying decorated tree map*

$$\mathcal{T}_n\colon\ \pi_0\mathsf{Grop}_n(M;\mathrm{U}) \twoheadrightarrow \mathbb{Z}[\mathrm{Tree}_{\pi_1 M}(n)].$$

This is a *surjection* of sets (see Proposition 7.16). In other words, any linear combination of $\pi_1 M$-decorated trees is realised by a grope forest on U.

Furthermore, in Proposition 8.5 we extend the map from Theorem D to

$$\psi\colon \mathsf{Grop}_n(M;\mathrm{U}) \to \mathsf{H}_n(M).$$

Remark 1.10. *Let us point out that although we restrict only to gropes in* 3*-manifolds, there should exist a generalisation for any* $d \geq 3$*. Namely, one simply replaces the model* 3*-ball* B_Γ *by a* d*-ball containing the* 2*-complex* G_Γ*, so that a thick grope is still an embedding* $\mathsf{B}_\Gamma \hookrightarrow M$ *such that neighbourhoods of caps intersect* K *in single points. To construct* $\psi(\mathbf{G}) \in \Omega^{n(d-3)}\mathsf{H}_n(M)$ *one uses that the intersection point has a* $(d-1)$*-dimensional normal disk, giving an* $n(d-2)$*-family of arcs.*

Interlude: About the geometric calculus. By the geometric calculus we mean a geometric approach to the theory of finite type invariants, either using claspers or gropes. We refer the reader to Section 7 for all notions related to this theory necessary for our main result, Theorem E. We will not assume familiarity with it and we will prove all needed results.

We discuss the geometric calculus further in Section 10 and there we *do rely* on the existing background. We synthesise certain known results which were scattered throughout the literature and also fill in some gaps. In particular, there is a map $\mathcal{R}_n\colon \mathbb{Z}[\mathrm{Tree}_{\pi_1 M}(n)] \to \mathbb{K}_n(M;\mathrm{U})/\sim_{n+1}$ related both to $\partial^\perp$ and $\mathcal{T}_n$, and we use it to show that the target is a *an abelian group for any* 3*-manifold* M *and* $n \geq 1$. See Section 2.2.1 for the precise statements.

§3 *The underlying tree is detected in the Taylor tower*

The first step on the journey between the homotopy theory of punctured knots and the geometry of gropes was to translate them both to the language of decorated trees: for $\dim M = 3$ these trees at the same time underlie gropes and also generate the group of components of the Taylor layers. It remains to show their compatibility via the map

$$\mathsf{Grop}_{n-1}(M;\mathrm{U}) \xrightarrow{\psi} \mathsf{H}_{n-1}(M) \xrightarrow{\mathsf{e}_n} \mathsf{F}_n(M).$$

Theorem E (Main Theorem)**.** *For $\mathbf{G} \in \mathsf{Grop}^1_{n-1}(M;\mathrm{U})$ the connected component of the point $\mathsf{e}_n\psi(\mathbf{G}) \in \pi_0\mathsf{F}_n(M)$ is given by the class of its underlying tree $[\mathcal{T}_{n-1}(\mathbf{G})] \in \mathsf{Lie}_{\pi_1 M}(n-1)$.*

More explicitly, for a thick grope $\mathbf{G}\colon \mathsf{B}_\Gamma \to M$ on U with the underlying tree $\varepsilon\Gamma^{g_{\underline{n-1}}}$, we have

$$\left[\mathsf{e}_n\psi(\mathbf{G})\right] = \left[\varepsilon\Gamma^{g_{\underline{n-1}}}\right] \quad \in \pi_0\mathsf{F}_n(M) \cong \mathsf{Lie}_{\pi_1 M}(n-1).$$

We prove this in Section 9 using Corollary 1.4 from above: it is enough to show that the Samelson product $\Gamma(m_i^{\varepsilon_i g_i})\colon \mathbb{S}^{n-1} \to \Omega M_{\underline{n-1}}$ is homotopic to the map

$$\mathcal{D}\big(\chi\mathsf{e}_n\psi(\mathbf{G})\big)^{\underline{n-1}}\colon\ \mathbb{S}^{n-1} \to \Omega M_{\underline{n-1}}.$$

This is just the initial coordinate of $\mathcal{D}\big(\chi\mathsf{e}_n\psi(\mathbf{G})\big) \in \Omega^{n-1}\operatorname{tofib}(\Omega M_\bullet, \Omega\lambda)$. The maps $\mathcal{D}$ and χ were constructed in Theorem C. The idea of the proof is to use inductive descriptions of both Samelson products (see Lemma A.5) and thick gropes, to reduce to checking that $\mathcal{D}\big(\mathsf{e}_n\psi(\mathbf{G})\big)^{\underline{n-1}}$ is homotopic to a certain pointwise commutator map. A crucial step for this reduction is the description of the map χ in Section 6 as

$$(\chi f)^{\underline{n-1}} = \mathop{\boxplus}_{S\subseteq\underline{n-1}} (f^{\underline{n-1}})^{h^S}.$$

This is a map on $\mathbb{S}^{n-1}$ obtained by gluing together along faces 2^{n-1} different maps $(f^{\underline{n-1}})^{h^S}$, each defined on I^{n-1} as a certain 'h^S-reflection' of the original map $f^{\underline{n-1}}$ across a face of I^{n-1}.

Therefore, every generator of $\pi_0\mathsf{F}_n(M)$ is in the image of $\pi_0\mathsf{e}_n$. However, Theorem B claims that $\pi_0\mathsf{e}_n$ is a surjection of sets, so we need to extend Theorem E to realise linear combinations as well.

Theorem F. *For a grope forest $\mathbf{F} \in \mathsf{Grop}_{n-1}(M;\mathrm{U})$ we have*

$$\left[\mathsf{e}_n\psi(\mathbf{F})\right] = \left[\mathcal{T}_{n-1}(\mathbf{F})\right] \quad \in \pi_0\mathsf{F}_n(M) \cong \mathsf{Lie}_{\pi_1 M}(n-1).$$

In other words, the following diagram of sets commutes

$$\begin{tikzcd}
\pi_0\mathsf{Grop}_{n-1}(M;\mathrm{U}) \arrow[r, "\mathcal{T}_{n-1}"] \arrow[d, "\pi_0\psi"'] & \mathbb{Z}[\mathrm{Tree}_{\pi_1 M}(n-1)] \arrow[d, two heads, "(\mathrm{mod}\ AS, IHX)"] \\
\pi_0\mathsf{H}_{n-1}(M) \arrow[r, "\pi_0\mathsf{e}_n"] & \pi_0\mathsf{F}_n(M)
\end{tikzcd} \tag{1.5}$$

For the proof of this theorem see the end of Section 9. We can now prove Theorem B.

Proof of Theorem B. Since by Proposition 7.16 the underlying decorated tree map $\mathcal{T}_{n-1}$ is surjective, the commutative diagram of Theorem F implies $\pi_0\mathsf{e}_n$ is as well. $\square$

Let us remark that more general gropes and ψ mentioned in Remark 1.10 would give points $\mathsf{e}_n\psi(\mathbf{G}) \in \Omega^{(n-1)(d-3)}\mathsf{F}_n(M)$, and the method of our proofs should readily extend to show surjectivity of ev_n on the first non-vanishing group $\pi_{(n-1)(d-3)}\mathsf{F}_n(M)$ of the Taylor layer for $\mathcal{K}(M)$. We plan to provide details in future work, and give a brief discussion in Section 2.3.

2 Geometric realisations of trees

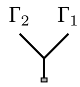
In Section 2.1 we define several variants of trees. In Section 2.2 we state our results about the geometric realisation of trees in 3-manifolds, and relate this to the homotopy spectral sequence for the Taylor tower. Finally, we discuss applications beyond dimension three in Section 2.3.

2.1 Trees

2.1.1 Lie trees. Fix a finite nonempty set S and an integer $d \geq 2$.

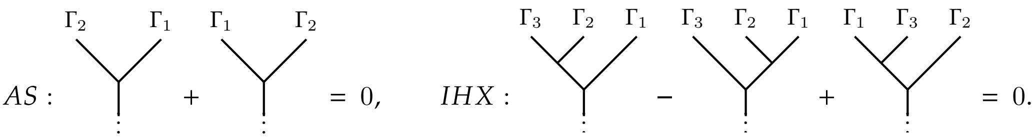
Definition 2.1. *A (vertex-oriented uni-trivalent) tree is a connected simply connected graph with vertices of valence three or one and with cyclic order of the edges incident to each trivalent vertex, called the vertex orientation. In the pictures this is specified by the positive orientation of the plane.*

A rooted tree $\Gamma \in \mathrm{Tree}(S)$ is a tree with one distinguished univalent vertex (the root) and all other univalent vertices (the leaves) labelled in bijective manner by the set S.

We define the grafting[10] *of two trees $\Gamma_j \in \mathrm{Tree}(S_j)$ for $j = 1, 2$ as the tree* 

$\in \mathrm{Tree}(S_1 \sqcup S_2)$ *obtained by gluing the two roots together and 'sprouting' a new edge with a new root.*

The group of Lie trees $\mathsf{Lie}(S) := {\mathbb{Z}[\mathrm{Tree}(S)]}/{AS, IHX}$ is defined as the quotient of the free abelian group on the set of rooted trees by the following relations, where the dots represent the remaining unchanged part of an arbitrary tree:



(2.1)

We will relate Lie trees to words (Lie monomials) in the free Lie algebra.

Definition 2.2. *Let $\mathbb{L}_d(S) = \mathbb{L}(x^k : k \in S)$ be the free $\mathbb{Z}$-graded Lie algebra over $\mathbb{Z}$, where each x^k has degree $|x^k| = d - 2$. Thus, the degree of a word $w \in \mathbb{L}_d(S)$ is $|w| = (d-2)l_w$ where l_w is the length of w, that is, the total number of letters in w.*

The normalised Lie algebra $\mathsf{N}\mathbb{L}_d(S)$ is the Lie subalgebra of $\mathbb{L}_d(S)$ generated by the words in which every letter appears at least once.[11] *Let $\mathsf{Lie}_d(S) \subseteq \mathsf{N}\mathbb{L}_d(S)$ be its subgroup generated by the words in which each letter appears exactly once. This is precisely the degree $|S|(d-2)$ part of $\mathsf{N}\mathbb{L}_d(S)$.*

If $d = 2$ one can assign to a tree $\Gamma \in \mathsf{Lie}(S)$ a Lie word $\omega_2(\Gamma) \in \mathsf{Lie}_2(S)$ using vertex orientations, so that the grafting of trees precisely corresponds to the Lie bracket. This gives an isomorphism $\mathsf{Lie}(S) \cong \mathsf{Lie}_2(S)$ since relations (2.1) correspond to the antisymmetry and Jacobi relations in $\mathsf{Lie}_2(S)$.

However, for a general $d \geq 2$ Lie words satisfy the *graded* antisymmetry and Jacobi relations:

$$\begin{aligned} &[w_1, w_2] + (-1)^{|w_1||w_2|}[w_2, w_1] = 0, \\ &[w_1, [w_2, w_3]] - [[w_1, w_2], w_3] - (-1)^{|w_1||w_2|}[w_2, [w_1, w_3]] = 0, \end{aligned} \tag{2.2}$$

while the relations (2.1) – which are inspired by applications in geometric topology (see [CST07] for example) – never involve graded signs. We have learned from [Con08] that the correspondence can nevertheless be obtained as follows (compare also [Rob04]).

---

[10] Let us warn the reader that in the context of operads one usually grafts the root of one tree into the leaf of another; strictly speaking, we are performing the 'full grafting' of two trees onto the corolla of degree 2.

[11] That is, $\mathsf{N}\mathbb{L}_d(S) := \bigcap_{k \in S} \ker(\jmath^k : \mathbb{L}_d(S) \to \mathbb{L}_d(S \setminus k))$, where $\jmath^k$ replaces each appearance of x^k by zero.

Lemma 2.3. *If S is ordered, there is an isomorphism of abelian groups*

$$\omega_d\colon\ \mathsf{Lie}(S) \xrightarrow{\cong} \mathsf{Lie}_d(S)$$

defined inductively on $|S|$ by $\overset{i}{|} \mapsto x^i$ and for $S = S_1 \sqcup S_2$ and $\Gamma_j \in \mathrm{Tree}(S_j)$ by

$$\overset{\Gamma_2\quad\Gamma_1}{\curlyvee} \mapsto (-1)^{(1|2)_d}\big[\omega_d(\Gamma_1), \omega_d(\Gamma_2)\big].$$

Here $(1|2)_d := (1|2)\cdot(d-2)$ with $(1|2) := \big|\big\{(i_1, i_2) \in S_1 \times S_2 : i_1 > i_2\big\}\big|$.

Hence, one can think of graded Lie words also as Lie trees, but keeping in mind that for odd d the isomorphism ω_d introduces a sign. For the proof of the lemma see the end of Appendix A.

For $\underline{n} := \{1, \dots, n\}$ we write $\mathrm{Tree}(n) := \mathrm{Tree}(\underline{n})$ and $\mathsf{Lie}(n) := \mathsf{Lie}(\underline{n})$. Their elements can alternatively be drawn in the plane as in Figure 2: the root and leaves are attached to a fixed horizontal line according to their increasing label, with the root labelled by 0. The vertex orientation is still induced from the plane; we might have some edges intersecting, but this is not part of the data.

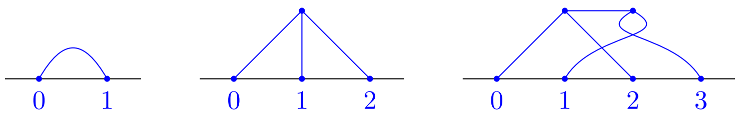


Figure 2. The trees $\omega\colon \overset{i}{|} \mapsto x^i$, $\overset{2\ 1}{\curlyvee} \mapsto [x^1, x^2]$, $\overset{1\ 3\ 2}{\curlyvee} \mapsto (-1)^{d-2}[x^2, (-1)^{d-2}[x^3, x^1]]$ drawn in the plane.

Using the AS and IHX relations repeatedly one can show that $\mathsf{Lie}(n) \cong \mathbb{Z}^{(n-1)!}$, with a basis given by trees from Figure 3 (ignoring red decorations for now) for various permutations $\sigma \in \mathcal{S}_{n-1}$. These trees correspond to left-normed Lie words $[x^{\sigma(1)}, [x^{\sigma(2)}, [\dots[x^{\sigma(n-1)}, x^n]\dots]]]$.

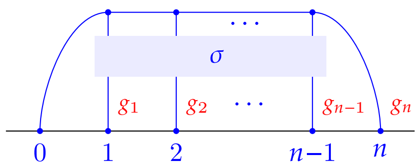


Figure 3. A left-normed tree $\Gamma^{g_{\underline{n}}} \in \mathrm{Tree}_{\pi_1 M}(n)$, with $g_{\underline{n}} := (g_1, \dots, g_n) \in (\pi_1 M)^n$ and $\sigma \in \mathcal{S}_{n-1}$.

However, $\mathsf{Lie}(n)$ is an interesting $\mathcal{S}_n$-representation, by permuting the leaf labels, giving the arity n of the *Lie operad* $\mathsf{Lie}(\bullet)$. Actually, it naturally *extends* to an $\mathcal{S}_{n+1}$-representation by permuting all the labels $\{0, 1, \dots, n\}$; this is related to the cyclic operad structure on $\mathsf{Lie}(\bullet)$, see Remark B.5.

Furthermore, Lemma 2.3 implies that $\mathsf{Lie}_d(n) \cong \mathsf{Lie}(n) \otimes \mathrm{sgn}_{n+1}$ as representations of $\mathcal{S}_{n+1}$, where sgn_{n+1} is the sign representation. More explicitly, $\sigma \in \mathcal{S}_{n+1}$ acts on a word given as $w = \omega_d(\Gamma)$ for some tree $\Gamma \in \mathsf{Lie}(n)$, by $\sigma_*(\omega_d(\Gamma)) := (\mathrm{sgn}\,\sigma)\,\omega_d(\sigma_*\Gamma)$. See [Rob04, Prop. 3.4] for details.

2.1.2 Decorated trees. For manifolds with non-trivial fundamental group $\pi_1 M$ we will need to consider more general trees. Let π be a set and S, d fixed as above. We write $\pi^S := \mathrm{Map}(S, \pi)$, so $\pi^{\underline{n}} = \pi^n$ is the cartesian product. If $\pi = \pi_1 M$, then we assume $d := \dim M$ by convention.

Definition 2.4. *Let $\mathrm{Tree}_\pi(S) := \mathrm{Tree}(S) \times \pi^S$ be the set of rooted trees whose leaves are labelled bijectively by S, and additionally for each $i \in S$ the edge incident to the leaf i is assigned an element $g_i \in \pi$, called a* decoration*. We denote elements of $\mathrm{Tree}_\pi(S)$ by Γ^{g_S} where $\Gamma \in \mathrm{Tree}(S)$ and $g_S := (g_i)_{i\in S} \in \pi^S$, and call them π-*decorated trees*.*

Definition 2.5. *The group* $\mathsf{Lie}_\pi(S)$ *of* π-*decorated Lie trees is defined as the quotient of* $\mathbb{Z}[\mathrm{Tree}_\pi(S)]$ *by the relations analogous to* AS, IHX *from* (2.1)*, which respect decorations in the natural way.*

The map forgetting the decoration $\mathsf{Lie}_\pi(S) \to \mathsf{Lie}(S)$ is an isomorphism if $\pi = \{1\}$. Similarly as above, $\mathsf{Lie}_\pi(n) \cong \big(\mathbb{Z}[\pi^n]\big)^{(n-1)!}$ with the basis of left-normed π-decorated trees from Figure 3. Analogously to Lemma 2.3 there is an isomorphism of $\mathsf{Lie}_\pi(S)$ onto the subgroup of the free Lie algebra $\mathbb{L}\big((x^i)^g : i \in S, g \in \pi, |(x^i)^g| = d-2\big)$ of words in which each $i \in S$ appears exactly once.

If π is a group, there is an action of $\sigma \in \mathcal{S}_{n+1}$ on $\mathsf{Lie}_\pi(n)$ by

$$\sigma_*(\Gamma^{g_{\underline{n}}}) \;:=\; \big(\sigma_*\Gamma\big)^{\sigma_*(g_{\underline{n}})}$$

using the already mentioned action on $\mathsf{Lie}(n)$ and the following one on π^n. Let σ act naturally on the set $[n] := \{0, 1, \ldots, n\}$, then define $g_0 = 1 \in \pi$ and

$$\sigma_*(g_{\underline{n}}) = (g_{\sigma^{-1}(0)})^{-1} \cdot \big(g_{\sigma^{-1}(1)}, \ldots, g_{\sigma^{-1}(n)}\big). \tag{2.3}$$

This is well defined since there is a bijection $\pi^n \to {\pi^{[n]}}\big/{\Delta(\pi)}$, where Δ is the diagonal left action of π, given by $g_{\underline{n}} \mapsto [(1, g_{\underline{n}})]$ and its inverse by $[g_{[n]}] \mapsto (g_0^{-1} \cdot g_1, \ldots, g_0^{-1} \cdot g_n)$. As the target has a natural action by $\mathcal{S}_{n+1}$, we obtain an action on π^n which is precisely given by the formula (2.3).

Definition 2.6. *For* $\sigma \in \mathcal{S}_{n+1}$ *we denote by* σ_* *the induced action on* $\mathsf{Lie}_\pi(n)$*, and for a transposition* $(i\ j) \in \mathcal{S}_{n+1}$ *and* $T \in \mathsf{Lie}_\pi(n)$ *we denote* $T^{i,j} := (i\ j)_*(T)$.

The motivation for this action comes from the way we interpret decorations when $\pi = \pi_1 M$. Namely, a $\pi_1 M$-decorated tree Γ^{g_S} can be viewed as a *homotopy class of a map* $x\colon \Gamma \to M$ which takes the root and leaves to some fixed arc K in M (a knot in practice).

The decoration $g_i \in \pi_1 M$ for the i-th leaf is the homotopy class of the loop γ_i, which goes from $x(0)$ (the basepoint) to the leaf $x(i)$ along the unique path in the tree connecting the i-th leaf and the root, then back from $x(i)$ to $x(0)$ along K. More precisely, the basepoint of M is fixed in some $p_0 \in K$ and the described loop γ_i should be conjugated by the piece of K between p_0 and $x(i)$.

For example, the action of $(0\,k)$ makes the k-th leaf of T the new root in $T^{0,k}$. Thus, if $g_i = [\gamma_i]$ are the old decorations, the new decoration for the i-th leaf in $T^{0,k}$ is homotopic to $\gamma_k^{-1} \cdot \gamma_i$.

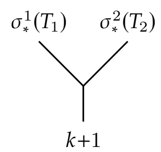
Remark 2.7. *For* $\pi = \pi_1 M$ *this action of* $\mathcal{S}_3$ *on* $\mathsf{Lie}_\pi(2) \cong \Lambda_1(\pi, 3) \cong \mathbb{Z}[\pi^2]$ *appears in the work of Schneiderman and Teichner [ST04], see the discussion around Theorem 3 there.*

Moreover, the group $\mathsf{Lie}_\pi(n)$ *is precisely equal to* $\Lambda_{n-1}(\pi, n+1)$ *from their more recent work [ST14], where the more general groups* $\Lambda_n(\pi, m)$ *were used as targets for obstruction invariants for pulling apart* m *surfaces in* M*; see [ST14, Lem. 2.1] for this identification.*

2.1.3 Jacobi trees.

We will need the following auxiliary notion.

Definition 2.8. *Assume* $T \in \mathrm{Tree}_\pi(n)$ *is obtained by grafting together* $T_j \in \mathrm{Tree}_\pi(S_j)$ *for* $j = 1, 2$*, so that for some* $k \in S_1$ *we have* $k+1 \in S_2$*. Consider the cycles* $\sigma^1 := (0\,1 \cdots k{+}1)$ *and* $\sigma^2 := (1 \cdots k)$ *in* $\mathcal{S}_{n+1}$ *and note that* $\sigma^1(S_1) \cap \sigma^2(S_2) = \{k{+}1\}$*. Define the* k-*replanting of* T *as the* π-*decorated tree*

$T[k] :=$ 

$\in \mathrm{Tree}_\pi(n),$

obtained by grafting together the (unrooted) trees $\sigma^j_*(T_j) \in \mathrm{Tree}(\sigma^j(S_j))$ *along their leaves* $k{+}1$.

Definition 2.9. *Define the abelian group of* Jacobi trees *in a d-manifold M by*

$$\mathcal{A}_1^T(M) := \mathsf{Lie}_{\pi_1 M}(1) \big/ {}_{1}\big|^{1} \qquad \textit{and for } n \geq 2 \textit{ by} \qquad \mathcal{A}_n^T(M) := \mathsf{Lie}_{\pi_1 M}(n) \big/ STU^2_{\pi_1 M}$$

where the relation $STU^2_{\pi_1 M}$ is defined by

$$STU^2_{\pi_1 M}: \quad T - T^{k,k+1} \quad = \quad T[k] - T[k]^{0,1} \tag{2.4}$$

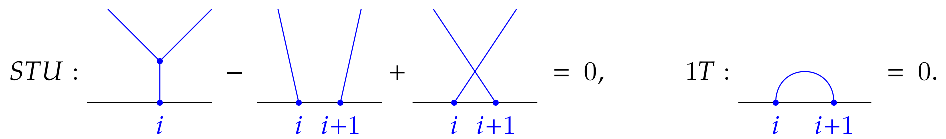
for any tree $T \in \mathrm{Tree}_{\pi_1 M}(n)$ that satisfies conditions of Definition 2.8.

Note that $\mathcal{A}_1^T(M) \cong \mathbb{Z}[\pi_1 M \backslash \{1\}]$, so for M simply connected we have $\mathcal{A}_1^T(M) = 0$. The calculations with the spectral sequence indicate that when $\pi_{d-1} M \neq 0$ apart from $STU^2_{\pi_1 M}$ one should perhaps introduce additional relations to $\mathcal{A}_n^T(M)$. See comments after Corollary 2.18.

2.1.4 Jacobi diagrams. In the theory of finite type invariants for $M = I^3$ one more generally considers Jacobi diagrams, which are uni-trivalent graphs with univalent vertices labelled by $0, \dots, |u| - 1$ (the leaves) and vertex-oriented trivalent vertices (see Definition 2.1).

The degree of a diagram $\frac{|u|+|t|}{2}$ is the half of the total number of vertices[12] and one uses the same convention as in Figure 2 to draw them in the plane (but there is no root now).

Definition 2.10. *For $n \geq 0$ define $\mathcal{A}_n$ as the quotient of the $\mathbb{Z}$-linear span of the set of Jacobi diagrams of degree n by the linear combinations of diagrams which locally look like*



(2.5)

Conant introduced in [Con08] the STU^2 relation on $\mathsf{Lie}(n)$ for odd d by

$$STU^2_{\{1\}}: \quad STU(D, v_k) \quad = \quad STU(D, v_0). \tag{2.6}$$

This uses two different applications of the STU relation on the same Jacobi diagram D, which has degree n and exactly one loop (i.e. the first Betti number $\beta_1(D) = 1$) as in Figure 4. That is, we apply the STU relation to the vertices v_0 and v_k respectively, assuming they lie on the loop of D and they are neighbours of the leaf 0 or k respectively.

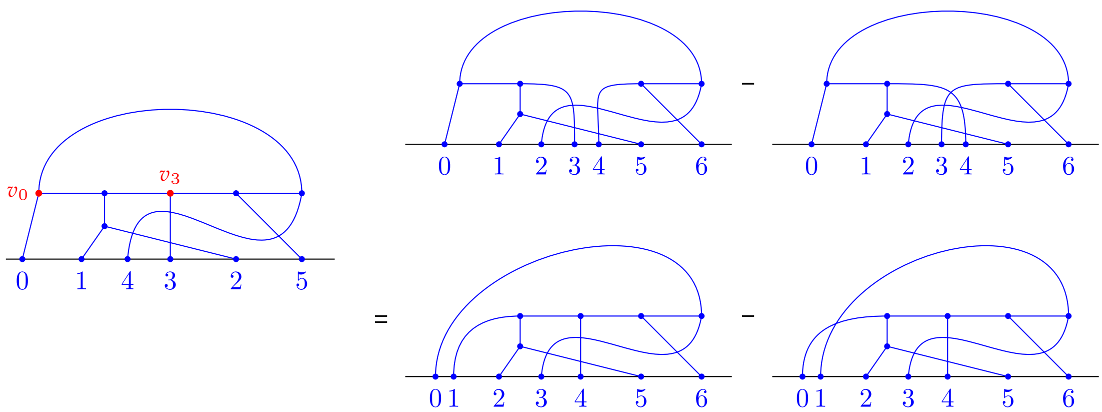


Figure 4. *Left*: A 1-loop graph D with $n = 6$ and $k = 3$. *Right*: The corresponding $STU^2_{\{1\}}$ relation.

[12] This is an integer since $|u| + 3|t| = 2|\mathrm{edges}|$.

LEMMA 2.11. *Our relation* (2.4) *agrees with Conant's* (2.6) *for* $M = I^d$ *for* d *odd. Therefore, our group* $\mathcal{A}_n^T := \mathcal{A}_n^T(I^3)$ *is precisely his* $\mathcal{A}_n^I$*.*

Proof. Indeed, (2.4) can be rewritten as (2.6): if T denotes the first term of $STU(D, v_k)$, then the first term of $STU(D, v_0)$ is obtained by gluing back leaves k and $k+1$ of T but separating the grafting at vertex v_0 in two different ways – this is exactly the k-th replanting $T[k]$. The other terms are clearly $T^{k,k+1}$ and $T[k]^{0,1}$.

Actually, Conant more generally considers $STU(D, v_k) = STU(D, v_j)$ for vertices v_j, v_k which lie on the loop and which are neighbours of the leaves $j, k \in \{0, 1, \dots, n\}$ respectively. This is implied by (2.6). Namely, we can assume that the distance of the root to the unique loop of D is one, so that we have $STU(D, v_j) = STU(D, v_0) = STU(D, v_k)$. Indeed, in the IHX relation (2.1) assume v_0 is the vertex joining Γ_2 and Γ_3 and the root 0 is in Γ_1. Then one can see that two terms have the distance of the root to the loop smaller than the third term. Thus, we proceed by induction. □

Using the interpretation of $\pi_1 M$-decorated trees as maps $\Gamma \to M$ one can give a description analogous to (2.6) for any M. For this one should consider maps of 1-loop Jacobi diagrams $x\colon D \to M$ taking univalent vertices to a fixed arc K. Picking some leaves j, k adjacent to the loop and declaring j for the root, there is a unique way to assign $g_i \in \pi_1 M$ to any leaf $i \neq k$: go from $x(j)$ to $x(i)$ along the shortest path in D which does not pass through v_k, and then back along K. For k there are two possible group elements, which differ by the homotopy class of the loop of D.

Remark 2.12. *Note that in* (2.4) *the map* $(k\,k{+}1)_*$ *just exchanges the labels, but* $(0\,1)_*$ *has the effect of exchanging the two labels and also pre-multiplying all decorations by the inverse of*

$$g_1\,(\Gamma[k]) = g_{k+1}(\Gamma) \cdot g_k(\Gamma)^{-1}.$$

This class precisely corresponds to the homotopy class of the unique loop of D*.*

Remark 2.13. *To our knowledge Jacobi diagrams have not been studied in the literature for knots in arbitrary* 3*-manifolds. However, in [GK04] similar decorated diagrams were considered, and in [Vas98] certain generalised chord diagrams, called* $[i]_M$*-routes: this as a pair of a classical chord diagram and a map* $\mathbb{S}^1 \to M$ *sending the endpoints of a chord to the same point in* M*.*

Finite type invariants of knots in general 3*-manifolds were studied in [Kal98; Vas98; Gor99]. Configuration space integrals for links in rational homology* 3*-spheres were given in [BC98; BC99] and a universal Kontsevich-type invariant of links in* 3*-manifolds in [LMO98].*

2.1.5 The Hopf algebra of Jacobi diagrams. We now survey certain results about algebraic structures related to Jacobi diagrams, and show how in the geometric approach to the finite type theory one can reduce to considering trees only.

The sum $\mathcal{A} = \bigoplus_{n \geq 0} \mathcal{A}_n$ has a structure of a commutative and cocommutative Hopf algebra over $\mathbb{Z}$: the product concatanates horizontal lines of two diagrams,[13] and the coproduct Δ sends a diagram to the sum of all possible ways of separating its connected components into two groups.[14] The augmentation $\epsilon\colon \mathcal{A} \to \mathbb{Z}$ sends the empty diagram to 1 and any other diagram to 0.

There are two natural objects associated to $\mathcal{A}$: its group of indecomposables $\mathcal{A}^I := {}^{I(\mathcal{A})}\!/\!_{I(\mathcal{A})^2}$ where $I(\mathcal{A}) := \ker(\epsilon)$ is the augmentation ideal, and its Lie algebra $\mathfrak{pr}(\mathcal{A})$ of primitive elements (those $X \in \mathcal{A}$ for which $\Delta(X) = 1 \otimes X + X \otimes 1$), but the Lie bracket is trivial when $\mathcal{A}$ is commutative. Every primitive diagram is in $I(\mathcal{A})$, so there is a canonical map $\pi\colon \mathfrak{pr}(\mathcal{A}) \to \mathcal{A}^I$.

[13] Although $\mathcal{A}$ has an obvious grading making it into a graded Hopf algebra, the product is *not* graded commutative.
[14] The horizontal line is not part of the diagram (*connected* is sometimes called internally connected).

Since $\mathcal{A}$ is connected, commutative and cocommutative $\pi \otimes \mathbb{Q}\colon \mathfrak{pr}(\mathcal{A} \otimes \mathbb{Q}) \to \mathcal{A}^I \otimes \mathbb{Q}$ is an isomorphism by Milnor and Moore [MM65, Cor. 4.18]. Moreover, another classical result of theirs [MM65, Thm. 5.16] says that $\mathcal{A}$ is rationally the symmetric algebra generated by the primitives

$$Sym\, \mathfrak{pr}(\mathcal{A} \otimes \mathbb{Q}) \hookrightarrow\!\!\!\!\rightarrow \mathcal{A} \otimes \mathbb{Q}. \tag{2.7}$$

Note that *every connected Jacobi diagram is primitive* by definition. Moreover, Bar-Natan defined a 'PBW' isomorphism with the open diagrams – similar Hopf algebra of diagrams in which univalent vertices are not attached to the line – to show this is everything.

Theorem 2.14 ([Bar95a][15]). *The space $\mathfrak{pr}(\mathcal{A} \otimes \mathbb{Q})$ is spanned by connected Jacobi diagrams.*

However, it is an open and interesting question if there are torsion elements in $\mathcal{A}$, but Bar-Natan's isomorphism requires rational coefficients. Nevertheless, we have the following observation.

Lemma 2.15. *As an algebra $\mathcal{A}$ is generated by connected Jacobi diagrams. Moreover, every connected Jacobi diagram is a linear combination of diagrams which are trees.*

Proof. The first claim is the standard fact each Jacobi diagram D can be written as a *linear combination of products of connected diagrams*. To see this, start with the leftmost component of D and use the STU relation to swap away the first leaf which does not belong to this component. Repeat until all leaves of the component come first, and then continue with the other components.

For the second statement (see also [CV97]) start with a connected diagram D which has $\beta_1(D) = k \geq 0$ loops and express it as a linear combination of diagrams with $k-1$ loops: first apply IHX as in the proof of Lemma 2.11 to get diagrams with at least one leaf neighbour on a loop of D, then apply STU to this vertex. Continue until $k = 0$, which is a linear combination of trees. □

Therefore, $\mathcal{A}$ is primitively generated, meaning that $Sym\, \mathfrak{pr}(\mathcal{A}) \twoheadrightarrow \mathcal{A}$ is surjective. It follows from (2.7) that the kernel in each degree is torsion. Moreover, we saw that $\mathcal{A}$ is actually generated by trees, but the submodule of trees is not closed under the STU relation. A crucial result is the recognition due to Conant that the STU^2 relation is the appropriate replacement.

Theorem 2.16 ([Con08][16]). *There is a natural isomorphism of graded abelian groups*

$$C\colon \mathcal{A}^T \hookrightarrow\!\!\!\!\rightarrow \mathcal{A}^I.$$

Namely, C sends a Jacobi tree to its class viewed as a Jacobi diagram modulo STU and $I(\mathcal{A})^2$. Since the STU^2 is a consequence of STU, this is well-defined. For the same reason, the map

$$P\colon \mathcal{A}^T \to \mathfrak{pr}(\mathcal{A}) \subseteq \mathcal{A} \tag{2.8}$$

which sends a Jacobi tree to its class in $\mathcal{A}$ is well-defined. As trees are primitive, P indeed has image in $\mathfrak{pr}\,\mathcal{A}$. Moreover, we clearly have that Conant's isomorphism is the composite

$$\begin{tikzcd} \mathcal{A}^T \arrow[r, "P"] \arrow[rr, bend left, hook, two heads, "C"] & \mathfrak{pr}(\mathcal{A}) \arrow[r, "\pi"] & \mathcal{A}^I \end{tikzcd}$$

Corollary 2.17. *The map P is injective, π is surjective, and rationally both are isomorphisms.*

See Theorem G3 below, Section 7.1 and Appendix B for the role of $\mathcal{A}$ in the Vassiliev theory.

[15] In [Oht02, Lem. 6.11] this was claimed over $\mathbb{Z}$, but the proof has a gap. Another argument over $\mathbb{Q}$ using (2.7) was given in [CDM12, Thm. 5.5.1], but a possibility was omitted that a polynomial in connected diagrams is primitive.
[16] In [Con08] this was shown for $C \otimes \mathbb{Q}$, but [BCKS17] check that the proof applies integrally.

2.2 Further results

2.2.1 The realisation map. Assume now that M is a 3-manifold and recall that we denote by $\mathbb{K}(M) := \pi_0\mathcal{K}(M)$ the set of isotopy classes of long knots in M.

In Section 10 we will define the mentioned equivalence relation $\sim_n$ on $\mathbb{K}(M)$ in terms of grope forests, following [CT04b; CT04a]. Then for $n \geq 1$ we denote by $\mathbb{K}_n(M;\mathrm{U}) := \{K \in \mathbb{K}(M) \,|\, K \sim_n \mathrm{U}\}$ the set of knots which are n-equivalent to U. Since $K \sim_{n+1} \mathrm{U} \implies K \sim_n \mathrm{U}$ (see Theorem 10.3), this is a decreasing filtration of $\mathbb{K}(M)$ and there is an exact sequence of sets

$$\mathbb{K}_{n+1}(M;\mathrm{U}) \hookrightarrow \mathbb{K}_n(M;\mathrm{U}) \twoheadrightarrow \mathbb{K}_n(M;\mathrm{U})/{\sim_{n+1}}$$

This is the Gusarov–Habiro filtration, which is a geometric analogue of the Vassiliev–Gusarov filtration $\mathcal{V}_n(M) \subseteq \mathbb{Z}[\mathbb{K}(M)]$. See Section 7.1 for a comparison. We study the associated graded sets in Section 10.2, following the previous works [Hab00; CT04a; Oht02].

Theorem G1. *There is a structure of an abelian group on the set* $\mathbb{K}_n(M;\mathrm{U})/{\sim_{n+1}}$ *and a morphism* $\mathcal{R}_n^T$ *of abelian groups fitting into a commutative diagram of sets*

$$\begin{tikzcd}
\pi_0\mathsf{Grop}_n(M;\mathrm{U}) \arrow[r, two heads, "\mathcal{T}_n"] \arrow[d, two heads, "\partial^\perp"'] & \mathbb{Z}[\mathrm{Tree}_{\pi_1 M}(n)] \arrow[d, two heads, "\mathcal{R}_n^T"] \\
\mathbb{K}_n(M;\mathrm{U}) \arrow[r, two heads, "mod\ \sim_{n+1}"] & \mathbb{K}_n(M;\mathrm{U})/{\sim_{n+1}}
\end{tikzcd}$$

We prove this in Theorems 10.5 and 10.7.

If $M = I\times\Sigma$ for a compact surface Σ one has a well-defined operation of connected sum on $\mathbb{K}(I\times\Sigma)$. We check in Proposition 10.11 that our group structure on $\mathbb{K}_n(I\times\Sigma;\mathrm{U})/{\sim_{n+1}}$ coincides with the one induced from the monoid $\mathbb{K}(I\times\Sigma)$. This case was studied for string links in [Hab00, Lem. 5.5].

In Section 10.3 we then relate our realisation map to the group of Jacobi trees.

Theorem G2. *The map* $\mathcal{R}_n^T$ *vanishes on AS, IHX and* $STU^2_{\pi_1 M}$ *relations, so gives a surjection of abelian groups*

$$\mathcal{R}_n^T\colon\ \mathcal{A}_n^T(M) \twoheadrightarrow \mathbb{K}_n(M;\mathrm{U})/{\sim_{n+1}}$$

In particular, for $M = I^3$ this map is related to some existing realisation maps.

Theorem G3. *There is a commutative diagram of abelian groups*

$$\begin{tikzcd}
\mathcal{A}_n^T \arrow[r, hook, "P"'] \arrow[d, two heads, "\mathcal{R}_n^T"'] \arrow[rrr, bend left, two heads, "C"] & \mathrm{pr}(\mathcal{A})_n \arrow[r, hook] & \mathcal{A}_n \arrow[r, two heads] \arrow[d, two heads, "\mathcal{R}_n"] & \mathcal{A}_n^I \arrow[d, two heads, "\mathcal{R}_n^I"] \\
\mathbb{K}_n(I^3)/{\sim_{n+1}} \arrow[rr, "K \mapsto K-\mathrm{U}"] & & \mathcal{V}_n/\mathcal{V}_{n+1} \arrow[r, "cs_n"] & \mathbb{K}_n(I^3)/{\sim_{n+1}}
\end{tikzcd}$$

where $\mathcal{R}_n$ *is the classical map using crossing changes along chords (see Section 7.1),* $\mathcal{R}_n^I$ *was defined in [CT04a] so that the right square commutes, and* cs_n *sends addition to the connected sum.*

The upper part of the diagram commutes by Lemma 2.17, so it only remains to check that the left square does as well. In other words, $\mathcal{R}_n^T$ can be seen as the 'tree part' of $\mathcal{R}_n$, or its primitive version; note that the horizontal composites are basically identity maps, so $\mathcal{R}_n^T$ is the same as $\mathcal{R}_n^I$.

2.2.2 The diagram. For a 3-manifold M we can collect our results in the following diagram

$$\begin{tikzcd}
\pi_0\mathsf{Grop}_n(M;\mathrm{U}) \arrow[rr, two heads, "\mathcal{T}_n"] \arrow[d, "\pi_0\psi"] \arrow[ddd, bend right=60, "\partial^\perp"'] & & \mathbb{Z}[\mathrm{Tree}_{\pi_1 M}(n)] \arrow[d, two heads, "(\mathrm{mod}\ AS, IHX)"] \\
\pi_0\mathsf{H}_n(M) \arrow[rr, "\pi_0\mathsf{e}_{n+1}"] & & \mathsf{Lie}_{\pi_1 M}(n) = \pi_0\mathsf{F}_{n+1}(M) \arrow[dl, two heads, "STU^2_{\pi_1 M}"] \arrow[dd, two heads, "\substack{\mathrm{mod}\\ \mathrm{im}\,\pi_0\delta}"] \\
& \mathcal{A}^T_n(M) \arrow[dl, two heads, "\mathcal{R}^T_n"'] & \\
\mathbb{K}_n(M;\mathrm{U})/_{\sim_{n+1}} \arrow[rr, "\overline{e}_{n+1}"] & & \ker(\pi_0 p_{n+1}) \subseteq \pi_0\mathsf{P}_{n+1}(M)
\end{tikzcd} \tag{2.9}$$

All objects here are abelian groups except that $\pi_0\mathsf{Grop}_n(M;\mathrm{U})$ and $\pi_0\mathsf{H}_n(M)$ are only sets, as well as possibly

$$\ker(\pi_0 p_{n+1}) := (\pi_0 p_{n+1})^{-1}([\mathsf{ev}_n \mathrm{U}])$$

in general (but for $M = I^3$ this is an abelian group). The right vertical map is the quotient by the image on π_0 of the connecting map $\delta\colon \Omega\mathsf{P}_n(M) \to \mathsf{F}_{n+1}(M)$ for the fibration p_{n+1}.

The bottom horizontal map $\overline{e}_{n+1}$ is defined as as the map induced on the (set-theoretic) kernels

$$\begin{tikzcd}
\mathbb{K}_n(M;\mathrm{U})/_{\sim_{n+1}} \arrow[r, hook] \arrow[d, dashed, "\overline{e}_{n+1}"'] & \mathbb{K}(M)/_{\sim_{n+1}} \arrow[r, two heads] \arrow[d, "\pi_0\mathsf{ev}_{n+1}"] & \mathbb{K}(M)/_{\sim_n} \arrow[d, "\pi_0\mathsf{ev}_n"] \\
\ker(\pi_0 p_{n+1}) \arrow[r, hook] & \pi_0\mathsf{P}_{n+1}(M) \arrow[r, two heads] & \pi_0\mathsf{P}_n(M)
\end{tikzcd} \tag{2.10}$$

using that $\pi_0\mathsf{ev}_n$ factors though the quotient by $\sim_n$, which is a corollary of Theorem D, see (1.4).

Put differently, (1.4) says that $\pi_0\mathsf{ev}_n$ vanishes on $\mathbb{K}_n(M;\mathrm{U})$, so $\mathbb{K}_n(M;\mathrm{U}) \subseteq \mathrm{im}\big(\pi_0\mathsf{H}_n(M) \to \mathbb{K}(M)\big)$. Observe that Conjecture 1 precisely claims that this inclusion is an equality for $M = I^3$: if $\mathsf{ev}_n K$ for some knot K is in the path component of $\mathsf{ev}_n\mathrm{U}$, then there exists a path between them induced from a grope forest. Thus, on the left side of (2.9) there is no vertical map in general.

Corollary 2.18. *The diagram (2.9) commutes.*

Proof. The subdiagram comprised of arrows labelled in red commutes by Theorem G1. The upper rectangle commutes by Theorem F.

It remains to check that the right-angle triangle on the right commutes.

Let $F \in \mathbb{Z}[\mathrm{Tree}_{\pi_1 M}(n)]$ and denote by $[F] \in \mathcal{A}^T_n(M)$ its class. By the surjectivity of $\mathcal{T}_n$ we can find $\mathbf{F} \in \mathsf{Grop}_n(M;\mathrm{U})$ with

$$\mathcal{T}_n(\mathbf{F}) = F.$$

Let $K = \partial^\perp(\mathbf{F})$ and note that $[K] = \mathcal{R}^T_n[F]$. Then we have

$$\overline{e}_{n+1}\big(\mathcal{R}^T_n[F]\big) = [\mathsf{ev}_{n+1}(K)] = [\mathsf{e}_{n+1}\psi(\mathbf{F})] = [F] \quad (\mathrm{mod}\ \ \mathrm{im}\,\delta_*).$$

Here the second equality holds since $\mathsf{ev}_{n+1}(K) = i \circ \mathsf{e}_{n+1} \circ \psi(\mathbf{F})$, where $i\colon \mathsf{F}_{n+1}(M) \to \mathsf{P}_{n+1}(M)$, by definition, see (1.2). The last equality follows from the commutativity of the upper rectangle. □

2.2.3 Consequences for classical knots. We now consider $M = I^3$ and deduce the corollaries which we announced in the introduction.

Firstly, it follows from Conant's Theorem 2.28, which we state in the next section, that if we put $M = I^3$ in diagram (2.9), then the map $\mathrm{mod}\pi_0\delta$ factors through the group of Jacobi trees $\mathcal{A}_n^T$.

Therefore, Corollary 2.18 gives the following commutative triangle

$$\begin{tikzcd} & \mathcal{A}_n^T \arrow[dl, two heads, "\mathcal{R}_n^T"'] \arrow[dr, two heads, "\substack{\mathrm{mod}\\ d^{*>1}}"] & \\ \mathbb{K}_n(I^3)/_{\sim_{n+1}} \arrow[rr, two heads, "\overline{e}_{n+1}"] & & \ker(\pi_0 p_{n+1}) \end{tikzcd} \tag{2.11}$$

Actually, here $\mathcal{A}_n^T = E^2_{-(n+1),(n+1)}(I^3)$ and $\ker(\pi_0 p_{n+1}) = E^\infty_{-(n+1),(n+1)}(I^3)$ are terms on the diagonal of the spectral sequence and $d^{*>1}$ are higher differentials, see Section 2.3.

From this we can deduce Corollary 1.2: if for some $n \geq 1$ the map on the right in (2.11) is an isomorphism, then the other two maps are isomorphisms as well. More generally, if A is a torsion-free abelian group and the map $\mathcal{A}_n^T \otimes A \to \ker(\pi_0 p_{n+1}) \otimes A$ is an isomorphism, then both $\mathcal{R}_n^T \otimes A$ and $\overline{e}_{n+1} \otimes A$ are isomorphisms.

If for some A this is the case for all degrees below some $n+1$, then $\pi_0 \mathsf{ev}_{n+1}$ is a universal additive Vassiliev invariant of type $\leq n$ over A, meaning that there is an isomorphism

$$\pi_0 \mathsf{ev}_{n+1} \otimes A\colon\ \mathbb{K}(I^3)/_{\sim_{n+1}} \otimes A \xrightarrow{\cong} \pi_0 \mathsf{P}_{n+1}(I^3) \otimes A. \tag{2.12}$$

Indeed, this follows by induction from tensoring the sequences in (2.10) by A and using its flatness.

From this we concluded in Corollary 1.3 that the isomorphism (2.12) holds rationally, and p-adically in a range. This uses appropriate results from [BH20] (see also Remark 2.20) which determine that those higher differentials $d^{*>1}$ are trivial in certain cases, so

$$\mathcal{A}_n^T \otimes \mathbb{Q} \cong \ker(\pi_0 p_{n+1}) \otimes \mathbb{Q}, \quad \mathcal{A}_n^T \otimes \mathbb{Z}_p \cong \ker(\pi_0 p_{n+1}) \otimes \mathbb{Z}_p, \ \text{ if } n \leq p-2.$$

To deduce the integral result, we observe that the kernels of both $\mathcal{R}_n^T$ and $\overline{e}_{n+1}$ must consist of torsion elements. But by [Gus94] and [Man16, Sec. 3.5] the group $\mathcal{A}_n^T$ is torsion-free for $n \leq 6$.

Lastly, note that conversely, if there is a non-trivial higher differential hitting the diagonal, then not both $\mathcal{R}_n^T \otimes A$ and $\overline{e}_{n+1} \otimes A$ can be injective.

Remark 2.19. *There exists an inverse z_n to $\mathcal{R}_n^T \otimes \mathbb{Q}$ obtained as the logarithm of either the Kontsevich integral [Kon93] or the Bott–Taubes integrals [BT94; AF97] (see Section 7.1).*

Hence, $\overline{e}_{n+1} \otimes \mathbb{Q}$ agrees with these invariants, implying that the configuration space integrals factor through the embedding calculus tower:

$$\begin{tikzcd} & \bigoplus\limits_{1\leq k\leq n} \mathcal{A}_k^T \otimes \mathbb{Q} \arrow[dl, two heads, "\mathcal{R}_{\leq n}^T"] & \\ \mathbb{K}(I^3)/_{\sim_{n+1}} \otimes \mathbb{Q} \arrow[ur, bend left, "z_{\leq n}"] \arrow[rr, hook, two heads, "\pi_0 \mathsf{ev}_{n+1} \otimes \mathbb{Q}"'] & & \pi_0 \mathsf{P}_{n+1}(I^3) \otimes \mathbb{Q} \arrow[ul] \end{tikzcd}$$

where the map on the right is given by some splittings over $\mathbb{Q}$, making the diagram commute.

Remark 2.20. *Let us remark that the collapse of the spectral sequence $\mathrm{E}^*_{-n,t}(I^d) \otimes \mathbb{Q}$ which converges to the rational homotopy groups of $\mathcal{K}(I^d)$ was shown earlier by [ALTV08] but only for $d \geq 4$.*

The collapse of the corresponding homology *spectral sequences for the Taylor tower of $\mathcal{K}(I^d)$ for any $d \geq 3$ was shown by [LTV10; Son13; Mor15]. However, it is not clear if those arguments can be extended to show that the homotopy spectral sequence collapses also for $d = 3$. This follows from the results of [FTW17], and more directly from [BH20].*

The rational collapse along the diagonal is also used in the following argument of Goodwillie, which we include for completeness.

Proposition 2.21 (Goodwillie). *The set $\pi_0\mathsf{P}_\infty(I^3)$ is uncountable, so the Taylor tower does not converge to $\mathcal{K}(I^3)$, i.e. the map $\mathsf{ev}_\infty \colon \mathcal{K}(I^3) \to \mathsf{P}_\infty(I^3) := \lim \pi_0\mathsf{P}_n(I^3)$ is* not *a weak equivalence.*

Proof. We claim that $\pi_0\mathsf{P}_\infty(I^3)$ is uncountable, while $\pi_0\mathcal{K}(I^3)$ is countable. We have a surjection of sets $\pi_0\mathsf{P}_\infty(I^3) \twoheadrightarrow \lim \pi_0\mathsf{P}_n(I^3)$, so it is enough to show that $\lim \pi_0\mathsf{P}_n(I^3)$ is uncountable.

Indeed, $\pi_0 p_{n+1} \colon \pi_0\mathsf{P}_{n+1}(I^3) \twoheadrightarrow \pi_0\mathsf{P}_n(I^3)$ is surjective for every $n \geq 1$, but not injective since we saw that $\ker(\pi_0 p_{n+1}) \otimes \mathbb{Q} = \mathcal{A}_n^T \otimes \mathbb{Q}$, and these groups are non-trivial for all $n \geq 2$. □

However, we could take limits in the diagram (2.10). Then Milnor's $\lim^1$-sequence together with the fact $\lim^1 \left(\mathbb{K}(I^3)/\sim_n\right) = 0$ since maps in that tower are surjective, gives an exact sequence

$$\lim \left(\ker \pi_0\mathsf{ev}_n\right) \hookrightarrow \lim \mathbb{K}(I^3)/\sim_n \xrightarrow{\overline{\mathsf{ev}}_\infty} \lim \pi_0\mathsf{P}_n(I^3) \twoheadrightarrow \lim^1 \left(\ker \pi_0\mathsf{ev}_n\right). \tag{2.13}$$

If Conjecture 1 is true, then $\overline{\mathsf{ev}}_\infty$ is an isomorphism. See also Section 7.1.

Remark 2.22. *In [KST] we construct a simplicial space $\mathcal{K}_n(I^3)$ whose space of 0-simplices is $\mathcal{K}(I^3)$ and the space of 1-simplices is a space of gropes of degree n, and such that ev_n extends to a continuous map $\mathcal{K}_n(I^3) \to \mathsf{P}_n(I^3)$. We reformulate the injectivity part of Conjecture 1 as a simpler statement about this map and actually hope to prove that this is a homotopy equivalence, giving a very different and geometric description of $\mathsf{P}_n(I^3)$.*

Finally, any two group structures on $\pi_0\mathsf{T}_n\mathcal{K}(I^3)$ respecting the connected sum of knots must agree.

Corollary 2.23. *Two group structures on the set of components of Taylor stages constructed by [BW18] and [BCKS17] are equivalent, that is, $\pi_0\mathsf{T}_n^{BW} \cong \pi_0 AM_n$ as abelian groups.*

Proof. The models are weakly equivalent, so there is a bijection of sets $f \colon \pi_0 AM_n \to \pi_0 BW_n$ so that $f \circ \pi_0 ev_n = \pi_0\mathsf{ev}_n$. Since $\pi_0 ev_n$ is a *surjective* monoid map, for $x_i \in \pi_0 AM_n$ we find $K_i \in \mathbb{K}$ with $\pi_0 ev_n(K_i) = x_i$; then $x_1 + x_2 = \pi_0 ev_n(K_1 \# K_2)$. Using that $\pi_0\mathsf{ev}_n$ is also a monoid homomorphism we have $f(x_1 + x_2) = \pi_0\mathsf{ev}_n(K_1 \# K_1) = \pi_0\mathsf{ev}_n(K_1) + \pi_0\mathsf{ev}_n(K_2) = f(x_1) + f(x_2)$. □

Examples

Let us now see some examples.

Example 2.24. *Let $n = 2$. The grope in Figure 1 shows that the trefoil is 2-equivalent to the unknot. Actually, every knot is 2-equivalent to the unknot (see, for example, [MN89]), so*

$$\mathbb{K}(I^3)/\sim_2 = \{0\}.$$

Moreover, [BCSS05] show that $\mathsf{P}_2(I^3) \simeq *$, confirming Conjecture 1 in degree $n = 2$. △

Example 2.25. *Therefore, the first non-trivial knot invariant obtained from the calculus is:*

$$\pi_0\mathsf{ev}_3 \colon \mathbb{K} \longrightarrow \pi_0\mathsf{P}_3(I^3) \cong \pi_0\mathsf{F}_3(I^3) \cong \mathbb{Z}.$$

In [BCKS17] this was studied via linking of certain 'colinearity submanifolds' of configuration spaces, and shown that it agrees with the unique Vassiliev invariant v_2 of type ≤ 2 whose value on the trefoil is 1.[17] *Here unique can be understood as universal.*

Our approach lifts this calculation to fibres $\mathsf{e}_2 \colon \mathsf{H}_2(I^3) \longrightarrow \mathsf{F}_3(I^3)$.

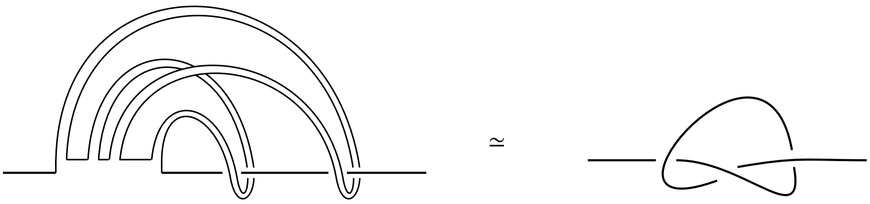
Namely, since by the previous example for any $K \in \mathbb{K}$ we have $K \sim_2 \mathrm{U}$, there exists a grope forest $\mathbf{F}$ of degree 2 from K to the unknot. By the extension of Theorem D for grope forests we get a point

$$\psi(\mathbf{F}) \in \mathsf{H}_2(I^3).$$

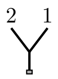
Thus, $\pi_0\mathsf{ev}_3(K)$ is simply the class

$$[\mathsf{e}_3\psi(\mathbf{F})] \in \pi_0\mathsf{F}_3(I^3).$$

For example, for K equal to the trefoil, we can use the grope $\mathbf{G}$ from Figure 1 which is modelled on the unique tree of degree 2, since $K = \partial^{\perp}\mathbf{G}$ is precisely the trefoil

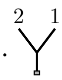


Then Theorem E shows that

$$[\mathsf{e}_3\psi(\mathbf{G})] =$$  $$\in \mathsf{Lie}(2).$$

is precisely the class of that tree in $\mathsf{Lie}(2)$. Actually, doing the computation explicitly in this example is a warm-up problem for the proof of the theorem, see Example 5.10.

Since the value of v_2 on trefoil is one, and this is the unique such invariant, this reproves

$$\pi_0\mathsf{ev}_3([K]) = v_2(K) \cdot$$ 

If for computing $v_2(K)$ one would use the Hopf invariant $\mathsf{Lie}(2) \subseteq \pi_3(\mathbb{S}^2 \vee \mathbb{S}^2) \longrightarrow \mathbb{Z}$, given as the linking number $\mathrm{lk}(f^{-1}(pt_1), f^{-1}(pt_2))$ for an appropriate representative f of the desired homotopy class, then one is very close to the colinearity story from [BCSS05].

Note that STU^2 relation is empty in this degree and $\mathcal{A}_2^T = \mathsf{Lie}(2) = E^{\infty}_{-3,3}$. △

Example 2.26. *The dimensions of the rational vector space of primitives were computed by Kneissler [Kne97] up to degree 12 and are given as follows.*

n	*1*	*2*	*3*	*4*	*5*	*6*	*7*	*8*	*9*	*10*	*11*	*12*
$\dim \mathfrak{pr}(\mathcal{A} \otimes \mathbb{Q})_n$	1	1	1	2	3	5	8	12	18	27	39	55

It was shown in [Das00] that $\dim \mathfrak{pr}(\mathcal{A} \otimes \mathbb{Q})_n > \exp(c\sqrt{n})$ for any constant $c < \pi\sqrt{2/3}$.

However, we expect that the computation of the groups of indecomposables $\mathcal{A}_n^T$ has smaller complexity, but to our knowledge this has yet not been pursued in the literature. Moreover, studying directly STU^2 relation rather than STU could lead to finding possible torsion in these groups. △

[17] This is v_2, the second coefficient of the Conway polynomial. It is an integral lift of the Arf invariant.

2.3 Beyond dimension three

The spectral sequence

Let M again be of arbitrary dimension $d \geq 3$. For a tower of pointed fibrations there is an associated homotopy spectral sequence, built out of long exact sequences for the homotopy groups of a fibration, see [BK72; GJ09]. Since $p_n\colon \mathsf{P}_n(M) \to \mathsf{P}_{n-1}(M)$ are surjective fibrations by Proposition 3.10, they have such an associate sequence, which is not 'fringed'.

The first page is given by $E^1_{-n,t} := \pi_{t-n}\mathsf{F}_n(M)$ which is by Corollary 5.2 isomorphic to

$$E^1_{-n,t} \cong \bigoplus_{w\in \mathsf{N'B}(n-1)} \pi_t\Sigma^{1+l_w(d-2)}(\Omega M)^{\wedge l'_w}$$

and the first differential

$$\begin{array}{ccc} E^1_{-n,t}(M) & \xrightarrow{d^1_{-n,t}} & E^1_{-(n+1),t}(M) \\ \| & & \| \\ \pi_{t-n}\mathsf{F}_n(M) & \longrightarrow & \pi_{t-n-1}\mathsf{F}_{n+1}(M) \end{array} \tag{2.14}$$

is induced from the composition of the inclusion and the connecting map

$$\Omega\mathsf{F}_n(M) \hookrightarrow \Omega\mathsf{P}_n(M) \xrightarrow{\delta} \mathsf{F}_{n+1}(M).$$

This spectral sequence was studied in [Sin09, Thm. 7.1], where a vanishing slope was determined. We recover that computation and also find the terms on this slope.

Corollary 2.27 (of Theorem C)**.** *The group $E^1_{-(n+1),t}$ vanishes for $t \leq n(d-2)$, and for each $l = n, n+1, \dots$ all entries in the strip $1 + l(d-2) \leq t \leq (l+1)(d-2)$ are generated by Samelson products using words of length at most l in which all letters appear.*

In particular, the first non-vanishing slope is given by

$$E^1_{-(n+1),1+n(d-2)}(M) \cong \mathsf{Lie}_{\pi_1 M}(n).$$

This extends the calculations of Scannell and Sinha [SS02] for $M = I^d$. They moreover give a description of the differential d^1, which is then used by Conant to compute the second page along the first non-vanishing slope.

Theorem 2.28 ([Con08])**.** *For $M = I^d$ with odd d the image of $\mathrm{im}(d^1_{-n,1+n(d-2)}) \subsetneq \mathsf{Lie}(n)$ is precisely spanned by the $STU^2_{\{1\}}$ relations, $n \geq 2$. Therefore, there is an isomorphism*

$$\mathcal{A}^T_n(I^d) \hookrightarrow\!\!\!\!\rightarrow E^2_{-(n+1),1+n(d-2)}(I^d).$$

Remark 2.29. *By the Milnor–Moore theorem [MM65] for $d \geq 4$ the Hurewicz map*

$$h\colon \pi_*(\mathcal{K}(I^d)) \otimes \mathbb{Q} \longrightarrow \mathfrak{pr}H_*(\mathcal{K}(I^d);\mathbb{Q})$$

is an isomorphism of Lie algebras where the source has the Samelson bracket (see Appendix A) and the target is the primitives of the connected Hopf algebra $H_*(\mathcal{K}(I^d);\mathbb{Q})$. This however fails for $\pi_0\mathcal{K}(I^3) = \mathbb{K}(I^3)$, which is instead the set of monoidlike elements in $H_0(\mathcal{K}(I^3);\mathbb{Z}) = \mathbb{Z}[\mathbb{K}(I^3)]$.

Similarly, [LT09] show that for $d \geq 4$ the E^2 page of the rational homotopy spectral sequence for $\mathcal{K}(I^d)$ is the primitives of the E^2 page of its homology spectral sequence.

We *claim* that Conant's proof extends to show that for any manifold M of dimension $d \geq 3$ the $STU^2_{\pi_1 M}$ relations (2.4) are *contained in* $\operatorname{im}(d^1_{-n,1+n(d-2)}) \subseteq \mathsf{Lie}_{\pi_1 M}(n)$.

This would imply that for $n \geq 2$ there is a map

$$\mathcal{A}^T_n(M) \xrightarrow[]{\substack{\text{mod rest of}\\ \operatorname{im}(d^1)}} E^2_{-(n+1),1+n(d-2)}(M). \tag{2.15}$$

Moreover, we claim that this map is an isomorphism if M is contractible. We only outline the proof of these claims in Appendix C, as they will not be used in the rest of the thesis.

Note that for $d = 3$ the map (2.15) is in general just a map of sets, since $\pi_1 \mathsf{F}_n(M)$ acts on the set $\pi_0 \mathsf{F}_{n+1}(M)$, and the quotient by $\operatorname{im}(d^1)$ is the set of orbits.

On the other hand, let us note that for a general M there might be more elements in the image of $d^1_{-n,1+n(d-2)}$ coming from $\pi_{d-1}M$, since these elements contribute to $\pi_{1+n(d-2)}\Sigma^{1+(n-1)(d-2)}(\Omega M)^{\wedge l'_w}$.

For $d = 3$ such relations might be relevant for the Gusarov–Habiro filtration as well, since they might also be in the kernel of $\mathcal{R}^T \colon \mathcal{A}^T_n(M) \twoheadrightarrow {}^{\mathbb{K}_n(M;\mathrm{U})}\!/\!_{\sim_{n+1}}$. This should be compared with a similar observation [Vas98, §1.4].

Realising trees in arbitrary dimensions

For M of dimension $d \geq 4$ the map

$$\pi_{n(d-3)}\mathsf{ev}_{n+1} \colon \pi_{n(d-3)}\mathcal{K}(M) \to \pi_{n(d-3)}\mathsf{P}_{n+1}(M). \tag{2.16}$$

is an isomorphism for any $n \geq 1$, since by the Goodwillie–Klein theorem ev_{n+1} is $(n+1)(d-3)$-connected. On the other hand, there is a short exact sequence

$$E^\infty_{-(n+1),t}(M) = {}^{\mathsf{Lie}_{\pi_1 M}(n)}\!/\!_{\operatorname{im}(\delta_*)} \hookrightarrow \pi_{n(d-3)}\mathsf{P}_{n+1}(M) \xrightarrow{p_{n+1}} \pi_{n(d-3)}\mathsf{P}_n(M).$$

Recall that in Remark 1.10 we have indicated a construction of maps $\mathbb{S}^{n(d-3)} \to \mathcal{K}(M)$ using gropes, realising the classes in this kernel (see also the end of Section 1). One could try to use this approach to reprove that $e_{n+1} \colon \ker(\pi_{n(d-3)}\mathsf{ev}_n) \to {}^{\mathsf{Lie}_{\pi_1 M}(n)}\!/\!_{\operatorname{im}(\delta_*)}$ is injective as well.

Furthermore, it is another interesting (and even harder) problem to extend this further and realise classes in $\pi_{n(d-3)}\mathsf{P}_n(M)$, or in $\pi_k \mathsf{F}_n(M)$ in the range $k \in [(n-1)(d-3), n(d-3)]$. This, roughly speaking, corresponds to graphs of higher homological degree in the appropriate graph complex. For example, if M is a 4-manifold the grope construction sketched above should realise all classes in $\pi_{n-1}\mathsf{F}_n(M)$, and then there is just one more step: to geometrically realise classes in $\pi_n \mathsf{F}_n(M)$ corresponding to '1-loop diagrams'.

Remark 2.30. *A construction of non-trivial classes in $H_{n(d-3)}(\mathcal{K}(I^d);\mathbb{Z})$ for $n \geq 2$ was given by Cattaneo, Cotta-Ramusino and Longoni [CCL02], using 'resolutions' of double points, analogously as in Vassiliev–Gusarov filtration. The next step is somewhat similar to the work of Sakai [Sak08] and Pelatt and Sinha [PS17] who realise certain classes in $H_{3(d-3)+1}(\mathcal{K}(I^d);\mathbb{Z})$ for d even. Let us also mention that the Taylor tower for $\mathcal{K}(I^d)$ was studied in [LTV10; ALTV08; LV14; Tur10].*

As a first step, we plan to study the image of $\delta \colon \Omega\mathsf{P}_1(M) \to \mathsf{F}_2(M)$ on homotopy groups, so that

$${}^{\mathbb{Z}[\pi_1 M]}\!/\!_{\operatorname{im}(\delta_*)} \hookrightarrow \pi_{d-3}\mathcal{K}(M) \cong \pi_{d-3}\mathsf{P}_2(M) \twoheadrightarrow \pi_{d-2}M.$$

We believe that for $M = (\mathbb{S}^1 \times \mathbb{S}^{d-1}) \setminus \mathbb{B}^d$ we will find $\operatorname{im}(\delta_*) = \langle \overset{1}{\underset{\square}{\big|}}{}^{1}, \overset{1}{\underset{\square}{\big|}}{}^{g} - (-1)^d \overset{1}{\underset{\square}{\big|}}{}^{g^{-1}} \rangle$, and this would recover a computation of [BG19].

The outline

In Part II we discuss the punctured knots model $\mathsf{P}_n(M)$ for M any manifold of dimension $d \geq 3$ and with non-empty boundary, and prove Theorem C.

The model is introduced in Section 3 and in Section 4 the layers are shown to be loop spaces. We determine their homotopy type in Section 5, where we also describe geometrically the generators of the first non-trivial homotopy group. In Section 5.3 we outline the strategy of proof of the main theorem and give a sketch of the proof on an example. Section 6 is devoted to proofs of the main technical tools: we define explicit homotopy equivalences χ from total fibres of certain cubes to iterated loop spaces.

This part ends with Appendix A which provides background on Samelson products and contains two important lemmas which describe more precisely their inductive behaviour.

– § –

In Part III we are concerned with 3-manifolds. Firstly, Section 7.1 surveys the general theory of finite type invariants, and Section 7.2 presents a self-contained account of gropes. In Section 8 we prove Theorem D and its extension for grope forests. Section 8.2 describes points $\mathsf{e}_n\psi(\mathbf{G})$ explicitly.

Finally, the main Theorems E and F are proven in Section 9. The proof of Theorem E will be by induction: after proving the induction base, we will show two auxiliary lemmas, from which the induction step will quickly follow.

– § –

Finally, Part IV is devoted to further topics. In Section 10 we discuss the geometric calculus: we briefly review the calculus with claspers in Section 10.1, and then use it study the n-equivalence relation and the realisation map. We prove Theorems G1, G2 and G3 in Section 10.2.

The thesis ends with two appendices. In Appendix B we survey the theory of finite type invariants of pure braid groups. Namely, much of the finite type theory can also be can be transferred to that case. Although this is not used in the rest of this thesis, we include it for completeness and since we believe the reader might benefit from understanding the interplay of the classical and geometric approaches in that setting.

In Appendix C we finish the proof that the projection maps p_n in the Taylor tower are surjections, by proving Proposition 3.9, and also outline a proof of our claims (2.15) from Section 2.3 about the image of the first differential in the homotopy spectral sequence.

– § –

Throughout the thesis we aim to make both the homotopy theory and geometry accessible without assuming much background. We hope that all potentially confusing notation and technical proofs can be understood with the help of accompanying examples and pictures.

In particular, the mutually related Examples 3.1, 5.9, 5.10, and 8.7 all describe the lowest degree computation for a 3-manifold M, which is also the base case of the induction in the proof of Theorem E. The induction step is outlined in Example 5.11.

See Examples 10.9 and 10.10 for the Gusarov-Habiro filtration, apart from the already presented Examples 2.24, 2.25 and 2.26.

For background reading on these topics we recommend, apart from the references mentioned in the introduction and throughout the thesis, also the expository article [ŠV19] for the Goodwillie–Weiss calculus and the thesis [Shi19] for a viewpoint similar to ours.

Notation

Notation 1 (Spaces).

- *Let $I := [0,1]$ denote the unit interval, $\mathscr{P}X$ the space of free paths $[0,1] \to X$ in a space X, and $\mathscr{P}_*X$ the subspace of paths that start at the basepoint $* \in X$.*
- *For $\gamma \in \mathscr{P}X$ we write $\gamma\colon \gamma(0) \rightsquigarrow \gamma(1) \subseteq X$, to denote its endpoints. The inverse path is γ^{-1}, which we also sometimes denote by γ_{1-t}. The concatenation of loops will be denoted by $\gamma \cdot \eta$, and the commutator by $[\gamma, \eta] := \gamma \cdot \eta \cdot \gamma^{-1} \cdot \eta^{-1}$.*
- *ΣX is the reduced suspension of X and ΩX is its based loop space.*
- *If M is an oriented manifold, then $-M$ is the same manifold but oppositely oriented. All manifolds M have* non-empty boundary. *We denote by $\mathbb{S}M \subseteq TM$ the unit tangent bundle.*

Notation 2 (Categories).

- *A* diagram *over a small category $\mathcal{C}$ is a functor $X_\bullet\colon \mathcal{C} \to \mathsf{Top}$ to the category of topological spaces. Let $\mathsf{Top}^{\mathcal{C}}$ denote the category of diagrams over $\mathcal{C}$.*
- *Let $[n] = \{0,1,2,\dots,n\}$ and $\underline{n} := \{1,2,\dots,n\}$. For a finite ordered set S the cube category $\mathcal{P}(S)$ is the poset of all subsets of S; the punctured cube category $\mathcal{P}_\emptyset[n]$ is the poset of all non-empty subsets of $[n]$.*
- *Let Δ^S be the simplex whose vertices are indexed by the set S, and let $(C^{bar}\Delta)^S$ be the cone on the barycentric subdivision of Δ^S, see Figure 26.*
- *There are levelwise homeomorphisms of punctured cubical diagrams $|\mathcal{P}_\emptyset[n] \downarrow \bullet| \cong \Delta^\bullet$ and of cubical diagrams $|\mathcal{P}\underline{n} \downarrow \bullet| \cong I^\bullet$ and also $\hbar^\bullet\colon I^\bullet \to (C^{bar}\Delta)^\bullet$, see (3.5).*
- *$\mathcal{S}_n$ is the symmetric group on n letters.*
- *For $\mathbb{L}$, $\mathsf{N}\mathbb{L}$, Lie see Section 2.1.*
- *$\mathsf{B}(S)$ is a Hall basis for the free Lie algebra $\mathbb{L}(S)$; for $\mathsf{N'B}(n)$ see Theorem 5.4.*

Notation 3 (Main objects).

$\mathcal{K}(M)$	– *the space of knots in M, see (1.1)*
U	– *an arbitrarily chosen basepoint in $\mathcal{K}(M)$*
$\mathsf{P}_n(M)$,	*also $\mathsf{F}_n(M), \mathsf{H}_n(M)$ and maps $p_n, \mathsf{ev}_n, \mathsf{e}_n$ – the punctured knots model, see (1.2)*
$\mathscr{F}_S, \mathscr{F}^n_S$	– *Def. 3.13*
M_{0S}, M_S	– *Lem. 4.1*
$\mathbb{B}, \mathbb{S}$	– *a d-ball and a $(d-1)$-sphere*
$\vartheta_{(R_1,R_2)}$	– *the map $X^{R_1 \cup R_2} \to X^{R_1} \times X^{R_2}$ which exchanges the coordinates*
$\mathbb{D}$	– *a 2-disk*
$\Gamma, \Gamma^{g_{\underline{n-1}}}$	*a tree and a π-decorated tree, Sec. 2.1*
G_Γ	– *an abstract grope modelled on Γ, Def. 7.9*
$\mathcal{G}$	– *a grope cobordism, Def. 7.10*
$\mathbf{G}$	– *a thick grope, Def. 7.13*
$\mathbf{F}$	– *a grope forest, Def. 7.14*
$(\varepsilon_i, \gamma_i)_{i \in \underline{n}}$	– *the underlying decoration of a thick grope, Def. 7.12;*
$\mathcal{A}^T_n$	– *the group of Jacobi trees, Def. 2.10*
$\mathcal{T}_n$	– *the underlying tree map, Prop. 7.16*
$\mathcal{R}^T_n$	– *the realisation map, Thm. 10.5*
$\mathsf{Grop}_n(M;\mathrm{U})$	– *the space of gropes forests, Def. 7.15*
$\mathbb{K}_n(M;\mathrm{U})$	– *the subset of $\mathbb{K}(M) := \pi_0\mathcal{K}(M)$ of knots which are n-equivalent to U*

See also Notation 4 for the notation related to the punctured knots model, and Notation 5 and 6 for manifolds M_{0S} and $M \vee \mathbb{S}_S$ respectively.

Preliminaries on homotopy limits

We will need the notion of a homotopy limit of a diagram $X_\bullet \in \mathsf{Top}^{\mathcal{C}}$; for an introduction see [BK72; MV15]. This is the space $\operatorname{holim}(X_\bullet) \in \mathsf{Top}$, also written $\operatorname{holim}_{c\in\mathcal{C}} X_c$, defined as the mapping space

$$\mathrm{Map}_{\mathsf{Top}^{\mathcal{C}}}\big(|\mathcal{C}\downarrow\bullet|, X_\bullet\big).$$

Firstly, $|\mathcal{C}\downarrow\bullet| \in \mathsf{Top}^{\mathcal{C}}$ is the diagram which sends $c \in \mathcal{C}$ to the topological space obtained as the classifying space of a certain category $(\mathcal{C}\downarrow c)$ (called the overcategory). Namely, the objects of this category are morphisms $c' \to c$ in $\mathcal{C}$, and its arrows are triangles over c in $\mathcal{C}$.

Recall that the classifying space $|\mathcal{D}|$ of a category $\mathcal{D}$ is the geometric realisation of the nerve of $\mathcal{D}$ – the simplicial set whose k-simplices are sets of k-composable arrows in $\mathcal{D}$.

Finally, the mapping space between two objects in $\mathsf{Top}^{\mathcal{C}}$ is defined as the set of natural transformations between the two diagrams and is seen as a subspace of $\prod_{c\in\mathcal{C}} \mathrm{Map}\big(|\mathcal{C}\downarrow c|, X_c\big)$ from which it inherits the topology. In other words, a point $f \in \operatorname{holim}(X_\bullet)$ consists of a collection of maps $f^c \colon |\mathcal{C}\downarrow c| \to X_c$ which are compatible with respect to the morphisms in $\mathcal{C}$.

The crucial property of a homotopy limit is its *homotopy invariance*: if $X_\bullet \to Y_\bullet$ is a map of diagrams such that each $X_c \to Y_c$ is a weak equivalence, then the induced map $\operatorname{holim} X_\bullet \to \operatorname{holim} Y_\bullet$ is a weak equivalence as well.

– § –

In particular, a punctured $(n+1)$-cube is a diagram $X_\bullet$ over $\mathcal{P}_\emptyset[n]$, the poset of non-empty subsets of $[n] := \{0, 1, \dots, n\}$. Thus, $X_\bullet$ consists of a collection of spaces X_S for $\emptyset \neq S \subseteq [n]$ and mutually compatible maps $x_S^k \colon X_S \to X_{S\cup k}$ for $k \in [n] \setminus S$.

We have that $|\mathcal{P}_\emptyset[n] \downarrow S| \cong \Delta^S$ is the simplex spanned by the vertex set S, i.e. this nerve is the simplicial set obtained by barycentric subdivision of the standard $(|S|-1)$-simplex, see Figure 26. The maps in this diagram correspond to inclusions $\iota_R^{S\setminus R} \colon \Delta^R \hookrightarrow \Delta^S$ for $R \subseteq S$ of the face whose barycentric coordinates in $S \setminus R$ are zero. Therefore, we have

$$\operatorname{holim}(X_\bullet) = \mathrm{Map}_{\mathsf{Top}^{\mathcal{P}_\emptyset[n]}}\big(\Delta^\bullet, X_\bullet\big).$$

So a point $f \in \operatorname{holim}(X_\bullet)$ consists of a collection $f^S \colon \Delta^S \to X_S$ such that for all $k \not\ni S \subseteq [n]$

$$\begin{array}{ccc} \Delta^S & \xrightarrow{\iota_S^k} & \Delta^{S\cup k} \\ {\scriptstyle f^S}\downarrow & & \downarrow{\scriptstyle f^{S\cup k}} \\ X_S & \xrightarrow{x_S^k} & X_{S\cup k} \end{array}$$

commutes. Similarly, an n-cube is a diagram over $\mathcal{P}\underline{n}$, the poset of *all* subsets of $\underline{n} := \{1, \dots, n\}$. For the n-cube $S \mapsto |\mathcal{P}\underline{n} \downarrow S| \cong I^S$ is a cube whose coordinates are indexed by S, and the map $\iota_R^{S\setminus R} \colon I^R \hookrightarrow I^S$ for $R \subseteq S \subseteq \underline{n}$ is the inclusion of the face whose coordinates in $S \setminus R$ are zero.

Actually, for $Y_\bullet \in \mathsf{Top}^{\mathcal{P}\underline{n}}$ we have $\operatorname{holim}(Y_\bullet) \simeq Y_\emptyset$, since $\emptyset \in \mathcal{P}\underline{n}$ is the initial object.

However, one can take the homotopy limit of the punctured n-cube when $Y_\emptyset$ is omitted, and compare this to $Y_\emptyset$. More precisely, we define the total homotopy fibre of $Y_\bullet$ as the homotopy fibre of the natural map

$$c \colon Y_\emptyset \longrightarrow \operatorname*{holim}_{S\in\mathcal{P}_\emptyset[n]}(Y_S).$$

We will show in Lemma 3.7 that $f \in \operatorname{tofib}(Y_\bullet)$ can also be given as a suitable collection $f^S \colon I^S \to Y_S$.

Part II

The embedding calculus for knots in a general manifold

Throughout this part M is a *connected compact smooth manifold of dimension* $d \geq 3$ *with non-empty boundary.* Recall that we fix $b\colon [0,\epsilon) \sqcup (1-\epsilon, 1] \hookrightarrow M$ and consider the space

$$\mathcal{K}(M) := \mathcal{E}\mathrm{mb}_\partial(I, M) := \{\, f : I \hookrightarrow M \mid f \equiv b \text{ near } \partial I \,\}$$

whose elements we simply call *knots.* We choose an arbitrary knot $\mathrm{U} \in \mathcal{K}(M)$ for our basepoint.

– § –

Section 3 introduces the punctured model for $\mathcal{K}(M)$ and its basic properties.

In Section 4 we express the Taylor layers as iterated loop spaces, using the map χ.

Section 5 describes the homotopy types of layers, using some preliminaries from Appendix A.

Section 6 provides deferred proofs related to the delooping map χ.

Appendix A introduces Samelson products and shows their inductive nature.

3 The punctured knots model

The n-th Taylor approximation of $\mathcal{K}(M)$, for $n \geq 0$, is defined as the homotopy limit

$$\mathsf{T}_n(M) := \operatorname*{holim}_{U \in \mathcal{O}_n(I)^{op}} \mathcal{E}\mathrm{mb}_\partial(U, M).$$

The category $\mathcal{O}_n(I)^{op}$ is the poset of those open subsets U of I which are homeomorphic to the union of at most n open intervals and the collar of ∂I. The space $\mathcal{E}\mathrm{mb}_\partial(U, M)$ of embeddings $U \hookrightarrow M$, which near ∂I agree with a fixed embedding $b\colon [0, \epsilon) \sqcup (1 - \epsilon, 1] \hookrightarrow M$, is equipped with the Whitney C^∞ topology. The maps in the diagram are restrictions of embeddings to submanifolds.

Now, as observed by Goodwillie, computing this homotopy limit over a certain *finite subposet* gives a homotopy equivalent space which we now define; see [MV15, Example 10.2.18] for a proof.

Namely, note that U is of the shape $I \setminus V$, where $V \subseteq I \setminus \partial I$ consists of at most $n + 1$ closed subintervals. The desired subposet contains only sets $I \setminus J_S$ where $J_S := \bigsqcup_{i \in S} J_i$, for some $\emptyset \neq S \subseteq [n] := \{0, 1, \dots, n\}$ and for a fixed collection of disjoint closed subintervals $J_i = [L_i, R_i] \subseteq I$ increasingly converging to a fixed point $R_\infty < 1$.

Note that this poset is equivalent to the punctured cube category $\mathcal{P}_\emptyset[n]$, and its opposite is isomorphic to it. Thus, we have a punctured cubical diagram $\big(\mathcal{E}\mathrm{mb}_\partial(I \setminus J_\bullet, M), r\big)$, where the restriction map $r^k_S\colon \mathcal{E}\mathrm{mb}_\partial(I \setminus J_S, M) \to \mathcal{E}\mathrm{mb}_\partial(I \setminus J_{S \cup \{k\}}, M)$ introduces a 'puncture' at J_k for $k \notin S$. Then the space

$$\mathsf{P}_n(M) := \operatorname*{holim}_{S \in \mathcal{P}_\emptyset[n]} \mathcal{E}\mathrm{mb}_\partial(I \setminus J_S, M) \tag{3.1}$$

is called the $\mathsf{punctured\ knots\ model}$ for $\mathsf{T}_n\mathcal{K}(M)$ – as elements of $\mathcal{E}\mathrm{mb}_\partial(I \setminus J_S, M)$ indeed look like knots which have punctures at J_i, for $i \in S$.

By the definition of this homotopy limit in the preliminaries section, a point $f \in \mathsf{P}_n(M)$ consists of a compatible collection $\{f^S\}_{\emptyset \neq S \subseteq [n]}$ where each f^S is a Δ^S-family of knots punctured at J_S. In other words, f consists of n once-punctured knots, for each two of them – so $\binom{n}{2}$ in total – an isotopy between their restrictions to twice-punctured knots, then $\binom{n}{3}$ two-parameter isotopies of thrice-punctured knots connecting restrictions of respective isotopies of twice-punctured knots, etc.

Example 3.1. *In degree $n = 2$ the space $\mathsf{P}_2(M)$ is the homotopy limit of the punctured 3-cube*

$$\begin{tikzcd}
 & \mathcal{E}\mathrm{mb}_\partial(I \setminus J_{12}, M) \arrow[rr] & & \mathcal{E}\mathrm{mb}_\partial(I \setminus J_{012}, M) \\
\mathcal{E}\mathrm{mb}_\partial(I \setminus J_2, M) \arrow[ur] \arrow[rr] & & \mathcal{E}\mathrm{mb}_\partial(I \setminus J_{02}, M) \arrow[ur] & \\
 & \mathcal{E}\mathrm{mb}_\partial(I \setminus J_1, M) \arrow[uu] \arrow[rr] & & \mathcal{E}\mathrm{mb}_\partial(I \setminus J_{01}, M) \arrow[uu] \\
\mathsf{P}_2(M) \arrow[u, dotted] \arrow[ur, dotted] \arrow[rr, dotted] & & \mathcal{E}\mathrm{mb}_\partial(I \setminus J_0, M) \arrow[uu] \arrow[ur] &
\end{tikzcd}$$

Remark 3.2. *The condition $f \equiv b$ near ∂I for $f \in \mathcal{E}\mathrm{mb}_\partial(I \setminus J_S, M)$ (also for $\mathcal{K}(M)$) can be replaced by the requirement that f is 'flat' outside of $[\mathrm{L}_0, \mathrm{R}_\infty]$, that is, it agrees with $\mathrm{U} \in \mathcal{K}(M)$ on $I \setminus [\mathrm{L}_0, \mathrm{R}_\infty]$. This clearly gives equivalent spaces.*

Notation 4. *To save space we shall denote $\mathcal{E}\mathrm{mb}_\partial(I \setminus J_S, M)$ by $\mathcal{E}_S$ and write $\mathcal{E}^n_\bullet = \{\mathcal{E}_S\}_{S \in \mathcal{P}_\emptyset[n]}$, where the ambient manifold M will be clear from the context.*

We will also simply write $\mathcal{E}_{Sk} := \mathcal{E}_{S \cup \{k\}}$. We equip each $\mathcal{E}_S$ with the basepoint $\mathrm{U}_{\widehat{S}}$ and note that $r^k_S\colon \mathcal{E}_S \to \mathcal{E}_{Sk}$ with $k \notin S \subseteq [n]$ is a based map. Hence, the basepoint $\mathsf{P}_n(M) := \operatorname{holim} \mathcal{E}^n_\bullet$ is $\mathsf{ev}_n\mathrm{U}$.

Using $[n-1] \subseteq [n]$ we consider two inclusions $\mathcal{P}_\emptyset[n-1] \hookrightarrow \mathcal{P}_\emptyset[n]$ given by $\mathrm{Id} : S \mapsto S$ and $\mathrm{Id} \cup n : S \mapsto S \cup n$. The punctured n-cube $\mathcal{E}^n_\bullet \circ \mathrm{Id}$ is precisely $\mathcal{E}^{n-1}_\bullet$. Let us denote[18] *the other cube $\mathcal{E}^n_\bullet \circ (\mathrm{Id} \cup n) \colon S \mapsto \mathcal{E}\mathrm{mb}_\partial(I \setminus J_{Sn}, M)$ by $\mathcal{E}^n_{\bullet \cup n}$. Hence, our punctured $(n+1)$-cube decomposes as*

$$\mathcal{E}^n_\bullet = \begin{tikzcd} \mathcal{E}_n \arrow[r, "r^\bullet_n"] & \mathcal{E}^n_{\bullet \cup n} \\ & \mathcal{E}^{n-1}_\bullet \arrow[u, "r^n_\bullet"'] \end{tikzcd} \tag{3.2}$$

Note that the upper row forms an n-cube, which we denote $\mathcal{E}^n_{\bullet \cup n}$, but with the index now in $\mathcal{P}[n-1]$.

For $K \in \mathcal{K}(M)$ and $S \in \mathcal{P}_\emptyset[n]$ we denote by $K_{\widehat{S}} := K|_{I \setminus J_S} \in \mathcal{E}_S$ the knot K punctured at J_i, $i \in S$.

For two indices $i, j \in [n]$ we define $W_{ij} := (R_i, L_{j+1})$, so that for $\emptyset \neq S = \{i_1 < i_2 < \cdots < i_d\} \subseteq [n]$ we have $\mathrm{U}_{\widehat{S}} = W_{-\infty} \sqcup W_{0i_1} \sqcup W_{i_1 i_2} \sqcup \cdots \sqcup W_{i_d n} \sqcup W_\infty$. Here by abuse of notation W_{ij} is both in the source I and in the image $\mathrm{U} \subseteq M$. By Remark 3.2 we assume $f(W_{\pm\infty}) = W_{\pm\infty}$ for any $f \in \mathcal{E}_S$. Lastly, denote by w_i the midpoint of the interval $W_{i,i+1}$

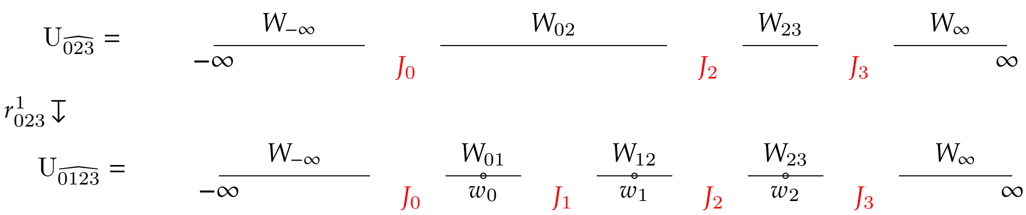


Figure 5. Examples of $\mathrm{U}_{\widehat{S}}$ and the restriction map r^j_S for $n = 3, S = \{0, 2, 3\}, j = 1$.

Given $K \in \mathcal{K}(M)$ various restrictions $K_{\widehat{S}}$ are mutually compatible, so assemble to give a map $\mathcal{K}(M) \longrightarrow \lim \mathcal{E}_\bullet$. Composing it with the canonical map from the limit to the homotopy limit gives the evaluation map

$$\begin{tikzcd} \mathcal{K}(M) \arrow[r, "\cong"] \arrow[rr, bend left, "\mathsf{ev}_n"] & \lim \mathcal{E}^n_\bullet \arrow[r, "\mathsf{const}"] & \operatorname{holim} \mathcal{E}^n_\bullet = \mathsf{P}_n(M). \end{tikzcd}$$

More explicitly, for $S \in \mathcal{P}_\emptyset[n]$ it is the constant family:

$$\mathsf{ev}_n(K)^S \colon \Delta^S \longrightarrow \mathcal{E}_S, \quad \vec{t} \mapsto K_{\widehat{S}}$$

Actually, for $n \geq 2$ there is a homeomorphism $\mathcal{K}(M) \cong \lim \mathcal{E}^n_\bullet$. This follows since having at least three different punctures ensures that all $f^S \in \mathcal{E}_S$ are pairwise disjoint, apart from agreeing on intersections. However, for $n = 1$ this does not hold, since $f^{\{0\}}|_{J_1}$ and $f^{\{1\}}|_{J_0}$ potentially intersect. Instead, we shall see below that $\lim \mathcal{E}^1_\bullet \simeq \mathsf{P}_1(M)$.

Remark 3.3. *By a family version of the isotopy extension theorem, r^k_S is a fibre bundle [Pal60]. In particular, it is a Serre fibration, whose fibre is the space of embeddings of J_k into M which miss the punctured unknot $\mathrm{U}_{\widehat{Sk}}$, namely $\mathrm{fib}(r^k_S) = \mathcal{E}\mathrm{mb}_\partial(J_k, M \setminus \mathrm{U}_{\widehat{Sk}})$.*

The zeroth Taylor stage. Given $K \in \mathcal{E}_i$ for some $i \geq 0$ we can start 'shortening' its both ends until only the flat parts $W_{-\infty}$ and W_∞ remain. In other words:

Lemma 3.4. *Each $\mathcal{E}_i = \mathcal{E}\mathrm{mb}_\partial(I \setminus J_i, M)$ is contractible. Hence, $\mathsf{P}_0(M) = \mathcal{E}_0$ is as well.*

[18] In [BCKS17] this is denoted as restriction to subdiagram $\mathcal{P}_{n+} \subseteq \mathcal{P}_\emptyset[n]$.

What we roughly described above is actually a deformation retraction $h_t\colon \mathcal{E}_i \to \mathcal{E}_i$ onto $\mathrm{U}_{\widehat{i}} \in \mathcal{E}_i$. Namely, for $t \in [0,1]$ let $tJ_i := [L_0 + t(L_i - L_0), R_\infty - t(R_\infty - R_i)]$ and consider

$$\mathsf{pull}_t\colon I \setminus J_i \xrightarrow{\cong} I \setminus tJ_i \hookrightarrow I \setminus J_i.$$

Precomposing each $f \in \mathcal{E}_i$ with this map gives the desired homotopy between $h_1(f) = \mathsf{pull}_1 \circ f = f$ and $h_0(f) = \mathsf{pull}_0 \circ f = W_{-\infty} \sqcup W_\infty$. The latter is not quite our basepoint, but we can postcompose h_t with a diffeomorphism $\mathsf{resc}^i_t\colon M \to M$ which squeezes the tubular neighbourhood of $\mathrm{U}|_{tJ_i}$ (a d-ball) back to a neighbourhood of $\mathrm{U}|_{J_i}$. We will use similar maps in Section 4.2.

The first Taylor stage. As we mentioned above, the limit of the diagram

$$\mathcal{E}^1_\bullet = \begin{tikzcd} \mathcal{E}\mathrm{mb}_\partial(I \setminus J_1, M) \arrow[r] & \mathcal{E}\mathrm{mb}_\partial(I \setminus J_{01}, M) \\ & \mathcal{E}\mathrm{mb}_\partial(I \setminus J_0, M) \arrow[u] \end{tikzcd} \tag{3.3}$$

is not homeomorphic to the space of knots. Instead, it is given as

$$\lim \mathcal{E}^1_\bullet = \{ (f^0, f^1) \mid f^0_{I\setminus J_{01}} = f^1_{I\setminus J_{01}} \} = \{K \in \mathcal{I}\mathrm{mm}_\partial(I, M) \mid K_{\widehat{0}}, K_{\widehat{1}} \text{ are embeddings}\}$$

– the space of those immersions which are embeddings when restricted to $I \setminus J_0$ or $I \setminus J_1$. Actually, since *both maps in the diagram* $\mathcal{E}^1_\bullet$ *are fibrations* (see Remark 3.3), the limit is equivalent to the homotopy limit.[19] Hence we have the upper row in the commutative diagram

$$\begin{tikzcd} \mathcal{K}(M) \arrow[r] \arrow[d, hook, "\iota"] \arrow[rr, bend left, "\mathsf{ev}_1"] & \lim \mathcal{E}^1_\bullet \arrow[r, "\mathsf{const}", "\simeq"'] \arrow[d, hook, "\iota"] & \operatorname{holim} \mathcal{E}^1_\bullet =: \mathsf{P}_1(M) \arrow[d, "\simeq"] \arrow[r, "\simeq"] & \Omega(\mathbb{S}M) \\ \mathcal{I}mm_\partial(I, M) \arrow[r, equal] & \lim \mathcal{I}^1_\bullet \arrow[r, "\simeq", "Smale"'] & \operatorname{holim} \mathcal{I}^1_\bullet \arrow[ur] \end{tikzcd} \tag{3.4}$$

Let us now explain the rest of the diagram. As mentioned in the preliminaries, the homotopy limit can be computed from any levelwise homotopy equivalent diagram:

$$\mathcal{E}^1_\bullet \quad\simeq\quad \begin{tikzcd} \mathcal{I}\mathrm{mm}_\partial(I \setminus J_1, M) \arrow[r] & \mathcal{I}\mathrm{mm}_\partial(I \setminus J_{01}, M) \\ & \mathcal{I}\mathrm{mm}_\partial(I \setminus J_0, M) \arrow[u] \end{tikzcd} \quad\simeq\quad \begin{tikzcd} \mathcal{P}_*(\mathbb{S}M) \arrow[r, "|_{W_{01}}"] & \mathcal{P}(\mathbb{S}M) \\ & \mathcal{P}_*(\mathbb{S}M) \arrow[u, "|_{W_{01}}"'] \end{tikzcd}$$

The first equivalence is induced from the weak equivalences $\mathcal{E}\mathrm{mb}(V, M) \to \mathcal{I}\mathrm{mm}(V, M)$ for V a disjoint union of disks. The second equivalence is induced from the unit derivative maps, giving paths in the unit tangent bundle $\mathbb{S}M$. Here $\mathcal{P}\mathbb{S}M \simeq \mathbb{S}M$ and $\mathcal{P}_*\mathbb{S}M \simeq *$. One can check that the homotopy limit of the rightmost diagram is $\Omega(\mathbb{S}M)$, so one has the triangle in (3.4).

On the other hand, the strict limit in the middle diagram is clearly $\lim \mathcal{I}^1_\bullet \cong \mathcal{I}\mathrm{mm}_\partial(I, M)$. The fact that this is also *its homotopy limit* is non-trivial: by a theorem of Smale [Sma58] the restriction maps for immersions are *also fibrations*. This also implies that immersions form a polynomial functor of degree at most 1, that is, $\mathsf{T}_n\mathcal{I}mm_\partial(I, M) \simeq \mathcal{I}mm_\partial(I, M)$ for all $n \geq 1$. Here we similarly define $\mathsf{T}_n\mathcal{I}mm_\partial(I, M) := \operatorname{holim} \mathcal{I}^n_\bullet$, using $\mathcal{I}^n_S := \mathcal{I}\mathrm{mm}_\partial(I \setminus J_S, M)$. See [Wei05; GW99].

However, to obtain $\mathsf{P}_1(M) \simeq \Omega(\mathbb{S}M)$ we did not need Smale's result. Finally, observe that as a consequence of this discussion the inclusion $\iota\colon \lim \mathcal{E}^1_\bullet \hookrightarrow \lim \mathcal{I}^1_\bullet$ of 'special' immersions into all immersions is – maybe surprisingly – a weak equivalence.

[19] Warning: although all maps in cubes for higher n are also fibrations, one cannot conclude that $\operatorname{holim} \mathcal{E}^n_\bullet \simeq \lim \mathcal{E}^n_\bullet$, as is the case for $n = 1$. Namely, for $n \geq 2$ this is not enough to make an n-cube 'fibrant'.

3.1 Projection maps are surjective fibrations

Let $p_n\colon \mathsf{P}_n(M) \to \mathsf{P}_{n-1}(M)$ be the map induced *by forgetting the last puncture* J_n, that is, the map induced on homotopy limits from the inclusion of diagrams $\mathcal{E}^{n-1}_\bullet \subseteq \mathcal{E}^n_\bullet$ (see Notation 4). We clearly have $p_n \circ \mathsf{ev}_n = \mathsf{ev}_{n-1}$, so p_n respects the basepoints $p_n(\mathsf{ev}_n \mathrm{U}) = \mathsf{ev}_{n-1}\mathrm{U}$.

Proposition 3.5. *The map $p_n\colon \mathsf{P}_n(M) \to \mathsf{P}_{n-1}(M)$ is a fibration for each $n \geq 1$. Moreover, its fibre $\mathsf{F}_n(M) := \mathrm{fib}_{\mathsf{ev}_{n-1}\mathrm{U}}(p_n)$ is homeomorphic to the total homotopy fibre of the n-cube $\mathcal{E}^n_{\bullet\cup n}$.*

Before proving this, we recall the notion of a total homotopy fibre and its properties.

Definition 3.6. *The total homotopy fibre of an n-cube $(C_\bullet, r)\colon \mathscr{P}[n-1] \to \mathsf{Top}_*$ is the space*

$$\mathrm{tofib}(C_\bullet) := \mathrm{hofib}_{c(\mathrm{U}_\emptyset)}\Big(C_\emptyset \xrightarrow{c} \mathrm{holim}(C|_{\mathscr{P}_0[n-1]})\Big).$$

Here $\mathrm{U}_S \in C_S$ are the basepoints and c is the natural map sending $x \in C_\emptyset$ to the collection of constant maps $c(x)^S$, each equal to the image of x under $r^S_\emptyset\colon C_\emptyset \to C_S$. This factors as

$$\begin{tikzcd}
C_\emptyset = \lim C \arrow[r, "c"] \arrow[d, "\mathsf{const}"', "\simeq"] & \mathrm{holim}(C|_{\mathscr{P}_0[n-1]}) \\
\mathrm{holim}\, C \arrow[ur, "\overline{c}"'] &
\end{tikzcd}$$

where $\overline{c}$ is the restriction map to the homotopy limit of a subdiagram and const is the canonical map from the limit to the homotopy limit. Since C has the initial object, const is a weak equivalence. Hence, $\mathrm{hofib}(c)$ and $\mathrm{hofib}(\overline{c})$ are weakly equivalent. Even something stronger is true.

Lemma 3.7. *The map $\overline{c}$ is a fibration and its fibre $\mathrm{fib}_{c(\mathrm{U}_\emptyset)}(\overline{c})$ is homeomorphic to $\mathrm{tofib}(C_\bullet)$.*

Proof. See [Goo92] for several descriptions of total homotopy fibres and inspiration for this proof. Consider the mapping path space[20] E_c of c. The natural projection $p\colon E_c \to \mathrm{holim}(C|_{\mathscr{P}_0[n-1]})$ is a fibration and $\mathrm{fib}_{c(\mathrm{U}_\emptyset)}(p) = \mathrm{hofib}_{c(\mathrm{U}_\emptyset)}(c)$, and the latter is our definition of $\mathrm{tofib}(C_\bullet)$.

We will construct a *homeomorphism* $q\colon E_c \to \mathrm{holim}\, C$ and a commutative diagram:

$$\begin{tikzcd}
 & C_\emptyset \arrow[dl, "\simeq"'] \arrow[d] \arrow[dr, "c"] & \\
E_c \arrow[rr, "p"] \arrow[dr, dotted, "q"'] & & \mathrm{holim}(C|_{\mathscr{P}_0[n-1]}) \\
 & \mathrm{holim}\, C \arrow[ur, "\overline{c}"'] &
\end{tikzcd}$$

It will immediately follow that $\overline{c}$ is a fibration as well (as the composition of a fibration and a homeomorphism) with the fibre homeomorphic to $\mathrm{tofib}(C_\bullet)$.

Let $(x, \gamma) \in E_c$, so $x \in C_\emptyset$ and $\gamma\colon I \to \mathrm{holim}\, C|_{\mathscr{P}_0[n-1]}$ with $\gamma(0) = c(x)$. Equivalently, γ is a collection of maps $\gamma(-)^S\colon I \times \Delta^S \to C_S$ for $S \neq \emptyset$, which is on $\{0\} \times \Delta^S$ constantly equal to $r^S_\emptyset(x)$.

Hence, $\gamma(-)^S$ factors through the quotient by $\{0\} \times \Delta^S$, so is a map on the cone $\mathcal{C}\Delta^S$. Let us define $\mathcal{C}\Delta^\emptyset := I^0$ and $\gamma(-)^\emptyset = x\colon \mathcal{C}\Delta^\emptyset \to C_\emptyset$. Then our point gives a map of cubical diagrams

$$\gamma(-)^\bullet\colon (\mathcal{C}^{bar}\Delta)^\bullet \to C_\bullet$$

where $(\mathcal{C}^{bar}\Delta)^S$ is defined as the simplicial complex obtained from $\mathcal{C}\Delta^S$ by the barycentric subdivision[21] of its face $\{1\} \times \Delta^S$, and the maps in the cube are face inclusions.

[20] Aka mapping cocylinder: for a map $f\colon X \to Y$ this is $E_f := \mathrm{holim}(X \to Y \leftarrow \mathscr{P}Y) = \{\, (x, \gamma) \in X \times \mathscr{P}Y \mid \gamma(0) = f(x)\,\}$, and is a usual way of turning f into a fibration $p\colon E_f \to Y$. Actually $\mathrm{hofib}_{\mathrm{U}}(f)$ is precisely defined as $\mathrm{fib}_{\mathrm{U}}(p)$.

[21] If we do not subdivide, we get $(\mathcal{C}\Delta)^S \cong \Delta^{S \cup n}$, where n is a new index labelling the cone point.

Using the homeomorphism $|\mathcal{P}[n]\downarrow\bullet|\cong I^\bullet$ from the preliminaries, one constructs a levelwise homeomorphism of cubes

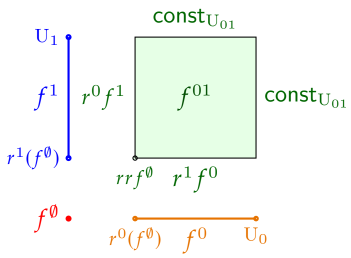
$$\hbar^\bullet\colon I^\bullet\to(\mathcal{C}^{bar}\Delta)^\bullet. \tag{3.5}$$

This maps the initial vertex of the cube to the cone point, and the 1-faces to the barycentrically subdivided simplex. We omit writing out its explicit definition.

Finally, define $q\colon E_c\to\operatorname{holim}\mathsf{C}$ by $q(x,\gamma):=\gamma(-)^\bullet\circ\hbar^\bullet$. This is also a homeomorphism, and makes the diagram above commute. □

Therefore, a point in $\mathrm{tofib}(c)\cong\mathrm{fib}_{c(\mathrm{U}_\emptyset)}(\overline{c})$ consists of a collection of maps $f^S\colon I^S\to\mathsf{C}_S$ for $S\subseteq[n-1]$, which send the 1-faces $\partial_1 I^S\subseteq I^S$ to the basepoint $\mathrm{U}_S\in\mathsf{C}_S$ and are compatible on the 0-faces, that is, $r^k_s\circ f^S=f^{Sk}|_{t_k=1}$. For $n=2$ we present this pictorially as follows.

$$f\in\mathrm{tofib}\left(\begin{tikzcd} \mathsf{C}_1 \arrow[r,"r^0"] & \mathsf{C}_{01}\\ \mathsf{C}_\emptyset \arrow[u,"r^1"] \arrow[r,"r^0"] & \mathsf{C}^0 \arrow[u,"r^1"'] \end{tikzcd}\right)\iff$$



(3.6)

Proof of Proposition 3.5. Using the decomposition of $\mathcal{E}^n_\bullet$ into subcubes from (3.2) and the fact that the homotopy limits can be computed 'iteratively', we obtain a homeomorphism:[22]

$$\mathsf{P}_n(M)=\operatorname{holim}\left(\begin{tikzcd} \mathcal{E}_n \arrow[r,"r^\bullet_n"] & \mathcal{E}^n_{\bullet\cup n}\\ & \mathcal{E}^{n-1}_\bullet \arrow[u,"r^n_\bullet"'] \end{tikzcd}\right)\cong\operatorname{holim}\left(\begin{tikzcd} \mathcal{E}_n \arrow[r,"c"] & \operatorname*{holim}_{\mathcal{P}_\emptyset[n-1]}(\mathcal{E}^n_{\bullet\cup n})\\ & \mathsf{P}_{n-1}(M) \arrow[u,"r^n_*"'] \end{tikzcd}\right) \tag{3.7}$$

Thus, $\mathsf{P}_n(M)$ is the homotopy limit of the diagram on the right which has only two maps – so a homotopy pullback. The map c is an analogue of ev_{n-1} but for J_n-punctured knots $\mathcal{E}_n:=\mathcal{E}mb_\partial(I\setminus J_n,M)$, while $r^n_*\colon\mathsf{P}_{n-1}(M)\to\operatorname{holim}_{\mathcal{P}_\emptyset[n-1]}(\mathcal{E}^n_{\bullet\cup n})$ is the induced map on the homotopy limits from the maps r^n_S, so it punctures at J_n every punctured knot in the family.

The homotopy pullback is homeomorphic to the *pullback* of the same diagram with c replaced by a fibration. By the proof of Lemma 3.7, the path fibration $E_c\to\operatorname{holim}(\mathcal{E}^n_{\bullet\cup n})$ is equivalent to the fibration $\overline{c}$, so we have a (strict) pullback square:

$$\begin{tikzcd} \operatorname*{holim}_{\mathcal{P}[n-1]}(\mathcal{E}^n_{\bullet\cup n}) \arrow[r,"\overline{c}"] & \operatorname*{holim}_{\mathcal{P}_\emptyset[n-1]}(\mathcal{E}^n_{\bullet\cup n})\\ \mathsf{P}_n(M) \arrow[u,dashed] \arrow[r,dashed,"p_n"] & \mathsf{P}_{n-1}(M) \arrow[u,"r^n_*"'] \end{tikzcd} \tag{3.8}$$

Since $\overline{c}$ is a fibration, p_n is as well ('pullbacks preserve fibrations') and the fibres are homeomorphic:

$$\mathsf{F}_n(M):=\mathrm{fib}_{\mathsf{ev}_{n-1}\mathrm{U}}(p_n)\;\cong\;\mathrm{fib}_{c(\mathrm{U}_{\overline{n}})}(\overline{c})\cong\mathrm{tofib}(\mathcal{E}^n_{\bullet\cup n}).$$ □

We see from the proof that (3.7) can be taken as a definition of the n-th Taylor stage:

$$\mathsf{P}_n(M)\cong\operatorname{holim}\left(\mathcal{E}_n\xrightarrow{c}\mathsf{BF}_n(M)\xleftarrow{r^n_*}\mathsf{P}_{n-1}(M)\right) \tag{3.9}$$

[22] To prove this one uses homeomorphisms $\Delta^{S\cup n}\cong\mathcal{C}\Delta^S$ which assemble into a map $(\mathcal{C}\Delta)^\bullet\to\Delta^\bullet$ (see Footnote 21); for details see [Goo92] or [MV15, Lemma 5.3.6].

where we denote $\mathsf{BF}_n(M) := \operatorname*{holim}_{\mathcal{P}_\emptyset[n-1]}(\mathcal{E}^n_{\bullet\cup n})$. The following corollary explains this notation.

Corollary 3.8. *There is a commutative diagram in with vertical inclusions weak equivalences*

$$\begin{tikzcd} \Omega(\mathsf{BF}_n(M)) \arrow[r, hook] \arrow[d, hook, "\simeq"] & \operatorname{hofib}(r^n_*) \arrow[d, hook, "\simeq"] \\ \mathsf{F}_n(M) \arrow[r, hook] & \mathsf{P}_n(M) \end{tikzcd}$$

Indeed, $\mathsf{P}_n(M) \simeq \operatorname{holim}(* \to \mathsf{BF}_n(M) \leftarrow \mathsf{P}_{n-1}(M))$ and $\mathsf{F}_n(M) \simeq \operatorname{hofib}(* \to \mathsf{BF}_n(M))$ since $\mathcal{E}_n \simeq *$ by Lemma 3.4. We will prove the next result in Appendix C using the results of Sections 4 and 5.

Proposition 3.9. *The space $\mathsf{BF}_n(M)$ is connected.*

Corollary 3.10. *The fibration p_n is surjective.*

Proof. Consider the homotopy fibre sequence $\mathsf{P}_n(M) \xrightarrow{p_n} \mathsf{P}_{n-1}(M) \xrightarrow{r^n_*} \mathsf{BF}_n(M)$. The proposition implies surjectivity of $\operatorname{hofib}(r^n_*) \to \mathsf{P}_{n-1}(M)$ (as for each $x \in \mathsf{P}_{n-1}(M)$ there exists a path from $r^n_*(x)$ to the basepoint in $\mathsf{BF}_n(M)$), so p_n is surjective as well. □

This surjectivity was proven for $M = I^3$ in [BCKS17, Theorem 5.13] (in the model AM_n).

Remark 3.11. *One can try to use Corollary 3.8 to show that $\mathsf{P}_n(I^3)$ is a double loop space for $n \geq 2$. Namely, we will see in Section 4 that $\mathsf{BF}_n(I^3)$ is an $(n-1)$-fold loop space, so by induction it would suffice to show that r^n_* is a map of double loop spaces. Such deloopings were constructed in other models by [Tur14] and [BW18], but this approach might be simpler. We plan to investigate if they also exist for some other manifolds M.*

3.2 Homotopy fibres of the evaluation and projection maps

Recall that $\mathsf{H}_{n-1}(M)$ was defined in (1.2) as the homotopy fibre of the map $\mathsf{ev}_{n-1} \colon \mathcal{K}(M) \to \mathsf{P}_{n-1}(M)$ over the basepoint $\mathsf{ev}_{n-1}\mathrm{U}$. Since $\mathcal{K}(M) = \mathcal{E}\mathrm{mb}_\partial(I, M) = \mathcal{E}_\emptyset$, that homotopy fibre is by definition the total fibre of the n-cube $\mathcal{E}_S$, where $S \subseteq [n-1]$ is now allowed to be empty:

$$\mathsf{H}_{n-1}(M) \cong \operatorname*{tofib}_{\mathcal{P}[n-1]}(\mathcal{E}^{n-1}_\bullet).$$

Since in Proposition 3.5 we found $\mathsf{F}_n(M) \cong \operatorname{tofib}_{\mathcal{P}[n-1]}(\mathcal{E}^n_{\bullet\cup n})$, let us define

$$\mathsf{e}_n \colon \mathsf{H}_{n-1}(M) \to \mathsf{F}_n(M)$$

as the map induced on total homotopy fibres from the map of n-cubes $r^n_\bullet \colon \mathcal{E}^{n-1}_\bullet \to \mathcal{E}^n_{\bullet\cup n}$. This again 'punctures at J_n every punctured knot in the family'. Using different descriptions of total homotopy fibres from the proof of Lemma 3.7 we immediately have the following.

Lemma 3.12. *The composition $\mathsf{H}_{n-1}(M) \xrightarrow{\mathsf{e}_n} \mathsf{F}_n(M) \hookrightarrow \operatorname{hofib}(p_n)$ agrees with the canonical map $l_n \colon \mathsf{H}_{n-1}(M) \to \operatorname{hofib}(p_n)$ induced from the evaluation map $l_n(K, \eta) = (\mathsf{ev}_n K, \eta)$.*

Note that one of the vertices of the cube computing $\mathsf{H}_{n-1}(M)$ is the space of knots itself. This is in contrast to the cube for $\mathsf{F}_n(M)$, in which the piece J_n is always absent – precisely this will allow us to compute its homotopy type in the next two sections.

The total homotopy fibre of an n-cube can also be computed 'iteratively', by first taking homotopy fibres in one arbitrary direction and then finding the total fibre of the resulting $(n-1)$-cube. This is similar to the comment in Footnote 22, and uses $I^n = I \times I^{n-1}$. See [Goo92; MV15] for a proof.

For the first direction we will choose the one which 'punctures at zero', that is, we take homotopy fibres of r^0_S. Since by Remark 3.3 these maps are fibrations, we can instead take the actual fibres.

Definition 3.13. *For each* $S \subseteq \underline{n-1} := \{1, 2, \dots, n-1\}$ *define*

$$\mathscr{F}_S := \mathrm{fib}\left(r^0_S \colon \mathcal{E}_S \to \mathcal{E}_{0S}\right) \quad \textit{and} \quad \mathscr{F}^n_S := \mathrm{fib}\left(r^0_{Sn} \colon \mathcal{E}_{Sn} \to \mathcal{E}_{0Sn}\right).$$

The basepoint of $\mathcal{E}_S$ is $\mathrm{U}_{\widehat{S}} := \mathrm{U}_{I \setminus J_S}$, so writing the first fibre out, we get

$$\begin{aligned} \mathscr{F}_S &= \mathrm{fib}_{\mathrm{U}_{\widehat{0S}}}\left(r^0_S \colon \mathcal{E}\mathrm{mb}_\partial(I \setminus J_S, M) \to \mathcal{E}\mathrm{mb}_\partial(I \setminus J_{0S}, M)\right) \\ &= (r^0_S)^{-1}(\mathrm{U}_{\widehat{0S}}) = \left\{ K : I \setminus J_S \hookrightarrow M \mid K_{I \setminus J_{\widehat{0S}}} = \mathrm{U}_{\widehat{0S}} \right\} \cong \mathcal{E}\mathrm{mb}_\partial(J_0, M \setminus \mathrm{U}_{\widehat{0S}}). \end{aligned}$$

Thus, $\mathscr{F}_S$ is the space of embeddings with fixed boundary of the arc J_0 into the complement in M of the punctured unknot $\mathrm{U}_{\widehat{0S}}$. See Figure 6. Moreover, $(\mathscr{F}_\bullet, r)$ is an $(n-1)$-cube, with restriction maps r^k_S from before, $k \notin S \subseteq \underline{n-1}$. Similarly for $\mathscr{F}^n_S \cong \mathcal{E}\mathrm{mb}_\partial(J_0, M \setminus \mathrm{U}_{\widehat{0Sn}})$ with maps r^k_{Sn}. We will, however, simply write $r^k_S \colon \mathscr{F}^n_S \to \mathscr{F}^n_{Sk}$ here as well, since n is clear from the context.

Moreover, we have a commutative diagram

$$\begin{tikzcd} \mathsf{H}_{n-1}(M) \cong \underset{S \subseteq [n-1]}{\mathrm{tofib}}\,(\mathcal{E}_S) \cong \underset{S \subseteq \underline{n-1}}{\mathrm{tofib}}\left(\mathrm{hofib}(r^0_S)\right) \arrow[d, "\mathsf{e}_n"'] & \underset{S \subseteq \underline{n-1}}{\mathrm{tofib}}\left(\mathscr{F}_S\right) \arrow[l, hook', "\simeq"'] \arrow[d] \\ \mathsf{F}_n(M) \cong \underset{S \subseteq [n-1]}{\mathrm{tofib}}\,(\mathcal{E}_{Sn}) \cong \underset{S \subseteq \underline{n-1}}{\mathrm{tofib}}\left(\mathrm{hofib}(r^0_{Sn})\right) & \underset{S \subseteq \underline{n-1}}{\mathrm{tofib}}\left(\mathscr{F}^n_S\right) \arrow[l, hook', "\simeq"'] \end{tikzcd} \tag{3.10}$$

where the vertical map on the right is induced from $r^n_S \colon \mathscr{F}_S \to \mathscr{F}^n_S$.

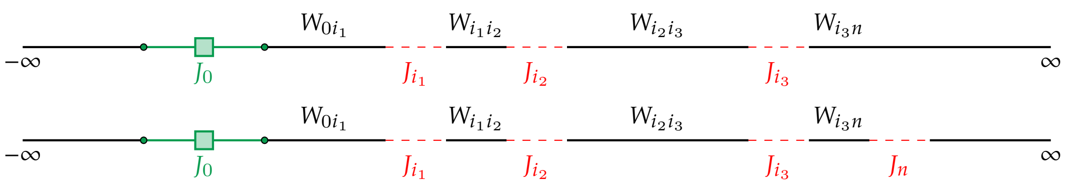


Figure 6. A point in $\mathscr{F}_S$ and $\mathscr{F}^n_S$ respectively, for $S = \{i_1, i_2, i_3\} \subseteq \underline{n-1}$. The small square on J_0 denotes that there some knotting, as well as linking with the rest of the black open intervals, can occur.

In the next section we will see that $\mathscr{F}^n_S$ can equivalently be described as the space of embeddings of the arc J_0 in the complement of the balls as depicted in Figure 7: the lower point there corresponds to the lower point from Figure 6 for $n = 6$ and $i_1 = 2, i_2 = 3, i_3 = 5$.

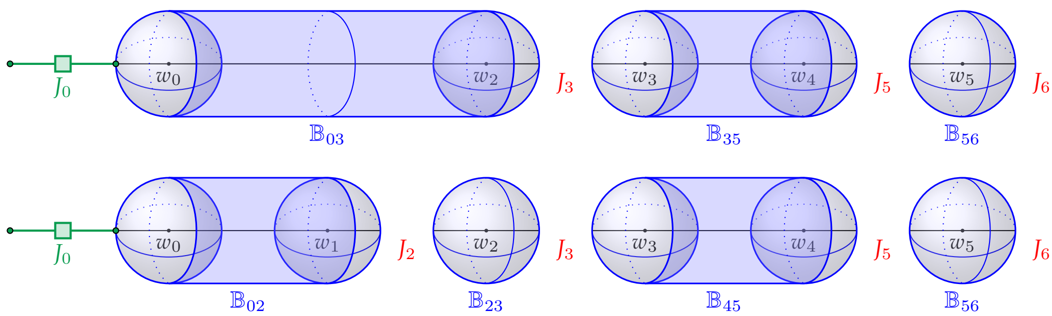


Figure 7. For $n = 6$ the manifold M_{035} (resp. M_{0235}) is the complement of the three (four) balls. The map $\rho^2_{04} : M_{035} \to M_{0235}$ adds the material $\mathbb{B}_{13} \setminus (\mathbb{B}_{12} \cup \mathbb{B}_{23}) = \mathbb{B}_{03} \setminus (\mathbb{B}_{02} \cup \mathbb{B}_{23})$.

4 Delooping the layers

The goal of this and the next section is to determine the homotopy type of the Taylor layer $\mathsf{F}_n(M) \simeq \mathrm{tofib}(\mathscr{F}^n_\bullet, r)$ for $n \geq 1$. Such computations go back to [GW99, Section 5] for the case when M has the homotopy type of a suspension, and also [BCKS17] for $M = I^3$. However, as mentioned in the introduction, those results did not suffice for our purposes as we need *a geometric interpretation* of the homotopy classes: for the discussion in Section 9 it will be crucial to determine the class in $\pi_0\mathsf{F}_n(M)$ of a geometrically described point $x \in \mathsf{F}_n(M)$, for $d = 3$.

We saw that the space $\mathscr{F}^n_S$ consists of embeddings $J_0 \hookrightarrow M \setminus \mathrm{U}_{\widehat{0Sn}}$. We can remove the pieces $W_{\pm\infty}$ of the punctured unknot (see Notation 4), which are the *same* for all S, by shrinking them to a collar of ∂M and then removing their small neighbourhoods. We still write M for this manifold.

Furthermore, writing $S = \{i_1 < \cdots < i_m\}$ for $m \geq 1$ and by convention $i_0 := 0, i_{m+1} := n$, we will enlarge the pieces $W_{i_p i_{p+1}}$ of $\mathrm{U}_{\widehat{0Sn}}$ into d-dimensional balls $\mathbb{B}_{i_p i_{p+1}} \subseteq M$, as follows (see Figure 7).

Notation 5. *Firstly, let $\mathbb{S}_i := \mathbb{S}^{d-1}_i \subseteq M$ be the $(d-1)$-dimensional sphere with the diameter $W_{i,i+1}$ for $0 \leq i \leq n-1$. Then for $1 \leq p \leq m$ let $\mathbb{S}_{i_p i_{p+1}} \subseteq M$ be the ellipsoid consisting of the cylinder $[w_{i_p}, w_{i_{p+1}-1}] \times \mathbb{S}^{d-2}$ together with the west hemisphere of $\mathbb{S}_{i_p}$ and the east of $\mathbb{S}_{i_{p+1}-1}$.*

Let $\mathbb{B}_{i_p i_{p+1}}$ to be the region interior to this ellipsoid (so it contains $W_{i_p i_{p+1}}$). Finally, let

$$M_{0S} := M \setminus \Big(\mathbb{B}_{0i_1} \sqcup \mathbb{B}_{i_1 i_2} \sqcup \cdots \sqcup \mathbb{B}_{i_m n}\Big).$$

Lemma 4.1. *For each $S \subseteq \underline{n-1}$ there is a homeomorphism $\mathscr{F}^n_S \cong \mathcal{E}\mathrm{mb}_\partial(J_0, M_{0S})$ and for $k \notin S$ the map $r^k_S\colon \mathscr{F}^n_S \to \mathscr{F}^n_{Sk}$ corresponds to the composition with the inclusion*

$$\rho^k_S : M_{0S} \longleftrightarrow M_{0Sk} = M_{0S} \cup \big(\mathbb{B}_{k-1,k+1} \setminus (\mathbb{B}_{k-1,k} \sqcup \mathbb{B}_{k,k+1})\big).$$

From now on we use this description of the cube $(\mathscr{F}^n_\bullet, r)$. To identify its total homotopy fibre, our strategy is to first provide a homotopy equivalence χ to an $(n-1)$-fold loop space (Section 4.1), and then deloop once more (Section 4.2). The homotopy type of $\mathsf{F}_n(M)$ is computed in Section 5, its first non-trivial homotopy group in Section 5.1, and its generators in Section 5.2.

Example 4.2. *Our approach is motivated by the following observation about the diagram*

$$\begin{tikzcd}
\mathcal{E}\mathrm{mb}_\partial(I \setminus J_1, M) \arrow[r, "r^0_1"] & \mathcal{E}\mathrm{mb}_\partial(I \setminus J_{01}, M) \\
\lim \mathcal{E}^1 \arrow[u, dotted] \arrow[r, dotted, "p"] & \mathsf{P}_0 \arrow[u, "r^1_0"']
\end{tikzcd}$$

as in (3.3). In order to determine the homotopy type $\mathsf{F}_1(M) := \mathrm{fib}(p) = \mathrm{fib}(r^0_1) \cong \mathcal{E}\mathrm{mb}_\partial(J_0, M \setminus \mathrm{U}_{\widehat{01}})$, we use that Smale's derivative maps give weak equivalences:

$$\begin{tikzcd}
\mathsf{F}_1(M) \arrow[r, dashed] \arrow[d, hook] & \mathcal{E}\mathrm{mb}_\partial(I \setminus J_1, M) \arrow[r, "r^0_1"] \arrow[d, hook, "\simeq"'] & \mathcal{E}\mathrm{mb}_\partial(I \setminus J_{01}, M) \arrow[d, hook, "\simeq"'] \\
\mathcal{I}\mathrm{mm}_\partial(J_0, M) \arrow[r, dashed] \arrow[d] & \mathcal{I}\mathrm{mm}_\partial(I \setminus J_1, M) \arrow[r, "r^0_1"] \arrow[d, "\simeq"', "\mathcal{D}_{[L_0, w_{01}]}"] & \mathcal{I}\mathrm{mm}_\partial(I \setminus J_{01}, M) \arrow[d, "\simeq"', "\mathcal{D}_{w_{01}}"] \\
\Omega\mathbb{S}M \arrow[r, dashed] & \mathscr{P}_*\mathbb{S}M \arrow[r] & \mathbb{S}M
\end{tikzcd}$$

Hence, $\mathsf{F}_1(M) \simeq \mathcal{I}\mathrm{mm}_\partial(J_0, M) \simeq \Omega\mathbb{S}M$. Note how the disjointness condition with $\mathrm{U}_{\widehat{01}}$ is lost when we pass to immersions. See Section 5.3.1 for more examples. △

4.1 The initial delooping

THEOREM 4.3. *For the n-th layer $\mathsf{F}_n(M) \simeq \operatorname{tofib}(\mathscr{F}^n_\bullet, r)$ of the Taylor tower for $\mathcal{K}(M)$, $n \geq 1$, there is a contravariant $(n-1)$-cube $(\mathscr{F}^n_\bullet, l)$ and an explicit homotopy equivalence*

$$\chi\colon \underset{\mathscr{P}(\underline{n-1})}{\operatorname{tofib}} \left(\mathscr{F}^n_\bullet, r\right) \xrightarrow{\sim} \Omega^{n-1} \underset{\mathscr{P}(\underline{n-1})^{\mathrm{op}}}{\operatorname{tofib}} \left(\mathscr{F}^n_\bullet, l\right).$$

We prove this using Proposition 4.8, which says that such a homotopy equivalence exists for any cube which has an $(n-1)$-*fold left homotopy inverse.* After we define this notion and state that proposition, we proceed to construct maps l^k_S giving such an inverse $(\mathscr{F}^n_\bullet, l)$ for our cube $(\mathscr{F}^n_\bullet, r)$. All proofs about left homotopy inverses are deferred to Section 6.

A left homotopy inverse for a map $r\colon X \to Y$ is a map $l\colon Y \to X$ such that $l \circ r \simeq \mathrm{Id}_X$. One could also call l a retraction up to homotopy and for our purposes it will be crucial to specify a homotopy h from Id to $l \circ r$. This can be summarised by:

$$\begin{tikzcd} & X \\ X \arrow[ur, "\mathrm{Id}"] \arrow[r, "r"'] & Y \arrow[u, "l"'] \arrow[ul, phantom, "\Downarrow h"] \end{tikzcd} \tag{4.1}$$

Note that l gives a section in the long exact sequence of homotopy groups for r, so we get split short exact sequences

$$0 \longrightarrow \pi_* X \underset{l_*}{\overset{r_*}{\rightleftarrows}} \pi_* Y \longrightarrow \pi_{*-1} \operatorname{hofib}(r) \longrightarrow 0 \tag{4.2}$$

and $\pi_{*-1} \operatorname{hofib}(r) \cong \pi_* \operatorname{hofib}(l) \cong \ker(l_*)$. Actually, something stronger is true.

LEMMA 4.4. *Given the data of (4.1) there are inverse homotopy equivalences*

$$\chi\colon \operatorname{hofib}(r) \underset{\sim}{\rightleftarrows} \Omega \operatorname{hofib}(l)\colon \chi^{-1}$$

One can generalise this from 1-cubes (maps), to diagrams over $\mathscr{P}\underline{m}$ for $m \geq 1$ as follows.

Definition 4.5. *Let $R_\bullet = \mathsf{C}_{\bullet \not\ni m} \xrightarrow{r^m} \mathsf{C}_{\bullet \ni m}$ be an m-cube with $m \geq 1$, seen as a 1-cube of $(m-1)$-cubes. A* left homotopy inverse *for $R_\bullet$ is the data of a diagram:*

$$\begin{tikzcd} & \mathsf{C}_{\bullet \not\ni m} \\ \mathsf{C}_{\bullet \not\ni m} \arrow[ur, "\mathrm{Id}"] \arrow[r, "r^m"'] & \mathsf{C}_{\bullet \ni m} \arrow[u, "l^m"'] \arrow[ul, phantom, "\Downarrow h^m"] \end{tikzcd} \tag{4.3}$$

In more detail, it consists of

(1) an m-cube $L_\bullet = \mathsf{C}_{\bullet \ni m} \xrightarrow{l^m} \mathsf{C}_{\bullet \not\ni m}$ and

(2) for each $S \subseteq \underline{m-1}$ a homotopy $h^m_S\colon \mathrm{Id}_{\mathsf{C}_S} \rightsquigarrow l^m_S \circ r^m_S$, that are mutually compatible in the sense that $h^m_\bullet(t)\colon \mathsf{C}_{\bullet \not\ni m} \to \mathsf{C}_{\bullet \not\ni m}$ is an m-cube for each fixed $0 \leq t \leq 1$.

LEMMA 4.6. *Given the data of (4.3), there are inverse homotopy equivalences*

$$\chi_m\colon \operatorname{tofib}(R_\bullet) \underset{\sim}{\rightleftarrows} \Omega \operatorname{tofib}(L_\bullet) : (\chi_m)^{-1}$$

To repeat this procedure and get a homotopy equivalence from the total fibre of an m-cube to an m-fold loop space, we need a left homotopy inverse l^k_S for each r^k_S. We also need suitable conditions for homotopies h^k_S, in order to avoid obtaining cubes which are commutative only up to homotopy.

Definition 4.7. *An m-fold left homotopy inverse for an m-cube $D^m := (C_\bullet, r)$ is given as follows.*

(1) For each $S \subseteq \underline{m}$ and $k \in \underline{m} \setminus S$ a map $l^k_S : C_{Sk} \to C_S$ is given such that

$$l^k_S \circ l^i_{Sk} = l^i_S \circ l^k_{Si}, \quad \forall i \notin S,\ i \neq k \tag{4.4}$$

$$l^k_{Si} \circ r^i_{Sk} = r^i_S \circ l^k_S, \quad \forall i \notin S,\ k > Si := S \cup \{i\}. \tag{4.5}$$

These equations ensure that for $0 \leq k \leq m$ there is a well-defined m-cube D^k obtained from D^m by replacing the arrows r^i_S by l^i_S for $k+1 \leq i \leq m$.[23] *In particular, $D^0 = (C_\bullet, l)$.*

(2) For each $0 \leq k \leq m$ and $t \in [0,1]$ a map of diagrams

$$h^k_\bullet(t) : D^k_{\bullet\not\ni k} \to D^k_{\bullet\not\ni k} \tag{4.6}$$

is given, such that $h^k_\bullet(0) = \mathrm{Id}$ and $h^k_\bullet(1) = l^k_\bullet \circ r^k_\bullet$.

For $k = m, \dots, 0$ we can write the cube D^k as $D^k_{\bullet\not\ni k} \xrightarrow{r^k_\bullet} D^k_{\bullet\ni k}$ and then define $D^{k-1} := D^k_{\bullet\ni k} \xrightarrow{l^k_\bullet} D^k_{\bullet\not\ni k}$. Hence D^k is a diagram over $\mathcal{P}(\underline{m-k}) \times \mathcal{P}^{op}(\underline{m} \setminus \underline{m-k})$; in particular, D^0 is a contravariant cube. However, all these categories are isomorphic to $\mathcal{P}(\underline{m})$ if we appropriately rename the vertices. Thus, an m-fold left homotopy inverse for D^m is given by the following data for each $0 \leq k \leq m$:

$$\begin{tikzcd} & D^k_{\bullet\not\ni k} \\ D^k_{\bullet\not\ni k} \arrow[ur, "\mathrm{Id}"] \arrow[r, "r^k_\bullet"'] \arrow[ur, phantom, shift right=3, "\Downarrow h^k_\bullet"] & D^k_{\bullet\ni k} \arrow[u, "l^k_\bullet"'] \end{tikzcd} \tag{4.7}$$

Proposition 4.8. *Given the data of (4.7) there is a sequence of homotopy equivalences*

$$\chi\colon \operatorname{tofib}(D^m) \xrightarrow[\sim]{\chi_m} \Omega \operatorname{tofib}(D^{m-1}) \xrightarrow[\sim]{\chi_{m-1}} \Omega^2 \operatorname{tofib}(D^{m-2}) \xrightarrow[\sim]{\chi_{m-2}} \cdots \xrightarrow[\sim]{\chi_1} \Omega^m \operatorname{tofib}(D^0). \tag{4.8}$$

Moreover, the homotopy inverse is given by $\chi^{-1}\colon \Omega^m \operatorname{tofib}(D^0) \xrightarrow{\Omega^m \mathsf{forg}} \Omega^m C_{\underline{m}} \hookrightarrow \operatorname{tofib}(D^m)$, where

$$\mathsf{forg}\colon \operatorname{tofib}(D^0) \longrightarrow C_{\underline{m}}, \qquad \left\{f^{\underline{m}\setminus S} : I^S \to C_{\underline{m}\setminus S}\right\} \mapsto f^{\underline{m}}.$$

It easily follows for $D^0 = (C_\bullet, l)$ as above that the entrywise homotopy groups form a contravariant m-cube $\pi_* D^0 = (\pi_* C_\bullet, \pi_* l)$ in graded groups (with $* > 0$), which has a *right m-fold inverse*. Thus, we have the following analogue of (4.2):

$$\pi_*\Big(\operatorname{tofib}(D^0)\Big) \cong \bigcap_{k\in\underline{m}} \ker\left(\pi_* l^k_{\underline{m}\setminus k}\right) \xhookrightarrow{\quad \mathsf{forg} \quad} \pi_* C_{\underline{m}}. \tag{4.9}$$

For proofs of all these results see Section 6; in Proposition 6.6 we will also give an explicit description of χ, used later in Section 9. Let us now turn to applying them in our situation.

Theorem 4.3 will follow from Proposition 4.8 once we construct an $(n-1)$-fold left homotopy inverse $(\mathscr{F}^n_S, l^k_S)$ for $(\mathscr{F}^n_S, r^k_S)$. By Lemma 4.1 the latter is obtained by applying $\mathcal{E}\mathrm{mb}_\partial(J_0, -)$ to (M_{0S}, ρ^k_S), which is also a cube: ρ^k-maps commute as they add mutually disjoint pieces $\mathbb{B}_{k-1,k+1} \setminus (\mathbb{B}_{k-1} \cup \mathbb{B}_k)$.

Theorem 4.9. *The $(n-1)$-cube (M_{0S}, ρ^k_S) has an $(n-1)$-fold left homotopy inverse (M_{0S}, λ^k_S).*

This implies Theorem 4.3. Namely, we construct the desired $(\mathscr{F}^n_S, l^k_S)$ by applying $\mathcal{E}\mathrm{mb}_\partial(J_0, -)$ to (M_{0S}, λ^k_S), i.e. let $l^k_S = \lambda^k_S \circ -$. It is clear that this gives a cube and that l^k_S and r^k_S also satisfy conditions (4.4) and (4.5). Similarly, $h^k_\bullet \circ -$ uses $h^k_\bullet\colon \lambda^k_\bullet \circ \rho^k_\bullet \rightsquigarrow \mathrm{Id}$ and so satisfies (4.6).

[23] We see D^k as an $(m-k)$-cube of k-cubes; maps in k-cubes are r-maps, while maps between them are l-maps.

To prove Theorem 4.9 we first define for each ρ^k_S a left homotopy inverse λ^k_S in the sense of (4.1), and then revisit the construction to ensure that all conditions of Definition 4.7 are satisfied.

LEMMA 4.10. *For $k \notin S \subseteq \underline{n-1}$ the map ρ^k_S has a left homotopy inverse $\lambda^k_S : M_{0Sk} \to M_{0S}$.*

Proof. Let $S > k := \{j \in S : j > k\}$ and let $i_{p+1} := \min\{(S > k) \cup \{n\}\}$ be the smallest index in S which is bigger than k, or n if that set is empty. Consider the inclusion map

$$e_{ki_{p+1}} : M_{0Sk} \hookrightarrow M_{0Sk} \cup \mathbb{B}_{ki_{p+1}}$$

which adds back the ball $\mathbb{B}_{ki_{p+1}}$. We visualise $e_{ki_{p+1}}$ by erasing $\mathbb{B}_{ki_{p+1}}$ from the picture as in Figure 8.

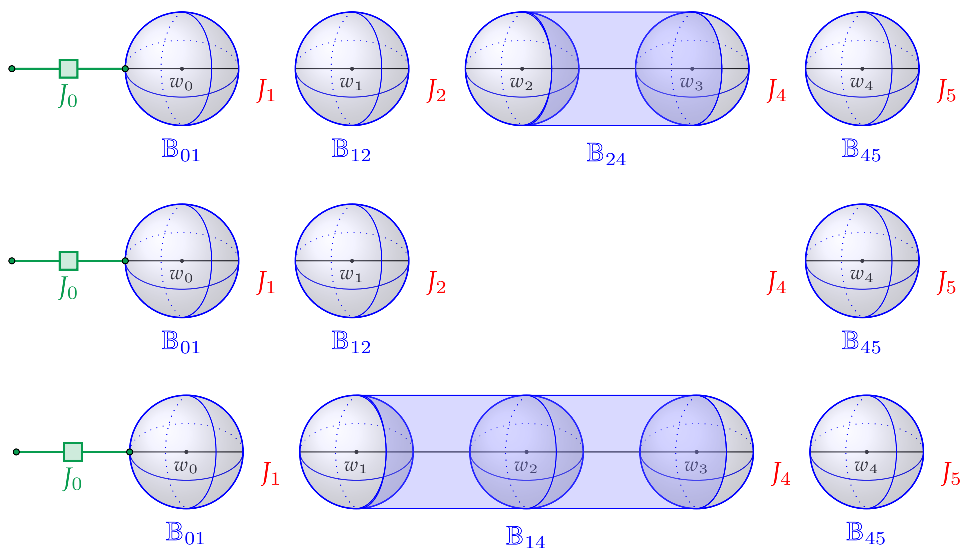


Figure 8. The map λ^k_S for $n = 5, S = \{1, 4\}, k = 2, i_p = 1, i_{p+1} = 4$ takes top M_{0124} to the bottom M_{014}. From the top to the middle apply e_{24}, and from the middle to the bottom the diffeomorphism $\mathsf{drag}^2_4(1)$.

Observe that $M_{0Sk} \cup \mathbb{B}_{ki_{p+1}}$ and M_{0S} are isotopic as submanifolds of M by an ambient isotopy

$$\mathsf{drag}^k_{S>k}(t) \colon M \to M, \quad \mathsf{drag}^k_{S>k}(0) = \mathrm{Id}_M, \quad \mathsf{drag}^k_{S>k}(1)(M_{0Sk} \cup \mathbb{B}_{ki_{p+1}}) = M_{0S},$$

which, loosely speaking, *elongates $\mathbb{B}_{i_pk}$ by gradually dragging the right hemisphere of $\mathbb{S}_{k-1}$ to the right, until it equals the right hemisphere of $\mathbb{S}_{i_{p+1}-1}$.* We will define a specific parametrisation in the proof of Theorem 4.9 below (it will indeed depend on $S > k$ and not only on i_{p+1}).

Now let $d^k_S(t) := \mathsf{drag}^k_{S>k}(t)|_{M_{0Sk}\cup\mathbb{B}_{ki_{p+1}}}$ and define

$$\lambda^k_S := d^k_S(1) \circ e_{ki_{p+1}} : M_{0Sk} \to M_{0S}.$$

It remains to provide a homotopy h^k_S between $\mathrm{Id}_{M_{0S}}$ and the composite

$$\begin{tikzcd}
\lambda^k_S \circ \rho^k_S \colon M_{0S} \arrow[r, hook, "\rho^k_S"] & M_{0Sk} \arrow[r, hook, "e_{ki_{p+1}}"] \arrow[d, equal] & M_{0Sk} \cup \mathbb{B}_{ki_{p+1}} \arrow[r, "d^k_S(1)"] \arrow[d, equal] & M_{0S} \\
& M_{0S} \cup \big(\mathbb{B}_{i_pi_{p+1}} \setminus (\mathbb{B}_{i_pk} \cup \mathbb{B}_{ki_{p+1}})\big) \arrow[r, "\cup\mathbb{B}_{ki_{p+1}}"] & M_{0S} \cup \big(\mathbb{B}_{i_pi_{p+1}} \setminus \mathbb{B}_{i_pk}\big) &
\end{tikzcd}$$

The composition of the first two maps adds to M_{0S} the material $\mathbb{B}_{i_pi_{p+1}} \setminus \mathbb{B}_{i_pk}$, which is diffeomorphic to a ball.[24] Adding this material gradually gives an isotopy $\mathsf{add}_t \colon M_{0S} \hookrightarrow M$ such that $\mathrm{im}(\mathsf{add}_0) =$

[24] We use here the fact that $\mathbb{B}_{k-1,k+1} \setminus (\mathbb{B}_{k-1} \cup \mathbb{B}_k) = \mathbb{B}_{i_pi_{p+1}} \setminus (\mathbb{B}_{i_pk} \cup \mathbb{B}_{ki_{p+1}})$.

M_{0S} and $\mathrm{im}(\mathsf{add}_1) = M_{0Sk} \cup \mathbb{B}_{ki_{p+1}}$. We can parametrise this so that $\mathrm{im}(\mathsf{add}_t) = \mathrm{im}(d^k_S(t))$ for each $t \in [0,1]$, so the two isotopies can be composed into a desired homotopy

$$h^k_S(t)\colon \quad M_{0S} \xhookrightarrow{\mathsf{add}_t} \mathrm{im}(\mathsf{add}_t) \xrightarrow{\quad d^k_S(t) \quad} M_{0S}. \qquad \square$$

Proof of Theorem 4.9. We now ensure that the maps λ^k_S and h^k_S constructed in the previous proof satisfy conditions of Definition 4.7. We are still free to *specify a particular parametrisation* of the ambient isotopy $\mathsf{drag}^k_{S>k}(t)\colon M \to M$, which is given roughly as a 'dragging move', acting non-trivially only in a tubular neighbourhood of $W_{i_p i_{p+1}}$.

Firstly, for $S \subseteq \underline{n-1} \setminus \{i,k\}$ the conditions (4.5) and (4.4) respectively equivalent to having that the following left diagram commutes for $k > Si$ and the right diagram for, say, $i < k$:

$$\begin{tikzcd} M_{0Si} & M_{0Sik} \arrow[l, "\lambda^k_{Si}"'] \\ M_{0S} \arrow[u, "\rho^i_S"] & M_{0Sk} \arrow[l, "\lambda^k_S"] \arrow[u, "\rho^i_{Sk}"'] \end{tikzcd} \qquad \begin{tikzcd} M_{0Si} \arrow[d, "\lambda^i_S"'] & M_{0Sik} \arrow[l, "\lambda^k_{Si}"'] \arrow[d, "\lambda^i_{Sk}"] \\ M_{0S} & M_{0Sk} \arrow[l, "\lambda^k_S"] \end{tikzcd}$$

For the left diagram this is clear. Indeed, ρ^i_S and ρ^i_{Sk} both add the same material $\mathbb{B}_{i-1,i+1} \setminus (\mathbb{B}_{i-1} \cup \mathbb{B}_i)$ independently of the location of the other punctures, and as $k > Si$, both λ^k_S and λ^k_{Si} erase the ball $\mathbb{B}_{kn}$ and then use the same flow $\mathsf{drag}^k_{S>k} = \mathsf{drag}^k_{Si>k} = \mathsf{drag}^k_{\emptyset}$.

On the other hand, the commutativity of the right diagram will follow if we ensure that

$$\mathsf{drag}^i_{S>i}(1) \circ \mathsf{drag}^k_{Si>k}(1) = \mathsf{drag}^k_{S>k}(1) \circ \mathsf{drag}^i_{Sk>i}(1) \tag{4.10}$$

Lastly, the condition (4.6) is equivalent to having that for each $t \in [0,1]$ the following left square commutes if $i > k$ (clear since $\mathsf{drag}^i_{Sk>i}(t) = \mathsf{drag}^i_{S>i}(t)$) and the right square if $i < k$:

$$\begin{tikzcd} M_{0S} \arrow[r, "\rho^k_S"] \arrow[d, "h^i_S(t)"'] & M_{0Sk} \arrow[d, "h^i_{Sk}(t)"] \\ M_{0S} \arrow[r, "\rho^k_S"] & M_{0Sk} \end{tikzcd} \qquad \begin{tikzcd} M_{0S} \arrow[d, "h^i_S(t)"'] & M_{0Sk} \arrow[l, "\lambda^k_S"'] \arrow[d, "h^i_{Sk}(t)"] \\ M_{0S} & M_{0Sk} \arrow[l, "\lambda^k_S"] \end{tikzcd}$$

Therefore, we should ensure that

$$\mathsf{drag}^i_{S>i}(t) \circ \mathsf{drag}^k_{S>k}(1) = \mathsf{drag}^k_{S>k}(1) \circ \mathsf{drag}^i_{Sk>i}(t) \qquad \forall t \in [0,1] \tag{4.11}$$

Note that (4.10) follows from (4.11) by putting $t = 1$ and using $iS\!>k = S\!>k$, since $i < k$.

We now define parametrisations of $\mathsf{drag}^i_{S>i}$ inductively on $|S > i| \geq 0$ for $i \in \underline{n-1}$ and $S \subseteq \underline{n-1} \setminus \{i\}$. Pick each $\mathsf{drag}^i_{\emptyset}$ freely and assume for some $s \geq 0$ we chose $\mathsf{drag}^i_{S>i}$ for all $|S > i| < s$. Let now $|S' > i| = s$ for some $S' = Sk$ with $k := \min\{(S' > i) \cup \{n\}\}$. Then let

$$\mathsf{drag}^i_{S'>i}(t) := \mathsf{drag}^k_{S>k}(1)^{-1} \circ \mathsf{drag}^i_{S>i}(t) \circ \mathsf{drag}^k_{S>k}(1). \tag{4.12}$$

This finishes the definition. Let us check that (4.11) holds for any $S \subseteq \underline{n-1} \setminus \{i,k\}$ and $i < k$ by induction on $|i < S < k| \geq 0$. If there is no $i_p \in S$ with $i < i_p < k$, then (4.12) is precisely (4.11).

Otherwise, take the smallest such i_p so $S = Ri_p$. Apply (4.12) for $S' = (Rk)i_p$ and the induction hypothesis for $\mathsf{drag}^i_{Rk>i}(t)$ to get

$$\begin{aligned} \mathsf{drag}^i_{Sk>i}(t) &= \mathsf{drag}^{i_p}_{Rk>i_p}(1)^{-1} \circ \Big(\mathsf{drag}^k_{R>k}(1)^{-1} \circ \mathsf{drag}^i_{R>i}(t) \circ \mathsf{drag}^k_{R>k}(1)\Big) \circ \mathsf{drag}^{i_p}_{Rk>i_p}(1) \\ &= \mathsf{drag}^k_{Ri_p>k}(1)^{-1} \circ \Big(\mathsf{drag}^{i_p}_{R>i_p}(1)^{-1} \circ \mathsf{drag}^i_{R>i}(t) \circ \mathsf{drag}^{i_p}_{R>i_p}(1)\Big) \circ \mathsf{drag}^k_{Ri_p>k}(1). \end{aligned}$$

For the second equality we have used that $\mathsf{drag}^k_{R>k}(1) \circ \mathsf{drag}^{i_p}_{Rk>i_p}(1) = \mathsf{drag}^{i_p}_{R>i_p}(1) \circ \mathsf{drag}^k_{R>k}(1)$ again by the hypothesis. Now observe that $Ri_p > k = R > k$, so the last expression equals $\mathsf{drag}^k_{S>k}(1)^{-1} \circ \mathsf{drag}^i_{S>i}(t) \circ \mathsf{drag}^k_{S>k}(1)$, finishing the induction step. $\square$

4.2 The final delooping

Analogously as in Example 4.2 we have weak equivalences

$$\mathscr{F}^n_\emptyset := \mathscr{E}\mathrm{mb}_\partial(J_0, M_0) \hookrightarrow \mathscr{I}\mathrm{mm}_\partial(J_0, M) \xrightarrow{\mathscr{D}} \Omega \mathbb{S}M.$$

Recall from Notation 5 that $M_0 := M \setminus \mathbb{B}_{0n}$ and note that when passing to immersions we forget this disjointness condition for J_0 and $\mathbb{B}_{0n}$. We will now determine the homotopy type of each $\mathscr{F}^n_S$ using similar ideas. Let $M_\emptyset = M$ and for $S = \{i_1, \dots, i_m\} \subseteq \underline{n-1}$ let

$$M_S := M \setminus \big(\mathbb{B}_{i_1 i_2} \sqcup \cdots \sqcup \mathbb{B}_{i_m n}\big) = M_{0S} \cup \mathbb{B}_{0 i_1}. \tag{4.13}$$

The basepoint is at $p_0 \in M_S$, the midpoint of J_0. We now analogously consider inclusions

$$\mathscr{F}^n_S = \mathscr{E}\mathrm{mb}_\partial(J_0, M_{0S}) \hookrightarrow \mathscr{I}\mathrm{mm}_\partial(J_0, M_{0S}) \hookrightarrow \mathscr{I}\mathrm{mm}_\partial(J_0, M_S). \tag{4.14}$$

The unit derivative of an immersion $f\colon J_0 \looparrowright M_S$ is a path $\mathscr{D}f\colon I \longrightarrow \mathbb{S}M_S$ in the unit tangent bundle, whose endpoints $(L_0, \vec{e})$ and $(R_0, \vec{e})$ agree with those of $\mathrm{U}_{J_0} := \mathrm{U}|_{J_0}$. To make $\mathscr{D}f$ into a closed loop in $\mathbb{S}M_S$ we concatenate it with the unit derivative of any arc $\widetilde{\mathrm{U}_{J_0}}$, which agrees with U_{J_0} except near endpoints, at which its derivative is $-\vec{e}$ instead. See Figure 9 for an example.

Thus, $\mathscr{D}\widetilde{\mathrm{U}_{J_0}}$ followed by the path $\mathscr{D}f$ in reverse can be seen as a loop at $(p_0, \vec{e})$, so we have

$$\mathscr{D}_S\colon \mathscr{I}\mathrm{mm}_\partial(J_0, M_S) \xrightarrow{\sim} \Omega\big(\mathbb{S}M_S\big), \quad f \mapsto (\mathscr{D}\widetilde{\mathrm{U}_{J_0}}) \cdot (\mathscr{D}f)_{1-t} \tag{4.15}$$

By a theorem of Smale this map is a *weak equivalence* [Sma58].

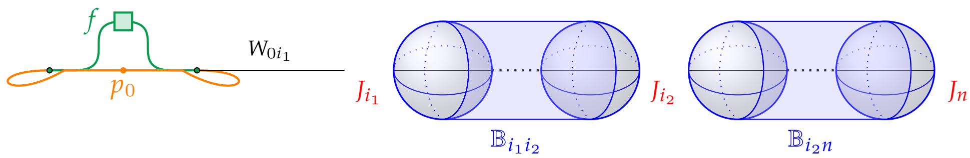


Figure 9. The manifold $M_{i_1 i_2}$ is the complement of $\mathbb{B}_{i_1 i_2} \sqcup \mathbb{B}_{i_2 n} \subseteq M$. A choice for the arc $\widetilde{\mathrm{U}}_{J_0}$ is in orange.

We define maps $\lambda^k_S\colon M_{Sk} \longrightarrow M_S$ for $k \notin S$ as in the proof of Lemma 4.10, since the presence of the index 0 was irrelevant there.[25] Similarly as before, this forms an $(n-1)$-cube $(M_\bullet, \lambda)$ and we let $(\Omega\mathbb{S}M_\bullet, \Omega\mathbb{S}\lambda)$ be the corresponding cube of loops on the unit tangent bundles.

THEOREM 4.11. *Composing* (4.15) *with the inclusions* (4.14) *gives the map* $\mathscr{D}_S\colon \mathscr{F}^n_S \to \Omega\mathbb{S}M_S$ *which is a homotopy equivalence for any* $S \subseteq \underline{n-1}$. *Hence, there is an equivalence of cubes*

$$\mathscr{D}_\bullet\colon \big(\mathscr{F}^n_\bullet, l\big) \xrightarrow{\sim} \big(\Omega\mathbb{S}M_\bullet, \Omega\mathbb{S}\lambda\big).$$

COROLLARY 4.12. *For* $n \geq 2$ *the map of cubes* $\mathbb{S}(M_\bullet) \to M_\bullet$ *forgetting the tangent data is a homotopy equivalence on total homotopy fibres, so there is a homotopy equivalence*

$$\mathscr{D}\colon \operatorname{tofib}\big(\mathscr{F}^n_\bullet, l\big) \xrightarrow{\sim} \operatorname{tofib}\big(\Omega M_\bullet, \Omega\lambda\big).$$

[25] But remembering that $\lambda^k_\emptyset\colon M \setminus \mathbb{B}_{kn} \to M$ not only adds the ball $\mathbb{B}_{kn}$, but also deforms M using the dragging map.

Proof of Corollary 4.12. The rows in the commutative diagram

$$\begin{tikzcd} \mathbb{S}^{d-1} \arrow[r] \arrow[d, equal] & \mathbb{S}(M_{Sk}) \arrow[r] \arrow[d, "\mathbb{S}\lambda^k_S"] & M_{Sk} \arrow[d, "\lambda^k_S"] \\ \mathbb{S}^{d-1} \arrow[r] & \mathbb{S}(M_S) \arrow[r] & M_S \end{tikzcd}$$

are fibre bundles, so comparing the vertical homotopy fibres gives $\mathrm{hofib}(\mathbb{S}\lambda^k_S) \simeq \mathrm{hofib}(\lambda^k_S)$. □

Remark 4.13. *With the tangent data now gone, define $\mathcal{D}_S \colon \mathscr{F}^n_S \to \Omega M_S$ using simply $\widetilde{\mathrm{U}}_{J_0} := \mathrm{U}_{J_0}$.*

Remark 4.14. *Actually, the maps $\mathcal{D}_S$ factor through spaces ΩM_{0S}, giving diagrams*

$$\begin{tikzcd} \mathscr{F}^n_{Sk} \arrow[r, "\mathcal{D}_{Sk}"] \arrow[d, dashed, shift left, "l^k_S"] & \Omega M_{0Sk} \arrow[r, hook, "\rho^0"] \arrow[d, dashed, shift left, "\Omega\lambda^k_S"] & \Omega M_{Sk} \arrow[d, dashed, "\Omega\lambda^k_S"] \\ \mathscr{F}^n_S \arrow[r, "\mathcal{D}_S"] \arrow[u, shift left, "r^k_S"] & \Omega M_{0S} \arrow[r, hook, "\rho^0"] \arrow[u, shift left, "\Omega\rho^k_S"] & \Omega M_S \end{tikzcd}$$

If either both upward or all downward arrows are omitted, the resulting diagram commutes. By the last corollary, the leftmost and the rightmost dashed maps form cubes with homotopy equivalent total fibres. By Theorem 4.9 we also have the cube $(\Omega M_{0\bullet}, \Omega\rho)$ and its $(n-1)$-fold left homotopy inverse $(\Omega M_{0\bullet}, \Omega\lambda)$.

However, it is important to point out that there are no ρ-maps *between spaces ΩM_S which would form a cube equivalent to our original cube $(\mathscr{F}^n_S, r^k_S)$. The reason lies in the fact that the information about the disjointness of J_0 with $\mathbb{B}_{0i_1}$ is lost when we pass from M_{0S} to M_S. More precisely, there are no maps $M_S \to M_{kS}$ when k is smaller than all indices in S, but otherwise we do have ρ^k_S. Actually, the homotopies $h^k_S(t)$ do restrict to M_S and also commute with $\mathcal{D}_S$ by construction.*

Proof of Theorem 4.11. We will identify $\mathcal{D}_S \colon \mathscr{F}^n_S \to \Omega\mathbb{S}M_S$ with the composite of two homotopy equivalences $\overline{\chi} \colon \mathscr{F}^n_S \to \Omega\,\mathrm{fib}(l^0_{Sn})$ and $\Omega\mathcal{D}_{w_{0i_1}} \colon \Omega\,\mathrm{fib}(l^0_{Sn}) \to \Omega(\mathbb{S}M_S)$. To construct the former we again use left homotopy inverses, recalling that $\mathscr{F}^n_S := \mathrm{fib}(r^0_{Sn})$ (see Section 3.2).

Lemma 4.15. *For $\emptyset \neq R \subseteq \underline{n}$ the map $r^0_R \colon \mathcal{E}_R \to \mathcal{E}_{0R}$ has a left homotopy inverse l^0_R which is a* fibration. *Moreover, the image of $\overline{\chi} \colon \mathscr{F}^n_S \hookrightarrow \mathrm{hofib}(r^0_{Sn}) \xrightarrow{\chi} \Omega\,\mathrm{hofib}(l^0_{Sn})$ lies in $\Omega\,\mathrm{fib}(l^0_{Sn})$.*

Proof. Given a point $K \colon I \setminus J_{0R} \hookrightarrow M$ in $\mathcal{E}_{0R}$ to get a point in $\mathcal{E}_R$ we need to 'define K on J_0'. To this end, consider a pulling map similar to the one used for retraction of $\mathcal{E}_i$ (see Lemma 3.4):

$$\mathsf{pull}\colon \quad I \setminus J_R \xrightarrow[\cong]{\mathsf{resc}} \Big(I \setminus J_R\Big) \setminus [L_0, L_{i_1}] = \Big(I \setminus J_{0R}\Big) \setminus W_{0i_1} \xhookrightarrow{incl} I \setminus J_{0R}$$

where $[L_0, L_{i_1}] = J_0 \cup W_{0i_1}$. The composite $K \circ \mathsf{pull} = K \circ incl \circ \mathsf{resc} = K_{\widehat{W_{0i_1}}} \circ \mathsf{resc}$ is a point in $\mathcal{E}_R$. However, this does not give a based map $\mathcal{E}_{0R} \to \mathcal{E}_R$ since $\mathrm{U}_{\widehat{0R}} \circ \mathsf{pull} \neq \mathrm{U}_{\widehat{R}}$. It becomes based if we postcompose with a diffeomorphism resc_{0i_1} of M which squeezes the region $[L_0, R_{i_1}] \times \mathbb{D}^{d-1}_\epsilon$ into $J_{i_1} \times \mathbb{D}^{d-1}_\epsilon$, as in the proofs of Lemmas 3.4 and 4.10.

Therefore, we let $l^0_R := \mathsf{resc}_{0i_1} \circ - \circ \mathsf{pull} \colon \mathcal{E}_{0R} \to \mathcal{E}_R$ and observe it is a fibration: the restriction map is a fibration by Remark 3.3, and both rescaling maps are diffeomorphisms.

Let us now define a homotopy h between $l^0_R \circ r^0_R$ and $\mathrm{Id}_{\mathcal{E}_R}$. Since for $K \in \mathcal{E}_R$ we have $l^0_R r^0_R(K) = \mathsf{resc}_{0i_1} \circ K_{\widehat{0}} \circ \mathsf{pull} = \mathsf{resc}_{0i_1} \circ K_{\widehat{J_0 \cup W_{0i_1}}} \circ \mathsf{resc}$, we can similarly let $h(K) := \mathsf{resc}_{ti_1} \circ K \circ \mathsf{pull}_t$ using

$$\mathsf{pull}_t \colon \ I \setminus J_R \xrightarrow[\cong]{\mathsf{resc}} (I \setminus J_R) \setminus \big[L_0 + t\cdot(L_{i_1} - L_0), L_{i_1}\big] \hookrightarrow I \setminus J_R,$$

which is a homotopy between $\mathrm{Id}_{I\setminus J_R}$ and pull, and an isotopy $\mathsf{resc}_{ti_1}: M \to M$ which makes h_t into a basepoint preserving homotopy: it squeezes $[L_0 + t\cdot(L_{i_1} - L_0), R_{i_1}] \times \mathbb{D}^{d-1}_\epsilon$ into $J_{i_1} \times \mathbb{D}^{d-1}_\epsilon$.

Now Lemma 4.4 gives the homotopy equivalence $\chi\colon \operatorname{hofib}(r^0_R) \to \operatorname{hofib}(l^0_R)$.

To prove the second claim we take $R = Sn$ and check that $\overline{\chi} := \chi|_{\operatorname{fib}(r^0_{Sn})}$ has image in $\Omega\operatorname{fib}(l^0_{Sn})$. For this it is enough to check that $\mathsf{forg}\circ\overline{\chi}\colon \mathscr{F}^n_S \to \Omega\mathcal{E}_{0Sn}$ lends in the subspace $\Omega\operatorname{fib}(l^0_{Sn}) \subseteq \Omega\mathcal{E}_{0Sn}$.

For $f \in \mathscr{F}^n_S$ the corresponding point under $\mathscr{F}^n_S \cong \operatorname{fib}(r^0_{Sn}) \subseteq \mathcal{E}_{Sn}$ is given by $\mathrm{U}_f := f \cup \mathrm{U}_{0Sn} \in \mathcal{E}_{Sn}$. Then by (6.4) from Section 6 we have

$$\mathsf{forg}\circ\overline{\chi}(f) = \mathsf{forg}\circ\chi(\mathrm{U}_f, \mathsf{const}_{\mathrm{U}_{0Sn}}) = r^0_{Sn} h_{1-t}(\mathrm{U}_f) \quad \in \Omega\mathcal{E}_{0Sn}.$$

We claim that $l^0_{Sn}(\mathsf{forg}\circ\overline{\chi}(f)) = \mathrm{U}_{\widehat{Sn}} \in \mathcal{E}_{Sn}$. Indeed, $h_t(\mathrm{U}_f) = \mathsf{resc}_{ti_1}\circ \mathrm{U}_f|_{[tL_0, L_{i_1}]}\circ\mathsf{resc}$ is different from U only on $[tL_0, L_{i_1}]$, but $l^0_{Sn} r^0_{Sn}(h_t(\mathrm{U}_f)) = \mathsf{resc}_{0i_1}\circ h_t(\mathrm{U}_f)_{\overline{J_0\cup W_{0i_1}}}\circ\mathsf{resc}$ only 'sees' the restriction to the complement of $J_0 \cup W_{0i_1} = [L_0, L_{i_1}]$ so it equals $\mathrm{U}_{\widehat{Sn}}$ for all $t \in [0,1]$. □

Therefore, we have the following diagram which commutes except that $incl\circ\mathsf{forg}\circ\chi \simeq \mathrm{Id}$.

$$\begin{tikzcd}
\mathscr{F}^n_S = \operatorname{fib}(r^0_{Sn}) \arrow[rr, dashed, "\overline{\chi}"] \arrow[d, hook, "\sim"] & & \Omega\operatorname{fib}(l^0_{Sn}) \arrow[r, "\mathcal{D}_{w_{0i_1}}"] \arrow[dl] \arrow[d, hook, "\sim"] & \Omega\mathbb{S}M_S \\
 & \Omega\mathcal{E}_{0Sn} \arrow[dl] & & \\
\operatorname{hofib}(r^0_{Sn}) \arrow[rr, "\chi", "\sim"'] & & \Omega\operatorname{hofib}(l^0_{Sn}) \arrow[ul, "\mathsf{forg}"'] &
\end{tikzcd}$$

The space $\operatorname{fib}(l^0_{Sn})$ consists of those $K\colon I\setminus J_{0Sn} \hookrightarrow M$ for which $l^0_{Sn}(K) = \mathrm{U}_{\widehat{Sn}}$, so they agree with U everywhere except possibly on $W_{0i_1} \subseteq I$. Since the derivative at the midpoint $\mathcal{D}_{w_{0i_1}}$ is a *homotopy equivalence for embeddings of disks with freely moving boundary*, we indeed get

$$\mathcal{D}_{w_{0i_1}}:\ \operatorname{fib}(l^0_{Sn}) \cong \mathcal{E}\mathrm{mb}\Big(W_{0i_1}, I^3 \setminus (W_{i_1i_2} \sqcup \cdots \sqcup W_{i_{m-1}i_m} \sqcup W_{i_m n})\Big) \simeq \mathcal{I}\mathrm{mm}(I, M_S) \simeq \mathbb{S}M_S.$$

Finally, let us check that $\Omega\mathcal{D}_{w_{0i_1}}\circ\overline{\chi}\colon \mathscr{F}^n_S \to \Omega\operatorname{fib}(l^0_{Sn}) \to \Omega\mathbb{S}M_S$ agrees with $\mathcal{D}_S$. For each $t\in[0,1]$ this is taking the derivative at $w_{0i_1} \in W_{0i_1}$ of the restriction of $r^0_{Sn}h_{1-t}(\mathrm{U}_f)$ to W_{0i_1}. As the time t increases, $r^0_{Sn}h_{1-t}(\mathrm{U}_f)$ has the piece W_{0i_1} travelling along U_f, by the definition of h. Thus, the point w_{0i_1} 'scans' the derivative of U_f in the manifold M_S. This is precisely $\mathcal{D}_S(f)$. □

Remark 4.16. *As mentioned in the introduction, the authors of [BCKS17] use Sinha's cosimplicial model* $AM_n(I^3) := \operatorname{holim}\mathsf{Conf}'_\bullet\langle M,\partial\rangle$*, where* $\mathsf{Conf}'_n\langle M\rangle$ *is a compactified configuration space of* n *points in* $\mathbb{S}M$ *[Sin09]. We can compare this to our approach via the homotopy-commutative diagram*

$$\begin{tikzcd}
\mathscr{F}^n_S \arrow[r, dashed] \arrow[d, "\sim"'] & \mathcal{E}_{Sn}(M) \arrow[r, shift left, "r^0_{Sn}"] \arrow[d, "\prod_{k=1}^m \mathcal{D}_{w_{i_pi_{p+1}}}"', "\sim"] & \mathcal{E}_{0Sn}(M) \arrow[l, shift left, "l^0_{Sn}"] \arrow[d, "\sim"', "\prod_{k=0}^m \mathcal{D}_{w_{i_pi_{p+1}}}"] & \operatorname{fib}(l^0_{Sn}) \arrow[l, dotted] \arrow[d, "\sim"] \\
\Omega\mathbb{S}M_S \arrow[r, dashed] & \mathsf{Conf}'_S\langle M,\partial\rangle \arrow[r, shift left, "d^0"] & \mathsf{Conf}'_{0S}\langle M,\partial\rangle \arrow[l, shift left, "s^0"] & \mathbb{S}M_S \arrow[l, dotted]
\end{tikzcd}$$

The codegeneracy s^k *forgets points, and models our left homotopy inverse* l^k_S *(the harder map in our approach). Our restriction map* r^k_S *is modelled by the coface map* d^k*, which doubles points and is the harder map in their approach since it requires a compactification.*

The authors then use the cosimplicial identity $s^k\circ d^k = \mathrm{Id}$*, i.e. that* s^k *is a strict left inverse for* d^k*, to compute* $\mathsf{F}_n(I^3)$*. Indeed, the homotopy type of* $\operatorname{fib}(s^0)$ *is easier to find as it was also easier for us to compute the homotopy type of* $\operatorname{fib}(l^0_{Sn})$ *rather than* $\operatorname{fib}(r^0_{Sn})$*.*

5 Homotopy type of the layers

Notation 6. *For $S = \{i_1, \dots, i_m\} \subseteq \underline{n-1}$ denote the wedge of $(d-1)$-spheres $\mathbb{S}_{i_p i_{p+1}} := \partial \mathbb{B}_{i_p i_{p+1}}$ by*

$$\mathbb{S}_S := \mathbb{S}_{i_1 i_2} \vee \cdots \vee \mathbb{S}_{i_m n}$$

See Notation 5 and Figure 7. Let $M \vee \mathbb{S}_\bullet$ be the $(n-1)$-cube with spaces $M \vee \mathbb{S}_S$ and maps

$$\mathsf{col}_S^k \colon M \vee \mathbb{S}_{Sk} \longrightarrow M \vee \mathbb{S}_S$$

given by the identity on all wedge factors except on the sphere labelled by ki_{p+1} which is collapsed onto the wedge point. Here $i_p < k < i_{p+1}$ are the closest neighbouring indices.

Lemma 5.1. *For $n \geq 2$ there is a homotopy equivalence $\mathsf{retr}_\bullet \colon (M_\bullet, \lambda) \to (M \vee \mathbb{S}_\bullet, \mathsf{col})$.*

Proof. Recall that $M_S := M \setminus \mathbb{B}_S$ for $\mathbb{B}_S := \mathbb{B}_{i_1 i_2} \sqcup \cdots \sqcup \mathbb{B}_{i_m n}$. Take a thin enough neighbourhood $V := \mathrm{U}|_{[L_1,1]} \times \mathbb{D}_\epsilon^{d-1} \subseteq M$ of U containing all balls $\mathbb{B}_{ij}$. Then $V \setminus \mathbb{B}_S$ is diffeomorphic to $(I^d)_S$, and this clearly retracts onto $\mathbb{S}_S$: first project vertically onto the 'collection of beads' on U (see Figure 9) and then contract $\mathrm{U}_{\widehat{S}}$ and some arcs on the spheres to get one wedge point at L_0.

Observe that $M = M' \cup V$ where $M' := (M \setminus V) \cup (\partial M \cap \partial V)$ is diffeomorphic to M. Thus, we can define a retraction $\mathsf{retr}_S \colon M_S = M' \cup (V \setminus \mathbb{B}_S) \to M' \vee \mathbb{S}_S$ by applying the above retraction on $V \setminus \mathbb{B}_S$ while also gradually contracting $\partial V \cap \partial M'$ onto the point $L_0 \in \partial M'$.

Finally, it is not hard to see that contractions can be chosen so that λ_S^k commutes with col_S^k. □

For a different proof see [GW99, Cor. 5.3]. The assumption $\partial M \neq \emptyset$ is essential for this lemma and it does not hold for closed manifolds. In Corollary 1.8 we used this to compute the homotopy groups of configuration spaces manifolds with non-empty boundary.

Corollary 5.2 (of Theorem 4.3, Corollary 4.12 and Lemma 5.1). *There are homotopy equivalences $\mathsf{F}_1(M) \simeq \Omega(\mathbb{S}M)$ and*

$$\mathsf{F}_n(M) \xrightarrow[\sim]{\chi} \Omega^{n-1}\,\mathrm{tofib}(\mathscr{F}_\bullet^n, l) \xrightarrow[\sim]{\mathscr{D}} \Omega^n\,\mathrm{tofib}(M_\bullet, \lambda) \xrightarrow[\sim]{\mathsf{retr}} \Omega^n\,\mathrm{tofib}(M \vee \mathbb{S}_\bullet, \mathsf{col}), \quad n \geq 2.$$

Assume now $n \geq 2$. By (4.9) and the comment after it there is a commutative diagram

$$\begin{tikzcd}
\pi_*\,\mathrm{tofib}\left(\mathscr{F}_\bullet^n, l\right) \arrow[r, hook, two heads, "\mathsf{retr}\mathscr{D}", "\cong"'] \arrow[d, hook, "\mathsf{forg}"'] & \pi_{*+1}\,\mathrm{tofib}\left(M \vee \mathbb{S}_\bullet, \mathsf{col}\right) \arrow[d, hook, "\mathsf{forg}"'] \\
\bigcap_{k=1}^{n-1} \ker(\pi_* l_{\underline{n-1}\setminus k}^k) \subseteq \pi_* \mathscr{F}_{\underline{n-1}}^n \arrow[r, "\mathsf{retr}\mathscr{D}_{n-1}"] & \pi_{*+1}\left(M \vee \mathbb{S}_{\underline{n-1}}\right) \supseteq \bigcap_{k=1}^{n-1} \ker(\pi_{*+1}\mathsf{col}_{\underline{n-1}\setminus k}^k)
\end{tikzcd} \tag{5.1}$$

However, we can actually precisely determine the homotopy type of $\mathsf{F}_n(M)$ in terms of ΩM – more precisely, in terms of suspensions of iterated smashes of ΩM with itself. This is Theorem 5.4 below. For its proof we will use some classical results which we now recall, referring the reader to Appendix A for more details.

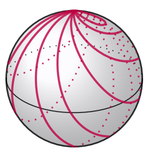


Figure 10. Several values $\eta_{\mathbb{S}_1}(t)$ of the canonical map $\eta_{\mathbb{S}_1} \colon \mathbb{S}^1 \to \Omega\mathbb{S}^2$.

Let $\iota_M\colon M \hookrightarrow M \vee \Sigma A$ and $\iota_{\Sigma A}\colon \Sigma A \hookrightarrow M \vee \Sigma A$ be the natural inclusions. Let $\eta_A\colon A \to \Omega\Sigma A$ be the unit of the loop-suspension adjunction, taking $a \in A$ to the loop $\theta \mapsto \theta \wedge a$. See Figure 10.

Consider the map $\Omega\iota_M\colon \Omega M \hookrightarrow \Omega(M \vee \Sigma A)$ and the composite

$$x_A\colon A \xrightarrow{\eta_A} \Omega\Sigma A \xhookrightarrow{\Omega\iota_{\Sigma A}} \Omega(M \vee \Sigma A). \tag{5.2}$$

We form their Samelson product (for the definition see Appendix A):

$$[x_A, \Omega\iota_M]\colon A \wedge \Omega M \to \Omega(M \vee \Sigma A).$$

LEMMA 5.3 ([Gra71; Spe71])**.** *For well-pointed spaces M and A there is a fibration sequence*

$$\Omega\Sigma\big(A \vee (A \wedge \Omega M)\big) \xrightarrow{\widetilde{x_A \vee [x_A, \Omega\iota_M]}} \Omega\big(M \vee \Sigma A\big) \underset{\Omega\iota_M}{\overset{\Omega\mathsf{col}_{\Sigma A}}{\rightleftarrows}} \Omega M$$

where the first map is the unique multiplicative extension of the map $x_A \vee [x_A, \Omega\iota_M]$ (see (A.6)). Moreover, this fibration of H-spaces has a section $\Omega\iota_M$, so it is trivial.

Applying this to $A = \mathbb{S}^{d-2}_S := \bigvee_{i\in S} \mathbb{S}^{d-2}_i$ for $S \subseteq \underline{n-1}$ gives a trivial fibration

$$\Omega\Sigma\Big(\bigvee_{i\in S} \mathbb{S}^{d-2}_i \vee \Big(\big(\bigvee_{i\in S} \mathbb{S}^{d-2}_i\big) \wedge \Omega M\Big)\Big) \xrightarrow{\mu_S} \Omega(M \vee \mathbb{S}_S) \xrightarrow{\Omega\mathsf{col}_{\mathbb{S}_S}} \Omega M \tag{5.3}$$

where μ_S is the multiplicative extension of $x_{\mathbb{S}^{d-2}_S} \vee [x_{\mathbb{S}^{d-2}_S}, \Omega\iota_M]$. Thus, $\Omega(M \vee \mathbb{S}_S) \simeq Z_S \times \Omega M$, where using the distributive property $(X_1 \vee X_2) \wedge Y = (X_1 \wedge Y) \vee (X_2 \wedge Y)$ we have

$$Z_S := \Omega\Sigma\Big(\bigvee_{i\in S} \mathbb{S}^{d-2}_i \vee \bigvee_{i\in S} (\mathbb{S}^{d-2}_i \wedge \Omega M)\Big).$$

Note that this is now a loop space on a wedge of spaces which are all suspensions, and in this case the Hilton–Milnor Theorem A.2 applies (which generalises Lemma 5.3): there is a weak equivalence

$$\prod_{w\in \mathsf{B}(S\sqcup S')} \Omega\Sigma w(\mathbb{S}_i, \mathbb{S}_{i'} \wedge \Omega M) \xrightarrow[\sim]{hm_S} Z_S \tag{5.4}$$

where $S' \cong S$ is another copy of S and $\mathsf{B}(S \sqcup S')$ is a *Hall basis* (see Remark A.3) for the free Lie algebra

$$\mathbb{L}(S \sqcup S') := \mathbb{L}(x^i : i \in S \sqcup S') = \mathbb{L}(x^i, x^{i'} : i \in S).$$

For a Lie word w in letters $x^i, x^{i'}$ the corresponding space $w(\mathbb{S}_i, \mathbb{S}_{i'} \wedge \Omega M)$ in (5.4) is obtained as an iterated smash product of spaces $\mathbb{S}_i$ and $\mathbb{S}_{i'} \wedge \Omega M$. In fact, if we denote the length of w as the sum $l_w = l^0_w + l'_w$ of the number of its letters from S and S' respectively, then

$$w(\mathbb{S}_i, \mathbb{S}_{i'} \wedge \Omega M) \cong (\mathbb{S}^{d-2}_i)^{\wedge l^0_w} \wedge (\mathbb{S}^{d-2}_{i'} \wedge \Omega M)^{\wedge l'_w} \cong \Sigma^{l_w(d-2)}(\Omega M)^{\wedge l'_w}.$$

using the associativity of the smash product. The Hilton–Milnor map hm_S in (5.4) is analogous to μ_S: it is the pointwise product of the multiplicative extensions $\widetilde{w}(x_{\mathbb{S}^{d-2}_i}, x_{\mathbb{S}^{d-2}_{i'} \wedge \Omega M})$ of the Samelson products according to $w \in \mathsf{B}(S \cup S')$ of the maps $x_{\mathbb{S}^{d-2}_i}\colon \mathbb{S}^{d-2}_i \to Z_S$ and $x_{\mathbb{S}^{d-2}_{i'} \wedge \Omega M}\colon \mathbb{S}^{d-2}_{i'} \wedge \Omega M \to Z_S$. This uses the notation (5.2). We will provide more details in (A.7).

Finally, observe that the composite

$$\prod_{w\in \mathsf{B}(S\sqcup S')} \Omega\Sigma w(\mathbb{S}_i, \mathbb{S}_{i'} \wedge \Omega M) \xrightarrow[\sim]{hm_S} Z_S \xrightarrow{\mu_S} \Omega(M \vee \mathbb{S}_S)$$

is given by $\mu_S \circ hm_S = \prod \widetilde{w}(\mu_S \circ x_{\mathbb{S}^{d-2}_i}, \mu_S \circ x_{\mathbb{S}^{d-2}_{i'} \wedge \Omega M})$.

Unravelling the definitions, this is the pointwise product of multiplicative extensions of Samelson products of the maps

$$\begin{aligned} \mu_S \circ x_{\mathbb{S}_i^{d-2}} &\equiv \quad \mathbb{S}_i^{d-2} \xrightarrow{\quad \eta_{\mathbb{S}_i} \quad} \Omega\mathbb{S}_i \xrightarrow{\quad \widetilde{x_{\mathbb{S}_S^{d-2}}} \quad} \Omega(M \vee \mathbb{S}_S), \\ \mu_S \circ x_{\mathbb{S}_{i'}^{d-2} \wedge \Omega M} &\equiv \quad \mathbb{S}_{i'}^{d-2} \wedge \Omega M \xrightarrow{\eta_{\mathbb{S}_{i'}} \wedge \Omega M} \Omega(\mathbb{S}_{i'} \wedge \Omega M) \xrightarrow{\quad [x_{\mathbb{S}_S^{d-2}}, \widetilde{\Omega\iota_M}] \quad} \Omega(M \vee \mathbb{S}_S). \end{aligned} \tag{5.5}$$

We denote the first composite simply by

$$x_i \colon \mathbb{S}_i^{d-2} \to \Omega(M \vee \mathbb{S}_S),$$

as the set S should be clear from the context. Its value at $\vec{t} \in \mathbb{S}^{d-2}$ is the loop $\eta_{\mathbb{S}_i}(\vec{t}) \subseteq \mathbb{S}_i \subseteq M \vee \mathbb{S}_S$, as depicted in Figure 10 for $d = 3$.

The lower composite in (5.5) sends $\vec{t} \wedge \gamma \in \mathbb{S}_{i'}^{d-2} \wedge \Omega M$ to the loop in $M \vee \mathbb{S}_S$ which is the commutator of the loops $x_i(\vec{t})$ and $\iota_M\gamma \colon \mathbb{S}^1 \to M \hookrightarrow M \vee \mathbb{S}_S$. This is precisely the Samelson product

$$[x_i, \Omega\iota_M] \colon \mathbb{S}_i^{d-2} \to \Omega(M \vee \mathbb{S}_S).$$

Theorem 5.4. *For each $n \geq 2$ there is a weak equivalence*

$$\prod_{w \in \mathsf{N}'\mathsf{B}(\underline{n-1})} \Omega\Sigma^{1+l_w(d-2)}(\Omega M)^{\wedge l'_w} \xrightarrow[\sim]{\mu \circ hm} \operatorname{tofib}\big(\Omega(M \vee \mathbb{S}_\bullet), \Omega\mathsf{col}\big), \tag{5.6}$$

where $\mathsf{N}'\mathsf{B}(\underline{n-1})$ denotes the sub-basis of $\mathsf{B}(\underline{n-1} \cup \underline{n-1}')$ consisting precisely of those words in which for every $i \in \underline{n-1}$ at least one of the letters x^i or $x^{i'}$ appears. Therefore,

$$\mathsf{F}_n(M) \simeq \prod_{w \in \mathsf{N}'\mathsf{B}(\underline{n-1})} \Omega^n\Sigma^{1+(d-2)l_w}(\Omega M)^{\wedge l'_w}.$$

Proof. From the naturality of equivalences (5.3) and (5.4) it follows that there is an equivalence of contravariant $(n-1)$-cubes

$$\Big(\Omega M \times \prod_{w \in \mathsf{B}(S \sqcup S')} \Omega\Sigma^{1+l_w(d-2)}(\Omega M)^{\wedge l'_w},\ \mathsf{proj}_S^k\Big) \xrightarrow{\Omega\iota_M \times \mu \circ hm} \Big(\Omega\big(M \vee \mathbb{S}_S\big),\ \Omega\mathsf{col}_S^k\Big).$$

We will show that the total homotopy fibre of the first cube is the desired product over $\mathsf{N}'\mathsf{B}(\underline{n-1})$.

The map proj_S^k for $k \in S$ is a projection onto the factors corresponding to those words $w \in \mathsf{B}(S \sqcup S')$ which also belong to $\mathsf{B}((S \setminus k) \sqcup (S \setminus k)')$. These are precisely the words in which neither x^k nor $x^{k'}$ appears. Now, one clearly has $\operatorname{hofib}(\mathsf{proj}_{01}^1 \colon A_0 \times A_{01} \to A_0) \simeq A_{01}$ and more generally:

$$\operatorname*{tofib}_{S \subseteq \underline{n-1}} \Big(A_0 \times \prod_{T \subseteq S} A_T, \mathsf{proj}\Big) \simeq A_{\underline{n-1}}.$$

This follows by induction from the iterative description of total fibres, see [MV15, Ex. 5.5.5].

Therefore, the total homotopy fibre of the first cube is precisely the factor of the space at the vertex $\underline{n-1}$ which is indexed by the words in which for each $i \in \underline{n-1}$ at least one of x^i, $x^{i'}$ appears. □

In Section 5.1 we will now compute the lowest non-vanishing homotopy group of $\mathsf{F}_n(M)$ and describe its generators as maps to $\operatorname{tofib}\Omega(M \vee \mathbb{S}_\bullet)$. Then in Section 5.2 we will discuss transforming this into direct maps to $\mathsf{F}_n(M)$ and in Section 5.3 we will present a strategy how to avoid this. This will be used in Section 6 for the main proofs. We end this section with some examples in 5.3.1.

5.1 The first non-trivial homotopy group

In Section 2.1 we defined the group $\mathsf{Lie}_{\pi_1(M)}(n-1)$ generated by decorated trees $\Gamma^{g_{\underline{n-1}}} \in \mathrm{Tree}_{\pi_1 M}(n-1)$, which are pairs $(\Gamma, g_{\underline{n-1}})$ of an undecorated tree $\Gamma \in \mathrm{Tree}(n-1)$ and a tuple of decorations $g_i \in \pi_1 M$ with $i \in \underline{n-1}$. In view of Corollary 5.2 we can restate Theorem C as follows.

Theorem 5.5. *For each $n \geq 2$ the space $\mathrm{tofib}\,\Omega(M \vee \mathbb{S}_\bullet)$ is $((n-1)(d-2)-1)$-connected and the first non-trivial homotopy group admits an isomorphism*

$$\mathsf{Lie}_{\pi_1 M}(n-1) \xrightarrow[\cong]{W} \pi_{(n-1)(d-2)}\,\mathrm{tofib}\,\Omega(M \vee \mathbb{S}_\bullet),$$

where W maps a decorated tree $\Gamma^{g_{\underline{n-1}}}$ to the homotopy class $\Gamma\big(x_i^{g_i}\big)$ of the canonical extension to the total fibre of the Samelson product

$$\Gamma\big(x_i^{\gamma_i}\big)\colon\ \mathbb{S}^{(n-1)(d-2)} \longrightarrow \Omega(M \vee \mathbb{S}_{\underline{n-1}}). \tag{5.7}$$

Remark 5.6. *Some explanations are in order. The map x_i was introduced in (5.5). For $\gamma_i \in \Omega M$ we denote $\gamma_i\colon\ \mathbb{S}^0 \xrightarrow{\gamma_i} \Omega M \xrightarrow{\Omega\iota_M} \Omega(M \vee \mathbb{S}_{\underline{n-1}})$ abusing the notation. The map $x_i^{\gamma_i}\colon \mathbb{S}_i^{d-2} \to \Omega(M \vee \mathbb{S}_{\underline{n-1}})$ is defined as the pointwise conjugate (see Appendix A)*

$$\vec{t} \mapsto x_i^{\gamma_i}(\vec{t}) := \gamma_i \cdot x_i(\vec{t}) \cdot \gamma_i^{-1}. \tag{5.8}$$

If $g_i := [\gamma_i] \in \pi_1 M$, let $x_i^{g_i}$ be the homotopy class of $x_i^{\gamma_i}$ (for $g_i = 1$ this is just the class of x_i). Finally, for $\Gamma \in \mathrm{Tree}(n-1)$ the Samelson product (5.7) is defined in (A.8).

Since $\Sigma^k X$ is $(k-1)$-connected for any X, it follows from Theorem 5.4 that $\mathrm{tofib}(M \vee \mathbb{S}_\bullet)$ is $((n-1)(d-2)-1)$-connected. By (5.1) forg_* is injective, so the first non-trivial homotopy group is a subgroup

$$\mathsf{forg}_*\colon \pi_{(n-1)(d-2)}\,\mathrm{tofib}\,\Omega(M \vee \mathbb{S}_\bullet) \hookrightarrow \pi_{(n-1)(d-2)}\Omega(M \vee \mathbb{S}_{\underline{n-1}}).$$

Proposition 5.7. *The group $\mathrm{im}(\mathsf{forg}_*)$ is the free abelian group on the set*

$$\Big\{w(x_i, [x_i, g_i]) \ :\ w(x^i, x^{i'}) \in \mathsf{N'B}(\underline{n-1}),\ l_w = n-1,\ g_i \in \pi_1 M \setminus \{1\}\Big\}$$

where $[x_i, g_i]$ is the homotopy class of the Samelson product of x_i and $\gamma_i\colon \mathbb{S}^0 \to \Omega(M \vee \mathbb{S}_{\underline{n-1}})$.

Proof. Using (5.3) and (5.4), and the proof of Theorem 5.4 we see

$$\mathrm{im}(\mathsf{forg}_*) \cong \bigoplus_{w \in \mathsf{N'B}(\underline{n-1})} \pi_{(n-1)(d-2)}\Omega\Sigma^{1+l_w(d-2)}(\Omega M)^{l'_w}$$

The groups $\pi_{1+(n-1)(d-2)}\big(\Sigma^{1+l_w(d-2)}(\Omega M)^{\wedge l'_w}\big)$ are trivial if $l_w > n-1$, so let $l_w = n-1$.

For $k \geq 2$ and a space X the Hurewicz theorem gives $\pi_k(\Sigma^k X) \cong H_k(\Sigma^k X) \cong \widetilde{H}_0(X) \cong \mathbb{Z}[\pi_0(X) \setminus \{*\}]$, the free abelian group on the set of non-basepoint components of X; if X is connected, $\mathbb{Z}[\emptyset] = \{0\}$ by convention. Hence, $\pi_k(\Sigma^k X)$ is generated by k-fold suspensions of non-trivial based maps $\mathbb{S}^0 \to X$. In our case

$$\pi_0\big((\Omega M)^{\wedge l'_w}\big) \setminus \{*\} = \big(\pi_0(\Omega M) \setminus \{*\}\big)^{l'_w} = \big(\pi_1 M \setminus \{1\}\big)^{l'_w}.$$

If $l'_w = 0$, this equals $\{1\}$ for any M (since $(\Omega M)^{\wedge 0} = \mathbb{S}^0$ is the unit of the smash product).

Thus, $\pi_{1+(n-1)(d-2)}\big(\Sigma^{1+(n-1)(d-2)}(\Omega M)^{\wedge l'_w}\big)$ is isomorphic to $\mathbb{Z}[\big(\pi_1 M \setminus \{1\}\big)^{l'_w}]$ and a generating map orresponding to a tuple $(g_1, \dots, g_{l'_w})$ is the iterated suspension $q_\gamma := \Sigma^{1+(n-1)(d-2)}(\wedge\gamma_i)$ of the map $\wedge\gamma_i\colon \mathbb{S}^0 = (\mathbb{S}^0)^{\wedge n-1} \to w(\mathbb{S}^0, \Omega M) = (\Omega M)^{\wedge l'_w}$. This is obtained by smashing together $\mathrm{Id}\colon \mathbb{S}^0 \to \mathbb{S}^0$ for each x^i and a representative $\gamma_i\colon \mathbb{S}^0 \to \Omega M$ of the class $g_i \neq 1$, for each $x^{i'}$.

Thus, there is an isomorphism $\mathrm{im}(\mathsf{forg}_*) \cong \bigoplus_{w\in \mathsf{N'B}(\underline{n-1}), l_w=n-1} \mathbb{Z}[(\pi_1 M\setminus\{1\})^{l'_w}]$, and using the description of $\mu_{\underline{n-1}}\circ hm_{\underline{n-1}}$ from (5.5), the generating maps are of the shape

$$\mathbb{S}^{(n-1)(d-2)} \xrightarrow{\widehat{q}_\gamma} \Omega\Sigma w(\mathbb{S}_i, \mathbb{S}_{i'}\wedge\Omega M) \xrightarrow{\widetilde{w}(x_i,[x_i,\Omega\iota_M])} \Omega(M\vee\mathbb{S}_{\underline{n-1}}) \tag{5.9}$$

where $\widehat{q}_\gamma$ is the adjoint of q_γ. It remains to prove that this composite agrees with $w(x_i,[x_i,\gamma_i])$. This is the content of the following lemma. □

Lemma 5.8. *The map $\widetilde{w}(x_i,[x_i,\Omega\iota_M])\circ\widehat{q}_\gamma$ agrees with the Samelson product $w(x_i,[x_i,\gamma_i])$.*

For example, for $l'_w=0$ we have the word $w(x^i)$, and the map $\widehat{q}_\gamma=\eta\colon \mathbb{S}^{(n-1)(d-2)}\to\Omega\Sigma\mathbb{S}^{(n-1)(d-2)}$ is simply the loop-suspension adjunction unit, so $\widetilde{w}(x_i,[x_i,\Omega\iota_M])\circ\widehat{q}_\gamma = w(x_i)$ by definition.

Proof. For $\vec{t}_i\in\mathbb{S}^{d-2}_i$ and $\wedge\vec{t}_i\in w(\mathbb{S}^{d-2},\mathbb{S}^{d-2})\cong\mathbb{S}^{(n-1)(d-2)}$ the definition of the previous proof is

$$\widehat{q}_\gamma(\wedge\vec{t}_i) \;=\; \theta\mapsto\theta\wedge q_\gamma(\wedge\vec{t}_i) \;=\; \theta\mapsto\theta\wedge\bigwedge\vec{t}_i\wedge\gamma_i \quad\in\Omega\Sigma w(\mathbb{S}_i,\mathbb{S}_{i'}\wedge\Omega M).$$

Recall that for $i\in\underline{n-1}$ we have $\gamma_i=\mathrm{Id}$ so $\vec{t}_i\wedge\gamma_i=\vec{t}_i$. Moreover, $\widetilde{w}(\theta\mapsto\theta\wedge y):=\theta\mapsto w(y)(\theta)$ by definition of a multiplicative extension in (A.6). Therefore,

$$\widetilde{w}(x_i,[x_i,\Omega\iota_M])\Big(\widehat{q}_\gamma(\wedge\vec{t}_i)\Big)=\theta\mapsto w\big(x_i,[x_i,\Omega\iota_M]\big)\Big(\bigwedge\vec{t}_i\wedge\gamma_i\Big)(\theta) \;=\; w\big(x_i(\vec{t}_i),[x_i(\vec{t}_i),\gamma_i]\big)(\theta).$$

By the definition of the Samelson product, this loop in $M\vee\mathbb{S}_{\underline{n-1}}$ is the commutator of the loops $x_i(\vec{t}_i)$ and $[x_i,\Omega\iota_M](\vec{t}_i\wedge\gamma_i)=[x_i(\vec{t}_i),\Omega\iota_M\gamma_i]$, but we have denoted $\Omega\iota_M\gamma_i$ simply by γ_i. □

Therefore, the desired group $\pi_{(n-1)(d-2)}\,\mathrm{tofib}\,\Omega\big(M\vee\mathbb{S}_\bullet\big)$ is generated by the homotopy classes of the canonical extensions to the total fibre of maps $w(x_i,[x_i,\gamma_i])$, for $w\in\mathsf{N'B}(\underline{n-1})$ and non-trivial $\gamma_i\in\Omega M$. The extension is obtained by null-homotoping the image of this map in all other vertices.

Note that for the Samelson product $w(x_i,[x_i,\gamma_i])\colon w(\mathbb{S}^{d-2},\mathbb{S}^{d-2})\to\Omega(M\vee\mathbb{S}_{\underline{n-1}})$ to be defined on a sphere we need to precompose it by a homeomorphism $\vartheta_w\colon\mathbb{S}^{(n-1)(d-2)}\to w(\mathbb{S}^{d-2},\mathbb{S}^{d-2})$. This is explained in Appendix A.

Proof of Theorem C. As in the statement of the theorem, for $\Gamma^{g_{\underline{n-1}}}\in\mathsf{Lie}_{\pi_1 M}(n-1)$ with $g_i=[\gamma_1]$ we define $W(\Gamma^{g_{\underline{n-1}}})$ as the canonical extension to the total fibre of the Samelson product

$$\Gamma(x_i^{\gamma_i})\colon\mathbb{S}^{(n-1)(d-2)}\to w(\mathbb{S}^{d-2})\to\Omega M_{\underline{n-1}}.$$

We then linearly extend to $\mathbb{Z}[\mathrm{Tree}_{\pi_1 M}(n-1)]$. Thanks to the graded antisymmetry and Jacobi relations for Samelson products this vanishes on the relations AS, IHX – the check is the same as in the proof of Lemma 2.3. Hence, we get a well-defined map of abelian groups

$$W\colon\ \mathsf{Lie}_{\pi_1 M}(n-1)\to\pi_{(n-1)(d-2)}\,\mathrm{tofib}\,\Omega(M\vee\mathbb{S}_{\underline{n-1}}).$$

To prove that this is surjective, we check that any $w(x_i,[x_i,g_i])$ is in the image. Let us define $S'_w:=\{i\in\underline{n-1} : x^{i'} \text{ appears in } w\}$ and S_w similarly, so that $S_w\sqcup S'_w=\underline{n-1}$, since letters in w do not repeat. Using the identity

$$[x_i,g_i]=x_i-x_i^{g_i}\quad\in\pi_{d-2}\Omega(M\vee\mathbb{S}_{n-1}).$$

from (A.3) and the linearity of the Samelson bracket, we can expand $w(x_i,[x_i,g_i])=w(x_i,x_i-x_i^{g_i})$ as the sum of elements $(-1)^{|\sigma|}w^\sigma(x_i,x_i^{g_i})$ for $\sigma\subseteq S'_w$, where w^σ is obtained from w by replacing $x^{i'}$ with x^i if $i'\in\sigma$.

But now observe that since $w^{S'_w}$ has no primes left, we have $w^{S'_w}(x^i)\in\mathsf{Lie}_d(n-1)$, the group of Lie words of length $n-1$ in which each letter has degree $d-2$ and appears exactly once.

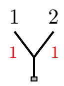
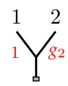
By Lemma 2.3 there is an isomorphism $\omega_d\colon \mathsf{Lie}(S) \to \mathsf{Lie}_d(S)$, so let $\Gamma := \omega_d^{-1}(w^{S'_w})$. Then by Lemma A.5 we have $w^{S'_w}(x_i, x_i^{g_i}) = w^{S'_w}(x_i) \simeq \Gamma(x_i)$. More generally

$$w^\sigma(x_i, x_i^{g_i}) = \Gamma(x_i^{g_i^\sigma})$$

where $g_i^\sigma = g_i$ for $i \in S'_w \setminus \sigma$ and otherwise $g_i = 1$. Therefore, W is indeed surjective:

$$w(x_i, [x_i, g_i]) = \sum_{\sigma \subseteq S'_w} (-1)^{|\sigma|} w^\sigma(x_i, x_i^{g_i}) = \sum_{\sigma \subseteq S'_w} (-1)^{|\sigma|} \Gamma(x_i^{g_i^\sigma}) = W\Big(\sum_{\sigma \subseteq S'_w} \Gamma^{g^\sigma_{\underline{n-1}}}\Big).$$

Lastly, define $W^{-1}\colon \pi_{(n-1)(d-2)}\,\mathrm{tofib}\,\Omega\big(M \vee \mathbb{S}_\bullet\big) \to \mathsf{Lie}_{\pi_1 M}(n-1)$ by $W^{-1}(w^\sigma(x_i, x_i^{g_i})) := \Gamma^{g^\sigma_{\underline{n-1}}}$ for $\Gamma \in \mathsf{NB}(\underline{n-1}) \subseteq \mathsf{Lie}(n-1)$ and extending linearly, then composing with the projection to $\mathsf{Lie}_{\pi_1 M}(n-1)$. This is well-defined, since ω_d^{-1} is an isomorphism. For example,

$W^{-1}[[x_2, g_2], x_1] = W^{-1}\big([x_2, x_1] - [x_2^{g_2}, x_1]\big) = (-1)^{d-2}$  $- (-1)^{d-2}$  $\in \mathsf{Lie}_{\pi_1 M}(2).$

Finally, we have $W \circ W^{-1} = \mathrm{Id}$ and $W^{-1} \circ W = \mathrm{Id}$ by construction. □

5.2 The generating maps

At this point it is not clear what the generating maps $\mathbb{S}^{(n-1)(d-3)} \to \mathsf{F}_n(M)$ are, since to explicitly find the inverse of the isomorphism $(\mathsf{retr} \circ \mathcal{D} \circ \chi)_*\colon \pi_{(n-1)(d-3)}\mathsf{F}_n(M) \to \pi_{(n-1)(d-2)}\,\mathrm{tofib}\,\Omega(M \vee \mathbb{S}_\bullet)$, for the equivalences retr, $\mathcal{D}$ and χ from Corollary 5.2.

5.2.1 The retraction. At least for $\mathsf{retr}\colon \mathrm{tofib}\,\Omega M_\bullet \to \mathrm{tofib}\,\Omega(M \vee \mathbb{S}_\bullet)$ this is not hard to do. Firstly, we can pick an explicit lift $m_i\colon \mathbb{S}^{d-2} \to \Omega M_{\underline{n-1}}$ of the map $x_i\colon \mathbb{S}^{d-2} \to \Omega(M \vee \mathbb{S}_{\underline{n-1}})$: namely, the $(d-2)$-parameter 'swing of a lasso' around the d-ball $\mathbb{B}_i \subseteq M$. See Figure 11 for $d = 3$. Indeed, using the definition of retr in Lemma 5.1 this family og loops covers the 2-sphere $\mathbb{S}_1$ exactly once, so we have $\mathsf{retr} \circ m_i \simeq x_i$. Compare with Figure 10.

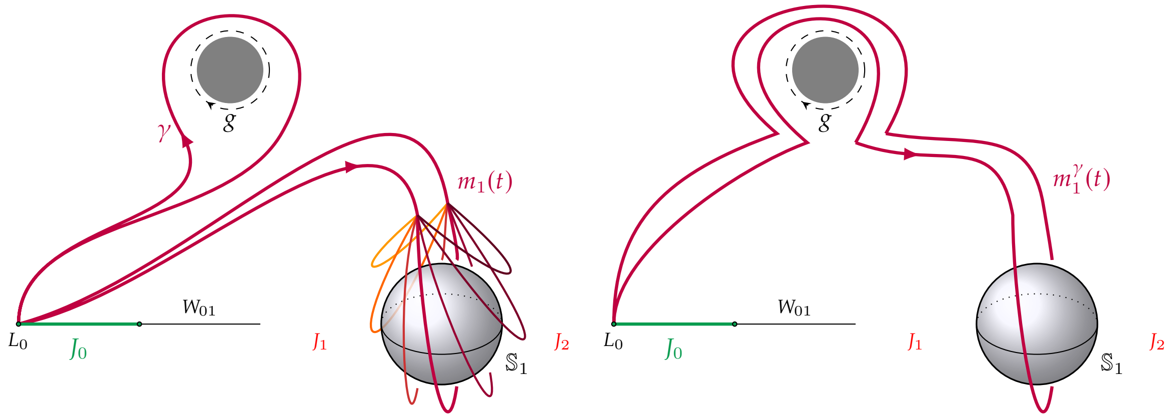


Figure 11. Both pictures show a part of a 3-manifold M with the basepoint L_0. *Left*: A representative γ of $1 \neq g \in \pi_1(M)$ is depicted as a loop around the grey 'hole in M', and the 1-parameter family $m_1(t) \in \Omega M_1$ for several $t \in \mathbb{S}^1$ is depicted by a gradient of colours. *Right*: One value $m_1^\gamma(t) = \gamma m_1(t)\gamma^{-1} \in \Omega M_1$.

The map $m_i^{-1}\colon \mathbb{S}^{d-2} \to \Omega M_{\underline{n-1}}$ is obtained by reversing orientations of all loops in the family, and this is equivalent to performing a twist as in Figure 12. Moreover, any $g_i \in \pi_1 M$ can be realised by a loop γ_i in M that misses all balls $\mathbb{B}_1, \dots, \mathbb{B}_{n-1}$, so defines $\gamma_i\colon \mathbb{S}^0 \to \Omega M_{\underline{n-1}}$. Thus, we can define $m_i^{\varepsilon_i\gamma_i}\colon \mathbb{S}^{d-2} \to \Omega M_{\underline{n-1}}$ as the pointwise conjugate of $m_i^{\varepsilon_i}$ by γ_i.

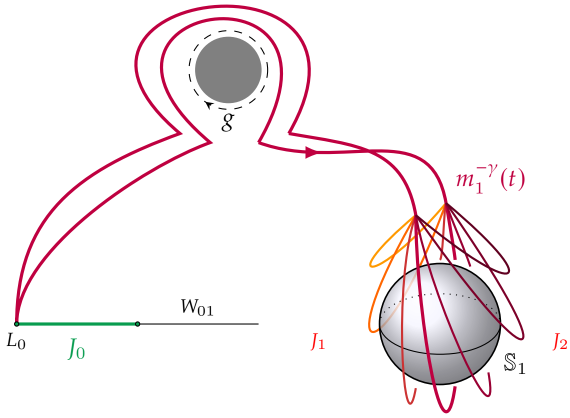


Figure 12. The family $m_1^{-\gamma}\colon \mathbb{S}^1 \to \Omega M_1$.

Finally, as the target is a loop space, we have Samelson products

$$\Gamma(m_i^{\gamma_i})\colon \mathbb{S}^{(n-1)(d-2)} \longrightarrow \Omega M_{\underline{n-1}} \tag{5.10}$$

See Figure 13 for $n = 3$. Since $\mathsf{forg}_*\colon \pi_{(n-1)(d-2)}\,\mathrm{tofib}\,\Omega M_\bullet \longrightarrow \pi_{(n-1)(d-2)}\Omega M_{\underline{n-1}}$ is also injective, the generators of the first group are represented by the extensions of the maps (5.10) to the total fibre using the canonical null-homotopies of m_i – by 'pulling up' through the ball $\mathbb{B}_i$.

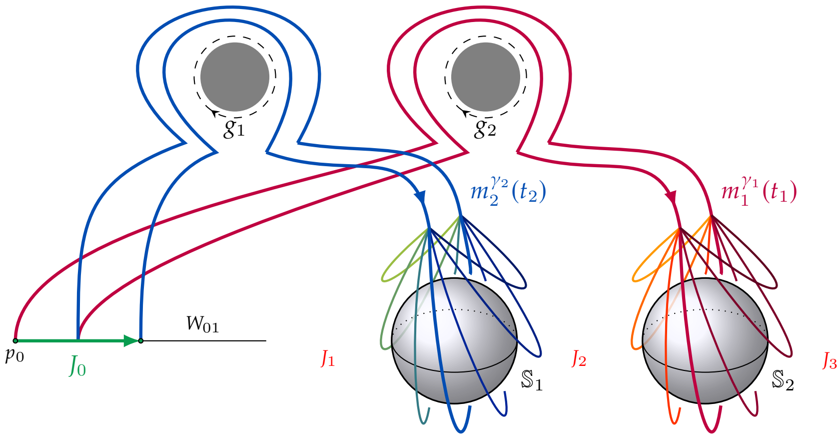


Figure 13. The value of $\overset{2\;\;1}{\curlyvee}(m_1^{\gamma_1}, m_2^{\gamma_2}) = [m_1^{\gamma_1}, m_2^{\gamma_2}]\colon \mathbb{S}^2 \to \Omega M_{12}$ at $(t_1, t_2) \in \mathbb{S}^1 \wedge \mathbb{S}^1 = \mathbb{S}^2$ is the commutator of the depicted loops $m_1^{\gamma_1}(t_1)$ and $m_2^{\gamma_2}(t_2)$.

5.2.2 The derivative. Consider now $\mathcal{D}_{\underline{n-1}}\colon \mathscr{F}^n_{\underline{n-1}} \longrightarrow \Omega M_{\underline{n-1}}$ which closes up $J_0 \hookrightarrow M_{\underline{n-1}}$ into a loop based at p_0 (the tangent vector is actually forgotten, see Remark 4.13). There is an obvious lift $\varphi_i\colon \mathbb{S}^{d-2} \longrightarrow \mathscr{F}^n_{\underline{n-1}}$ of m_i by ensuring that each loop $m_i(\vec{t}) \in \Omega M_{\underline{n-1}}$ is embedded and changing it to an arc from L_0 to R_0.

We can also ensure that different φ_i for $i \in \underline{n-1}$ are mutually disjoint. Furthermore, γ_i can be chosen to be embedded in $M_{\underline{n-1}}$, so we may define $\varphi_i^{\gamma_i}\colon \mathbb{S}^{d-2} \longrightarrow \mathscr{F}^n_{\underline{n-1}}$ as an *embedded conjugate*, by slightly pushing copies of γ_i off of each other. See Figure 14 for $d = 3$.

Similarly, we need to define Samelson products $\Gamma(\varphi_i^{\gamma_i})$ using an *embedded analogue of commutators*. This is not immediate: the problem is that $\mathscr{F}^n_{\underline{n-1}}$ is not an H-space in an obvious way, as concatenation of arcs $J_0 \hookrightarrow M_{\underline{n-1}}$ might result in a non-embedded arc. If this has been done, the generators of $\pi_{(n-1)(d-2)}\,\mathrm{tofib}(\mathscr{F}^n_\bullet, l)$ would be canonical extensions of $\Gamma(\varphi_i^{\gamma_i})$, again by (5.1).

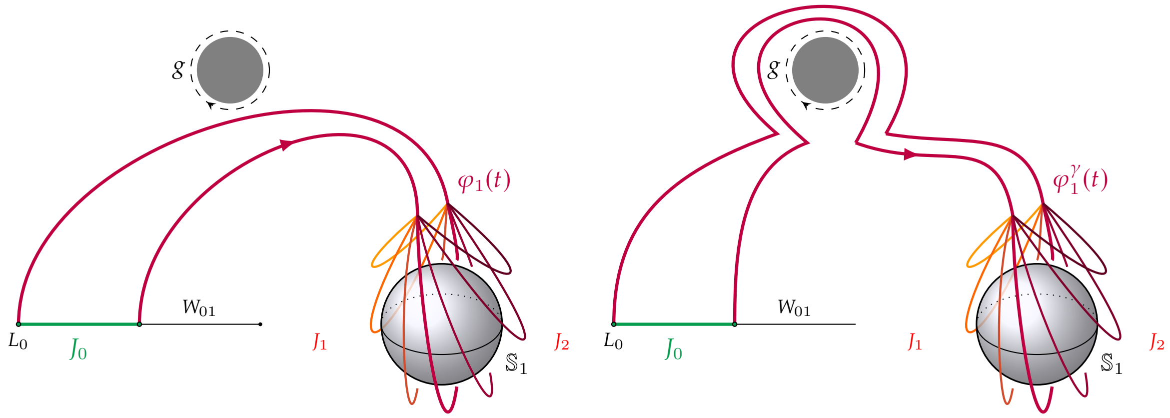


Figure 14. The 1-parameter families of arcs $\varphi_1(t) \in \mathscr{F}_1^2$ and $\varphi_1^\gamma(t) \in \mathscr{F}_1^2$ for several values of $t \in \mathbb{S}^1$.

5.2.3 The delooping map. If such embedded commutators had been constructed, then the map $\chi^{-1}\colon \Omega^{n-1}\,\mathrm{tofib}(\mathscr{F}^n_\bullet, l) \to \mathrm{tofib}(\mathscr{F}^n_\bullet, r)$ would be very easy: it is given as the composition of the map forg which forgets all null-homotopies, and the inclusion $\Omega^{n-1}\mathscr{F}^n_{\underline{n-1}} \hookrightarrow \mathrm{tofib}(\mathscr{F}^n_\bullet, r)$.

We do not, however, pursue defining those embedded commutators directly, since we will not need them: for $d = 3$ we will in Section 8 directly construct points $\psi(\mathbf{G}) \in \mathsf{H}_n(M)$ using *gropes* – which can indeed be seen as embedded commutators, see Remark 7.11 – and then prove that $\chi\mathsf{e}_n(\psi(\mathbf{G}))\colon \mathbb{S}^{(n-1)(d-2)} \to \mathrm{tofib}(\mathscr{F}^n_\bullet, l)$ are precisely the generators.

We will using the following simplification.

5.3 The strategy

Suppose that for a given map $f\colon \mathbb{S}^{(n-1)(d-3)} \to \mathsf{F}_n(M)$ we want to prove that its homotopy class corresponds to a class $\varepsilon\Gamma^{g_{\underline{n-1}}} \in \mathsf{Lie}_{\pi_1 M}(n-1)$ for $\varepsilon \in \{\pm 1\}$ under the isomorphism

$$W^{-1}(\mathsf{retr}\mathscr{D}\chi)_*\colon \pi_{(n-1)(d-3)}\mathsf{F}_n(M) \to \mathsf{Lie}_{\pi_1 M}(n-1)$$

from Theorem C. By the preceding discussion in Section 5.2, this is equivalent to considering the composite

$$\mathscr{D}\chi(f)\colon\ \mathbb{S}^{(n-1)(d-3)} \to \Omega^{n-1}\,\mathrm{tofib}\,\Omega M_\bullet$$

and checking that the homotopy class of its adjoint $\mathbb{S}^{(n-1)(d-2)} \to \mathrm{tofib}\,\Omega(M_\bullet)$ is the class of the canonical extension of $\varepsilon\Gamma(m_i^{g_i})$.

Actually, we saw that is instead enough to simply check this for the initial vertex[26]

$$\mathscr{D}_{\underline{n-1}}\,(\chi f)^{\underline{n-1}} \ \simeq\ \varepsilon\Gamma(m_i^{\gamma_i}):\quad \mathbb{S}^{(n-1)(d-2)} \to \Omega M_{\underline{n-1}}$$

We now claim $\varepsilon\Gamma(m_i^{\gamma_i}) \simeq \Gamma(m_i^{\varepsilon_i\gamma_i})$, for any tuple $\varepsilon_i \in \{\pm 1\}$ such that $\prod_{i=1}^{n-1} \varepsilon_i = \varepsilon$. Namely, define

$$m_i^{\varepsilon_i\gamma_i}(\vec{t}) := \gamma_i \cdot m_i(\vec{t})^{\varepsilon_i} \cdot \gamma_i^{-1},$$

where $m_i(\vec{t})^{-1}$ is the inverse of the loop $m_i(\vec{t}) \in \Omega M_{\underline{n-1}}$. Then $m_i^{\varepsilon_i\gamma_i} \simeq \varepsilon_i m_i^{\gamma_i}$ are homotopic maps by the Eckmann–Hilton argument, and $\Gamma(m_i^{\varepsilon_i\gamma_i}) \simeq \varepsilon\Gamma(m_i^{\gamma_i})$ by the bilinearity of Samelson products. See Appendix A for details.

[26] Recall that $\mathsf{forg}\mathscr{D}\chi(f) = (\mathscr{D}\chi f)^{\underline{n-1}} = \mathscr{D}_{\underline{n-1}}\,(\chi f)^{\underline{n-1}}$.

To prove Theorem E in Section 9 we will exactly show that for the point $f_{\mathbf{G}} = \mathsf{e}_n(\psi(\mathbf{G})) \in \mathsf{F}_n(M)$ coming from a thick grope $\mathbf{G}\colon \mathsf{B}_\Gamma \to M$ on U with the signed decoration $(\varepsilon_i, \gamma_i)_{\underline{n-1}}$ we have

$$\mathscr{D}_{\underline{n-1}}\left(\chi f_{\mathbf{G}}\right)^{\underline{n-1}} \simeq \Gamma(m_i^{\varepsilon_i\gamma_i}): \quad \mathbb{S}^{(n-1)(d-2)} \to \Omega M_{\underline{n-1}} \tag{5.11}$$

where $d = 3$. The proof will be based on the fact that both $\psi(\mathbf{G})$ and Samelson products are constructed inductively. For the former see Section 8 and for the latter see Lemma A.5.

Furthermore, for the proof of Theorem F we will use that $\sum_{l=1}^N \varepsilon_l \Gamma_l^{g^l_{\underline{n-1}}}$ is represented by the following pointwise product – again by the Eckmann–Hilton argument:

$$\prod_{1\leq i\leq N} \Gamma_l(m_i^{\varepsilon_i^l\gamma_i^l})\colon\ \mathbb{S}^{(n-1)(d-2)} \to \Omega M_{\underline{n-1}}, \quad \vec{t} \mapsto \Gamma_1(m_i^{\varepsilon_i^1\gamma_i^1})(\vec{t})\cdots\Gamma_N(m_i^{\varepsilon_i^N\gamma_i^N})(\vec{t}).$$

5.3.1 Examples Let us now illustrate our discussion so far on a couple of examples.

Example 5.9 ($n = 2$). *The punctured cube $\mathcal{E}^2_\bullet$ computing $\mathsf{P}_2(M)$ was displayed in Example 3.1. On one hand, $\mathsf{F}_2(M) \simeq \mathrm{tofib}(\mathscr{F}^2_S)$ is the total homotopy fibre of the top square:*

$$\begin{tikzcd}
& \mathscr{F}^2_1 \arrow[r, dashed] & \mathcal{E}\mathrm{mb}_\partial(I\setminus J_{12}, M) \arrow[rr, "r^0_1"] & & \mathcal{E}\mathrm{mb}_\partial(I\setminus J_{012}, M) \\
\mathscr{F}^2_\emptyset \arrow[r, dashed] & \mathcal{E}\mathrm{mb}_\partial(I\setminus J_2, M) \arrow[ur, "r^1_2"] \arrow[rr, "r^0_\emptyset"] & & \mathcal{E}\mathrm{mb}_\partial(I\setminus J_{02}, M) \arrow[ur, "r^1_{02}"'] &
\end{tikzcd}$$

On the other hand, if we complete $\mathcal{E}^2_\bullet$ with the initial vertex $\mathcal{K}(M) := \mathcal{E}\mathrm{mb}_\partial(I, M)$, then $\mathsf{H}_1 \simeq \mathrm{tofib}(\mathscr{F}_S)$ is the total fibre of the bottom square:

$$\begin{tikzcd}
& \mathscr{F}_1 \arrow[r, dashed] & \mathcal{E}\mathrm{mb}_\partial(I\setminus J_1, M) \arrow[rr, "r^0_1"] & & \mathcal{E}\mathrm{mb}_\partial(I\setminus J_{01}, M) \\
\mathscr{F}_\emptyset \arrow[r, dashed] & \mathcal{E}\mathrm{mb}_\partial(I, M) \arrow[ur, "r^1_\emptyset"] \arrow[rr, "r^0_\emptyset"] & & \mathcal{E}\mathrm{mb}_\partial(I\setminus J_0, M) \arrow[ur, "r^1_0"'] &
\end{tikzcd}$$

and the map $\mathsf{e}_2\colon \mathsf{H}_1(M) \to \mathsf{F}_2(M)$ is the obvious upward map (see Section 3.2).

Now by Theorem 4.3, we have

$$\mathsf{F}_2(M) \simeq \mathrm{hofib}\left(r^1_\emptyset\colon \mathscr{F}^2_\emptyset \to \mathscr{F}^2_1\right) \xrightarrow[\sim]{\chi} \Omega\,\mathrm{hofib}\left(l^1_\emptyset\colon \mathscr{F}^2_1 \to \mathscr{F}^2_\emptyset\right)$$

The map $l^1_\emptyset$ corresponds to $\lambda^1_\emptyset\colon M_1 = M\setminus\mathbb{B}_{12} \to M_\emptyset \cong M$ which adds back the ball $\mathbb{B}_{12}$ and rescales using the map drag*, see the proof of Lemma 4.10.*

By Corollary 4.12 the derivative and by Lemma 5.1 the retraction induce the equivalence

$$\xrightarrow[\sim]{\mathscr{D}} \Omega\,\mathrm{hofib}\left(\Omega M_1 \xrightarrow{\Omega\lambda^1_\emptyset} \Omega M_\emptyset\right) \xrightarrow[\sim]{\mathsf{retr}} \Omega\,\mathrm{hofib}\left(\Omega(M\vee\mathbb{S}_1) \xrightarrow{\Omega\mathsf{col}^1_\emptyset} \Omega M\right)$$

Finally, $\mathrm{hofib}(\Omega\mathsf{col}^1_\emptyset) \simeq \Omega(\mathbb{S}_1 \vee (\mathbb{S}_1 \wedge \Omega M))$ *by the Grey-Spencer Lemma 5.3, so we have*

$$\begin{aligned}
\pi_{d-3}\mathsf{F}_2(M) &\cong \pi_{d-2}\,\mathrm{hofib}(l^1_\emptyset) \cong \pi_{d-2}\,\mathrm{hofib}(\Omega\lambda^1_\emptyset) \cong \pi_{d-2}\,\mathrm{hofib}(\Omega\mathsf{col}^1_\emptyset)\\
&\cong \pi_{d-2}\Omega(\mathbb{S}_1\vee(\mathbb{S}_1\wedge\Omega M))) \cong \pi_{d-1}\mathbb{S}^{d-1} \oplus \pi_{d-1}\left(\Sigma^{d-1}\Omega M\right)\\
&\cong \mathbb{Z}\{x_1\} \oplus \bigoplus_{1\neq g\in\pi_1 M} \mathbb{Z}\{[x_1, g_1]\} \xrightarrow{W^{-1}} \mathsf{Lie}_{\pi_1 M}(1) \cong \mathbb{Z}[\pi_1 M]
\end{aligned}$$

using the isomorphism $W^{-1}x_1 = \overset{1}{\lfloor}{}^{1}$, $W^{-1}[x_1, g_1] = W^{-1}x_1 - W^{-1}x_1^{g_1} = \overset{1}{\lfloor}{}^{1} - \overset{1}{\lfloor}{}^{g}$. The generators for $\mathrm{hofib}(\Omega\mathsf{col}^1_\emptyset)$ *are the canonical extensions of x_1 and x_1^g, while for* $\mathrm{hofib}(\Omega\lambda^1_\emptyset)$ *they are the extensions of m_1 and m_1^γ. See Figure 11.*

The generators for $\mathrm{hofib}(l^1_\emptyset)$ *are the extensions of* φ_1 *and* φ_1^γ *(Figure 14). For example, the extension of* $\varphi_1^\gamma\colon \mathbb{S}^{d-2} \to \mathscr{F}^2_1$ *to* $\mathrm{hofib}(l^1_\emptyset)$ *uses the family of obvious null-homotopies of* $l^1_\emptyset(\varphi_1^\gamma)$ *across the* d*-ball* $\mathbb{B}_1$*.* △

Example 5.10 ($n = 3$)**.** *For the punctured 4-cube* $\mathcal{E}^3_\bullet$*, we can draw its top subcube* $\mathcal{E}^3_{\bullet\cup 3}$*:*

$$\begin{tikzcd}
& \mathscr{F}^3_{12} \arrow[rr, dashed] & & \mathcal{E}\mathrm{mb}_\partial(I\setminus J_{123}, M) \arrow[rr] & & \mathcal{E}\mathrm{mb}_\partial(I\setminus J_{0123}, M) \\
\mathscr{F}^3_{2} \arrow[rr, dashed] & & \mathcal{E}\mathrm{mb}_\partial(I\setminus J_{23}, M) \arrow[rr] \arrow[ur] & & \mathcal{E}\mathrm{mb}_\partial(I\setminus J_{023}, M) \arrow[ur] & \\
& \mathscr{F}^3_{1} \arrow[rr, dashed] & & \mathcal{E}\mathrm{mb}_\partial(I\setminus J_{13}, M) \arrow[rr] \arrow[uu] & & \mathcal{E}\mathrm{mb}_\partial(I\setminus J_{013}, M) \arrow[uu] \\
\mathscr{F}^3_{\emptyset} \arrow[rr, dashed] & & \mathcal{E}\mathrm{mb}_\partial(I\setminus J_{3}, M) \arrow[rr] \arrow[uu] \arrow[ur] & & \mathcal{E}\mathrm{mb}_\partial(I\setminus J_{03}, M) \arrow[uu] \arrow[ur] &
\end{tikzcd}$$

where the dashed arrows are fibres. We apply Theorems 4.3 and 4.11 to get homotopy equivalences

$$\mathsf{F}_3(M) = \mathrm{tofib}\left(\begin{tikzcd} \mathscr{F}^3_1 \arrow[r] & \mathscr{F}^3_{12} \\ \mathscr{F}^3_\emptyset \arrow[r] \arrow[u] & \mathscr{F}^3_2 \arrow[u] \end{tikzcd}\right) \xrightarrow{\chi} \Omega^2\,\mathrm{tofib}\left(\begin{tikzcd} \mathscr{F}^3_1 \arrow[d] & \mathscr{F}^3_{12} \arrow[l] \arrow[d] \\ \mathscr{F}^3_\emptyset & \mathscr{F}^3_2 \arrow[l] \end{tikzcd}\right) \xrightarrow{\mathcal{D}} \Omega^2\,\mathrm{tofib}\left(\begin{tikzcd} \Omega M_1 \arrow[d] & \Omega M_{12} \arrow[l] \arrow[d] \\ \Omega M & \Omega M_2 \arrow[l] \end{tikzcd}\right)$$

$$\xrightarrow{\mathsf{retr}} \Omega^2\,\mathrm{tofib}\left(\begin{tikzcd} \Omega(M\vee\mathbb{S}_1) \arrow[d] & \Omega(M\vee\mathbb{S}_1\vee\mathbb{S}_2) \arrow[l] \arrow[d] \\ \Omega M & \Omega(M\vee\mathbb{S}_2) \arrow[l] \end{tikzcd}\right) \simeq \Omega^2 \prod_{w\in\mathsf{N}'\mathsf{B}(\{1,2\})} \Omega\Sigma^{1+l_w(d-2)}(\Omega M)^{\wedge l'_w}$$

Hence, the first non-trivial homotopy group is $\mathsf{Lie}_{\pi_1 M}(2)$ *in degree* $2(d-2)$*, and for the last total fibre in the first row the generating maps are the canonical extensions of the maps*

$$\mathsf{forg}(\mathsf{retr})_*^{-1} W\left(\overset{2\quad 1}{{}_{g_2}\mathsf{Y}_{g_1}}\right) = \overset{2\ \ 1}{\mathsf{Y}}(m_1^{g_1}, m_2^{g_2}) = \left[m_1^{g_1}, m_2^{g_2}\right] \in \pi_2\Omega M_{12}. \tag{5.12}$$

△

Example 5.11 (Sketch of the proof of Theorem E for $n = 3$)**.** *Assume* $\mathcal{T}_2(\mathbf{G}) = \overset{2\quad 1}{{}_{g_2}\mathsf{Y}_{g_1}}$ *for a thick grope* $\mathbf{G}$ *in a* 3*-manifold* M*, using the underling forest map from Proposition 7.16. The construction in Section 8.2 produces the point*

$$\mathsf{e}_3\psi(\mathbf{G}) = \begin{pmatrix} \Psi^{\mathbf{G}}(-)^{\{1\}}_{J_0} & \Psi^{\mathbf{G}}(-)^{\{12\}}_{J_0} \\ \mathbf{G}(a_0^\perp) & \Psi^{\mathbf{G}}(-)^{\{2\}}_{J_0} \end{pmatrix} \in \mathsf{F}_3(M)$$

and so we obtain a class $\mathsf{forg}(\mathcal{D}\chi\mathsf{e}_3\psi(\mathbf{G})) \in \pi_2\Omega M_{12}$*. Then Theorem E asserts that this class agrees with* (5.12)*. One can visualise this by comparing Figure 13 with Figure 20.*

A close look at the definition of χ *implies that* $(\chi\mathsf{e}_3\psi(\mathbf{G}))^{\{12\}}$ *is obtained from the square-family of loops* $\Psi^{\mathbf{G}}(-)^{\{12\}}_{J_0}$ *by 'reflections relative to the balls* $\mathbb{B}_1$ *and* $\mathbb{B}_2$*', see Proposition 6.6.*

In Lemma 9.2 we will show that $\mathcal{D}_{12}\Psi^{\mathbf{G}}(-)^{\{12\}}_{J_0}\colon I^2 \to \mathscr{F}^3_{12} \to \Omega M_{12}$ *is homotopic to the commutator of certain loops corresponding to degree* 1 *gropes out of which* $\mathbf{G}$ *is built (the two caps of* $\mathbf{G}$*). On the other hand, the Samelson product* $[m_1^{\gamma_1}, m_2^{\gamma_2}]\colon \mathbb{S}^2 \to \Omega M_{12}$ *is also defined inductively in terms of commutators. Hence, we will be able finish the proof by induction.* △

6 On left homotopy inverses

In this section we prove Lemmas 4.4 and 4.6, and Propositions 4.8 and 6.6.

Proof of Lemma 4.4. Consider the commutative square

$$\begin{tikzcd} X \arrow[r, "l \circ r"] \arrow[d, equal] & X \\ X \arrow[r, "r"] & Y \arrow[u, "l"'] \end{tikzcd} \tag{6.1}$$

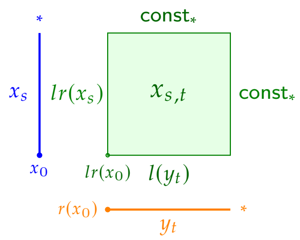
Its total homotopy fibre Z is according to Lemma 3.7 given by

$$\left\{(x_0, x_s, y_t, x_{s,t}) \in X \times \mathscr{P}_*X \times \mathscr{P}_*Y \times X^{I^2} \,\middle|\, x_s : x_0 \rightsquigarrow *, y_t : r(x_0) \rightsquigarrow *, x_{s,t} : lr(x_s) \cdot l(y_t) \rightsquigarrow \mathsf{const}_*\right\}$$

where $\cdot$ is path concatenation and the square $x_{s,t} : I^2 \longrightarrow X$ can be viewed as a path of paths in two different ways, or as a path of loops – from its zero-edges to its one-edges, see the picture in (6.2).

In this description Z can easily be seen as the iterated homotopy fibre in two different ways, that is, in the next diagram all rows and columns are homotopy fibre sequences:

$$\begin{tikzcd} X \times_{l \circ r} \mathscr{P}_*X \arrow[r, dashed] & X \arrow[r, "l \circ r"] & X \\ \mathrm{hofib}(r) \arrow[u, dashed] \arrow[r, dashed] & X \arrow[u, equal] \arrow[r, "r"] & Y \arrow[u, "l"'] \\ Z \arrow[u, dotted, "p_1", "\simeq"'] \arrow[r, dotted, "p_2"] & \mathscr{P}_*X \arrow[u, dashed] \arrow[r, dashed] & \mathrm{hofib}(l) \arrow[u, dashed] \end{tikzcd}$$



(6.2)

The two dotted maps are $p_1(x_0, x_s, y_t, x_{s,t}) = (x_0, y_t)$ and $p_2(x_0, x_s, y_t, x_{s,t}) = (x_0, x_s)$. Since $lr \simeq \mathrm{Id}_X$, the homotopy fibre $\mathrm{hofib}(lr) = X \times_{lr} \mathscr{P}_*X$ is contractible, so p_1 is a weak equivalence. On the other hand, the path space $\mathscr{P}_*X = \mathrm{hofib}(\mathrm{Id}_X)$ is also contractible, so we immediately have

$$\chi^{-1} : \quad \Omega\,\mathrm{hofib}(l) \xrightarrow[\sim]{\delta_z} Z \xrightarrow[\sim]{p_1} \mathrm{hofib}(r).$$

However, we now determine an explicit homotopy inverse χ by finding inverses p_1^{-1} and δ_z^{-1}.

To define p_1^{-1}: $\mathrm{hofib}(r) \longrightarrow Z$ first recall there is a chosen homotopy $h : X \times I \longrightarrow X$ from Id to lr. Thus, for $(x_0, y_t) \in \mathrm{hofib}(r)$ we have a path $h_t(x_0) : x_0 \rightsquigarrow lr(x_0)$, and since $y_0 = r(x_0)$, this can be concatenated with $l(y_t)$. Also, for each $t \in [0,1]$ we have a path $h_s(ly_t) : l(y_t) \rightsquigarrow lrl(y_t)$. We let

$$p_1^{-1}(x_0, y_t) = \Big(\; x_0, \quad h_s(x_0) \cdot l(y_s), \quad y_t, \quad h_s(h_t(x_0)) \widetilde{\boxplus} h_s(ly_t) \Big) \in Z.$$

The square $h_s(h_t(x_0)) \widetilde{\boxplus} h_s(ly_t)$ in X is obtained by identifying the two edges $h_t(x_0) \equiv h_s(x_0)$ of the square $(s,t) \mapsto h_s(h_t(x_0))$ to get a bigon, to which $(s,t) \mapsto h_s(ly_t)$ is glued along the common edge $h_s(lr(x_0))$. We reshape this to a square and see it as a path from $lr\big(h_s(x_0) \cdot l(y_s)\big) \cdot ly_t$ to const_*.

Since clearly $p_1 \circ p_1^{-1} = \mathrm{Id}$ and p_1 is a weak equivalence, p_1^{-1} is a homotopy inverse for p_1 (alternatively, there is a homotopy $p_1^{-1} \circ p_1 \simeq \mathrm{Id}$ by gradually introducing back the coordinate x_s).

The map $\delta_z^{-1} : Z \longrightarrow \Omega\,\mathrm{hofib}(l)$ comes from comparing the bottom raw in the diagram (6.2) to the fibre sequence $\Omega\,\mathrm{hofib}(l) \longrightarrow \mathscr{P}_*\,\mathrm{hofib}(l) \longrightarrow \mathrm{hofib}(l)$. We define it by

$$\delta_z^{-1}(x_0, x_s, y_t, x_{s,t}) = \Big\{\; t \;\mapsto\; \big(r(x_{1-t}) \cdot y_t,\; lr(x_{s \geq t}) \boxplus x_{s,t}\big) \Big\}.$$

where x_{1-t} is the inverse of the path x_t and $x_{s \geq t}$ is the square $(s,t) \mapsto x_{1-t}|_{t \in [0,1-s]}$.

Since $\delta_z^{-1} \circ \delta_z(y_t, x_{s,t}) = (r(\mathsf{const}_*) \cdot y_t, lr(\mathsf{const}_*)_{\leq t} \cdot x_{s,t}) = (y_t, x_{s,t})$, the map δ_z^{-1} is indeed a homotopy inverse for δ_z, by the same argument as above.

Hence, the map $\chi := \delta_Z^{-1} \circ p_1^{-1}\colon\ \mathrm{hofib}(r) \longrightarrow \Omega\,\mathrm{hofib}(l)$ is given by

$$\chi(x_0, y_t) \ = \Big\{\, t \ \mapsto \ \Big(r\Big(h_s(x_0)\cdot l(y_s)\Big)_{s=1-t} \cdot y_t,\quad lr\Big(h_s(x_0)\cdot l(y_s)\Big)_{s\geq t} \boxminus \big(h_s(h_t x_0)\widetilde{\boxminus} h_s(l y_t)\big)\Big)\,\Big\}$$

and is the desired homotopy inverse to χ^{-1}. $\square$

Remark 6.1. *All triangles in the following diagram commute*

$$\begin{tikzcd}
\{t \mapsto y_t\} \in & \Omega Y \arrow[rr, hook, "\delta"] & & \mathrm{hofib}(r) \arrow[d, shift right, red, "p_1^{-1}"'] \arrow[dll, red, "\chi"] & \ni (*, y_t) \\
\{t \mapsto (y_t, x_{s,t})\} \in & \Omega\,\mathrm{hofib}(l) \arrow[u, "\mathsf{forg}"] \arrow[urr, "\chi^{-1}"] \arrow[rr, shift right, "\delta_z"'] & & Z \arrow[u, shift right, "p_1"'] \arrow[ll, shift right, red, "\delta_z^{-1}"'] & \ni (*, \mathsf{const}_*, y_t, x_{s,t})
\end{tikzcd} \tag{6.3}$$

We simplify the expression for χ using the following notation.

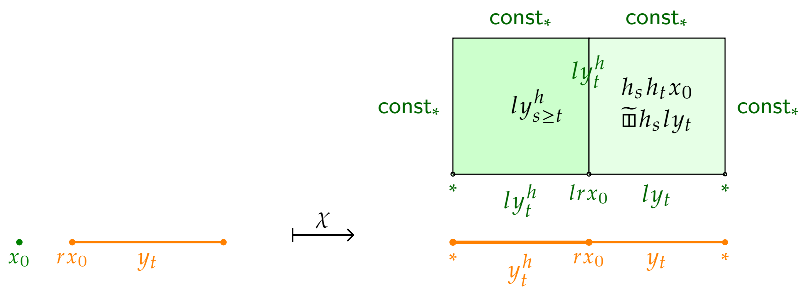
Definition 6.2. *In the situation of the previous proof let us define the h-reflection of y by*

$$y_t^h := r\big(h_s(x_0)\cdot l y_s\big)_{s=1-t}$$

Note that this is a path from $*$ to $rx_0 \in Y$. We now rewrite χ as

$$\chi(x_0, y_t) = \Big(\, y_t^h \cdot y_t,\ l y^h_{s\geq t} \boxminus \big(h_s h_t x_0 \widetilde{\boxminus} h_s l y_t\big)\,\Big). \tag{6.4}$$

and represent it pictorially by (note how the path y_t gets 'reflected' across its starting point)



(6.5)

As a word of caution, note that the composite map $\Omega Y \hookrightarrow \mathrm{hofib}(r) \xrightarrow{\chi} \Omega\,\mathrm{hofib}(l)$ is not a loop map: $\chi(*, y_t) = (rly_{1-t}\cdot y_t,\ lrly_{s\geq t} \boxminus h_s l y_t)$. When attempting to prove Proposition 4.8 by induction, one might run into needing that a similar map is a loop map, which is not the case. However, instead of delooping from 'below' (first delooping $\mathscr{F}_S^n$ for example), we need to start delooping from 'above', using the following lemma.

Proof of Lemma 4.6. We have two 1-cubes of $(m-1)$-cubes, namely the original cube $R_\bullet$ which uses maps r_S^m and the cube $L_\bullet$ which uses l_S^m instead, so we can write

$$R_\bullet: \qquad \mathsf{C}_{\bullet\not\ni m} \underset{l^m}{\overset{r^m}{\rightleftarrows}} \mathsf{C}_{\bullet\ni m} \qquad : L_\bullet$$

Their total fibres can be computed as the homotopy fibres of the induced maps

$$\mathrm{tofib}(R_\bullet) \dashrightarrow \mathrm{tofib}(\mathsf{C}_{\bullet\not\ni m}) \underset{l_*^m}{\overset{r_*^m}{\rightleftarrows}} \mathrm{tofib}(\mathsf{C}_{\bullet\ni m}) \dashleftarrow \mathrm{tofib}(L_\bullet)$$

We claim that $l_*^m \circ r_*^m = (l^m \circ r^m)_*$ is homotopic to Id. Indeed, by the condition (2) of Definition 4.5 for each $t \in [0,1]$ the homotopies $h_S^m(t)\colon l_S^m \circ r_S^m \rightsquigarrow \mathrm{Id}$ assemble into a map of cubes

$$h_\bullet^m(t)\colon \mathsf{C}_{\bullet\not\ni m} \to \mathsf{C}_{\bullet\not\ni m}$$

Hence, the induced map $h_*^m(t)$ on the total fibres is precisely a homotopy $(l^m \circ r^m)_* \rightsquigarrow \mathrm{Id}$.

Therefore, we can simply apply the preceding Lemma 4.4 to the left homotopy inverse l_*^m and the homotopy h_*^m to obtain the desired homotopy equivalence

$$\chi_m \colon \operatorname{tofib}(R_\bullet) \cong \operatorname{hofib}\left(r_*^m\right) \xrightarrow{\simeq} \Omega \operatorname{hofib}\left(l_*^m\right) \cong \Omega \operatorname{tofib}(L_\bullet). \qquad \square$$

Proof of Proposition 4.8. We will construct for each $0 \le k \le m-1$ a homotopy equivalence $\chi_{m-k} \colon \operatorname{tofib}(D^{m-k}) \to \Omega \operatorname{tofib}(D^{m-k-1})$, with the case $k = 0$ covered in the previous lemma. The argument is actually the same: conditions (4.4) and (4.5) in Definition 4.7 of an m-fold homotopy inverse ensure that for each k we have two 1-cubes of $(m-1)$-cubes:

$$D^{m-k}\colon \qquad D^{m-k}_{\bullet\not\ni m-k} \underset{l^{m-k}}{\overset{r^{m-k}}{\rightleftarrows}} D^{m-k}_{\bullet\ni m-k} \qquad \colon D^{m-k-1}$$

Moreover, the condition (4.6) ensures that $h_\bullet^{m-k}(t)$ is for each $t \in [0,1]$ a map of cubes, so $h_*^{m-k} \colon l_*^{m-k} \circ r_*^{m-k} \rightsquigarrow \mathrm{Id}_{D^{m-k}}$ witnesses that l_*^{m-k} is a left homotopy inverse. Therefore, by Lemma 4.4

$$\chi_{m-k} \colon \operatorname{tofib}(D^{m-k}) \cong \operatorname{hofib}\left(r_*^{m-k}\right) \xrightarrow{\sim} \Omega \operatorname{hofib}\left(l_*^{m-k}\right) \cong \Omega \operatorname{tofib}(D^{m-k-1})$$

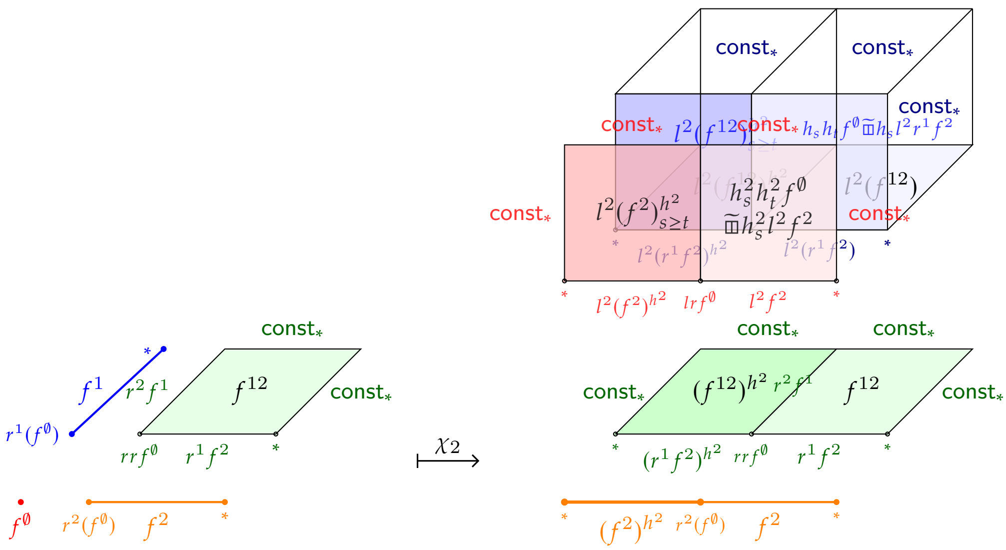
and the composite $\chi := \chi_1 \circ \cdots \circ \chi_m \colon \operatorname{tofib}(C_\bullet, r) \xrightarrow{\sim} \Omega^m \operatorname{tofib}(C_\bullet, l)$ is the desired equivalence. $\square$

A description of χ in terms of reflections of cubes

The first delooping. Let us first describe $\chi_m f \in \Omega \operatorname{tofib}(D^{m-1})$ for a point $f \in \operatorname{tofib}(R_\bullet)_{S \subseteq \underline{m}}$. The case $m = 1$ is Lemma 4.4 and picture (6.5). For $m = 2$ we have

$$R_\bullet = D^2_{\not\ni 2} \xrightarrow{r^2} D^2_{\ni 2} := \begin{tikzcd} C^1 \arrow[r, "r^2"] & C^{12} \\ C^\emptyset \arrow[u, "r^1"] \arrow[r, "r^2"] & C^2 \arrow[u, "r^1"'] \end{tikzcd} \qquad L_\bullet = D^2_{\not\ni 2} \xleftarrow{l^2} D^2_{\ni 2} := \begin{tikzcd} C^1 & C^{12} \arrow[l, "l^2"'] \\ C^\emptyset \arrow[u, "r^1"] & C^2 \arrow[l, "l^2"] \arrow[u, "r^1"'] \end{tikzcd} \qquad (6.6)$$

and $\chi_2 \colon \operatorname{hofib}(r_*^2) \to \Omega \operatorname{hofib}(l_*^2)$ is depicted in (6.7), with the colours indicating the ambient spaces from (6.6). Note that f^1 is itself discarded, but used in the rest of the diagram. For example, $(f^{12})^{h^2} := r^2\left(h_s^2(f^1) \boxplus_2 l^2 f^{12}\right)$, where we introduce notation $\boxplus_2$ for the concatenation $\cdot$ along the second coordinate.



$$(6.7)$$

Remark 6.3. *Observe that $\chi_2(f)$ is a well-defined point in $\Omega\,\mathrm{tofib}(L_\bullet)$ thanks to the conditions of Definition 4.5. For example, the orange line is indeed mapped to the bottom green line:*

$$r^1(f^2)^{h^2} = r^1r^2\big(h_s^2(f^\emptyset)\cdot l^2 f^2\big) = r^2r^1\big(h_s^2(f^\emptyset)\cdot l^2 f^2\big) = r^2\big(h_s^2(r^1 f^\emptyset)\cdot l^2(r^1 f^2)\big) = (r^1 f^2)^{h^2}$$

since r^1 commutes with l^2 by condition (1) *and with h_s^2 by condition* (2) *of the definition.*

For a general $m \geq 1$, let us denote $f_{t_m}^{Pm}(t_{p\in P}) := f^{Pm}(t_{p\in P}, t_m) \in C_{Pm}$ and rewrite f as

$$\Big(\ \{f^P\}_{P\subseteq \underline{m-1}},\ \{f_{t_m}^{Pm}\}_{P\subseteq \underline{m-1}}\ \Big) \in \mathrm{hofib}(r_P^m).$$

Then $\chi_m(f) \in \Omega\,\mathrm{hofib}(l^m)$ is given by

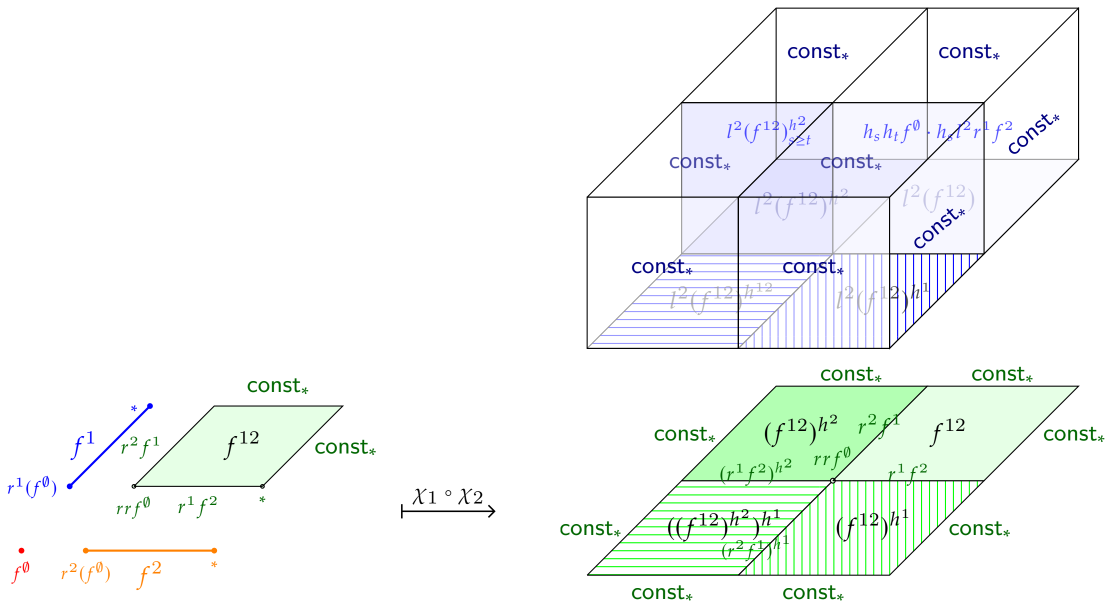
$$\chi_m(f^P, f_{t_m}^{Pm}) = \Big(\ (f^{Pm})_{t_m}^{h^m} \boxplus_m f_{t_m}^{Pm},\quad l^m(f^{Pm})_{s\geq t_m}^{h^m} \boxplus h_s^m h_{t_m}^m f^P \boxplus h_s^m l^m f_{t_m}^{Pm}\ \Big), \tag{6.8}$$

where $\boxplus_m$ denotes concatenation in the t_m-direction and $(f^{Pm})_{t_m}^{h^m}$ is the h^m-reflection as in Definition 6.2, namely reflection of f^{Pm} across the wall $I^P \times \{0\}$ in I^{Pm}. Explicitly,

$$(f^{Pm})_{t_m}^{h^m} := r^m\Big(\ h_s^m(f^P) \boxplus_m l^m(f_s^{Pm})\ \Big)_{s=1-t_m} \tag{6.9}$$

Therefore, we see that χ_m discards f^P for $P \subseteq \underline{m-1}$ but incorporates it into its first coordinate. The second coordinate of χ is another 'higher' layer of loops, in the spaces C^P.

The second delooping. Consider again $D^2 = R_\bullet$ from (6.6) and $\chi_1\chi_2(f) \in \Omega^2\,\mathrm{tofib}(D^0)$. The right part of (6.10) depicts its coordinates $S = \{1\}$ and $S = \{12\}$ (omitting $S = \emptyset, \{2\}$). Note that the large green square $\mathsf{forg}\circ\chi(f) = \chi_1\chi_2(f)^{\{12\}} \in \Omega^2 C_{\underline{2}}$ is obtained by gluing reflections of f^{12}.



$$\tag{6.10}$$

In order to generalise this observation we consider $m \geq 2$ and

$$\begin{aligned}\chi_{m-1}\chi_m(f) &= \chi_{m-1}\Big((f^{Pm})_{t_m}^{h^m} \boxplus_m f_{t_m}^{Pm}\ ,\ x^P\Big)_{P\subseteq\underline{m-1}}\\ &= \Big(\ \Big((f^{Rm-1m})_{t_m}^{h^m} \boxplus_m f_{t_m}^{Rm-1m}\Big)_{t_{m-1}}^{h^{m-1}} \boxplus_{m-1} \Big((f^{Rm-1m})_{t_m}^{h^m} \boxplus_m f_{t_m}^{Rm-1m}\Big)_{t_{m-1}},\\ &\qquad (x^{Rm-1})^{h^{m-1}} \boxplus_{m-1} x^{Rm-1},\ y^{Rm}\ \Big)_{R\subseteq\underline{m-2}}\end{aligned} \tag{6.11}$$

Here we have applied (6.8) twice and denoted by x and y the remaining irrelevant coordinates. The first coordinate is $(\chi_{m-1}\chi_m(f))^{Rm-1m} \in \Omega^2 C_{Rm-1m}$ where R runs through subsets of $\underline{m-2}$.

Lemma 6.4. $\big((f^{Rm-1m})^{h^m}_{t_m} \boxplus_m f^{Rm-1m}_{t_m}\big)^{h^{m-1}} = \big((f^{Rm-1m})^{h^m}_{t_m}\big)^{h^{m-1}} \boxplus_m \big(f^{Rm-1m}_{t_m}\big)^{h^{m-1}}$.

Proof. The left hand side is by (6.9) equal to r^{m-1} applied to the map (denoting $s := t_{m-1}$)

$$= h^{m-1}_s\Big((f^{Rm})^{h^m}_{t_m} \boxplus_m f^{Rm}_{t_m}\Big) \boxplus_{m-1} l^{m-1}\Big((f^{Rm-1m})^{h^m}_{t_m} \boxplus_m f^{Rm-1m}_{t_m}\Big)_s$$
$$= \Big(h^{m-1}_s(f^{Rm})^{h^m}_{t_m} \boxplus_m h^{m-1}_s f^{Rm}_{t_m}\Big) \boxplus_{m-1} \Big(l^{m-1}(f^{Rm-1m})^{h^m}_{t_m,s} \boxplus_m l^{m-1} f^{Rm-1m}_{t_m,s}\Big)$$

The concatenation in the t_{m-1}-direction can be interchanged with the one in the t_m-direction (this is another manifestation of the Eckmann–Hilton principle), so we obtain

$$= \Big(h^{m-1}_s(f^{Rm})^{h^m}_{t_m} \boxplus_{m-1} l^{m-1}(f^{Rm-1m})^{h^m}_{t_m,s}\Big) \boxplus_m \Big(h^{m-1}_s f^{Rm}_{t_m} \boxplus_{m-1} l^{m-1} f^{Rm-1m}_{t_m,s}\Big).$$

Finally, applying r^{m-1} gives the desired right hand side in the statement of the lemma. □

Therefore, we make the following definition.

Definition 6.5. *Fix $P \subseteq \underline{m}$ and let $f^P : I^P \to C_P$ for an m-cube $C_\bullet$. For $S \subseteq P$ we define a map $(f^P)^{h^S} : I^P \to C_P$ inductively on $|S| \leq |P|$ and call it the h^S-reflection of f^P.*

For $S = \emptyset$ we let $(f^P)^{h^\emptyset} := f^P$ and otherwise let $k = \min S$ and define

$$\big(f^P\big)^{h^S} := \Big(\big(f^P\big)^{h^{S\setminus k}}\Big)^{h^k}$$

using the definition of h^k-reflection from (6.9).

Note that $(f^P)^{h^S}$ is indeed a kind of a reflection of f^P across the 0-faces $\{0\}^S \times I^{P\setminus S} \subseteq \partial_0 I^P$. Indeed, the value of f^P on them agrees with the value of $(f^P)^{h^S}$ on the corresponding faces $\{1\}^S \times I^{P\setminus S} \subseteq \partial_1 I^P$. On the other hand, $(f^P)^{h^S}$ is constant on $\{0\}^S \times I^{P\setminus S} \subseteq \partial_0 I^P$.

Proposition 6.6. *For D^m as above, $\mathsf{forg} \circ \chi\colon \operatorname{tofib}(D^m) \to \Omega^m C_{\underline{m}}$ maps $f \in \operatorname{tofib}(D^m)$ to*

$$(\chi f)^{\underline{m}} = \boxplus_{S \subseteq \underline{m}} (f^{\underline{m}})^{h^S}$$

obtained by gluing together all h-reflections $(f^{\underline{m}})^{h^S}$ of $f^{\underline{m}}\colon I^m \to C_{\underline{m}}$ along the 0-faces of I^m.

Proof of Proposition 6.6. From (6.11) and Lemma 6.4 we conclude

$$\chi_{m-1}\chi_m(f)^{Rm-1m} = \Big(\big(f^{Rm-1m})^{h^m}\big)^{h^{m-1}} \boxplus_m \big(f^{Rm-1m})^{h^{m-1}}\Big) \boxplus_{m-1} \Big((f^{Rm-1m})^{h^m} \boxplus_m f^{Rm-1m}\Big)$$
$$= (f^{Rm-1m})^{h^{\{m-1,m\}}} \boxplus (f^{Rm-1m})^{h^{m-1}} \boxplus (f^{Rm-1m})^{h^m} \boxplus f^{Rm-1m}.$$

In the second line we simply omitted the brackets and used the symbol $\boxplus$ instead, since the operation $\boxplus_k$ glues unambiguously any two maps which have matching 0- and 1-faces indexed by k. Continuing in the manner of (6.11), we find

$$\chi_k \circ \cdots \circ \chi_{m-1}\chi_m(f)^{Rk\dots m-1m} = \boxplus_{S \subseteq \{k,\dots,m-1,m\}} (f^{Rk\dots m-1m})^{h^S}$$

so the coordinate of $\chi_1 \circ \cdots \circ \chi_m(f)$ corresponding to $\underline{m}$ is given as claimed by

$$(\chi f)^{\underline{m}} = \boxplus_{S \subseteq \underline{m}} (f^{\underline{m}})^{h^S}.$$ □

A Samelson products

In this section we provide a reminder on Samelson products and some of their properties; the main reference are [Whi78] and [Nei10].

Let G be a grouplike H-space, that is, an H-space whose multiplication $\cdot$ is homotopy associative and which has homotopy inverses, and we assume *these homotopies are specified as part of the data*. In our applications $G := \Omega(M \vee \bigvee_S \mathbb{S}^{d-1})$ with an inverse for $\gamma \in G$ given as the inverse loop $(\gamma^{-1})_t = \gamma_{1-t}$ and the canonical homotopy $\gamma \cdot \gamma^{-1} \rightsquigarrow \mathsf{const}_*$ given by $t \mapsto \gamma|_{[0,1-t]} \cdot \gamma^{-1}|_{[t,1]}$.

The homotopy groups $\pi_* G$ can be equipped with two associative operations – on one hand, the standard multiplication on homotopy groups of a space using the co-H-space structure on spheres (additive except on the fundamental group), and on the other hand, using the H-space structure on G to define the pointwise multiplication $f_1 \cdot f_2 \colon X_1 \times X_2 \to G \times G \to G$ of maps $f_j \colon X_j \to G$, and then if $X_1 = X_2 = \mathbb{S}^n$, precompose with the diagonal $\mathbb{S}^n \to \mathbb{S}^n \times \mathbb{S}^n$.

These operations give equivalent additive structure on $\pi_{>0} G$ (by the Eckmann–Hilton argument), but the latter also gives a group structure on $\pi_0 G$. Moreover, $\gamma \in G$ acts on a map $f \colon X \to G$ by pointwise conjugation $f^\gamma(x) := \gamma \cdot f(x) \cdot \gamma^{-1}$, and this defines an action of the group $\pi_0 G$ on the graded group $\pi_* G$. When G is a loop space this corresponds to the standard action of the fundamental group on the higher homotopy groups.

The $\mathsf{Samelson\ product}$ is a non-associative product of maps $f_j \colon X_j \to G$ for $j = 1, 2$, given by

$$[f_1, f_2] \colon X_1 \wedge X_2 \xrightarrow{f_1 \wedge f_2} G \wedge G \xrightarrow{[\cdot,\cdot]} G. \tag{A.1}$$

Here the commutator map $[\cdot,\cdot] : G \times G \to G$, given by $(x, y) \mapsto x \cdot y \cdot x^{-1} \cdot y^{-1}$, is null-homotopic on the wedge $G \vee G$, so factors through the smash product $G \wedge G := {}^{G \times G}\!/_{G \vee G}$. More precisely, since on the wedge one of the coordinates is equal to the basepoint, the word $[x, y]$ becomes of the shape $x \cdot x^{-1}$, for which there is a specified null-homotopy by the definition of a homotopy inverse.

Applying this to the case when each $X_j = \mathbb{S}^{n_j}$ is a sphere, and using homeomorphisms

$$\vartheta_{(n_1,n_2)} \colon \mathbb{S}^{n_1+n_2} \to \mathbb{S}^{n_1} \wedge \mathbb{S}^{n_2} \tag{A.2}$$

we get an operation $[\cdot,\cdot] : \pi_{n_1} G \times \pi_{n_2} G \to \pi_{n_1+n_2} G$. On $\pi_0 G$ this is just the group commutator, and there is an identity[27]

$$[f, \gamma] \simeq f - f^\gamma, \qquad f \in \pi_{>0} G\ ,\ \gamma \in \pi_0 G. \tag{A.3}$$

On the abelian group $\pi_{>0} G$ the Samelson bracket is bilinear and satisfies *graded* antisymmetry and Jacobi relations, making it into a graded Lie algebra over $\mathbb{Z}$. The origin of graded signs is in the fact that the coordinate exchange $\theta \colon \mathbb{S}^{n_1} \wedge \mathbb{S}^{n_2} \to \mathbb{S}^{n_2} \wedge \mathbb{S}^{n_1}$ induces the self-map $\vartheta^{-1}_{(n_2,n_1)} \circ \theta \circ \vartheta_{(n_1,n_2)}$ of $\mathbb{S}^{n_1+n_2}$ which has degree $(-1)^{n_1 n_2}$.

Actually, the action of $\pi_0 G$ on $\pi_{>0} G$ respects the grading and the Lie bracket

$$[f, g]^\gamma = [f^\gamma, g^\gamma], \qquad f, g \in \pi_{>0} G\ ,\ \gamma \in \pi_0 G,$$

so all this structure is encapsulated by saying that $\pi_{>0} G$ is a *graded Lie algebra over* $\mathbb{Z}[\pi_0 G]$.

Furthermore, the Hurewicz homomorphism $h \colon \pi_* G \to H_*(G; \mathbb{Z})$ takes the Samelson bracket to the graded commutator in the Pontrjagin Hopf algebra $H_*(G; \mathbb{Z})$. On $* > 0$ the image is contained in the primitives, while $\pi_0 G \to H_0(G; \mathbb{Z}) = \mathbb{Z}[\pi_0 G]$ is included as the grouplikes. For G connected, $h \colon \pi_* G \otimes \mathbb{Q} \cong \mathfrak{pr}\, H_*(G; \mathbb{Q})$ is an isomorphism of graded Lie algebras over $\mathbb{Q}$ [MM65].

---

[27] To see (A.3), plug $f_1 = f$ and $f_2 \colon \mathbb{S}^0 \to G$ into (A.1). The latter simply picks out a point $\gamma \in G$, so $[f, \gamma] = f \cdot (f^{-1})^\gamma$. Here f^{-1} is the pointwise inverse, which is homotopic to $-f$ by the mentioned Eckmann–Hilton argument.

One can iteratively form the Samelson product of maps $f_i\colon X_i \to G$ for $i \in S = \{i_1 < i_2 < \cdots < i_m\}$ according to a Lie word (a non-associative bracketing) $w(x^i)$ in the letters x^i, $i \in S$. To spell out this explicitly, we recursively define the space $w(X_i)$ and the map $w(f_i)\colon w(X_i) \to G$.

Firstly, for $k \in S$ let $x^k(X_i) := X_k$ and $x^k(f_i) := f_k$. Further, for $w = [w_1, w_2]$ let $w(X_i) = w_1(X_i) \bigwedge w_2(X_i)$ and define

$$w(f_i)\colon\ w(X_i) \xrightarrow{w_1(f_i) \bigwedge w_2(f_i)} G \wedge G \xrightarrow{[\cdot,\cdot]} G. \tag{A.4}$$

In particular, if $X_i = \mathbb{S}^{d-2}$ for all $i \in S$, to get a map from a sphere we need to precompose with some homeomorphism $\vartheta_{\sigma_w}\colon \mathbb{S}^{(d-2)l_w} \to w(\mathbb{S}^{d-2})$ similarly as in (A.2) (l_w is the word length of w).

The Hilton–Milnor theorem

Consider now $G = \Omega \bigvee_{i\in S} \Sigma X_i$. As in Section 5 we have the inclusion $\iota_i\colon \Sigma X_i \hookrightarrow \bigvee_{i\in S} \Sigma X_i$ and the canonical map $\eta_{X_i}\colon X_i \to \Omega\Sigma X_i$. Plugging into (A.4) the composite maps

$$x_i\colon\ X_i \xrightarrow{\eta_{X_i}} \Omega\Sigma X_i \xhookrightarrow{\Omega\iota_i} \Omega \bigvee_{i\in S} \Sigma X_i$$

gives the Samelson product

$$w(x_i)\colon\ w(X_i) \to \Omega \bigvee_{i\in S} \Sigma X_i. \tag{A.5}$$

Remark A.1. *For $G = \Omega Y$ the Samelson bracket on $\pi_*(\Omega Y) \cong \pi_{*+1}(Y)$ is adjoint to the Whitehead bracket on the latter group. The (generalised) Whitehead product of $f_i\colon \Sigma X_i \to Y$ is defined via*

$$[f_1, f_2]_W\colon\ \Sigma(X_1 \wedge X_2) \longrightarrow \Sigma X_1 \vee \Sigma X_2 \xrightarrow{f_1 \vee f_2} Y \vee Y \to Y,$$

where the last map is the fold and the first map can be explicitly defined, see [Whi78]. It is precisely the adjoint of the Samelson product $[x_1, x_2]\colon X_1 \wedge X_2 \to \Omega(\Sigma X_1 \vee \Sigma X_2)$ from (A.5). If $X_i = \mathbb{S}^{n_i-1}$ are spheres, this is the attaching map $\mathbb{S}^{n_1+n_2-1} \to \mathbb{S}^{n_1} \vee \mathbb{S}^{n_2}$ of the top cell in $\mathbb{S}^{n_1} \times \mathbb{S}^{n_2}$.

Actually, for $G = \Omega \bigvee_{i\in S} \Sigma X_i$ the Samelson products $w(x_i)$ 'generate the homotopy type of G'. A more precise statement is the Hilton–Milnor theorem below, for which we need a bit more notation. Firstly, since (A.5) is a map into a loop space, there is a unique multiplicative extension

$$\widetilde{w}(x_i)\colon\ \Omega\Sigma w(X_i) \longrightarrow \Omega \bigvee_{i\in S} \Sigma X_i. \tag{A.6}$$

Namely, for any space X the map $\eta_X\colon X \to \Omega\Sigma X$ is initial among all maps from X to a loop space, so any $f\colon X \to \Omega Z$ factors as the composition of η_X with $\widetilde{f} := \Omega(ev \circ \Sigma f)\colon \Omega\Sigma X \to \Omega\Sigma\Omega Z \to \Omega Z$. Explicitly, $\widetilde{f}\big(\theta \mapsto t_\theta \wedge a_\theta\big) = \theta \mapsto f(a_\theta)_{t_\theta}$ for $t_\theta \in \mathbb{S}^1$, $a_\theta \in X$ when θ ranges $\mathbb{S}^1$.

Moreover, given Lie words w_1 and w_2 we can take the pointwise product $\widetilde{w}_1(x_i) \cdot \widetilde{w}_1(x_i)$ (pointwise concatenate loops) as we saw above. Therefore, if $\mathsf{B}(S)$ denotes a Hall basis for the free Lie algebra $\mathbb{L}(S)$, we can define the map

$$hm := \prod_w \widetilde{w}\colon\ \prod_{w\in \mathsf{B}(S)} \Omega\Sigma w(X_i) \longrightarrow \Omega \bigvee_{i\in S} \Sigma X_i, \tag{A.7}$$

where on the source we use the product (Tikhonov) topology.

Theorem A.2 ([Hil55; Mil72; Gra71; Spe71])**.** *If for each $i \in S$ the space X_i is well-pointed and path-connected, then the map (A.7) is a weak homotopy equivalence.*

This can be proven by first iterating Gray–Spencer Lemma 5.3 to get a weak homotopy equivalence

$$\Omega\iota_A \times \bigvee_{i\geq 0}[x_A,[\overbrace{x_A,\dots,[x_A}, x_B]\dots]]\colon \; \Omega\Sigma A \times \Omega\Sigma \bigvee_{i\geq 0}\Big(A^{\wedge i}\wedge B\Big) \xrightarrow{\qquad\quad} \Omega\big(\Sigma A \vee \Sigma B\big),$$

and then using an inductive argument on the word length. See [Mil72, Thm. 4].

Remark A.3. *The set* $\mathsf{B}(S)$ *is a Hall basis for the usual,* ungraded, *free Lie algebra. This should not be confused with the fact that, if we put* $X_i = \mathbb{S}^{n_i}$ *with* $n_i \geq 2$, *then the theorem implies that* $\pi_*(\Omega \bigvee_S \mathbb{S}^{n_i+1})\otimes\mathbb{Q} \cong \mathbb{L}(x^{n_i} : i \in S)\otimes\mathbb{Q}$ *the* free graded Lie algebra.

Samelson products for trees

Let us now consider Samelson products for Lie words $w(x^i)$ in which each letter x^i, $i\in R$, appears exactly once, for a finite ordered set R. This is the ungraded case for now, with $|x^i| = 0$. Recall from Section 2.1 there is an isomorphism $\omega_2\colon \mathsf{Lie}(R) \to \mathsf{Lie}_2(R)$ (see also next subsection).

As mentioned above, given maps $f_i\colon \mathbb{S}^{d-2}\to G$ one obtains a map from a sphere by precomposing the Samelson product $w(f_i)\colon w(\mathbb{S}^{d-2}) \to G$ with $\vartheta_{\sigma_w}\colon \mathbb{S}^{(d-2)l_w} \to w(X_i)$, which permutes the factors according to the permutation σ_w corresponding to the word w. However, in the case when letters do not repeat we can instead define this map directly by induction.

LEMMA A.4. *The map* $w(f_i)\circ\vartheta_{\sigma_w}$ *for* $w = \omega_2(\Gamma)$ *is homotopic to the map* $\Gamma(f_i)$ *defined inductively by* $\overset{k}{|}(f_i) = f_k$ *and for* $\Gamma_j \in \mathrm{Tree}(R_j)$ *with* $R_1 \sqcup R_2 = R$ *by*

$$\overset{\Gamma_2\ \ \Gamma_1}{\curlyvee}(f_i)\colon\; (\mathbb{S}^{d-2})^{\wedge R} \xrightarrow{\;\vartheta_{(R_1,R_2)}\;} (\mathbb{S}^{d-2})^{\wedge R_1}\wedge(\mathbb{S}^{d-2})^{\wedge R_2} \xrightarrow{\;[\Gamma_1(f_i),\ \Gamma_2(f_i)]\;} G \tag{A.8}$$

where (R_1,R_2) *permutes the ordered set* R *into* $R_1\sqcup R_2 :=$ *first all indices of* R_1, *then of* R_2.

Proof. We have homotopies

$$w(f_i)\circ\vartheta_{\sigma_w} \simeq (\operatorname{sgn}\sigma_w)^{d-2}w(f_i), \qquad \Gamma(f_i) \;\simeq\; (-1)^{(1|2)_d}[\Gamma_1(f_i),\Gamma_2(f_i)]$$

since $\deg\vartheta_{(R_1,R_2)} = (-1)^{(1|2)_d}$, where $(1|2)_d := (d-2)\cdot|\{(i_1,i_2)\in R_1\times R_2 : i_1 > i_2\}|$ as in Lemma 2.3. The proof now follows by induction using that the sign of permutation satisfies the recursive formula

$$\operatorname{sgn}\sigma_w = (-1)^{(1|2)}\operatorname{sgn}\sigma_{w_1}\cdot\operatorname{sgn}\sigma_{w_2}. \qquad \square$$

In the proof of Theorem E in Section 9 we will need the following observation. Let $(M_S,\rho)_{S\subseteq R}$ be a cube with maps $\rho^k_S\colon M_S \to M_{Sk}$ and assume we are given maps $f_i\colon \mathbb{S}^{d-2}\to \Omega M_i$ for $i\in R$. For $S\subseteq R$ with $i\in S$ let us denote $f_{i,S} := \Omega\rho_i^{S\setminus i}\circ f_i\colon\; \mathbb{S}^{d-2} \longrightarrow \Omega M_i \longrightarrow \Omega M_S$. .

Note that the case $M_S = \vee_{i\in S}\Sigma X_i$ and $\rho_i := \iota_i$ is the setting of the Hilton–Milnor theorem.

LEMMA A.5. *The map* $[\Gamma_1(f_{i,R}),\Gamma_2(f_{i,R})]$ *as in* (A.8) *is obtained by* canonically *trivialising on the boundary the map*

$$x\colon (I^{d-2})^{R_1}\times(I^{d-2})^{R_2} \xrightarrow{\;\Gamma_1(f_{i,R_1})\times\Gamma_2(f_{i,R_1})\;} \Omega M_{R_1}\times\Omega M_{R_1} \xrightarrow{\;[\Omega\rho_{R_1}^{R\setminus R_1},\,\Omega\rho_{R_2}^{R\setminus R_2}]\;} \Omega M_R$$

More precisely, for each $\vec{t}\in\partial(I^{d-2})^R$ *we glue in the standard null-homotopy* $x(\vec{t})\cdot x(\vec{t})^{-1} \rightsquigarrow *$ *of loops in* ΩM_R *to extend* x *to a bigger cube on whose boundary it is constant.*

Here we are defining a map on $(\mathbb{S}^{d-2})^{\wedge R} \cong {(I^{d-2})^R}/_{\partial}$ by giving it on the cube $(I^{d-2})^R$ so that it is constant on the boundary. The proof of the lemma is clear from definitions. See Section 5.3 for how it will be used.

Proof of Lemma 2.3

We now prove that the map given by $\omega_d(\overset{i}{|}) = x^i$, $\omega_d(\Gamma) = \omega_\Gamma := (-1)^{(1|2)_d}[\omega_d(\Gamma_1), \omega_d(\Gamma_2)]$ is an isomorphism $\omega_d\colon \mathsf{Lie}(n-1) \to \mathsf{Lie}_d(n-1)$, as claimed in Section 2.1.

Proof of Lemma 2.3. We define ω_d by linearly extending the definition in the lemma and check it descends to the quotient by (2.1). We write $\omega_\Gamma := \omega_d(\Gamma)$ for short.

To this end, let ω_{AS} and ω_{IHX} be the images under ω_d of the linear combinations as in (2.1), but with roots instead of dots. It suffices to show that these are trivial, since then ω_d will also vanish on any tree in which AS or IHX appears as a subtree.

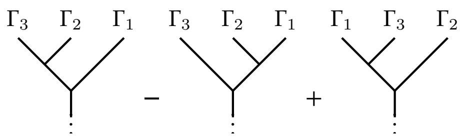
Firstly, using $|\omega_{\Gamma_j}| = |S_j|(d-2)$ and the obvious identity $(1|2)_d + (2|1)_d = |S_1||S_2|(d-2)$ we obtain:

$$\begin{aligned}
\omega_{AS} &= (-1)^{(1|2)_d}\left[\omega_{\Gamma_1}, \omega_{\Gamma_2}\right] + (-1)^{(2|1)_d}\left[\omega_{\Gamma_2}, \omega_{\Gamma_1}\right] \\
&= (-1)^{(1|2)_d}\Big(\left[\omega_{\Gamma_1}, \omega_{\Gamma_2}\right] + (-1)^{|S_1||S_2|(d-2)}\left[\omega_{\Gamma_2}, \omega_{\Gamma_1}\right]\Big) \\
&= (-1)^{(1|2)_d}\Big(\left[\omega_{\Gamma_1}, \omega_{\Gamma_2}\right] + (-1)^{|\omega_1||\omega_2|}\left[\omega_{\Gamma_2}, \omega_{\Gamma_1}\right]\Big)
\end{aligned}$$

which vanishes by the graded antisymmetry in $\mathsf{Lie}_d(S)$.

Secondly, recall that

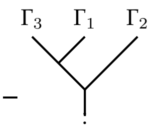
IHX :



$= 0.$

and note that by AS the last tree is equal to

$-$



Therefore, ω_{IHX} is equal to

$$\begin{aligned}
&(-1)^{(1|23)_d+(2|3)_d}\left[\omega_{\Gamma_1}, [\omega_{\Gamma_2}, \omega_{\Gamma_3}]\right] - (-1)^{(12|3)_d+(1|2)_d}\left[[\omega_{\Gamma_1}, \omega_{\Gamma_2}], \omega_{\Gamma_3}\right] - (-1)^{(2|13)_d+(1|3)_d}\left[\omega_{\Gamma_2}, [\omega_{\Gamma_1}, \omega_{\Gamma_3}]\right] \\
&= (-1)^{(1|2)_d+(1|3)_d+(2|3)_d}\Big(\left[\omega_{\Gamma_1}, [\omega_{\Gamma_2}, \omega_{\Gamma_3}]\right] - \left[[\omega_{\Gamma_1}, \omega_{\Gamma_2}], \omega_{\Gamma_3}\right] - (-1)^{(2|1)_d+(1|2)_d}\left[\omega_{\Gamma_2}, [\omega_{\Gamma_1}, \omega_{\Gamma_3}]\right]\Big)
\end{aligned}$$

where we have used the identities

$$\begin{aligned}
&(1|23) + (2|3) = (1|2) + (1|3) + (2|3) = (12|3) + (1|2), \\
&(2|13) + (1|3) = (2|1) + (2|3) + (1|3).
\end{aligned}$$

Now again plugging in $(2|13)_d + (1|3)_d = |\omega_{\Gamma_1}||\omega_{\Gamma_2}|$ we get that the terms in the parenthesis are precisely those of the graded Jacobi relation (2.2), which holds in $\mathsf{Lie}_d(S)$.

Finally, ω_d is clearly a surjection and an inverse ω_d^{-1} can be constructed in an analogous way – AS and IHX will imply it is well-defined modulo graded antisymmetry and Jacobi relations. $\square$

Part III

Comparing to the geometric calculus in dimension three

Throughout this part M is an oriented 3-manifold with non-empty boundary.

– § –

In Section 7 we explain how gropes relate to the theory of finite type invariants, define thick gropes and grope forests, and their underlying trees.

In Section 8 we prove Theorem D, namely, we construct a map $\psi\colon \mathsf{Grop}_n(M;\mathrm{U}) \to \mathsf{H}_n(M)$.

Finally, in Section 9 we prove main Theorems E and F.

7 Introduction to the geometric calculus

After briefly reviewing the *classical approach* to the finite type theory (for book treatments see [Oht02; CDM12]), and explaining what we mean by *the geometric calculus*, we will devote this section to our adaptation of the latter: we will define grope cobordisms and their modifications, thick gropes and grope forests, which are best suited for our purposes.

7.1 Classical versus geometric approach

In this introduction we restrict to the case of classical (long) knots $M = I^3$, and we denote by $\mathbb{K} := \pi_0\mathcal{K}(I^3)$ the monoid of knots with the operation $\#$ of connected sum.

A singular knot is an immersion $\sigma\colon I \looparrowright I^3$ with finitely many transverse double points, which agrees with U near boundary. By resolving double points of σ in all possible ways[28] we get a linear combination $K_\sigma \in \mathbb{Z}[\mathbb{K}]$. Depending on the minimal number $n \geq 1$ of double points this defines a decreasing filtration $\mathcal{V}_n \subseteq \mathbb{Z}[\mathbb{K}]$ of the monoid ring, with $\mathcal{V}_1$ precisely the augmentation ideal.

The associated graded of this filtration is related to the Hopf algebra of chord diagrams: those Jacobi diagrams from Definition 2.10 in Section 2.1.3 which have no trivalent vertices. Namely, for a singular knot σ with n double points one has n pairs of points on the source interval I which are identified by σ; we record each pair by a chord to get a chord diagram D_σ on I of $\deg(D_\sigma) = n$.

This assignment is surjective, but far from being injective. However, there is a well-defined map $\mathcal{R}_n$ which takes a chord diagram D to the class $[K_{\sigma(D)}] \in {}^{\mathcal{V}_n}\!/_{\mathcal{V}_{n+1}}$, where $\sigma(D)$ is any singular knot with the chord diagram $D_{\sigma(D)} = D$. One can check that this is well-defined and vanishes on diagrams which have an 'isolated chord', as $1T$ from (2.5) (since our knots are not framed) and on the $4T$ relations, certain linear combinations of four chord diagrams (coming from triple points).

Actually, $4T$ is a consequence of the relation STU from Definition 2.10, so there is a linear map

$$\mathbb{Z}[\textit{chord diagrams of deg } n]\big/_{4T,\,1T} \to \mathbb{Z}[\textit{Jacobi diagrams of deg } n]\big/_{STU,\,1T} =: \mathcal{A}_n \tag{7.1}$$

By an important result of [Bar95a] this is actually *an isomorphism.*[29] Hence, by the previous paragraph there is a surjection of finitely generated abelian groups called the realisation map

$$\mathcal{R}_n\colon\ \mathcal{A}_n \longrightarrow\!\!\!\!\rightarrow {}^{\mathcal{V}_n}\!/_{\mathcal{V}_{n+1}} \qquad\qquad D \mapsto [K_{\sigma(D)}]. \tag{7.2}$$

A knot invariant $v\colon \mathbb{K} \to T$ is of type $\leq n$ if its linear extension $\overline{v}\colon \mathbb{Z}[\mathbb{K}] \to T$ vanishes on $\mathcal{V}_{n+1}$. Here T is an abelian group and v is just a map of sets.

Definition 7.1. *Let R be a ring, A a graded R-module and $\widehat{A} := \prod_{n\geq 1} A_n$ its completion. A map $\zeta\colon \mathbb{K} \to \widehat{A}$ is a universal Vassiliev invariant over R if the linear extension $\overline{\zeta}\colon R[\mathbb{K}] \to \widehat{A}$ is a filtered R-linear map inducing an isomorphism of the associated graded R-modules. Equivalently,*

(1) $\zeta = \prod_{n\geq 1}\zeta_n$ and for each $n \geq 1$ the map ζ_n is an invariant of type $\leq n$,

(2) the restriction $\overline{\zeta}_n|_{\mathcal{V}_n}\colon {}^{\mathcal{V}_n}\!/_{\mathcal{V}_{n+1}} \otimes R \to A_n$ is an isomorphism.

We say that ζ is classical if the composite $\overline{\zeta}_n|_{\mathcal{V}_n} \circ (\mathcal{R}_n \otimes R)$ is the identity on $\mathcal{A}_n \otimes R = A_n$.

Lemma 7.2 (justifying the 'universality'). *If ζ is a universal Vassiliev invariant over R, then any invariant $v\colon \mathbb{K} \to T$ of type $\leq n$ with values in an R-module T can be written as a sum $\sum_{k=1}^{n} v_k \circ \overline{\zeta}_k$, where $v_k := \overline{v}|_{\mathcal{V}_k} \circ (\overline{\zeta}_k|_{\mathcal{V}_k})^{-1}\colon A_k \to T$, called the k-th symbol of v.*

[28] Two strands intersecting at a point can be pushed off each other in two different ways.

[29] In [Bar95a] rational coefficients are used, but the proof goes through over the integers unchanged.

Proof. Indeed, $v - v_n \circ \overline{\zeta}_n$ vanishes on $\mathcal{V}_n$, so it is an invariant of type $\leq n-1$ whose $(n-1)$-st symbol is equal to v_{n-1}, so we can proceed by induction. □

The Kontsevich integral, as well as the Bott–Taubes configuration space integrals [BT94; AF97], are classical universal Vassiliev invariant *over* $\mathbb{Q}$. It is an open problem if they agree, but some progress was made in [Poi02; Les02] (note that there may be several universal invariants over the same coefficient ring since only the 'bottom part' $\overline{\zeta}_n|_{\mathcal{V}_n}$ is determined). As a consequence,

$$\mathcal{R}_n \otimes \mathbb{Q} \colon \ \mathcal{A}_n \otimes \mathbb{Q} \xrightarrow{\cong} {}^{\mathcal{V}_n}\!/\!_{\mathcal{V}_{n+1}} \otimes \mathbb{Q}. \tag{7.3}$$

Remark 7.3. *Therefore, the kernel of $\mathcal{R}_n$ consists of torsion elements. It is an open problem if it is actually trivial – so that $\mathcal{R}_n$ is an isomorphism – and if any of these two groups has torsion.*

The Bar-Natan's isomorphism (7.1) gives more power to the theory as it is relatively easy to construct interesting invariants of Jacobi diagrams, called weight systems. For example, each trivalent vertex can be interpreted as the Lie bracket in a chosen semisimple Lie algebra and the horizontal line can be labelled by its representation yielding for each diagram a value in the ground field similarly as for the Reshetikhin-Turaev invariants. Actually, symbols of quantum invariants of knots are precisely such weight systems. By [Vog11] this is a strict subset of all weight systems.

However, introducing trivalent vertices raises the question of their *geometric* interpretation, as we had for chords. Several different answers are summarised in the following theorem.

Theorem 7.4. *For $K, K' \in \mathbb{K}$ and $n \geq 1$ the following are equivalent:*

(1) $K - K' \in \mathcal{V}_n$ or, equivalently, K and K' are not distinguished by any invariant of type $\leq n-1$;

(2) K' can be obtained from K by a finite sequence of infections by pure braids lying in the n-th lower central series subgroup;

(3) K' can be obtained from K by a surgery on a simple strict forest clasper *of degree n;*

(4) K' can be related to K by a finite sequence of simple capped genus one grope cobordisms *of degree n. In this case we say that K and K' are* n-equivalent *and write $K \sim_n K'$.*

The equivalence (1) ⇔ (2) is due to [Sta98], (1) ⇔ (3) are independently by [Gus00] and [Hab00, Thm. 3.17 & 6.18] and (3) ⇔ (4) by [CT04b, Thm. 4].

The idea behind all these descriptions is to view a crossing change as the simplest move, of degree one, in a whole *family of moves*. Namely, a chord guides a crossing change (a homotopy passing through the corresponding singular knot), while moves of higher degrees are certain iterations of the 'trivalent' move: grab three strands of the knot and tie them into the Borromean rings. We make this precise in the next section using the last approach of the theorem (see Remark 7.11).

Let us define the Gusarov–Habiro filtration $\mathbb{K}_n \subseteq \mathbb{K}$ as sumbonoids $\mathbb{K}_n := \{K \in \mathbb{K} : K \sim_n \mathrm{U}\}$. Then the theorem implies that it maps to the Vassiliev–Gusarov filtration:

$$\begin{tikzcd} & \mathbb{K}_n \arrow[r] \arrow[d, hook] & \mathcal{V}_n \arrow[d, hook] & \\ \pi_0\mathcal{K}(I^3) = & \mathbb{K} \arrow[r, "K \mapsto K - \mathrm{U}"] & \mathbb{Z}[\mathbb{K}] & = H_0(\mathcal{K}(I^3);\mathbb{Z}) \end{tikzcd} \tag{7.4}$$

This is what we call the *geometric approach*, as we are back to working with knots, instead of their linear combinations – or dually, their invariants $H^0(\mathcal{K}(I^3);T)$. In terms of invariants of finite type, the next lemma shows that we are restricting to the study of those which are additive, that is, monoid maps from $\mathbb{K}$ to abelian groups.

LEMMA 7.5. *An additive invariant is of type $\leq n-1$ if and only if it vanishes on $\mathbb{K}_n$. That is, $v\colon \mathbb{K} \to A$ is a monoid map and vanishes on $\mathbb{K}_n$ if and only if $\overline{v}\colon \mathbb{Z}[\mathbb{K}] \to A$ vanishes on $\mathcal{V}_1 \cdot \mathcal{V}_1 + \mathcal{V}_n$.*

Proof. Since $v(K_1 \# K_2) - v(K_1) - v(K_2) = \widehat{v}\big((K_1 - \mathrm{U})\#(K_2 - \mathrm{U})\big)$, v is a monoid map if and only if its linear extension $\widehat{v}$ vanishes on $\mathcal{V}_1 \cdot \mathcal{V}_1 \subseteq \mathbb{Z}[\mathbb{K}]$. On one hand, by Theorem 7.4 we have $\{K - \mathrm{U} : K \in \mathbb{K}_n\} \subseteq \mathcal{V}_n$ and on the other, $\mathcal{V}_n \subseteq \mathcal{V}_1 \cdot \mathcal{V}_1 + \{K - \mathrm{U} : K \in \mathbb{K}_n\}$ by a result of Habiro [Hab00, Thm. 6.17]. Since $v(K) = \widehat{v}(K - \mathrm{U})$, the claim follows. □

Furthermore, recall from Sections 2.1.5 and 2.2.1 that we can also pass from the Hopf algebra $\mathcal{A} := \prod_{n\geq 1} \mathcal{A}_n$ to its subgroup $\mathcal{A}^T \subseteq \mathcal{A}$ of Jacobi trees. Namely, there is an analogous realisation map $\mathcal{R}_n^T\colon \mathcal{A}_n^T \to {}^{\mathbb{K}_n}\!/\!{}_{\sim_{n+1}}$ for $n \geq 1$ (see Theorems G1 and G2), fitting into a commutative diagram

$$\begin{tikzcd} \mathcal{A}_n^T \arrow[r, hook] \arrow[d, two heads, "\mathcal{R}_n^T"'] & \mathcal{A}_n \arrow[d, two heads, "\mathcal{R}_n"] \\ {}^{\mathbb{K}_n}\!/\!{}_{\sim_{n+1}} \arrow[r, "K \mapsto K - \mathrm{U}"] & {}^{\mathcal{V}_n}\!/\!{}_{\mathcal{V}_{n+1}} \end{tikzcd}$$

by Theorem G3. Moreover, each ${}^{\mathbb{K}_n}\!/\!{}_{\sim_{n+1}}$ is a finitely generated abelian group and the map $\mathcal{R}_n^T$ is a homomorphism of groups [Gus00; Hab00]. For the proofs of these results see Section 10, in which we also treat the general case $\mathbb{K}(M) := \pi_0\mathcal{K}(M)$.

Our main discussion does not depend on them: for Theorems A–F we need only develop the notion of gropes, grope forests, and their underlying decorated trees, as is done in the next Section 7.2.

Let us now discuss the corresponding notion of a universal *additive* invariant over a ring R. Consider $\mathbb{K}$ as a filtered monoid with the Gusarov–Habiro filtration $\mathbb{K} = \mathbb{K}_0 \supseteq \mathbb{K}_1 \supseteq \cdots$.

Definition 7.6. *Let $A = F_0 \supseteq F_1 \supseteq \cdots$ be a filtered R-module and $\widehat{A} := \lim {}^{A}\!/\!{}_{F_n}$. A universal additive Vassiliev knot invariant over R is a map of* filtered monoids *$\zeta\colon \mathbb{K} \to \widehat{A}$ which induces an isomorphism on the associated graded R-modules, that is*

$$\zeta_n|_{\mathbb{K}_n} \otimes R\colon\ {}^{\mathbb{K}_n}\!/\!{}_{\sim_{n+1}} \otimes R \lhook\joinrel\twoheadrightarrow {}^{F_n}\!/\!{}_{F_{n+1}} \qquad \forall n \geq 0.$$

We say that ζ is classical if the composite $(\overline{\zeta}_n|_{\mathbb{K}_n} \otimes R) \circ (\mathcal{R}_n^T \otimes R)$ is the identity on $\mathcal{A}_n^T \otimes R = {}^{F_n}\!/\!{}_{F_{n+1}}$.

Remark 7.7. *Consider the completion of $\mathbb{K}$ over R with respect to the Gusarov–Habiro filtration*

$$\widehat{\mathbb{K}}_R := \lim \big({}^{\mathbb{K}}\!/\!{}_{\sim_n} \otimes R\big).$$

If ζ is a universal additive Vassiliev knot invariant over R then the induced map $\widehat{\zeta}\colon \widehat{\mathbb{K}}_R \to \widehat{A}$ is an isomorphism of complete filtered R-modules.

Similarly as before, a universal additive invariant ζ indeed satisfies a *universality property*: any additive invariant $v\colon \mathbb{K} \to T$ of type $\leq n$ with values in an R-module T is a sum $\sum_{k=1}^{n} v_k \circ \overline{\zeta}_k$.

Note however that this definition is more flexible than Definition 7.1, since the completion on $\widehat{A}$ is with respect to a filtration instead of a grading. For example, we could take $R = \mathbb{Z}$, $A = \mathbb{K}$ and the obvious map $\zeta\colon \mathbb{K} \to \lim {}^{\mathbb{K}}\!/\!{}_{\sim_n}$, which satisfies the conditions. This is precisely Habiro's universal additive invariant ν [Hab00, Thm. 6.17].

A universal additive Vassiliev invariant over $\mathbb{Q}$ can be given as the logarithm either of the Kontsevich or the Bott-Taubes integral Z from (7.3), which are both grouplike [Kon93; AF97]:

$$z := \log(Z)\colon \mathbb{K} \to \mathrm{pr}(\widehat{\mathcal{A} \otimes \mathbb{Q}}) \cong \widehat{\mathcal{A}^T \otimes \mathbb{Q}}.$$

Recall that Conjecture 1 claims that the evaluation map $\pi_0\mathsf{ev}_n$ factors through an isomorphism

$$\pi_0\mathsf{ev}_n\colon \mathbb{K}/\sim_n \to \pi_0\mathsf{P}_n(I^3), \quad \forall n \geq 1.$$

This is equivalent to the claim that the total evaluation map

$$e_\infty := \lim \pi_0\mathsf{ev}_n\colon \mathbb{K} \longrightarrow \lim \pi_0\mathsf{P}_n(I^3)$$

is a universal additive Vassiliev invariant over $\mathbb{Z}$ in the sense of Definition 7.6, where the filtration on the target is by abelian groups $F_k := \ker\big((\lim \pi_0\mathsf{P}_n(I^3)) \twoheadrightarrow \pi_0\mathsf{P}_k(I^3)\big)$. See also (2.13).

See Appendix B for a discussion of the finite type theory for pure braid groups, which closely parallels the content of this section, but is also simpler in certain regards. For example, the role of groups $\mathcal{A}^T$ of Jacobi trees is played by the Drinfeld-Kohno Lie algebra $\mathfrak{p}(m)$, which is torsion-free.

General 3-manifolds

The definition of the Vassiliev–Gusarov filtration $\mathcal{V}_n(M) \subseteq \mathbb{Z}[\mathbb{K}(M)]$ generalises from $M = I^3$ to any 3-manifold M completely analogously. Namely, we simply take singular knots in M and resolve their double points in all possible ways.

It is also straightforward to define the Gusarov–Habiro filtration $\mathbb{K}_n(M;\mathrm{U})$ on the set $\mathbb{K}(M)$, since claspers and gropes are defined in any M, as we will see in Section 7.2. The filtration is in general only by subsets, but in Section 10 we will show that $\mathbb{K}_n(M;\mathrm{U})/\sim_{n+1}$ is always an abelian group.

Moreover, the equivalence from Theorem 7.4 of the clasper version (3) and the grope version (4) was shown in [CT04b] for any 3-manifold M, so two knots are n-equivalent if there is either a sequence of claspers or grope cobordisms between them. However, it is still an open problem if they are equivalent to the Vassiliev version (1).

In other words, if we say that two knots $[K], [K'] \in \mathbb{K}(M)$ are $\mathcal{V}_n$-equivalent if their formal difference $[K] - [K'] \in \mathbb{Z}[\mathbb{K}(M)]$ lies in $\mathcal{V}_n(M)$, then the following is open unless $M = I^3$.

Conjecture 7.8 ([Hab00]). *Two knots in a 3-manifold M are $\mathcal{V}_n$-equivalent if and only if they are n-equivalent.*

Some open problems

(1) Are rational Vassiliev invariants complete: is it true that $\bigcap_{n=1}^{\infty} \mathcal{V}_n \otimes \mathbb{Q} = \emptyset$?
(2) Do Vassiliev invariants detect the unknot? Equivalently, is it true that $\bigcap_{n=1}^{\infty} \mathbb{K}_n = \{[\mathrm{U}]\}$?[30]
(3) Do Vassiliev invariants distinguish oriented knots?
(4) Can Vassiliev invariants distinguish a knot from its orientation reverse?
(5) Is the abelian group $\mathcal{V}_n/\mathcal{V}_{n+1}$ torsion-free for all $n \geq 1$?
(6) Is the abelian group $\mathcal{A}_n$ is torsion-free for all $n \geq 1$.[31]
(7) Do Kontsevich and Bott–Taubes integrals agree?
(8) Does Theorem 7.4 hold for knots in an arbitrary 3-manifold? (Conjecture 7.8)

See also Problems 1.92 (L-N) in Kirby's list [Kir78], and [CDM12] for a survey of partial progress on some of these problems.

[30] This would follow from the Volume Conjecture, see [MM01].
[31] This implies the preceding conjecture, see Remark 7.3.

7.2 Grope cobordisms, thick gropes and grope forests

7.2.1 Abstract gropes. For a finite non-empty set S we defined the set of (rooted vertex-oriented uni-trivalent) trees $\mathrm{Tree}(S)$ in Definition 2.1. Now we define certain 2-complexes modelled on such trees. Grope cobordisms will be their particular embeddings into a 3-manifold M.

Definition 7.9. *A punctured torus T is a genus one compact oriented surface with one boundary component ∂T, see Figure 15. We fix an oriented subarc $a_0 \subseteq \partial T$ and view T as the plumbing of two ordered bands b_1 and b_2. The core curve $\beta_j \subseteq b_j$ is oriented for $j = 1$ (2) in the same (opposite) manner as the boundary component of b_j which contains a part of a_0.*[32]

An abstract (capped) grope G_Γ modelled on $\Gamma \in \mathrm{Tree}(S)$ is a 2-complex with boundary $\partial G_\Gamma = a_0 \cup a_0^\perp$ built inductively on $|S|$ as follows.

- *For $S = \{i\}$ the only tree is $\Gamma = \overset{i}{|}$ and we let G_Γ simply be an oriented disk, the i-th cap, with a chosen oriented subarc a_0 of the boundary.*
- *For $|S| \geq 2$ any tree $\Gamma \in \mathrm{Tree}(S)$ is obtained by grafting two trees of lower degrees*
$$\Gamma = \overset{\Gamma_2 \quad \Gamma_1}{\curlyvee}, \qquad \Gamma_j \in \mathrm{Tree}(S_j), \quad S_1 \sqcup S_2 = S.$$
Thus, abstract gropes G_{Γ_1} and G_{Γ_2} are defined by the induction hypothesis. Let G_Γ be the result of attaching both of them to a single punctured torus T, called the bottom stage of G_Γ, via orientation-preserving homeomorphisms $\partial G_{\Gamma_j} \cong \beta_j \subseteq T$, for $j = 1, 2$. Moreover, let $\partial G_\Gamma := \partial T$ be the boundary of the bottom stage and $a_0 \subseteq \partial G_\Gamma$ the corresponding oriented subarc of ∂T.

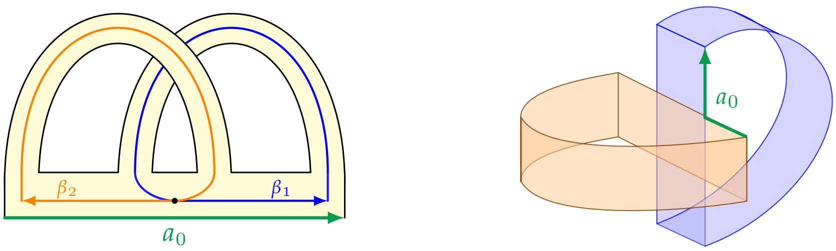


Figure 15. The model of a punctured torus as the plumbing of two bands.

Note that G_Γ has precisely $|S|$ caps (this is its degree), labelled bijectively by S. By a stage of a grope we mean any of the punctured tori or caps it contains; each stage of a grope is an oriented surface. Observe that a thickening of the 2-complex G_Γ, that is, the union of products of all stages with an interval, is homeomorphic to $\mathbb{B}^3$ (see also Figures 21 and 23).

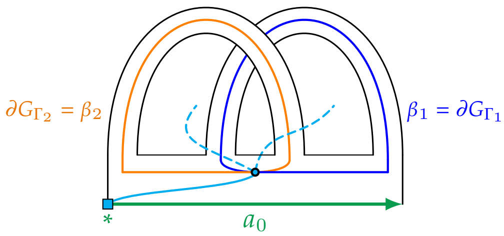


Figure 16. The underlying tree is obtained by gluing the light blue arcs for each stage.

Abstract gropes are just combinatorial objects: there is a 1–1 correspondence between them and rooted trees. In fact, the tree Γ on which G_Γ was modelled can be seen as its subset $\Gamma \subseteq G_\Gamma$, called

[32] This choice is made so that the boundary is homotopic to $[\beta_1, \beta_2] = \beta_1\beta_2\beta_1^{-1}\beta_2^{-1}$.

the underlying tree of G_Γ, as follows. The root of Γ is the initial point $*$ of $a_0 \subseteq \partial G_\Gamma$, and each trivalent vertex of Γ is the intersection point $\beta_1 \cap \beta_2$ in the corresponding grope stage. The leaves of Γ are the centres of caps. Finally, the edges are obtained at each stage as in Figure 16, and are cyclically ordered using the order (β_1, β_2), which agrees with the corresponding vertex orientation in Γ. This construction is equivalent to the one from [CST07, Def. 16 & Sec. 3.4].

7.2.2 Grope cobordisms. Recall that $K_{\widehat{0}}$ denotes the restriction of K to $I \setminus J_0$.

Definition 7.10. *Let $K \in \mathcal{K}(M)$ and $\Gamma \in \mathrm{Tree}(S)$ for a finite nonempty set $S \subseteq \mathbb{N}$. A (simple capped genus one) grope cobordism*[33] *on K modelled on Γ is is an embedding $\mathcal{G}\colon G_\Gamma \to M$ into the complement of K except that:*

- *$\mathcal{G}(a_0) \subseteq K(J_0)$ and the orientations of these arcs agree;*
- *for each $i \in S$, the i-th cap intersects $K_{\widehat{0}}$ transversely in exactly one point $p_i \in K_{\widehat{0}}$, which is the centre of the cap and which belongs to $K(J_i) \subseteq K_{\widehat{0}}$.*

We see $\mathcal{G}$ as a cobordism between K and the output knot $\partial^\perp\mathcal{G} := K_{\widehat{0}} \cup \mathcal{G}(a_0^\perp)$, smoothened at the corners and oriented compatibly with the orientation of $K_{\widehat{0}}$ (so $\mathcal{G}(a_0^\perp)$ is oriented oppositely in $\partial^\perp\mathcal{G}$ than as a subset of $\mathcal{G}$, as usual for oriented cobordisms). For examples see Figures 17, 18 and 20.

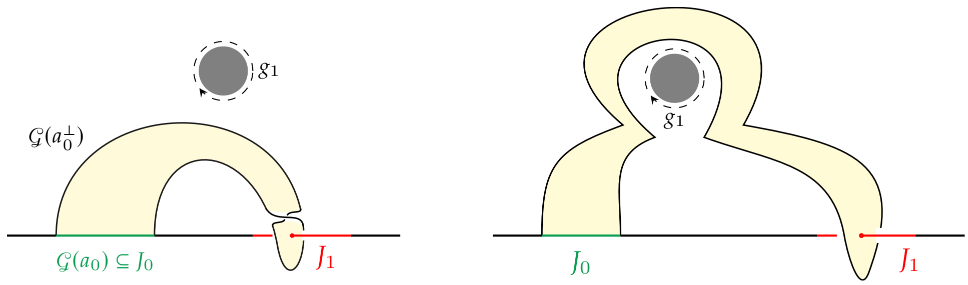


Figure 17. Two grope cobordisms of degree 1 on $K\colon I \hookrightarrow M$ (the horizontal line). In both cases $\partial^\perp\mathcal{G}$ is the union of black and red arcs; the left one is contained in $I^3 \subseteq M$ and is isotopic to the trefoil.

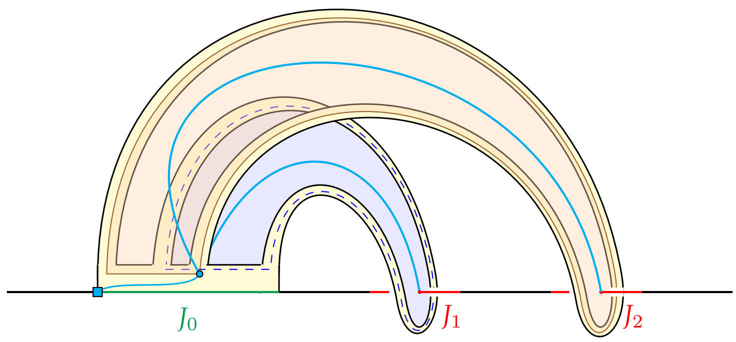


Figure 18. A grope cobordism $\mathcal{G}\colon G_\Gamma \to I^3$ on $K = \mathrm{U}$ with the underlying tree $\mathcal{G}($ $\overset{2\ \ 1}{\curlyvee}$ $)$ depicted in light blue. The knot $\partial^\perp\mathcal{G}$ is the union of $\mathrm{U}_{\widehat{0}}$ and the long black arc $\mathcal{G}(a_0^\perp)$.

Remark 7.11. *The crucial observation is that the arc $\mathcal{G}(a_0^\perp)$ is an 'embedded commutator' of the curves $\mathcal{G}(\beta_1)$ and $\mathcal{G}(\beta_2)$. For example, for $\mathcal{G}$ from Figure 18 the arc $\mathcal{G}(a_0^\perp)$ represents the commutator of the meridians of arcs $K(J_1)$ and $K(J_2)$, as for the Borromean link.*

[33] Non-simple, non-capped and higher genus gropes are also considered in the literature, but will not be needed in our discussion. However, grope forests defined below in Definition 7.14 are related to higher genus grope cobordisms.

Figure 19. *Left*: The knot $\partial^{\perp}\mathcal{G}$ from Figure 18. *Right*: 'Swinging' the bands of $\partial^{\perp}\mathcal{G}$ gives an isotopy which introduces twists into the bands; this is a standard projection of the right-handed trefoil where a Seifert surface is clearly visible. For the usual projection see Example 2.25.

We will see in Section 10.1 that the edges of the underlying tree of a grope can be framed in a unique way (using their framings in the surface stages) to get a clasper [CT04b]; this will also exhibit the connection to 'iterated' Borromoean links.

7.2.3 The underlying decorated tree. For a grope cobordism $\mathcal{G}\colon G_\Gamma \to M$ on a knot K we now extend its model tree $\Gamma \in \mathrm{Tree}(S)$ to a $\pi_1(M)$-decorated tree (from Definition 2.5).

Definition 7.12. *Let $\gamma_i^{\perp}\colon I \to M$ be the path from $K(L_0)$ to p_i obtained as the image under $\mathcal{G}$ of the unique path in the tree $\Gamma \subseteq G_\Gamma$ from the root to its i-th leaf. Let $[p_i, K(L_0)]$ be the image of K between $p_i \in K(J_i) \cap \mathcal{G}(G_\Gamma)$ and $K(L_0)$ (see Figure 22). Then we have a loop in M given by*

$$\gamma_i := \gamma_i^{\perp} \cup [p_i, K(L_0)]$$

Let $\varepsilon_i := \mathrm{sgn}(p_i) \in \{\pm\}$ be the sign of the intersection of $K(J_i)$ and the i-th cap of $\mathcal{G}$. The tuple $(\varepsilon_i, \gamma_i)_{i\in S}$ is called the signed decoration *of $\mathcal{G}$.*

Lastly, define the underlying decorated tree *of $\mathcal{G}$ by $\varepsilon\Gamma^{g_S} \in \mathbb{Z}[\mathrm{Tree}_{\pi_1(M)}(S)]$, where $\varepsilon := \prod_{i=1}^{n} \varepsilon_i$ and $g_S(\mathcal{G}) \in (\pi_1 M)^S$ is the tuple of classes $g_i = [\gamma_i] \in \pi_1 M$.*

In other words, γ_i is obtained by gluing two different paths from $K(L_0)$ to p_i: the obvious one along K, and the one that goes 'through the grope', following $\mathcal{G}(\Gamma) \subseteq \mathcal{G}(G_\Gamma) \subseteq M$, see Figure 18. For that example we have trivial group elements and $\varepsilon_1 = +1$, $\varepsilon_2 = -1$, while for Figure 20 we see $g_{\underline{2}} = (g_1, g_2)$ and $\varepsilon_1 = \varepsilon_2 = +1$. The signs of grope cobordisms in Figure 17 are respectively $\varepsilon(\mathcal{G}) = \varepsilon_1 = -1$ and $+1$, and for the latter the group element is computed in Figure 22.

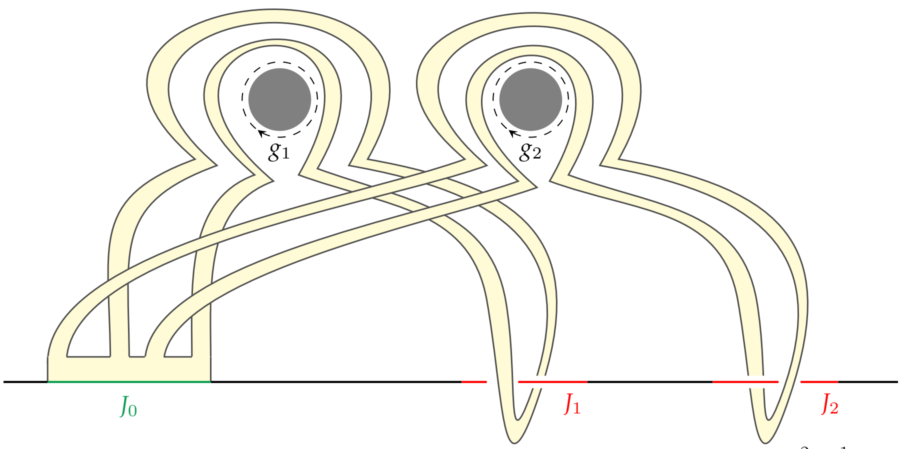
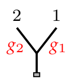


Figure 20. A grope cobordism $\mathcal{G}$ in a manifold M whose underlying decorated tree is  . If $M = I^3$ and K is the unknot, then $\partial^{\perp}\mathcal{G}$ is the figure eight knot.

7.2.4 Thick gropes. A regular neighbourhood of a grope cobordism $\mathcal{G}$ is diffeomorphic to a ball $\mathbf{G}\colon \mathbb{B}^3 \hookrightarrow M$, since inductively we are just thickening the punctured torus and attaching cancelling 3-dimensional 2-handles. The 3-ball $\mathbf{G}$ intersects the knot K in subarcs $\mathbf{G}(a_i) \subseteq J_i$, $1 \leq i \leq n$, which are neighbourhoods in K of the intersection points $p_i \in K(J_i)$, where $a_i \subseteq \mathbb{B}^3$ are some neatly embedded arcs (meaning $a_i \cap \partial\mathbb{B}^3 = \partial a_i$). See Figure 21.

It is convenient to fix a choice of such a neighbourhood $\mathbf{G}$ as follows; let us pick some $\varepsilon > 0$.

Definition 7.13. *A thick grope on $K \in \mathcal{K}(M)$ modelled on a tree $\Gamma \in \mathrm{Tree}(S)$ is an embedding*

$$\mathbf{G}\colon \mathsf{B}_\Gamma \hookrightarrow M$$

which does not intersect K except that $\mathbf{G}(a_i) \subseteq K(J_i)$ for certain arcs $a_i \subseteq \mathsf{B}_\Gamma$, $i \in \{0\} \sqcup S$. Here the model ball $\mathsf{B}_\Gamma \cong \mathbb{B}^3$, its set of arcs and a subset $G_\Gamma \subseteq \mathsf{B}_\Gamma$ are defined inductively on $|S|$ as follows.

For the induction base, we have $c = \overset{i}{|}$ and we define $\mathsf{B}_c := G_c \times I \cong \mathbb{D}^2 \times I$ and $G_c := G_c \times \{0\}$. The arc a_i is defined as the core $(0,0) \times I$ and the arc a_0 is the distinguished subarc of ∂G_c.

For $\Gamma = \overset{\Gamma_2 \ \Gamma_1}{\curlyvee}$ define B_Γ as the plumbing of the already defined model balls B_{Γ_1} and B_{Γ_2} along the respective squares $a_0 \times [-\varepsilon, \varepsilon] \subseteq \partial\mathsf{B}_{\Gamma_j}$ (by first swapping the two coordinates, as usual). Let $\{a_i\}_{i\in S}$ be the disjoint union of the sets of arcs for B_{Γ_1} and B_{Γ_2}.

Define the abstract grope $G_\Gamma \subseteq \mathsf{B}_\Gamma$ as the plumbing of the bands $\partial G_{\Gamma_j} \times [-\varepsilon, \varepsilon] \subseteq \partial\mathsf{B}_{\Gamma_j}$ along the squares $a_0 \times [-\varepsilon, \varepsilon]$. Finally, let a_0 for B_Γ be the distinguished arc in ∂G_Γ as in Definition 7.9.

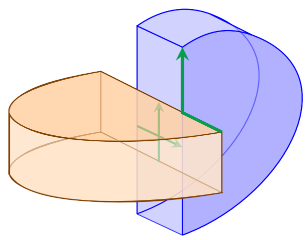


Figure 21. The plumbing of the blue ball B_{Γ_1} and the orange ball B_{Γ_2}.

Note that $\mathcal{G} := \mathbf{G}|_{G_\Gamma}$ is a grope cobordism on K in the sense of Definition 7.10. We can thus also define an underlying decorated tree $\varepsilon(\mathbf{G})\Gamma^{g(\mathbf{G})}$ of a thick grope as in Definition 7.12. Moreover, we define the output of $\mathbf{G}$ as the knot $\partial^\perp\mathbf{G} := \partial^\perp(\mathcal{G}) = K_{\widehat{0}} \cup \mathbf{G}(a_0^\perp)$, see Definition 7.9 and 7.10.

Conversely, for a given grope cobordism $\mathcal{G}$ and a choice of its regular neighbourhood, there is a unique thick grope $\mathbf{G}$ whose image is precisely that neighbourhood and $\mathbf{G}|_{G_\Gamma} = \mathcal{G}$.

7.2.5 Grope forests. Recall from Theorem 7.4 that two knots are n-equivalent if there exist a *sequence* of grope cobordisms between them. An analogue in our setting is a *disjoint collection of thick gropes* called a grope forest.

Definition 7.14. *A grope forest of degree n and cardinality $N \geq 1$ on a knot K is a map*

$$\mathbf{F} := \bigsqcup_{l=1}^{N} \mathbf{G}_l \colon \bigsqcup_{l=1}^{N} \mathsf{B}_{\Gamma_l} \hookrightarrow M$$

such that $\mathbf{G}_l\colon \mathsf{B}_{\Gamma_l} \hookrightarrow M$ are mutually disjoint thick gropes on K modelled on $\Gamma_l \in \mathrm{Tree}(n)$, and whose arcs $\mathbf{G}_l(a_0) \subseteq K(J_0)$ appear in $K(J_0)$ in the decreasing order of their indices $N \geq l \geq 1$.

The output knot $\partial^\perp\mathbf{F}$ is obtained from K by replacing each interval $\mathbf{G}_l(a_0)$ by the arc $\mathbf{G}(a_0^\perp)$ (the order in which replacements are done is irrelevant by the disjointness assumption).

Note that for a fixed $i \in \underline{n}$ we allow an arbitrary order of intersections of $K(J_i)$ with the i-th caps of different gropes, see Figure 22 for an example with $\mathrm{cap}_1(\mathbf{G}_1) < \mathrm{cap}_1(\mathbf{G}_2)$, but $\mathrm{cap}_2(\mathbf{G}_2) < \mathrm{cap}_2(\mathbf{G}_1)$.

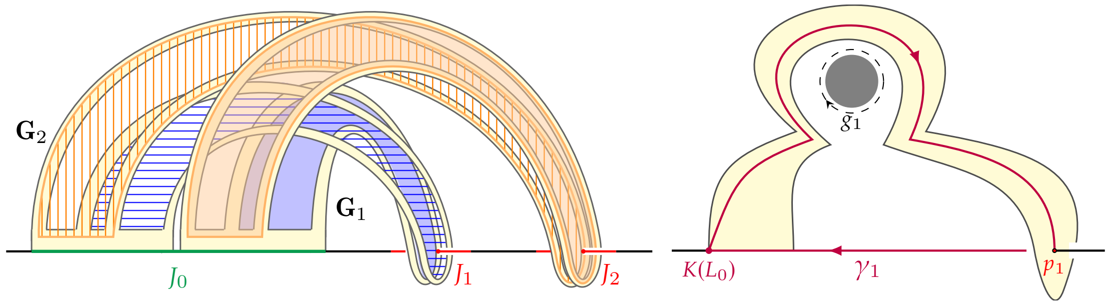


Figure 22. *Left*: A grope forest $\mathbf{F} = \mathbf{G}_1 \sqcup \mathbf{G}_2$ with $\mathcal{T}_2(\mathbf{F}) = 2\ {}^{1}\!\overset{2\quad 1}{\Upsilon}{}^{1}$ $\in \mathbb{Z}[\mathrm{Tree}_{\pi_1 M}(2)]$ is a thickening of the depicted 2-complex. *Right*: The homotopy class of $\gamma_1(\mathcal{G})$ is precisely $g_1 \in \pi_1 M$.

Grope forests are suitable for defining 'spaces of gropes' in a straightforward manner.

Definition 7.15. *Fix $K \in \mathcal{K}(M)$. The space of thick gropes on K modelled on $\Gamma \in \mathrm{Tree}(n)$ is the subspace $\mathcal{E}\mathrm{mb}_K(\mathsf{B}_\Gamma, M) \subseteq \mathcal{E}\mathrm{mb}(\mathbb{B}^3, M)$ of those embeddings satisfying conditions of Definition 7.13.*

Similarly, for $N \geq 1$ define $\mathcal{E}\mathrm{mb}_K(\bigsqcup_{l=1}^N \mathsf{B}_{\Gamma_l}, M) \subseteq \mathcal{E}\mathrm{mb}(\bigsqcup_N \mathbb{B}^3, M)$ to be the space of grope forests of cardinality N on K modelled on $(\Gamma_1, \dots, \Gamma_N)$ and let

$$\mathsf{Grop}_n^N(M;K) := \bigsqcup_{(\Gamma_1,\dots,\Gamma_N)\in\mathrm{Tree}(n)^N} \mathcal{E}\mathrm{mb}_K\left(\bigsqcup_{l=1}^{N} \mathsf{B}_{\Gamma_l}, M\right).$$

In particular, $\mathsf{Grop}_n^1(M;K)$ is the space of thick gropes on K. *Finally, the* space of all grope forests on K *is the disjoint union $\mathsf{Grop}_n(M;K) := \bigsqcup_{N\geq 1} \mathsf{Grop}_n^N(M;K)$.*

PROPOSITION 7.16. *There is a surjection of sets*

$$\mathcal{T}_n \colon \pi_0 \mathsf{Grop}_n(M;K) \twoheadrightarrow \mathbb{Z}[\mathrm{Tree}_{\pi_1 M}(n)],$$

which sends a grope forest $\bigsqcup_{l=1}^N \mathbf{G}_l \colon \bigsqcup_{l=1}^N \mathsf{B}_{\Gamma_l} \hookrightarrow M$ to the linear combination $\sum_{l=1}^N \varepsilon(\mathbf{G}_l) \cdot \Gamma_l^{g(\mathbf{G}_l)}$.

Proof. To prove that this map is well-defined, first consider $N = 1$. For a fixed tree Γ the only allowed isotopies of thick gropes modelled on Γ – that is, paths in the space $\mathcal{E}\mathrm{mb}_K(\mathsf{B}_\Gamma, M)$ – are those isotopies of the 3-ball $\mathsf{B}_\Gamma = \mathbb{B}^3$ which preserve the property that each special arc $a_i \subseteq \mathsf{B}_\Gamma$ is mapped into $K(J_i)$. Such an isotopy cannot change the homotopy classes $g_i(\mathbf{G}_l)$, so $\Gamma_l^{g(\mathbf{G}_l)}$ is an invariant. Similarly, the sign $\varepsilon_i(\mathbf{G}_l)$ as defined in Section 7.2.3 is positive if and only if the orientation $\mathbf{G}_l(a_i)$ agrees with the orientation of K. This is preserved during an isotopy.

An analogous argument applies to grope forests as well, considering one thick grope at a time.

For the surjectivity, let $\sum_{l=1}^N \varepsilon^l \Gamma_l^{g^l}$ be a linear combination of decorated trees, $\varepsilon^l \in \{\pm 1\}$. Any $g^l_{\underline{n-1}} \in (\pi_1 M)^{n-1}$ can be represented by a tuple of disjointly embedded loops $\gamma_i^l \subseteq M$. Thus, there is a map $\Gamma_l \to M$ which embeds the edges mutually disjointly, maps the i-th leaf to a point $p_i \in K(J_i)$ and has the associated path (from $K(L_0)$ to p_i along Γ and then back along K) isotopic to γ_i^l. Thicken this to a ball to get a thick grope $\mathbf{G}_l$, introducing a twist to one cap if $\varepsilon^l = -1$.

This can be done so that $\mathbf{G}_l$ are mutually disjoint (as they are neighbourhoods of 1-complexes), and that the order $\mathbf{G}_l(a_0)$ is decreasing with l, so this defines a desired grope forest. $\square$

8 Gropes and the Taylor tower

8.1 Gropes give paths in the Taylor tower

Let $\mathbf{G}$ be a thick grope in M on a knot K modelled on $\Gamma \in \mathrm{Tree}(n)$. According to Theorem D there is a path in $\mathsf{P}_n(M)$ between the evaluation of the output knot and of the original knot

$$\Psi^{\mathbf{G}} \colon \mathsf{ev}_n(\partial^{\perp}\mathbf{G}) \rightsquigarrow \mathsf{ev}_n(K).$$

In this section we prove this based on ideas from [KST], and also show there is a continuous map

$$\psi \colon \mathsf{Grop}^1_n(M;\mathrm{U}) \to \mathsf{H}_n(M), \quad \psi(\mathbf{G}) = (\partial^{\perp}\mathbf{G}, \Psi^{\mathbf{G}}). \tag{8.1}$$

We reformulate the theorem as the following proposition.

Recall that $f \in \mathsf{P}_n(M) := \operatorname{holim} \mathcal{E}_{\bullet}$ is given as a collection $f^S \colon \Delta^S \to \mathcal{E}\mathrm{mb}_{\partial}(I \setminus J_S, M)$ for $S \subseteq [n]$, which is compatible under inclusions $\iota_S \colon \Delta^S \hookrightarrow \Delta^{\underline{n}}$, see Notation 2. Recall also that K_{J_0} denotes the restriction of an arc K to $J_0 \subseteq I$, while $K_{\widehat{S}}$ denotes the restriction to $I \setminus J_S$.

Proposition 8.1. *For* $\mathbf{G}$ *as above there is a continuous map*

$$\mathscr{P}^{\mathbf{G}} \colon \Delta^{\underline{n}} \longrightarrow \mathrm{Map}_{\partial}\big([0,1], \mathcal{E}\mathrm{mb}_{\partial}(J_0, M)\big)\ ,\ \mathscr{P}^{\mathbf{G}}_u(0) = (\partial^{\perp}\mathbf{G})_{J_0}\ ,\ \mathscr{P}^{\mathbf{G}}_u(1) = K_{J_0},\ \forall u \in \Delta^{\underline{n}}$$

which gives a well-defined map $\Psi^{\mathbf{G}} \colon [0,1] \to \mathsf{P}_n(M)$ *taking* $\theta \in [0,1]$ *to*

$$\Psi^{\mathbf{G}}(\theta)^S \colon \Delta^S \to \mathcal{E}\mathrm{mb}_{\partial}(I \setminus J_S, M), \qquad \vec{t} \mapsto \begin{cases} K_{\widehat{S}}, & \text{if } 0 \in S, \\ K_{\widehat{0S}} \cup \mathscr{P}^{\mathbf{G}}_{\iota_S(\vec{t})}(\theta), & \text{if } 0 \notin S. \end{cases} \tag{8.2}$$

Let us outline the proof. Let $\mathcal{E}\mathrm{mb}_{\partial}(\mathbb{D}^2, \mathsf{B}_{\Gamma})$ denote the space of embeddings of disks in the model ball with the boundary condition $\partial\mathbb{D}^2 = \partial G_{\Gamma}$. Firstly, in Proposition 8.4 we construct a family of disks $\phi_{\Gamma} \colon \Delta^{\underline{n}} \longrightarrow \mathcal{E}\mathrm{mb}_{\partial}\big(\mathbb{D}^2, \mathsf{B}_{\Gamma}\big)$ satisfying certain condition (8.4). Then we choose a homeomorphism $[0,1] \times J_0 \to \mathbb{D}^2$. This gives an isotopy $j_{\theta} \colon J_0 \hookrightarrow \mathbb{D}^2$, $\theta \in [0,1]$, relative to the endpoints from one half of the boundary circle to the other across $\mathbb{D}^2$. Finally, for $u \in \Delta^{\underline{n}}$, $\theta \in [0,1]$ we define $\mathscr{P}^{\mathbf{G}}_u(\theta)$ as the composite

$$J_0 \xhookrightarrow{\ j_{\theta}\ } \mathbb{D}^2 \xhookrightarrow{\ \phi_{\Gamma}(u)\ } \mathsf{B}_{\Gamma} \xhookrightarrow{\ \mathbf{G}\ } M. \tag{8.3}$$

We will finish the proof by checking that $\Psi^{\mathbf{G}}$ is well-defined thanks to conditions (8.4). The continuity of (8.1) follows as well, since the space $\mathsf{Grop}^1_n(M;\mathrm{U})$ of thick gropes of degree n on U from Definition 7.15 was given the subspace topology $\mathsf{Grop}^1_n(M;\mathrm{U}) \subseteq \mathcal{E}\mathrm{mb}(\mathbb{B}^3, M)$.

The symmetric surgery

Let us first construct a 1-parameter family of disks $\mathbb{D}_u \subseteq \mathsf{B}_{\Gamma}$, $u \in \Delta^1$, for Γ an abstract grope modelled on the unique tree of degree $n = 2$ (Figure 23). This consists of a punctured torus (yellow) and two caps bounded by its core curves β_1 (blue) and β_2 (orange).

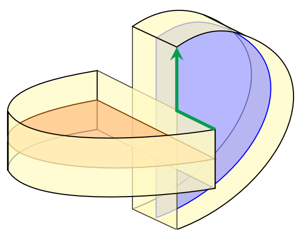
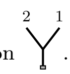


Figure 23. The abstract grope modelled on 

.

There is a classical construction of *ambient surgery* on a punctured torus $T \subseteq M$, using an embedded disk D whose interior is disjoint from T and with boundary a simple closed curve on T. Namely, we take out a neighbourhood of the curve $\partial D \subseteq T$ and glue to the newly created boundary two parallel copies of D, so that T is turned into an embedded disk.

Hence, when our abstract grope of degree 2 is embedded as a grope cobordism we can do two different ambient surgeries on it: on the first (respectively second) cap as depicted in the leftmost (rightmost) part of Figure 24. Note that the thick grope specifies concrete push-offs of caps.

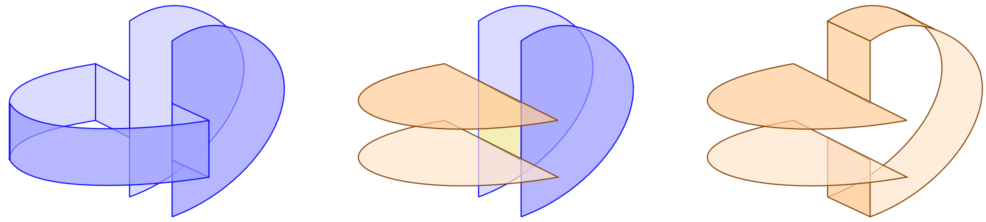


Figure 24. *Left*: The resulting disk $\mathbb{D}_1$ after the surgery along the cap 1 on G_Γ from Figure 23. *Middle*: The result of the symmetric surgery on G_Γ. *Right*: The result $\mathbb{D}_2$ of the surgery along the cap 2 on G_Γ.

In addition, one can do both surgeries at once, called the symmetric surgery (or contraction), as depicted in the middle part of Figure 24. The following lemma says that there actually exists a whole 1-parameter family of disks containing the three disks we have described.

LEMMA 8.2 (Symmetric Isotopy)**.** *For $\Gamma = \overset{2\ \ 1}{\curlyvee}$ there is an isotopy $\phi_\Gamma \colon [0,1] \to \mathcal{E}\mathrm{mb}_\partial(\mathbb{D}^2, \mathsf{B}_\Gamma)$ such that $\mathbb{D}_t$ for $t \in \{0,1\}$ is the surgery on G_Γ using the cap labelled by $1+t$.*

Proof. Recall that B_Γ is the model ball obtained by plumbing together $\mathsf{B}\overset{1}{\rfloor}$ and $\mathsf{B}\overset{2}{\rfloor}$. We now specify an isotopy from $\mathbb{D}_1 \subseteq \mathsf{B}_\Gamma$ to $\mathbb{D}_2 \subseteq \mathsf{B}_\Gamma$, which passes through the symmetric surgery, using Figure 24 as an accurate model of these disks.

First isotope the interior of the blue band of $\mathbb{D}_1$ by pushing it across the interior of the ball $\mathsf{B}\overset{2}{\rfloor}$, until we arrive at the symmetric surgery. In more detail, as t increases from 0 to $\frac{1}{2}$ we let the blue band 'stick more and more to the bottom and top orange disks', as shown in Figure 25, so that when $t = \frac{1}{2}$ the band has transformed into the union of the two orange disks and the yellow region.

The two 'sticking curves' (inside of the two orange disks, copies of the cap 2) are specified by an isotopy $j_\theta \colon J_0 \hookrightarrow \mathbb{D}^2$ which we fixed at the beginning of this section (also, smoothen the corners).

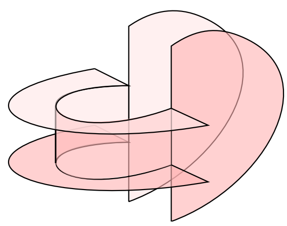


Figure 25. Disk $\mathbb{D}_t$ for some $t \in [0, \frac{1}{2}]$.

Symmetrically, for increasing $t \in [\frac{1}{2}, 1]$ the isotopy uses the ball $\mathsf{B}\overset{1}{\rfloor}$ to stretch the distinguished yellow region of the symmetric surgery, using the sticking curves on the blue disks as a guide, until reaching the position of the orange band for $t = 1$. $\square$

Remark 8.3. *It is precisely this isotopy that is a crucial ingredient for the connection between the geometric calculus and the Taylor tower. To construct paths in $\mathsf{P}_n(M)$ using claspers instead, it would be necessary to fix a 1-parameter family of homotopies of Borromean rings whenever one component is erased, but for trees of higher degrees these homotopies will increase in complexity. Specifying them explicitly would be cumbersome to do.*

Instead, gropes precisely keep track of all necessary homotopies in a canonical way, since they already contain all needed additional data, which is missing in the clasper picture. Moreover, we will use this exact choice of the isotopy in our crucial Lemma 9.2.

On the other hand, claspers are more convenient when one works modulo isotopy, see Section 10.

Families of disks

We now generalise the Symmetric Isotopy Lemma 8.2 to trees of any degree $n \geq 2$. We view Δ^S as the simplicial set obtained by barycentric subdivision from the standard simplex whose vertices were labelled by S (see Figure 26).

Figure 26. Examples of Δ^S for $S = \{2,3\}$ and $S = \underline{3}$.

Proposition 8.4. *Let a finite set $S \neq \emptyset$ and a tree $\Gamma \in \mathrm{Tree}(S)$ there is a continuous map*

$$\phi_\Gamma \colon \Delta^S \longrightarrow \mathcal{E}\mathrm{mb}_\partial(\mathbb{D}^2, \mathsf{B}_\Gamma)$$

describing a family $\mathbb{D}_u := \mathrm{im}\,\phi_\Gamma(u) \subseteq \mathsf{B}_\Gamma$ of neatly embedded disks in the model ball such that

$$(\forall i \in S) \quad \mathrm{int}(\mathbb{D}_u) \pitchfork a_i \neq \emptyset \implies i \in |\varsigma_u| \tag{8.4}$$

where $\varsigma_u \subseteq \Delta^S$ denotes the top dimensional simplex to which u belongs and $|\varsigma_u|$ its set of vertices.

Proof. We prove this by induction on $|S|$. For $|S| = 1$ we have $\Gamma = \overset{i}{|}$ and $|\Delta^S| = \Delta^0 = \{i\}$, so we need to construct only one disk $\mathbb{D}_i \subset \mathsf{B}_\Gamma$ whose boundary is the boundary of the grope and such that $\mathrm{int}(\mathbb{D}_i) \pitchfork a_1 \neq \emptyset$. Clearly, we can just let $\mathbb{D}_i := G_\Gamma$, since in this case the abstract grope is itself a disk, intersecting a_1 in one point.

Assume that we have defined the desired family for any tree of degree $< k$ for some $k \geq 2$, and consider S with $|S| = k$ and a tree $\Gamma \in \mathrm{Tree}(S)$ such that

$$\Gamma = \overset{\Gamma_2 \quad \Gamma_1}{\curlyvee}, \quad \Gamma_{\mathrm{j}} \in \mathrm{Tree}(S_{\mathrm{j}}),\ S = S_1 \sqcup S_2.$$

Pick $u \in \Delta^S$ and let us define $\mathbb{D}_u \subseteq \mathsf{B}_\Gamma$. Firstly, we identify $\Delta^S \cong \Delta^{S_1} \star \Delta^{S_2}$ with the join of the simplices $\Delta^{S_{\mathrm{j}}}$, so u is given as a linear combination

$$u = (1-t)u_1 + tu_2, \quad t \in [0,1],\ u_{\mathrm{j}} \in \Delta^{S_{\mathrm{j}}}.$$

The ball B_Γ is by definition the plumbing of the balls $\mathsf{B}_{\Gamma_{\mathrm{j}}}$ for $\mathrm{j} = 1, 2$, and since $1 \leq |S_{\mathrm{j}}| \leq |S| - 1$, by induction hypothesis we have maps $\phi_{\Gamma_{\mathrm{j}}}$ satisfying (8.4). In particular, we have disks $\mathbb{D}_{u_{\mathrm{j}}} \subseteq \mathsf{B}_{\Gamma_{\mathrm{j}}}$.

Let us pick some neat tubular neighbourhoods $\nu\mathbb{D}_{u_{\mathrm{j}}} \subseteq \mathsf{B}_{\Gamma_{\mathrm{j}}}$, so that $\partial(\nu\mathbb{D}_{u_{\mathrm{j}}}) \cap \partial\mathsf{B}_\Gamma = \partial G_{\Gamma_{\mathrm{j}}} \times [-\varepsilon, \varepsilon]$.

Then we can plumb $\nu\mathbb{D}_{u_1}$ and $\nu\mathbb{D}_{u_2}$ together along $a_0 \times [-\varepsilon, \varepsilon]$ and get a ball $\mathsf{B} \subseteq \mathsf{B}_\Gamma$ such that $G_\Gamma \subseteq \mathsf{B}$. Now by Lemma 8.2 there is an isotopy inside of B from the disk obtained by surgery on G_Γ along $\mathbb{D}_{u_1}$ to the disk obtained by surgery on G_Γ along $\mathbb{D}_{u_2}$.

Let $\mathbb{D}_u$ be the time t of that isotopy. Clearly $\partial\mathbb{D}_u = \partial G_\Gamma$. Let us show that the property (8.4) holds. Since $\mathbb{D}_u$ is contained in B, which is a sufficiently small neighbourhood of the disks $\mathbb{D}_{u_1}$ and $\mathbb{D}_{u_2}$, it will intersect an arc a_i only if one of those disks did. Hence, by the induction hypothesis i belongs either to $|\varsigma_{u_1}|$ or $|\varsigma_{u_2}|$, but $|\varsigma_u| = |\varsigma_{u_1}| \sqcup |\varsigma_{u_2}|$ by the definition of the join. $\square$

In particular, for $n = 2$ we have $u = (1-t)+2t = 1+t$ and so $\mathbb{D}_u = \mathbb{D}_{1+t}$ is precisely the isotopy from Lemma 8.2. Note how for an abstract grope of degree n each torus stage gives one independent parameter for the family, so there are $n-1$ parameters in total (remember that $|\Delta^{\underline{n}}| = \Delta^{n-1}$).

The end of the proof: isotopies across the disks

Proof of Proposition 8.1. As announced in (8.3) at the beginning of the section, we use the isotopy of the previous proposition for $S = \underline{n}$ and the given thick grope to define for $u \in \Delta^{\underline{n}}$ and $\theta \in [0,1]$

$$\mathscr{P}^{\mathbf{G}}_u(\theta)\colon\ J_0 \xhookrightarrow{j_\theta} \mathbb{D} \xhookrightarrow{\phi(u)} \mathsf{B}_\Gamma \xhookrightarrow{\mathbf{G}} M.$$

We clearly have $\mathscr{P}^{\mathbf{G}}_u(0) = (\partial^\perp\mathbf{G})_{J_0} = \mathbf{G}(a_0^\perp)$ and $\mathscr{P}^{\mathbf{G}}_u(1) = K_{J_0} = \mathbf{G}(a_0)$ for all $u \in \Delta^{\underline{n}}$. We claim that thanks to the condition (8.4), the map $\Psi^{\mathbf{G}}$ as defined in (8.2) is well-defined, that is

$$\Psi^{\mathbf{G}}(\theta)^S(\vec{t}) \ \in\ \mathscr{E}\mathrm{mb}_\partial(I \setminus J_S, M).$$

This is clear for $S \subseteq [n]$ such that $0 \in S$, since we then constantly have the punctured unknot $\mathrm{U}_{\widehat{S}}$. On the other hand, for $0 \notin S$ we need to check that for each $\vec{t} \in \Delta^S$ and $\theta \in [0,1]$ we have

$$\mathscr{P}^{\mathbf{G}}_u(\theta) \cap K_{\widehat{0S}} = \emptyset$$

where $u := \iota_S(\vec{t})$. Equivalently, if the interior of $\mathbf{G}(\mathbb{D}_u)$ intersects some $K(J_i)$, then $i \in S$.

Indeed, if $\mathrm{int}\mathbf{G}(\mathbb{D}_u) \cap K(J_i) \neq \emptyset$, then we must have $\mathrm{int}(\mathbb{D}_u) \cap a_i \neq \emptyset$, since $\mathbf{G}$ is an embedding. But then (8.4) implies that $i \in |\varsigma_u|$. As u is obtained by inclusion from the face Δ^S, the maximal simplex that contains it must be contained in Δ^S. Hence, $i \in |\varsigma_u| \subseteq S$. $\square$

The extension to grope forests

Let us now extend Theorem D to grope forest.

PROPOSITION 8.5. *For a grope forest* $\mathbf{F}$ *of degree* n *on* K *there exists a path* $\Psi^{\mathbf{F}}\colon [0,1] \to \mathsf{P}_n(M)$ *from* $\mathsf{ev}_n(\partial^\perp\mathbf{F})$ *to* $\mathsf{ev}_n K$. *Moreover, this defines a map on the space of all grope forests*

$$\psi\colon \mathsf{Grop}_n(M;\mathrm{U}) \to \mathsf{H}_n(M)$$

which extends the map ψ *from the space of thick gropes* $\mathsf{Grop}^1_n(M;\mathrm{U}) \subseteq \mathsf{Grop}_n(M;\mathrm{U})$.

Proof. If $\mathbf{F} = \bigsqcup_{l=1}^N \mathbf{G}_l\colon \bigsqcup_{l=1}^N \mathsf{B}_{\Gamma_l} \hookrightarrow M$, then each $\mathbf{G}_l$ can be viewed as a thick grope on K. Indeed, it has $\mathbf{G}_l(a_0) \subseteq K_{J_0}$ and the conditions for all the arcs a_i, $i \in \underline{n}$, are satisfied.

Therefore, by Theorem D we have a path $\Psi^{\mathbf{G}_l}$ in $\mathsf{P}_n(M)$ from $\mathsf{ev}_n(\partial^\perp\mathbf{G}_l)$ to $\mathsf{ev}_n K$, which was constructed in Proposition 8.1 using the arcs $\mathscr{P}^{\mathbf{G}_l}_u(\theta)\colon J_0 \hookrightarrow M \setminus K_{\widehat{0S}}$. For a fixed $\theta \in [0,1]$ and $S \subseteq \underline{n}$ these arcs are pairwise disjoint for varying $l = 1,\dots,N$, because of the mutual disjointness of $\mathbf{G}_l$. Hence, we can concatenate them to get an arc

$$\Psi^{\mathbf{F}}(\theta)^S_{J_0} := \Psi^{\mathbf{G}_1}(\theta)^S_{J_0} \cdot \Psi^{\mathbf{G}_2}(\theta)^S_{J_0} \cdots \Psi^{\mathbf{G}_N}(\theta)^S_{J_0} \ \in\ \mathscr{E}\mathrm{mb}(J_0, M \setminus K_{\widehat{0S}}).$$

We then define $\Psi^{\mathbf{F}}$ analogously to the definition of $\Psi^{\mathbf{G}}$ in (8.2), by letting

$$\Psi^{\mathbf{F}}(\theta)^S : \Delta^S \to \mathcal{E}\mathrm{mb}_\partial(I \setminus J_S, M), \qquad \vec{t} \mapsto K_{\widehat{0S}} \cup \Psi^{\mathbf{F}}(\theta)^S_{J_0}. \tag{8.5}$$

for $\theta \in [0,1]$ and $S \subset [n]$. As in the proof of Proposition 8.1, this is indeed a path $\mathsf{ev}_n(\partial^\perp \mathbf{F}) \rightsquigarrow \mathsf{ev}_n K$.

Finally, for $K := \mathrm{U}$ let $\psi(\mathbf{F}) := (\mathrm{U}, \Psi^{\mathbf{F}}) \in \mathsf{H}_n(M)$. To see that this is a continuous map on the space of grope forests, note that moving within a component in that space preserves the order of roots of thick gropes, so arcs always get concatenated in the same order. Since the topology is given as the subspace topology of the space $\mathcal{E}\mathrm{mb}(\bigsqcup_N \mathbb{B}^3, M)$, small deformations of grope forests lead to small deformations of each of the arcs, keeping them disjoint. □

Remark 8.6. *A perhaps more obvious choice for $\Psi^{\mathbf{F}}$ would simply be*

$$\Psi^{\mathbf{G}_1} \cdot \Psi^{\mathbf{G}_2} \cdots \Psi^{\mathbf{G}_N} : I \to \mathsf{P}_n(M),$$

the concatenation of the paths in $\mathsf{P}_n(M)$. This will actually give an equivalent point $\mathsf{e}_n(\psi\mathbf{F}) \in \mathsf{F}_n(M)$, essentially because $\mathsf{F}_n(M)$ is an iterated loop space and – while our definition was concatenation in the J_0-direction, this definition corresponds to the concatenation in the 'diagonal' Ω^{n-1} direction. However, our choice will make the proof of Theorem F straightforward.

We omit the proof, only indicating that the two choices $\mathcal{D}\chi\mathsf{e}_n(\psi\mathbf{F}) \in \Omega^n \operatorname{tofib}(M_\bullet, \rho)$ can be compared using the description of $\chi\mathsf{e}_n(\psi\mathbf{F})$ in terms of the h-reflections of Proposition 6.6.

Note that this discussion implies that concatenation of thick gropes into a grope forest can be seen as a partially defined H-space or E_1 structure on the space $\mathsf{H}_{n-1}(M)$.

Let us demonstrate the map Ψ on an example in the lowest degree.

Example 8.7 (degree 1)**.** *A grope cobordism $\mathcal{G}$ on K modelled on $\Gamma = \overset{1}{|}$ is simply a disk (see Figure 17 for examples) guiding a crossing change homotopy K_θ from $K_0 = \partial^\perp \mathbf{G}$ to $K_1 = K$. The corresponding thick grope $\mathbf{G}$ is a tubular neighbourhood of this disk.*

Its underlying decorated tree is a decorated chord $\overset{1}{|}{}^{g}$ for some element $g \in \pi_1(M)$.

The disk family in this case consists of a single disk $\mathbb{D} \subseteq \mathsf{B}_\Gamma$ and $\mathbf{G}(\mathbb{D}) = \mathcal{G} \subseteq M$. The map $\mathscr{P}^{\mathbf{G}} : \Delta^0 \to \mathrm{Map}_\partial\big([0,1], \mathcal{E}\mathrm{mb}_\partial(J_0, M)\big)$ swings the arc $\mathbf{G}(a_0^\perp)$ across $\mathbf{G}(\mathbb{D})$ to K_{J_0}. Note that the path through immersions $K_{\widehat{0}} \cup \mathscr{P}^{\mathbf{G}}(\theta)$ is precisely K_θ, $\theta \in [0,1]$.

The path $\Psi^{\mathbf{G}} : [0,1] \to \mathsf{P}_1(M) = \operatorname{holim}_{\mathscr{P}_\nu[1]} \mathcal{E}^1_\bullet$ is hence given by

$$\Psi^{\mathbf{G}}(\theta)^{\{0\}} : \Delta^0 \to \mathcal{E}\mathrm{mb}(I \setminus J_0, M), \quad pt \mapsto K_{\widehat{0}}$$
$$\Psi^{\mathbf{G}}(\theta)^{\{1\}} : \Delta^0 \to \mathcal{E}\mathrm{mb}(I \setminus J_1, M), \quad pt \mapsto (K_\theta)_{\widehat{1}}$$
$$\Psi^{\mathbf{G}}(\theta)^{\{01\}} : \Delta^1 \to \mathcal{E}\mathrm{mb}(I \setminus I_{01}, M), \quad t \mapsto K_{\widehat{01}}, \quad \forall t \in \Delta^1$$

Only $\Psi^{\mathbf{G}}(-)^{\{1\}} : \Delta^0 \to \mathcal{E}\mathrm{mb}_\partial(I \setminus J_1, M)$ is not constant with $\theta \in [0,1]$. It is the isotopy between $(\partial^\perp\mathbf{G})_{\widehat{1}}$ and $K_{\widehat{1}}$ – the crossing change homotopy, now unobstructed since J_1 is gone.

See also Figure 27 for the corresponding points $\psi(\mathbf{G}) \in \mathsf{H}_1(M)$ and $\mathsf{e}_2\psi(\mathbf{G}) \in \mathsf{F}_2(M)$. △

8.2 Gropes give points in the layers

Given a thick grope $\mathbf{G} \in \mathsf{Grop}_{n-1}(M; \mathrm{U})$ we obtain a point

$$\psi(\mathbf{G}) := (\partial^\perp \mathbf{G}, \Psi^{\mathbf{G}}) \in \mathsf{H}_{n-1}(M).$$

Since $\mathsf{H}_{n-1}(M) := \mathrm{hofib}(\mathsf{ev}_{n-1}) \cong \mathrm{tofib}_{S\subseteq[n-1]}(\mathcal{E}_S)$, in the latter coordinates this is given by

$$\psi(\mathbf{G})^S = \begin{cases} I^0 \xrightarrow{\partial^\perp \mathbf{G}} \mathcal{E}_\emptyset, & S = \emptyset \\ I^S \xrightarrow{\hbar^S} \mathcal{C}^{bar}(\Delta^S) \xrightarrow{\Psi^{\mathbf{G}}(-)^S} \mathcal{E}_S, & \emptyset \neq S \subseteq \underline{n-1} \end{cases}$$

where $\hbar^\bullet$ is the homeomorphism of cubes from (3.5), needed for the translation from the definition of a total fibre as a homotopy fibre to its description in terms of maps of cubes. In Section 3.2 we also saw that $\mathrm{tofib}_{S\subseteq[n-1]}\,\mathcal{E}_S$ is homotopy equivalent to its subspace $\mathrm{tofib}_{S\subseteq\underline{n-1}}\,\mathscr{F}_S$.

LEMMA 8.8. *$\psi(\mathbf{G})$ lies in the subspace* $\mathrm{tofib}(\mathscr{F}_S)$ *and in the coordinates $\mathscr{F}_S \cong \mathcal{E}\mathrm{mb}_\partial(J_0, M \setminus \mathrm{U}_{\widehat{0S}})$ it is given simply by restricting $\psi(\mathbf{G})^S$ to $J_0 \subseteq I$.*

Proof. It is enough to check that for $S \subseteq [n-1]$ with $S \ni 0$ the map $\psi(\mathbf{G})^S\colon I^S \to \mathcal{E}_S$ is constantly equal to $\mathrm{U}_{\widehat{S}}$ (since then the only non trivial part of $\psi(\mathbf{G})^S$ for $S \not\ni 0$ is $\psi(\mathbf{G})^S|_{J_0}$). However, this is clear from $\psi(\mathbf{G})^S := \Psi^{\mathbf{G}}(-)^S \circ \hbar^S$ and the very definition $\Psi^{\mathbf{G}}(\theta)^S = \mathrm{U}_{\widehat{S}}$ in (8.2). □

Recall that $\mathsf{F}_n(M)$ is also homotopy equivalent to its subspace $\mathrm{tofib}_{S\subseteq\underline{n-1}}(\mathscr{F}^n_S)$ (whose homotopy type we studied in Sections 4 and 5) and in (3.10) we saw that $\mathsf{e}_n\colon \mathsf{H}_{n-1}(M) \to \mathsf{F}_n(M)$ corresponds to the map $r^n_*\colon\ \mathrm{tofib}(\mathscr{F}_S) \to \mathrm{tofib}(\mathscr{F}^n_S)$ induced by postcomposition with $\rho^n_S\colon M \setminus \mathrm{U}_{\widehat{0S}} \hookrightarrow M \setminus \mathrm{U}_{\widehat{0Sn}}$.

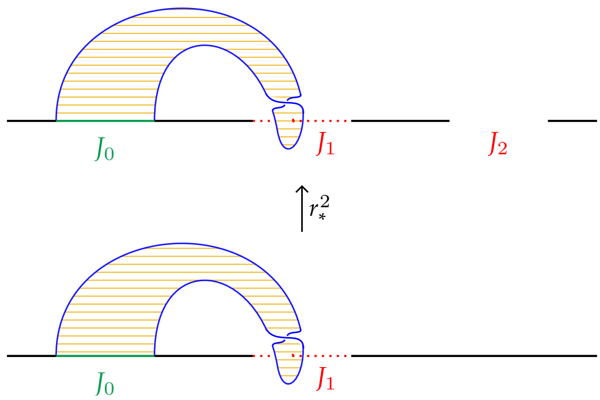


Figure 27. *Bottom*: A point $\psi(\mathbf{G}) \in \mathrm{tofib}(\mathscr{F}_S) = \mathsf{H}_1(M)$ consists of the blue arc $\psi(\mathbf{G})^\emptyset := \mathbf{G}(a_0^\perp) \in \mathscr{F}_\emptyset$ and the path $\psi(\mathbf{G})^1 := \Psi^{\mathbf{G}}(-)^1_{J_0} : I^1 \to \mathscr{F}_1$ across the yellow disk. *Top*: To get the point $\mathsf{e}_2(\psi(\mathbf{G})) \in \mathrm{tofib}(\mathscr{F}^2_S) = \mathsf{F}_1(M)$ we simply introduce one more puncture into the ambient space.

Hence, the image under the evaluation map of our grope point is (recalling that $(\partial^\perp\mathbf{G})_{J_0} = \mathbf{G}(a_0^\perp)$)

$$f_{\mathbf{G}} := \mathsf{e}_n\psi(\mathbf{G}) = \begin{cases} I^0 \xrightarrow{\mathbf{G}(a_0^\perp)} \mathscr{F}^n_\emptyset\ , & S = \emptyset, \\ I^S \xrightarrow{\hbar^S} \mathcal{C}^{bar}(\Delta^S) \xrightarrow{\Psi^{\mathbf{G}}(-)^S_{J_0}} \mathscr{F}^n_S\ , & \emptyset \neq S \subseteq \underline{n-1}. \end{cases} \tag{8.6}$$

Similarly, for $\mathbf{F} \in \mathsf{Grop}_{n-1}(M;\mathrm{U})$ the corresponding point in $\mathsf{F}_n(M)$ is given by

$$f_{\mathbf{F}} := \mathsf{e}_n\psi(\mathbf{F}) = \begin{cases} I^0 \xrightarrow{(\partial^\perp\mathbf{F})_{J_0}} \mathscr{F}^n_\emptyset\ , & S = \emptyset, \\ I^S \xrightarrow{\hbar^S} \mathcal{C}^{bar}(\Delta^S) \xrightarrow{\Psi^{\mathbf{G}_1}(-)^S_{J_0}\cdot\ldots\cdot\Psi^{\mathbf{G}_N}(-)^S_{J_0}} \mathscr{F}^n_S\ , & \emptyset \neq S \subseteq \underline{n-1}. \end{cases} \tag{8.7}$$

where $\Psi^{\mathbf{G}_l}(-)^S_{J_0}\colon \mathcal{C}^{bar}(\Delta^S) \to \mathscr{F}^n_S$ are concatenated pointwise, along their J_0 direction.

9 Proofs of Theorems E and F

Let $\mathbf{G}\colon \mathsf{B}_\Gamma \hookrightarrow M$ be a thick grope on U with the underlying decorated tree $\varepsilon\Gamma^{g_{\underline{n-1}}} \in \mathrm{Tree}(n-1)$. In the previous section we have constructed $\psi(\mathbf{G}) \in \mathsf{H}_{n-1}(M)$ and in (8.6) we described the point

$$f_{\mathbf{G}} \;:=\; \mathsf{e}_n\psi(\mathbf{G}) \quad \in \mathsf{F}_n(M).$$

In this section we prove Theorem E – namely, that

$$[f_{\mathbf{G}}] \;=\; [\varepsilon\Gamma^{g_{\underline{n-1}}}] \quad \in \pi_0\mathsf{F}_n(M) \cong \mathsf{Lie}_{\pi_1 M}(n-1).$$

In Section 5.3 we have reduced this to checking (5.11), that is

$$\mathscr{D}_{\underline{n-1}}\,(\chi f_{\mathbf{G}})^{\underline{n-1}} \;\simeq\; \Gamma(m_i^{\varepsilon_i\gamma_i})\colon \quad \mathbb{S}^{n-1} \to \Omega M_{\underline{n-1}}. \tag{9.1}$$

where $\varepsilon_i \in \{\pm 1\}$ and $\gamma_i \in \Omega M$ with $i \in \underline{n-1}$ are signed decorations of $\mathbf{G}$, and $g_i = [\gamma_i]$.

Remark 9.1 (A reminder)**.**

- *The map* $\chi\colon \mathsf{F}_n(M) \to \Omega^{n-1}\,\mathrm{tofib}(\mathscr{F}^n_\bullet, l)$ *was defined in Proposition 4.8 using left homotopy inverses* $l^k_S = (d^k_S(1)\circ e^k_S)\circ -$ *and homotopies* $h^k_s = (d^k_S(s)\circ \mathsf{add}_s)\circ -$ *constructed in Section 4.1. The map* $(\chi f_{\mathbf{G}})^{\underline{n-1}}\colon \mathbb{S}^{n-1} \to \mathscr{F}^n_{\underline{n-1}}$ *is simply the coordinate of* $\chi f_{\mathbf{G}}$ *indexed by* $\underline{n-1}$.
- *For* $S \subseteq \underline{n-1}$ *the map* $\mathscr{D}_S\colon \mathscr{F}^n_S \to \Omega M_S := \Omega(M \setminus \mathbb{B}_S)$ *which takes a punctured knot* $\kappa\colon J_0 \hookrightarrow M_S$ *to the loop obtained by concatenating* U_{J_0} *and the arc* κ *in reverse (see Remark 4.13).*
- *The map* $\Gamma(m_i^{\varepsilon_i\gamma_i})$ *on the right hand side of* (9.1) *is the Samelson product according to the word* $\omega_2(\Gamma)$ *of the maps* $m_i^{\varepsilon_i\gamma_i}\colon \mathbb{S}^1 \to \Omega M_{\underline{n-1}}$*. These are given by* $m_i^{\varepsilon_i\gamma_i}(\theta) := \gamma_i \cdot m_i(\theta)^{\varepsilon_i}\cdot\gamma_i^{-1}$*, where* $m_i\colon \mathbb{S}^1 \to \Omega M_{\underline{n-1}}$ *is the 'swing of a lasso' around* $\mathbb{B}_i$*. See Section 5.3 for details.*

Proof of Theorem E. We prove (9.1) by induction on $n \geq 2$ (for a proof sketch see Example 5.11).

The induction base. In this case $R = \{1\}$, $\Gamma = \overset{1}{|}$ and $\mathbf{G}$ it a thickening of a disk $\mathcal{G}$. We need to check that $\mathscr{D}_{\{1\}}(\chi f_{\mathbf{G}})^{\{1\}}\colon \mathbb{S}^1 \to \Omega M_1$ is homotopic to $m_1^{\varepsilon_1\gamma_1}\colon \mathbb{S}^1 \to \Omega M_1$.

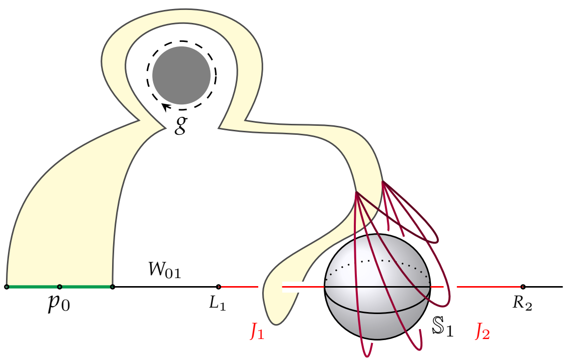


Figure 28. Merging Figures 17 and 11 together: a grope cobordism $\mathcal{G}$ and the family m_1.

Firstly, the loop $(\chi f_{\mathbf{G}})^{\{1\}} := \big(f_{\mathbf{G}}^{\{1\}}\big)^{h^1} \cdot f_{\mathbf{G}}^{\{1\}}$ is the concatenation of the path $f_{\mathbf{G}}^{\{1\}} := \Psi^{\mathbf{G}}(t)^1_{J_0}$ which is the isotopy across the disk $\mathcal{G}$ (see Example 8.7), and the path

$$\big(f_{\mathbf{G}}^{\{1\}}\big)^{h^1}_t := r^1_\emptyset\Big(\; h^1_\emptyset(s)(\mathbf{G}(a_0^\perp)) \cdot l^1_\emptyset\big(\Psi^{\mathbf{G}}(s)^1_{J_0}\big)\;\Big)_{t=1-s}$$

This is obtained by concatenating $h^1_\emptyset(-)(\mathbf{G}(a_0^\perp))$ with $l^1_\emptyset\big(\Psi^{\mathbf{G}}(-)^1_{J_0}\big)$ in $\mathscr{F}^2_\emptyset := \mathscr{E}\mathrm{mb}_\partial(J_0, M_0)$, then reverse this path and include it into $M_{01} = M_0 \cup \mathbb{B}_{01}$.

Recall from Lemma 4.10 that maps $l^1_\emptyset$ and $h^1_\emptyset$ act non-trivially only in the region $[L_1, R_2]\times\mathbb{D}^2 \subseteq M$.

Also recall that the isotopy $d^k_S(s)$ drags the east hemisphere of $\mathbb{B}_{01}$ to that of $\mathbb{S}_1$. Therefore, $h^1_\emptyset(s)(\mathbf{G}(a_0^\perp)) := d^1_\emptyset(s) \circ \mathsf{add}_s(\mathbf{G}(a_0^\perp))$ gradually 'drags to the right' the part of $\mathbf{G}(a_0^\perp)$ which is inside of this region, and the disk $l^1_\emptyset(\mathbf{G})$ agrees with $\mathcal{G}$ except having the tip shifted into J_2. So $l^1_\emptyset(\Psi^{\mathbf{G}}(s)^1_{J_0})$ moves the shifted arc $l^1_\emptyset(\mathbf{G}(a_0^\perp)) = h^1_\emptyset(1)(\mathbf{G}(a_0^\perp))$ back to U_{J_0} across the shifted disk $l^1_\emptyset(\mathbf{G})$. In other words, we use the puncture J_2 instead of J_1 to isotope $\mathbf{G}(a_0^\perp)$ back in analogous manner.

Applying $\mathcal{D}_1$ to this loop $(\chi f_{\mathbf{G}})^{\{1\}}$ allows us to homotope the part of the disk $\mathbf{G}$ which is in $M \setminus [L_1, R_2] \times \mathbb{D}^2$ (equal to the part of $l^1_\emptyset(\mathbf{G})$) onto its core arc (its underlying chord). Hence, we conclude that $\mathcal{D}_1(\chi f_{\mathbf{G}})^{\{1\}}$ is indeed homotopic to $\theta \mapsto \gamma_1 \cdot m_1(\theta)^{\varepsilon_1} \cdot \gamma_1^{-1}$.

Preliminaries for the induction step

It will be convenient to consider trees labelled by a finite set R.

(*setup*) Let $\mathbf{G}$ be a thick grope on U modelled on a tree $\Gamma \in \mathrm{Tree}(R)$ obtained by grafting together $\Gamma_1 \in \mathrm{Tree}(R_1)$ and $\Gamma_2 \in \mathrm{Tree}(R_2)$ with $R_1 \sqcup R_2 = R$. Let $\varepsilon_i \in \{\pm 1\}$ and $\gamma_i \in \Omega M$ with $i \in R$ be the signed decorations of $\mathbf{G}$.

In order to prove (9.1) for $R = \underline{n-1}$ we first simplify the map $\mathcal{D}_R\big(\chi f_{\mathbf{G}}\big)^R : \mathbb{S}^R \to \Omega M_R$ as follows. By Proposition 6.6 we have

$$\big(\chi f_{\mathbf{G}}\big)^R = \coprod_{S \subseteq R} \big(f^R_{\mathbf{G}}\big)^{h^S}.$$

In words, $(\chi f_{\mathbf{G}})^R : \mathbb{S}^R = I^R/\partial \to \mathscr{F}^{|R|+1}_R$ is obtained by gluing all h-reflections $\big(f^R_{\mathbf{G}}\big)^{h^S} : I^R \to \mathscr{F}^{|R|+1}_R$ along their 0-faces. These maps were defined inductively in Definition 6.5 by (for $k = \min S$)

$$\Big(\big(f^R_{\mathbf{G}}\big)^{h^{S\setminus k}}\Big)^{h^k} := r^k_{R\setminus k}\Big(h^k\Big(\big(f^{R\setminus k}_{\mathbf{G}}\big)^{h^{S\setminus k}}_s\Big) \boxplus_k l^k_{R\setminus k}\big(f^R_{\mathbf{G}}\big)^{h^{S\setminus k}}_s\Big). \tag{9.2}$$

Since $\mathcal{D}_R$ is applied pointwise, we obtain

$$\mathcal{D}_R\,\big(\chi f_{\mathbf{G}}\big)^R = \coprod_{S \subseteq R} \mathcal{D}_R\Big(\big(f^R_{\mathbf{G}}\big)^{h^S}\Big). \tag{9.3}$$

In the *Commutator Lemma* 9.2 we will show that $\mathcal{D}_R(f^R_{\mathbf{G}})$ is homotopic to a certain commutator map and in the *Reflections Lemma* 9.3 generalise this to all h^S-reflections $\mathcal{D}_R\big(f^R_{\mathbf{G}}\big)^{h^S}$. Having these homotopies collected in Corollary 9.4, we will be able to finish the proof of Theorem E.

The Commutator Lemma. For each $S \subseteq R$ we now study the map

$$\mathcal{D}_S f^S_{\mathbf{G}} : \quad I^S \xrightarrow{f^S_{\mathbf{G}}} \mathscr{F}^{|R|+1}_S \xrightarrow{\mathcal{D}_S} \Omega M_S$$

given by $\mathcal{D}_S f^S_{\mathbf{G}}(\vec{t}) = (\mathrm{U}_{J_0})_t \cdot (f^S_{\mathbf{G}}(\vec{t}))_{1-t}$ where $f^S_{\mathbf{G}}(\vec{t}) := \Psi^{\mathbf{G}}(\theta)^S_{J_0}(u)$ for $\hbar^S(\vec{t}) = (\theta, u) \in \mathcal{C}^{bar}(\Delta^S)$.

Using the inductive nature of Definition 7.13 we can write the thick grope $\mathbf{G}$ as the plumbing (see Figures 15 and 21) of two thick gropes $\mathbf{G}_\mathrm{j} := \mathbf{G}|_{\mathsf{B}_{\Gamma_\mathrm{j}}}$ modelled on trees Γ_j for $\mathrm{j} = 1, 2$.

More precisely, the boundary of the abstract grope $\partial G_{\Gamma_\mathrm{j}} = \beta_\mathrm{j}$ has its corresponding distinguished subarc $\beta^+_\mathrm{j} \subseteq \beta_\mathrm{j}$. Thus, the map $\mathbf{G}_\mathrm{j} : \mathsf{B}_{\Gamma_\mathrm{j}} \hookrightarrow M$ can be seen as a thick grope modelled on $\Gamma_\mathrm{j} \in \mathrm{Tree}(R_\mathrm{j})$ on the knot obtained from U as follows: replace $\mathbf{G}(a_0) \subseteq \mathrm{U}_{J_0}$ by the arc $\mathbf{G}(\beta^+_\mathrm{j})$, together with some arcs connecting their endpoints (the dotted arcs in the model $G_\Gamma \subseteq \mathsf{B}_\Gamma$ on the left of Figure 29). Observe that the newly produced knot is isotopic to U by an isotopy across the shaded region.

Thus, we can also isotope $\mathbf{G}_\mathrm{j}$, so that the boundary of its bottom stage is as in the right picture, and hence it is instead a thick grope from U to $\partial^\perp \mathbf{G}_\mathrm{j} := (\mathrm{U} \setminus \mathbf{G}(\beta^+_\mathrm{j})) \cup \mathbf{G}(\beta_\mathrm{j} \setminus \beta^+_\mathrm{j})$. Actually, for $\mathbf{G}_\mathrm{j}$ to be a grope on U we also need to reparametrise U so that punctures indeed have labels $1 \le i \le |R_j|$. Also, $\mathbf{G}_2$ should have the orientation of all stages reversed.

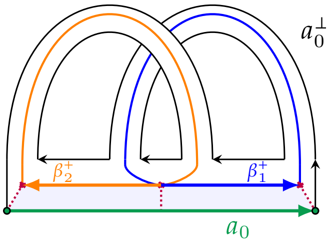


Figure 29. Modifying the bottom stage of a thick grope.

Thanks to these modifications we have points $\psi(\mathbf{G}_j) \in \mathsf{H}_{|R_j|}(M)$ for $j = 1, 2$. However, we now immediately reparametrise back to get the analogous maps $f^{S_j}_{\mathbf{G}_j} \colon I^{S_j} \to \mathscr{F}^{|R_j|+1}_{S_j}$ with $S_j := S \cap R_j$. In other words, although formally $\mathbf{G}_j$ are not thick gropes on U, we can easily switch back and forth between the viewpoints. Moreover, we define

$$\mathscr{D}_S f^{S_j}_{\mathbf{G}_j} \colon \; I^{S_j} \xrightarrow{\;f^{S_j}_{\mathbf{G}_j}\;} \mathscr{F}^{|R_j|+1}_{S_j} \xrightarrow{\mathscr{D}_{S_j}} \Omega M_{0S_j} \xrightarrow{\;\Omega\rho^0\rho\;} \Omega M_S, \tag{9.4}$$

recalling from Remark 4.14 that the last map is well-defined on the image of $\mathscr{D}_{S_j}$.

By the following result each loop $\mathscr{D}_R f^R_{\mathbf{G}}(\vec{t})$ is either the commutator of loops $\mathscr{D}_R f^{R_j}_{\mathbf{G}_j}(\vec{t}_j)$ or some time of a canonical null-homotopy. We use the convention $[0, \frac{1}{2}]^\emptyset = I^\emptyset$ and $[\frac{1}{2}, 1]^\emptyset = \emptyset$.

Lemma 9.2. *Assume $|R| \ge 2$. The map $\mathscr{D}_R f^R_{\mathbf{G}}$ is homotopic to the composition of the map $\vartheta_{(R_1,R_2)} \colon I^R \to I^{R_1} \times I^{R_2}$ which permutes the coordinates, and the map $C^R_{\mathbf{G}} \colon I^{R_1} \times I^{R_2} \to \Omega M_R$ given by*

$$C^R_{\mathbf{G}}(\vec{t}_1, \vec{t}_2) := \begin{cases} \left[\mathscr{D}_R f^{R_1}_{\mathbf{G}_1}(\vec{t}_1),\ \mathscr{D}_R f^{R_2}_{\mathbf{G}_2}(\vec{t}_2)\right] & ,\ (\vec{t}_1, \vec{t}_2) \in [0, \frac{1}{2}]^{R_1} \times [0, \frac{1}{2}]^{R_2} \\ \nu_{|\vec{t}_1|}\left(\mathscr{D}_R f^{R_2}_{\mathbf{G}_2}(\vec{t}_2)\right) & ,\ (\vec{t}_1, \vec{t}_2) \in [\frac{1}{2}, 1]^{R_1} \times [0, \frac{1}{2}]^{R_2} \\ \nu_{|\vec{t}_2|}\left(\mathscr{D}_R f^{R_1}_{\mathbf{G}_1}(\vec{t}_1)\right) & ,\ (\vec{t}_1, \vec{t}_2) \in [0, \frac{1}{2}]^{R_1} \times [\frac{1}{2}, 1]^{R_2} \\ \mathsf{const}_{p_0} & ,\ (\vec{t}_1, \vec{t}_2) \in [\frac{1}{2}, 1]^{R_1} \times [\frac{1}{2}, 1]^{R_2} \end{cases} \tag{9.5}$$

where $\nu_\theta(x)$ is the time θ of the canonical null-homotopy $x \cdot x^{-1} \rightsquigarrow \mathsf{const}_{p_0}$ for a loop $x \in \Omega M_R$. In Figure 30 these are shown as blue lines, and the subspace on which $C^R_{\mathbf{G}}$ is constant is contracted.

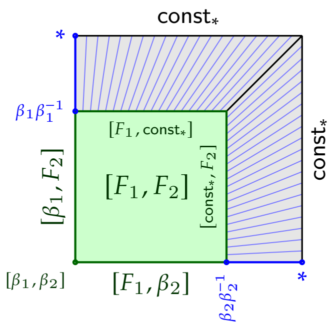


Figure 30. Schematic depiction of the map $C^R_{\mathbf{G}} \colon I^{R_1} \times I^{R_2} \to \Omega M_R$, with $F_j := \mathscr{D}_R f^{R_j}_{\mathbf{G}_j}$ for short.

Proof. Assume $R = \emptyset$. We have $f^\emptyset_{\mathbf{G}}(pt) = (\partial^\perp \mathbf{G})_{J_0} = \mathbf{G}(a_0^\perp)$ and $\mathscr{D}_\emptyset f^\emptyset_{\mathbf{G}}(pt) = (\mathrm{U}_{J_0})_t \cdot \mathbf{G}(a_0^\perp)_{1-t}$ is exactly the loop $\mathbf{G}(\partial G_\Gamma)$, the boundary of the bottom stage. Since the bottom stage is a punctured torus, it collapses onto the 1-skeleton. This homotopes the boundary onto the commutator $[\mathbf{G}(\beta_1), \mathbf{G}(\beta_2)] \in \Omega M_R$. Now each $\mathbf{G}(\beta_{\mathrm{j}}) = \mathbf{G}(\beta_{\mathrm{j}}^+) \cdot \mathbf{G}(\beta_{\mathrm{j}} \setminus \beta_{\mathrm{j}}^+)$ is precisely the loop $\mathscr{D}_\emptyset f^\emptyset_{\mathbf{G}_{\mathrm{j}}}(pt) := (\mathrm{U}_{J_0})_t \cdot \mathbf{G}_{\mathrm{j}}(a_0^\perp)_{1-t}$, so we conclude that $\mathscr{D}_\emptyset f^\emptyset_{\mathbf{G}}(pt)$ is homotopic to $\mathrm{C}^\emptyset_{\mathbf{G}}(pt)$ as claimed.

Assume now $R \neq \emptyset$ and recall that for $\hbar^R(\vec{t}) = (\theta, u) \in \mathcal{C}^{bar}(\Delta^R)$ the arc $f^R_{\mathbf{G}}(\vec{t}) := \Psi^{\mathbf{G}}(\theta)^R_{J_0}(u)$ is the time θ of an isotopy across the disk $\mathbf{G}(\mathbb{D}_u)$ (see Proposition 8.1): as $\theta \in [0,1]$ increases, the arc $a_0^\perp$ is being homotoped to a_0 across $\mathbb{D}_u$ using a foliation which we are still free to specify.

The disk $\mathbb{D}_u \subseteq \mathsf{B}_\Gamma$ was in turn defined as the time $t \in [0,1]$ of the *symmetric isotopy* (Lemma 8.2) between the two disks obtained by surgery on the bottom stage along $\mathbb{D}_{u_1} \subseteq \mathsf{B}_{\Gamma_1}$ or $\mathbb{D}_{u_2} \subseteq \mathsf{B}_{\Gamma_2}$ (see Proposition 8.4), where $u = (1-t)u_1 + tu_2 \in \Delta^R = \Delta^{R_1} \star \Delta^{R_2}$, with $u_{\mathrm{j}} \in \Delta^{R_{\mathrm{j}}}$. Without loss of generality, assume $t < \frac{1}{2}$, so $\mathbb{D}_u$ looks like in the left of Figure 31.

Here $\vec{t} \in I^R \cong \mathcal{C}^{bar}(\Delta^R) \cong \mathcal{C}^{bar}(\Delta^{R_1} \star \Delta^{R_2}) = \mathcal{C}^{bar}(\Delta^{R_1}) \times \mathcal{C}^{bar}(\Delta^{R_2})$ precisely gives $\hbar^{R_{\mathrm{j}}}(\vec{t}_{\mathrm{j}}) = (\theta, u_1)$.

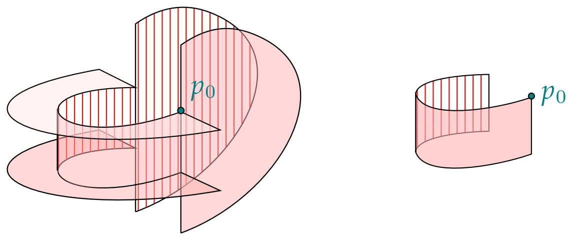


Figure 31. *Left*: Disk $\mathbb{D}_u$ for some $t < \frac{1}{2}$. Two vertical disks are copies of $\mathbb{D}_{u_1}$. *Right*: The band $b(u)$.

The loop $\mathscr{D}_R f^R_{\mathbf{G}}(\vec{t})$ is obtained by closing up the arc $\Psi^{\mathbf{G}}(\theta)^R_{J_0}(u)$ using for all $\vec{t}$ the same arc U_{J_0}. Thus, we can collapse this U_{J_0} to the basepoint p_0 throughout the whole family, so that $\mathscr{D}_R f^R_{\mathbf{G}}(\vec{t})$ becomes, for a fixed u, a basepoint preserving homotopy of the loop $\mathbf{G}(\partial G_\Gamma)$ to const_{p_0}.

We now *specify the foliation of* $\mathbb{D}_u$ in such manner that this homotopy is first done across the two parallel copies of $\mathbb{D}_{u_1}$ (vertical disks in Figure 31) and the two pieces of $\mathbb{D}_{u_2}$ (two regions lying flat), until for $\theta = \frac{1}{2}$ we have completely exhausted the parts of $\mathbb{D}_u$ which come from the caps. We are then left with a band $b(u)$ as on the right of Figure 31 and we let the *rest of the homotopy* be the 'vertical' contraction onto the vertical line containing p_0, followed by its collapse onto p_0.

To further simplify these homotopies we collapse throughout the family the remaining pieces of the *surgered torus* in $\mathbb{D}_u$ onto its skeleton. So 'parallel copies of curves' get identified similarly as for $R = \emptyset$. The final result is as on the left of Figure 32: for any $u \in \Delta^R$, $\theta \leq \frac{1}{2}$ our $\mathscr{D}_R f^R_{\mathbf{G}}(\vec{t})$ became the commutator of the loops $\mathscr{D}_R f^{R_{\mathrm{j}}}_{\mathbf{G}_{\mathrm{j}}}(\vec{t}_{\mathrm{j}}) = \mathscr{D}_R(\Psi^{\mathbf{G}_{\mathrm{j}}}(\theta_{\mathrm{j}})^{R_{\mathrm{j}}}_{J_0}(u_{\mathrm{j}}))$, with $\theta_1 \in [0,1]$ and $\theta_2 \in [0, c]$.

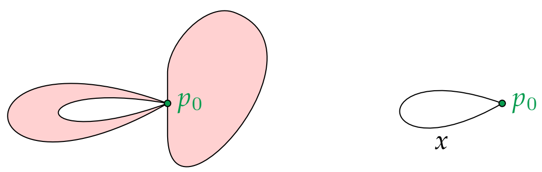


Figure 32. *Left*: Disk $\mathbb{D}_u$ after collapsing the punctured torus. *Right*: The band $b(u)$ after the collapse.

Here c is such that $\theta = \frac{1}{2}$ corresponds to $(\theta_1, \theta_2) = (1, c)$ and at this moment $\mathscr{D}_R f^{R_1}_{\mathbf{G}_1}(\vec{t}_1) = \mathsf{const}_{p_0}$, while $\mathscr{D}_R f^{R_2}_{\mathbf{G}_2}(\vec{t}_2)$ is the curve x on the right of Figure 32. Hence, for $\theta = \frac{1}{2}$ and a fixed u we have $\mathscr{D}_R f^R_{\mathbf{G}}(\vec{t}) = [\mathsf{const}_{p_0}, x]$ and our null-homotopy across $b(u)$ for $\theta \geq \frac{1}{2}$ indeed becomes the canonical null-homotopy $t \mapsto x_s|_{[0,t]} \cdot x_{1-s}|_{[1-t,1]}$ after the collapse. □

The Reflections Lemma. We now extend the previous result to describe each h^S-reflection

$$\mathcal{D}_R\big(f^R_{\mathbf{G}}\big)^{h^S}\colon\ I^R \xrightarrow{(f^R_{\mathbf{G}})^{h^S}} \mathscr{F}^{|R|+1}_R \xrightarrow{\mathcal{D}_R} \Omega M_R.$$

Lemma 9.3. *Assume $|R|\geq 2$ and $S\subseteq R$. The map $\mathcal{D}_R\big(f^R_{\mathbf{G}}\big)^{h^S}$ is homotopic to the composition of the map $\vartheta_{(R_1,R_2)}$ as before with the map $\big(C^R_{\mathbf{G}}\big)^{h^S}\colon I^{R_1}\times I^{R_2}\to\Omega M_R$ given by*

$$\big(C^R_{\mathbf{G}}\big)^{h^S}(\vec{t}_1,\vec{t}_2)=\begin{cases}\Big[\ \mathcal{D}_R\big(f^{R_1}_{\mathbf{G}_1}\big)^{h^{S\cap R_1}}(\vec{t}_1),\ \mathcal{D}_R\big(f^{R_2}_{\mathbf{G}_2}\big)^{h^{S\cap R_2}}(\vec{t}_2)\ \Big] & ,\ (\vec{t}_1,\vec{t}_2)\in[0,\tfrac12]^{R_1}\times[0,\tfrac12]^{R_2}\\ \nu_{|\vec{t}_1|}\Big(\mathcal{D}_R\big(f^{R_2}_{\mathbf{G}_2}\big)^{h^{S\cap R_2}}(\vec{t}_2)\Big) & ,\ (\vec{t}_1,\vec{t}_2)\in[\tfrac12,1]^{R_1}\times[0,\tfrac12]^{R_2}\\ \nu_{|\vec{t}_2|}\Big(\mathcal{D}_R\big(f^{R_1}_{\mathbf{G}_1}\big)^{h^{S\cap R_1}}(\vec{t}_1)\Big) & ,\ (\vec{t}_1,\vec{t}_2)\in[0,\tfrac12]^{R_1}\times[\tfrac12,1]^{R_2}\\ \mathsf{const}_{p_0} & ,\ (\vec{t}_1,\vec{t}_2)\in[\tfrac12,1]^{R_1}\times[\tfrac12,1]^{R_2}\end{cases}$$

Proof. The statement for $S=\emptyset$ is precisely the previous lemma (put $S:=R$ there).

Now assume $S\subseteq R$ is nonempty and that the statement is true inductively for all R' of cardinality $|R'|<|R|$ and any $S'\subseteq R$ of cardinality $|S'|<|S|$. Thus, letting $k:=\min S$ and $\underline{R}:=R\setminus k$ and $\underline{S}:=S\setminus k$, the statement is true for the pairs $(\underline{R},\underline{S})$ and $(R,\underline{S})$.

Using the defining formula for an h^S-reflection from (9.2), we compute

$$\begin{aligned}\mathcal{D}_R\big(f^R_{\mathbf{G}}\big)^{h^S} &= \mathcal{D}_R r^k_{\underline{R}}\Big(h^k\big(f^{\underline{R}}_{\mathbf{G}}\big)^{h^{\underline{S}}}\boxminus_k l^k_{\underline{R}}\big(f^R_{\mathbf{G}}\big)^{h^{\underline{S}}}\Big)\\ &= \Omega\rho^k_{\underline{R}}\circ\mathcal{D}_{\underline{R}}\Big(h^k\big(f^{\underline{R}}_{\mathbf{G}}\big)^{h^{\underline{S}}}\boxminus_k l^k_{\underline{R}}\big(f^R_{\mathbf{G}}\big)^{h^{\underline{S}}}\Big)\\ &= \Omega\rho^k_{\underline{R}}\Big(\mathcal{D}_{\underline{R}}\circ h^k\big(f^{\underline{R}}_{\mathbf{G}}\big)^{h^{\underline{S}}}\boxminus_k \mathcal{D}_{\underline{R}}\circ l^k_{\underline{R}}\big(f^R_{\mathbf{G}}\big)^{h^{\underline{S}}}\Big)\\ &= \Omega\rho^k_{\underline{R}}\Big(h^k\circ\mathcal{D}_{\underline{R}}\big(f^{\underline{R}}_{\mathbf{G}}\big)^{h^{\underline{S}}}\boxminus_k (\Omega\lambda^k_{\underline{R}})\circ\mathcal{D}_R\big(f^R_{\mathbf{G}}\big)^{h^{\underline{S}}}\Big).\end{aligned}\tag{9.6}$$

For the second equality we have used that $\rho^0\circ\mathcal{D}_R\circ r^k_{\underline{R}}=\rho^0\circ\Omega\rho^k_{\underline{R}}\circ\mathcal{D}_{\underline{R}}$ by Remark 4.14 (recall that we omit ρ^0 from notation), the third equality holds since $\mathcal{D}_R$ is applied pointwise, and for the last see again Remark 4.14. The induction hypothesis now implies

$$\mathcal{D}_R\big(f^R_{\mathbf{G}}\big)^{h^S}\simeq\Omega\rho^k_{\underline{R}}\Big(h^k\circ\big(C^{\underline{R}}_{\mathbf{G}}\big)^{h^{\underline{S}}}\circ\vartheta_{(\underline{R}_1,\underline{R}_2)}\ \boxminus_k\ \Omega\lambda^k_{\underline{R}}\circ\big(C^R_{\mathbf{G}}\big)^{h^{\underline{S}}}\circ\vartheta_{(R_1,R_2)}\Big)\tag{9.7}$$

and it remains to show that the last expression is equal to $(C^R_{\mathbf{G}})^{h^S}\circ\vartheta_{(R_1,R_2)}$.

To this end, assume without loss of generality that $k\in S\cap R_1$, and denote $\underline{R}_1=R_1\setminus k$ and $\underline{R}_2=R_2$. Then at $\vec{t}\in I^t$ we have

$$\Omega\rho^k_{\underline{R}}\Big(h^k(C^{\underline{R}}_{\mathbf{G}})^{h^{\underline{S}}}(\underline{\vec{t}_1},\vec{t}_2)\ \boxminus_k\ \Omega\lambda^k_{\underline{R}}(C^R_{\mathbf{G}})^{h^{\underline{S}}}(\vec{t}_1,\vec{t}_2)\Big).$$

Let us plug in the formulae for $(C^{\underline{R}}_{\mathbf{G}})^{h^{\underline{S}}}$ and $(C^R_{\mathbf{G}})^{h^{\underline{S}}}$ into (9.7). Observe that h^k and $\Omega\lambda^k_{\underline{R}}$ act *trivially* on the maps involving the grope $\mathbf{G}_2$, as those maps interact only with the punctures indexed by $S_2\not\ni k$. On the other hand, for $\vec{t}_1\in[0,\frac12]^{R_1}$ we will get maps

$$\begin{aligned}&h^k\circ\mathcal{D}_{\underline{R}}\big(f^{\underline{R}_1}_{\mathbf{G}_1}\big)^{h^{S\cap\underline{R}_1}}(\vec{t}_1)\boxminus_k(\Omega\lambda^k_{\underline{R}})\circ\mathcal{D}_R\big(f^{R_1}_{\mathbf{G}_1}\big)^{h^{\underline{S}\cap R_1}}(\vec{t}_1)\\ \text{and}\quad &h^k\circ\nu_{|\vec{t}_2|}\Big(\mathcal{D}_R\big(f^{R_1}_{\mathbf{G}_1}\big)^{h^{S\cap R_1}}(\vec{t}_1)\Big)\boxminus_k(\Omega\lambda^k_{\underline{R}})\circ\nu_{|\vec{t}_2|}\Big(\mathcal{D}_R\big(f^{R_1}_{\mathbf{G}_1}\big)^{h^{S\cap R_1}}(\vec{t}_1)\Big).\end{aligned}$$

Now the second expression is just $\nu_{|\vec{t}_2|}$ applied to the first, which is in turn equal to $\mathcal{D}_R\big(f^R_{\mathbf{G}_1}\big)^{h^{S\cap R_1}}(\vec{t}_1)$, by running the equalities from (9.6) in reverse.

Therefore, (9.7) indeed agrees with $(C^R_{\mathbf{G}})^{h^S}\circ\vartheta_{(R_1,R_2)}$. ∎

COROLLARY 9.4. *The homotopies from the previous lemma glue to a homotopy*

$$\mathcal{D}_R\left(\chi f_{\mathbf{G}}\right)^R = \boxplus_{S\subseteq R} \mathcal{D}_R\left(f^R_{\mathbf{G}}\right)^{h^S} \simeq \left(\boxplus_{S\subseteq R}\left(C^R_{\mathbf{G}}\right)^{h^S}\right)\circ\vartheta_{(R_1,R_2)}.$$

The end of the proof

Assume inductively that (9.1) is true for all $\mathbf{G}$ as in (*setup*) with $|R|<n-1$. Let $|R|=n-1$ and let us prove that $\Gamma(m_i^{\varepsilon_i\gamma_i})$ and $\mathcal{D}_R(\chi f_{\mathbf{G}})^R \simeq \left(\boxplus_{S\subseteq R}\left(C^R_{\mathbf{G}}\right)^{h^S}\right)\circ\vartheta_{(R_1,R_2)}$ are homotopic.

Firstly, $\mathbf{G}$ is the plumbing of thick gropes $\mathbf{G}_1$ and $\mathbf{G}_2$ modelled respectively on $\Gamma_{\mathrm{j}}\in\mathrm{Tree}(R_{\mathrm{j}})$ and with signed decorations $(\varepsilon_i,\gamma_i)_{i\in R_{\mathrm{j}}}$. Since both $|R_{\mathrm{j}}|<n-1$ the *induction hypothesis* implies that

$$\mathcal{D}_{R_{\mathrm{j}}}(\chi f_{\mathbf{G}_{\mathrm{j}}})^{R_{\mathrm{j}}} \simeq \Gamma_{\mathrm{j}}(m_i^{\varepsilon_i\gamma_i})\colon \quad (I^{R_{\mathrm{j}}},\partial)\longrightarrow(\Omega M_{R_{\mathrm{j}}},\mathsf{const}_*). \tag{9.8}$$

Secondly, in (A.8) we have defined $\Gamma(m_i^{\varepsilon_i\gamma_i})$ inductively by

$$\Gamma(m_i^{\varepsilon_i\gamma_i}) := \left[\Gamma_1(m_i^{\varepsilon_i\gamma_i}),\Gamma_2(m_i^{\varepsilon_i\gamma_i})\right]\circ\vartheta_{(R_1,R_2)}.$$

The first map in the formula is the Samelson product which was shown in Lemma A.5 to be obtained by canonically trivialising all the faces of the map[34]

$$I^{R_1}\times I^{R_2} \xrightarrow{\Gamma_1(m_i^{\varepsilon_i\gamma_i})\times\Gamma_2(m_i^{\varepsilon_i\gamma_i})} \Omega M_{R_1}\times\Omega M_{R_2} \xrightarrow{[\Omega\rho^{R\setminus R_1}_{R_1},\Omega\rho^{R\setminus R_2}_{R_2}]} \Omega M_R.$$

Plugging in (9.8) we get $\Gamma(m_i^{\varepsilon_i\gamma_i})\simeq w^{ind}\circ\vartheta_{(R_1,R_2)}$ for the map w^{ind} obtained by trivialising the faces of the map[35]

$$I^{R_1}\times I^{R_2} \xrightarrow{[\mathcal{D}_R(\chi f_{\mathbf{G}_1})^{R_1},\ \mathcal{D}_R(\chi f_{\mathbf{G}_2})^{R_2}]} \Omega M_R. \tag{9.9}$$

The map w^{ind} is depicted in Figure 33, with the map (9.9) given as the green square with the two coordinate axes $\vec{t}_{\mathrm{j}}\in I^{R_{\mathrm{j}}}$ (so it is an $(n-1)$-cube). Trivialising this on the boundary corresponds to putting the green square into a bigger one and filling in the intermediate region by null-homotopies $x\cdot x^{-1}\rightsquigarrow *$ along straight blue lines. Here $x\in\Omega M_R$ is some value of (9.9) on the boundary of the inner $(n-1)$-cube, and so w^{ind} is indeed constant on the boundary of the outer $(n-1)$-cube.

We now show that w^{ind} agrees with the map $\boxplus_{S\subseteq R}\left(C^R_{\mathbf{G}}\right)^{h^S}$, so Corollary 9.4 will finish the proof.

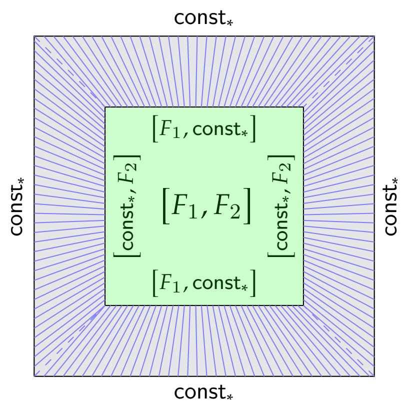


Figure 33. Schematic depiction of the map w^{ind}, where $F_{\mathrm{j}} := \mathcal{D}_R(\chi f_{\mathbf{G}_{\mathrm{j}}})^{R_{\mathrm{j}}}$ for short.

[34] More precisely, in that lemma we had $m_{i,R_{\mathrm{j}}} := \Omega\rho_i^{R_{\mathrm{j}}\setminus i}\circ m_i^{\varepsilon_i\gamma_i}$ if $i\in R_{\mathrm{j}}$, but we have already abused the notation when we decided to write $m_i := \Omega\rho_i^{S\setminus i}\circ\eta_{\mathbb{S}_i}$ (cf. (5.5)).

[35] Here we denote $\mathcal{D}_R = \Omega\rho^{R\setminus R_{\mathrm{j}}}_{R_{\mathrm{j}}}\circ\mathcal{D}_{R_{\mathrm{j}}}$ as in (9.4).

Let us first show this for the 'green parts' of Figures 30 and 33, i.e. on $[0,\frac{1}{2}]^{R_1}\times[0,\frac{1}{2}]^{R_2}$ we have

$$\begin{aligned} w^{ind} &:= \quad \big[\mathcal{D}_R(\chi f_{\mathbf{G}_1})^{R_1}, \mathcal{D}_R(\chi f_{\mathbf{G}_2})^{R_2}\big] \\ &= \Big[\boxplus_{S_1\subseteq R_1} \mathcal{D}_R\big(f^{R_1}_{\mathbf{G}_1}\big)^{h^{S_1}}, \boxplus_{S_2\subseteq R_2} \mathcal{D}_R\big(f^{R_2}_{\mathbf{G}_2}\big)^{h^{S_2}}\Big] \\ &= \boxplus_{S\subseteq R} \Big[\mathcal{D}_R\big(f^{R_1}_{\mathbf{G}_1}\big)^{h^{S\cap R_1}}, \mathcal{D}_R\big(f^{R_2}_{\mathbf{G}_2}\big)^{h^{S\cap R_2}}\Big] \quad =: \boxplus_{S\subseteq R} \big(C^R_{\mathbf{G}}\big)^{h^S} \end{aligned}$$

where the second equality is by (9.3), the third holds because the commutator bracket is applied pointwise and the last equality is by definition of $\big(C^R_{\mathbf{G}}\big)^{h^S}$ in Lemma 9.3.

Similarly, for $\vec{t}_1\in[0,\frac{1}{2}]^{R_1}$ we have a blue line null-homotopy, where $\vec{t}_2$ runs in $[\frac{1}{2},1]^{R_2}$, so

$$\begin{aligned} w^{ind}(\vec{t}_1,\vec{t}_2) &:= \nu_{|\vec{t}_2|}\Big(\boxplus_{S_1\subseteq R_1} \mathcal{D}_R\big(f^{R_1}_{\mathbf{G}_1}\big)^{h^{S_1}}(\vec{t}_1)\Big) \\ &= \boxplus_{S\subseteq R} \nu_{|\vec{t}_2|}\Big(\mathcal{D}_R\big(f^{R_1}_{\mathbf{G}_1}\big)^{h^{S\cap R_1}}(\vec{t}_1)\Big) \quad =: \boxplus_{S\subseteq R} \big(C^R_{\mathbf{G}}\big)^{h^S}(\vec{t}_1,\vec{t}_2). \qquad \square \end{aligned}$$

The proof of Theorem F

Proof. In Section 8.1 we have defined the extension $\psi\colon \mathsf{Grop}_{n-1}(M;\mathrm{U})\to \mathsf{H}_{n-1}(M)$ and in Proposition 7.16 the underlying tree map $\mathcal{T}_{n-1}\colon \pi_0\mathsf{Grop}_{n-1}(M;\mathrm{U})\to\mathbb{Z}[\mathrm{Tree}_{\pi_1 M}(n-1)]$. We now show that for a grope forest $\mathbf{F}\in\mathsf{Grop}_{n-1}(M;\mathrm{U})$ we have $[\mathsf{e}_n\psi(\mathbf{F})]=[\mathcal{T}_{n-1}(\mathbf{F})]\in\mathsf{Lie}_{\pi_1 M}(n-1)$.

In other words, for $\mathbf{F}=\bigsqcup_{l=1}^N \mathbf{G}_l\colon \bigsqcup_{l=1}^N \mathsf{B}_{\Gamma_l}\hookrightarrow M$ with $\mathcal{T}_{n-1}(\mathbf{G}_l)=\varepsilon^l\Gamma_l^{g^l}$, and denoting $f_{\mathbf{F}}:=\mathsf{e}_n\psi(\mathbf{F})$, we need to show

$$\big[f_{\mathbf{F}}\big]=\sum_{l=1}^N\Big[\varepsilon^l\Gamma_l^{g^l}\Big] \quad\in\pi_0\mathsf{F}_n(M)\cong\mathsf{Lie}_{\pi_1 M}(n-1).$$

This was reduced in Section 5.3 to proving that $\mathcal{D}_R(\chi f_{\mathbf{F}})^R\colon\mathbb{S}^{n-1}\to\Omega M_R$ is homotopic to a map realising the class on the right, namely, the pointwise product $\prod_{l=1}^N\Gamma_l(m_i^{\varepsilon_i^l\gamma_i^l})$ which takes $\vec{t}\in\mathbb{S}^{n-1}$ to the concatenation of the loops

$$\Gamma_l(m_i^{\varepsilon_i^l\gamma_i^l})(\vec{t})\ \in\ \Omega M_R,\quad 1\le l\le N.$$

Since each $\mathbf{G}_l$ is a thick grope on U with the underlying decorated tree $\mathcal{T}_{n-1}(\mathbf{G}_l)=\varepsilon^l\Gamma_l^{g^l}$, the maps $\Gamma_l(m_i^{\varepsilon_i^l\gamma_i^l})\simeq\mathcal{D}_R(\chi f_{\mathbf{G}_l})^R$ are homotopic by Theorem E. Hence, it remains to prove that $\mathcal{D}_R\big(\chi f_{\mathbf{F}}\big)^R$ is homotopic to the pointwise product $\prod_{l=1}^N\mathcal{D}_R\big(\chi f_{\mathbf{G}_l}\big)^R$.

Recall the definition of $f_{\mathbf{F}}$ in (8.7). Similarly as in the proof of the Commutator Lemma 9.2, there is a homotopy between $\mathcal{D}_R\big(f^R_{\mathbf{F}}\big)$ and the pointwise product of $\mathcal{D}_R(f^R_{\mathbf{G}_l})$ – since we can collapse U_{J_0} for all loops in the family. This extends to all h-reflections as in the Reflections Lemma 9.3 – there we had commutators of loops and here just their pointwise concatenations.

Therefore, using the same arguments as in the proof of Theorem E we can conclude

$$\begin{aligned} \mathcal{D}_R\big(\chi f_{\mathbf{F}}\big)^R &= \mathcal{D}_R\Big(\boxplus_{S\subseteq R}(f^R_{\mathbf{F}})^{h^S}\Big)=\boxplus_{S\subseteq R}\mathcal{D}_R\big(f^R_{\mathbf{F}}\big)^{h^S} \\ &\simeq \boxplus_{S\subseteq R}\prod_{l=1}^N\mathcal{D}_R\big(f^R_{\mathbf{G}_l}\big)^{h^S}=\prod_{l=1}^N\boxplus_{S\subseteq R}\mathcal{D}_R\big(f^R_{\mathbf{G}_l}\big)^{h^S}=\prod_{l=1}^N\mathcal{D}_R\big(\chi f_{\mathbf{G}_l}\big)^R. \qquad\square \end{aligned}$$

Part IV

Additional topics

In Section 10 we study the Gusarov–Habiro filtration of the set of (long) knots in a 3-manifold M with boundary, relating its associated graded sets to Jacobi trees via the realisation map. We prove Theorems G1, G2 and G3.

In Appendix B we survey the finite type theory of braids.

In Appendix C we prove Proposition 3.9 from Section 3.1, and also sketch the computation of the image of the d^1 differential in the first non-vanishing slope, as claimed in Section 2.3.

10 The Gusarov–Habiro filtration

In this section we discuss the geometric calculus for 3-manifolds. Firstly, in Section 10.1 we briefly review the theory of claspers. In Section 10.2 we introduce our variant of the n-equivalence relation, recall some of its properties and define the realisation map $\mathcal{R}^T$. Finally, in Section 10.3 we prove the statements about $\mathcal{R}^T$ which were announced in Section 2.2.1.

10.1 A short introduction to claspers

We have so far considered rooted vertex-oriented uni-trivalent trees, see Definition 2.1. Now let Γ be such a tree but without a distinguished root. Equivalently, Γ is a Jacobi diagram without loops.

A tree clasper C on a knot K modelled on Γ is the data of a map $C\colon \Gamma \to M$ which embeds all edges disjointly from each other and K, together with a framing on each edge and a choice of an embedded loop for each univalent vertex. These loops, called leaves of C, are embedded in $M \setminus (K \sqcup C(\Gamma))$ except that they attach to the univalent vertex of $C(\Gamma)$ as in Figure 34.

We say that a leaf of C is simple if it bounds a disk in $M \setminus C(\Gamma)$ which intersects K in precisely one point. We say that C is simple (or capped) if all its leaves are simple (for example, the clasper in Figure 34 is not simple), and that it is trivial if it has a leaf which bounds a disk in $M \setminus (K \sqcup C(\Gamma))$.

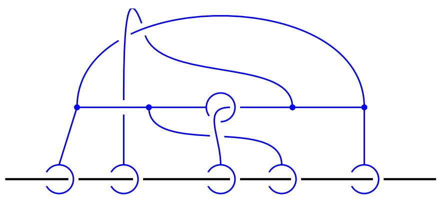


Figure 34. A clasper with one non-simple leaf, with the blackboard framing.

To a tree clasper C we assign a framed link L_C as in Figure 35: replace each edge by a Hopf link and each trivalent vertex by a copy of the Borromean rings. If C has at least one simple leaf, then the surgery on M along the framed link L_C gives a manifold diffeomorphic to M and under that identification K changes to some knot K^C in M. If C is trivial, K^C is isotopic to K. See [Hab00].

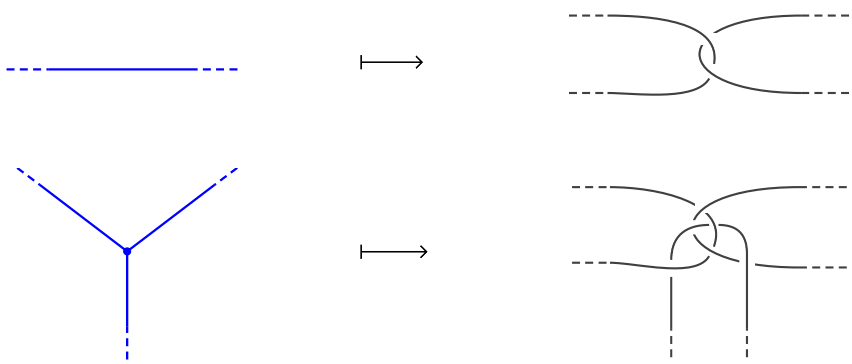


Figure 35. The construction of the associated link L_C for a tree clasper C.

Given a grope cobordism $\mathcal{G}\colon G_\Gamma \to M$ we now define, following Conant and Teichner, its underlying simple tree clasper $C(\mathcal{G})$. It is given as the image $\mathcal{G}(\Gamma)$ of the underlying tree $\Gamma \subseteq G_\Gamma$ (see Section 7.2), together with the framing of the edges induced from the corresponding surface stages, and the leaves given by small loops in caps of $\mathcal{G}$ around intersection points $p_i \in K$. Actually, [CT04b] considers more general *simple genus one* grope cobordisms; see Lemma 10.4 below for a comparison.

Theorem 10.1 ([CT04b, Thm. 23]). *The output knot $\partial^\perp \mathcal{G}$ of a simple genus one grope cobordism on K is isotopic to $K^{C(\mathcal{G})}$.*

Observe that claspers obtained from gropes are always simple. Moreover, tree claspers do not have a distinguished root, but given such a choice in a simple tree clasper, one can construct a grope with that underlying clasper. As explained in Remark 8.3, a grope contains additional data, the choice of which is crucial for obtaining a point in the Taylor layer. On the other hand, when interested only in the n-equivalence classes of knots, claspers are a simpler tool with combinatorial behaviour which we now outline.

Definition 10.2 ([Gus00; Hab00; CT04b]). *Two knots K and K' are n-equivalent $K \sim_n K'$ if there is a sequence of surgeries on simple tree claspers of degree n leading from K to K'. Equivalently, there is a sequence of simple genus one grope cobordisms of degree n between them.*

Note that for the definition of this relation simple tree claspers suffice. However, for proving its properties and studying the induced filtration non-simple tree claspers show useful. For example, they appear in the proof that n-equivalence implies $(n-1)$-equivalence, see the next section. Following Habiro, we introduce the notation of a box for three non-simple leaves as in Figure 36 (in all pictures, we use the blackboard framing).

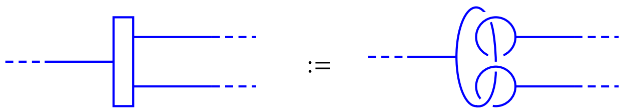


Figure 36. The box notation.

There are several useful moves which modify a tree clasper C of degree n, either corresponding to isotopies of the resulting knot K^C (we denote such a move by an arrow with $\simeq$), or so that K^C is changed within its $\sim_{n+1}$-equivalence class (denoted by an arrow with $\sim_{n+1}$).

The main tool in the first case is the zip construction, which moves a box 'through a trivalent vertex' as in Figure 37. The right picture depicts two tree claspers, one of which agrees with the initial tree clasper (in blue), while the other one agrees with it everywhere except for the additional box and a 'bad leaf' which links it with the first one. See [Hab00, Prop. 2.7, Move 11] and [Gus00, Thm. 6.3], where is is called 'the splitting of a variation'.

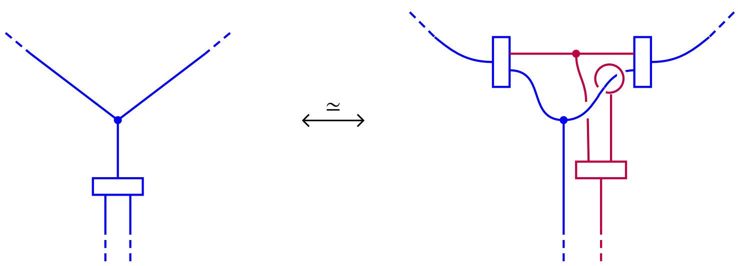


Figure 37. The zip construction.

However, if we are interested only in the class of K^C modulo $\sim_{n+1}$, we can modify this further. Namely, we continue the procedure of pushing the boxes through trivalent vertices down the tree. We obtain two tree claspers (a strict forest clasper of Habiro). We can then do crossing changes of each 'bad' red leaf with the blue clasper, since the difference corresponds to doing the surgery on a clasper of a higher degree (see item (4) in the proof of Theorem 10.5). This gives a trivial leaf, which can be erased together with its box [Hab00, Move 3] – we say that we are pruning the leaves off. The result consists of two identical copies of the initial clasper (stemming from the first box).

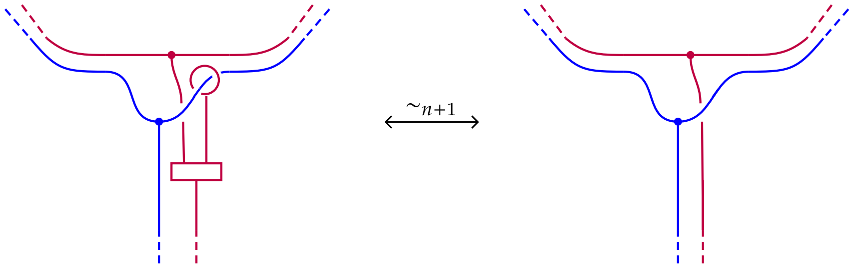


Figure 38. Pruning the leaves off.

Boxes naturally arise after performing either of the two crucial moves depicted in Figures 39; they will be used in the proof of Theorem G2. The sign on an edge denotes that the corresponding framing differs by a positive or negative half-twist from the blackboard framing. For the proof of the first move see [Gus00, Thm. 4.3] and for the second [Hab00, Prop. 2.7, Move 12].

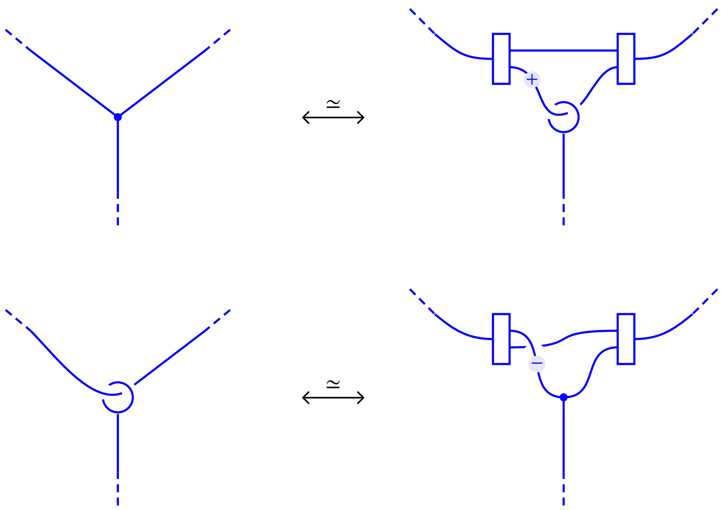


Figure 39. The moves of Gusarov and Habiro respectively.

Manipulations with claspers can be quite involved, so to save space we will only list needed results in the proof of Theorem 10.5, referring the reader to the work of Gusarov and Habiro for the proofs, which apply here verbatim. On the other hand, we will give a self-contained proof of Theorem G2 in Section 10.3, which uses only moves involving at most one non-simple leaf.

Moreover, in [CT04a] the authors more generally consider graph claspers, as $\mathcal{A}^I_n$ was not yet identified with $\mathcal{A}^T_n$ [Con08]. We will give a comparison in the proof of Theorem G3.

10.2 The n-equivalence relation and the primitive realisation map

Theorem 10.3 ([Gus00; Hab00]). *If $K \sim_n K'$ for some $n \geq 1$, then also $K \sim_{n-1} K'$.*

Sketch of the proof. It is enough to produce from a simple tree clasper C on K of degree n two simple tree claspers on K of degrees $n-1$, so that the result of the surgery on both of them is isotopic to K^C. Pick any trivalent vertex v in C which is a neighbour of a leaf. Apply Gusarov's move from Figure 39 on the vertex v so that the leaf edge is the vertical one in that figure.

Now do surgery only on that vertical edge, so that the edge of the clasper with which it links now 'goes around' K. Finally, zip down both boxes to get two tree claspers of degree $n-1$. When the 'blue clasper' is erased, the red clasper becomes simple, so doing surgery on both is a sequence of surgeries on simple tree claspers of degree $n-1$. □

Let $\mathcal{K}_n(M;\mathrm{U}) \subseteq \mathcal{K}(M)$ be the subspace of knots n-equivalent to U and $\mathbb{K}_n(M;\mathrm{U}) := \pi_0\mathcal{K}_n(M;\mathrm{U})$. Then by the theorem there is a decreasing filtration

$$\mathbb{K}(M) \supseteq \mathbb{K}_1(M;\mathrm{U}) \supseteq \cdots \supseteq \mathbb{K}_n(M;\mathrm{U}) \supseteq \cdots .$$

called the Gusarov–Habiro filtration. Let us now redefine the n-equivalence relation in terms of grope forests. Recall from Section 7.2.4 that for a grope forest $\mathbf{F}\colon \bigsqcup_{l=1}^{N} \mathsf{B}_{\Gamma_l} \to M$ on a knot K we have the output knot $\partial^\perp\mathbf{F} \in \mathcal{K}(M)$ obtained by replacing each $\mathbf{G}_l(a_0)$ by $\mathbf{G}_l(a_0^\perp)$.

Lemma 10.4. *Two knots are n-equivalent if and only if there exists a grope forest $\mathbf{F}$ of degree n on K, such that $\partial^\perp\mathbf{F}$ is isotopic to K'.*

Proof. The n-equivalence relation of [CT04b] is generated by isotopies and simple capped genus one grope cobordisms of degree n. However, their gropes are more general than ours: to fulfil the requirements of our definition a grope cobordism needs to attach to K inside of $K(J_0)$ and its i-th cap has to intersect K inside of $K(J_i)$.

The first condition is not actually a restriction, since a grope is equivalent to a clasper plus a choice of a root, so we can choose the root to always be the leftmost leaf of the clasper. To ensure the second condition, note that leaves do come in the desired order on K, so we need only slide them along K until they fall into the corresponding $K(J_i)$.

Therefore, $K \sim_n K'$ in the sense of [CT04b] if and only if there exists a sequence of thick gropes $\mathbf{G}_l$ of degree n between them, $1 \leq l \leq N$. We now turn this into a grope forest. Firstly, we can assume that $\mathbf{G}_l(a_0)$ is disjoint from $\mathbf{G}_{l-1}(a_0^\perp)$, since one can again slide it off if necessary. In addition, up to isotopy each $\mathbf{G}_l$ can be shrunk into an arbitrarily small neighbourhood of its underlying tree, and since these trees can be made disjoint (being 1-dimensional), we may assume each $\mathbf{G}_l$ is disjoint from all other thick gropes.

Hence, after a possible re-enumeration to ensure that $\mathbf{G}_l(a_0)$ come in the decreasing order, the union $\bigsqcup_{l=1}^{N} \mathbf{G}_l$ is precisely a grope forest. □

Interestingly, although grope forests correspond to a very restricted subclass of claspers, this class is closed under applications of the zip construction with pruning, since this produces claspers with parallel leaves. Note that in our definition of $\sim_n$ knots in $\mathcal{K}_n(M;\mathrm{U})$ differ from U only at J_0, so

$$\mathcal{K}_n(M;\mathrm{U}) \subseteq \mathcal{K}_0(M;\mathrm{U}) := \mathrm{fib}_{\mathsf{ev}_0\mathrm{U}}\big(\mathcal{K}(M) \to \mathsf{P}_0(M)\big) = \{K\colon I \hookrightarrow M \;:\; K|_{I\setminus J_0} = \mathrm{U}|_{I\setminus J_0}\}$$

The inclusion $\mathcal{K}_0(M;\mathrm{U}) \hookrightarrow \mathcal{K}(M)$ is a homotopy equivalence, since $\mathsf{P}_0(M) := \mathcal{E}\mathrm{mb}_\partial(I \setminus J_0, M)$ is contractible, by gradually shortening the free ends as in Lemma 3.4.

The primitive realisation map

It follows from Lemma 10.4 that the map which sends a grope forest $\mathbf{F}$ of degree $n \geq 1$ on U to its output $\partial^\perp\mathbf{F}$ is a continuous surjection

$$\partial^\perp\colon\ \mathsf{Grop}_n(M;\mathrm{U}) \twoheadrightarrow \mathcal{K}_n(M;\mathrm{U}).$$

On the other hand, recall from Proposition 7.16 that the underlying decorated tree map

$$\mathcal{T}_n\colon\ \pi_0\mathsf{Grop}_n(M;\mathrm{U}) \twoheadrightarrow \mathbb{Z}[\mathrm{Tree}_{\pi_1 M}(n)]$$

sends a grope forest $\mathbf{F}$ to the sum of the underlying trees of its constituent thick gropes. We now define the realisation map, mentioned in Sections 2.2.1 and 7.1.

THEOREM 10.5. *For $n \geq 1$ there exists a map $\mathcal{R}^T_n$ making the following diagram commute*

$$\begin{tikzcd} \pi_0\mathsf{Grop}_n(M;\mathrm{U}) \arrow[r, two heads, "\mathcal{T}_n"] \arrow[d, two heads, "\partial^\perp"'] & \mathbb{Z}[\mathrm{Tree}_{\pi_1 M}(n)] \arrow[d, two heads, "\mathcal{R}^T_n"] \\ \mathbb{K}_n(M;\mathrm{U}) \arrow[r, two heads, "mod\ \sim_{n+1}"] & \mathbb{K}_n(M;\mathrm{U})/\sim_{n+1} \end{tikzcd}$$

Proof. This is based on [Hab00, Thms. 4.3 & 4.7], but the formulation is closer to [CT04a, Lem. 2.1], where only $M = I^3$ was considered.

Pick $F \in \mathbb{Z}[\mathrm{Tree}_{\pi_1 M}(n)]$. We show that any embedding $\mathbf{F}\colon \bigsqcup_{l=1}^N \mathsf{B}_{\Gamma_l} \hookrightarrow M$ on U with $\mathcal{T}_n(\mathbf{F}) = F$ can be transformed – without changing the class of the knot $\partial^\perp\mathbf{F} \in \mathbb{K}_n(M;\mathrm{U})$ modulo $(n+1)$-equivalence – to one and the same collection of N disjoint thick gropes, namely the one that satisfies the following conditions.

(a) Thick gropes appear on U in any order, but with each root followed by all the leaves of the same grope, then the root and leaves of the next grope, and so on.

(b) Leaf edges of a thick grope with decorations $g^l_{\underline{n}} \in (\pi_1 M)^n$ are arbitrarily close to some pre-chosen representatives γ^l_i of g^l_i, so "not knotted", and all other edges are close to J_0.

(c) All edges have trivial framing.

(d) Thick gropes with the same underlying tree, but different sign, have been removed.

Note that this will finish the proof since it will imply that $[\partial^\perp\mathbf{F}] \in \mathbb{K}_n(M;\mathrm{U})/\sim_{n+1}$ depends only on the underlying decorated tree and not on a particular grope forest $\mathbf{F}$.

Firstly, as in the proof of Proposition 7.16, we can shrink $\mathbf{F}$ arbitrarily close to the 1-complex consisting of its underlying trees. Furthermore, by Theorem 10.1 the output knot of $\mathbf{F}$ is precisely the result of the clasper surgery on a collection of simple tree claspers obtained from that collection of the underlying trees.

We now show that one can ensure $(a)-(d)$ using manipulations with claspers. Namely, one can use moves from Figures 37 and 39 to prove that the following manipulations do not change the $(n+1)$-equivalence class of the output knot.

(1) Exchange the order along U of two leaves of two different[36] tree claspers [Hab00, Prop. 4.4].

(2) A crossing change of an edge of a tree clasper with U [Hab00, Prop. 4.5], [Gus00, Thm. 6.4].

[36] Note that two leaves of the same tree clasper are not allowed to exchange their order along U – this is part of the data of the underlying tree. This will instead give the STU^2 relation!

(3) A crossing change between two edges of two different tree claspers [Hab00, Prop. 4.6], [Gus00, Thm. 6.6].

(4) A crossing change between two edges (possibly the same) of the same tree clasper – because such a crossing change can be obtained using isotopies and crossing changes with U.

(5) A full twist on an edge – this reduces to doing a full twist on a leaf edge and this can again be done by passing an edge across U (see proof of [Hab00, Thm. 4.3]).

(6) Removing two tree claspers which have the same underlying tree, but differ by a half-twist on one leaf edge [Hab00, Thm. 4.7].

Observe that (a) follows from (1) and the fact that the leftmost leaves can be chosen for roots, (b) follows from $(2, 3, 4)$ and the fact that trees are contractible, (5) implies (c) and (6) implies (d). □

Therefore, we have a well-defined realisation map

$$\mathcal{R}_n^T\colon\ \mathbb{Z}[\mathrm{Tree}_{\pi_1 M}(n)] \twoheadrightarrow \mathbb{K}_n(M;\mathrm{U})/\!\sim_{n+1} \tag{10.1}$$

which, as a consequence of the proof, can be computed as follows.

COROLLARY 10.6. *Let $\#_{l=1}^N \mathbf{G}_l$ denote the collection of thick gropes with $\mathcal{T}_n(\mathbf{G}_l) := \varepsilon^l \Gamma_l^{g^l}$ satisfying $(a)-(d)$. Then we have*

$$\mathcal{R}_n^T\left(\sum_{l=1}^N \varepsilon^l \Gamma_l^{g^l}\right) := \mathrm{U}|_{[0,L_0]} \# \mathbf{G}_1(a_0^\perp) \# \mathbf{G}_2(a_0^\perp) \dots \# \mathbf{G}_N(a_0^\perp) \# \mathrm{U}|_{[R_0,1]}$$

Indeed, the output knot for this collection of thick gropes is by (a) a kind of a "connected sum": we first see a piece of U from 0 to L_0, concatenated with $\mathbf{G}_1(a_0^\perp)$, then $\mathbf{G}_2(a_0^\perp)$, and so on, until we see $\mathbf{G}_N(a_0^\perp)$ after which the rest of U follows. This also shows that our definition of $\mathcal{R}_n^T$ is very close to that of [Oht02, Theorem E.12] for $M = I^3$.

10.3 Properties of the primitive realisation map

The associated graded are abelian groups

The following proves the rest of Theorem G1.

THEOREM 10.7. *$\mathbb{K}_0(M;\mathrm{U})/\!\sim_1 \cong \pi_1 M$ and for $n \geq 1$ the set $\mathbb{K}_n(M;\mathrm{U})/\!\sim_{n+1}$ can be given abelian group structure, for which (10.1) is a group homomorphism.*

Proof. The first claim is clear since $\sim_1$ is generated by crossing changes. For $n \geq 1$ we use the following lemma, whose proof is immediate.

LEMMA 10.8. *Let $f\colon A \to S$ be a surjection of a group onto a set. If the equivalence relation $a_1 \sim_f a_2 \iff f(a_1) = f(a_2)$ is a congruence on A – that is, if $a_i \sim_f b_i$ for $i = 1, 2$ implies $a_1 + b_1 \sim_f a_2 + b_2$, then there is a group structure on S for which f is a homomorphism.*

Let us check that $\mathcal{R}_n^T$ indeed gives a congruence relation on $\mathbb{Z}[\mathrm{Tree}_{\pi_1 M}(n)]$.

Since this is abelian, we need only check that for $F_1, F_2, F_3 \in \mathbb{Z}[\mathrm{Tree}_{\pi_1 M}(n)]$ we have

$$\mathcal{R}_n^T(F_1) = \mathcal{R}_n^T(F_2) \implies \mathcal{R}_n^T(F_1 + F_3) = \mathcal{R}_n^T(F_2 + F_3).$$

For $i = 1, 2$ let $\mathbf{F}_i$ be a grope forest on U with $\mathcal{T}_n(\mathbf{F}_i) = F_i$.

Now pick a grope forest $\mathbf{F}_3$ on U with $\mathcal{T}_n(\mathbf{F}_3) = F_3$ and which is disjoint both from $\mathbf{F}_1$ and $\mathbf{F}_2$, and appears left to both of them. This is possible as thick gropes are neighbourhoods of 1-complexes.

The assumption $\mathcal{R}^T_n(F_1) = \mathcal{R}^T_n(F_2)$ means that $\partial^\perp \mathbf{F}_1 \sim_{n+1} \partial^\perp \mathbf{F}_2$. Now by the same argument, a forest clasper witnessing this $(n+1)$-equivalence can be chosen disjointly from $\mathbf{F}_3$. Hence, it also witnesses that $\partial^\perp(\mathbf{F}_1 \sqcup \mathbf{F}_3)$ and $\partial^\perp(\mathbf{F}_2 \sqcup \mathbf{F}_3)$ are $(n+1)$-equivalent, as desired.

Therefore, $\mathcal{R}^T_n \colon \mathbb{Z}[\mathrm{Tree}_{\pi_1 M}(n)] \to \mathbb{K}_n(M;\mathrm{U})/\sim_{n+1}$ is indeed a surjection of abelian groups. □

Example 10.9. *For $M = I^3$ and* U *the classical unknot we have*

$$\mathbb{K}(I^3) = \mathbb{K}_0(I^3;\mathrm{U}) = \mathbb{K}_1(I^3;\mathrm{U}), \qquad \mathbb{K}_0(I^3;\mathrm{U})/\sim_1 = \mathbb{K}_1(I^3;\mathrm{U})/\sim_2 \cong \{0\}$$

The last group is trivial as the quotient of $\mathbb{Z} = \mathbb{Z}[\{1\}]$ (the group ring of the trivial group) by $\overset{1}{|}{}^{1} = 0$, which is precisely the 1T relation.

Namely, any finger move in I^3, that is, a grope cobordism of degree 1, can be unknotted. The reason lies in the fact that modulo $\sim_2$ we can undo the twists and unknottings within the finger to obtain just the simplest 'flat' finger $\mathcal{G}$ as on the left picture of Figure 17, or its half-twist. This follows from moves (2) and (5) from the proof of Theorem 10.5. Finally, observe that the output knot $\partial^\perp\mathcal{G}$ for such a flat finger move is isotopic to the unknot.

On the other hand,

$$\mathbb{K}_2(I^3;\mathrm{U})/\sim_3 \cong \mathsf{Lie}(2) \cong \mathbb{Z}\{\overset{2\ \ 1}{Y}\}$$

is non-trivial. It is generated by the right-handed trefoil, see Figures 18 and 19. △

Example 10.10. *The group $\mathbb{K}_1(M;\mathrm{U})/\sim_2$ consists of 2-equivalence classes of knots which are homotopic to* U*. By the theorem it is a quotient of $\mathbb{Z}[\pi_1 M]$. The generator corresponding to $g \in \pi_1 M$ is given by the embedded loop obtained by the finger move along g as in Figure 17. Linear combinations $\sum_i g_i$ are by Corollary 10.6 appropriate 'connected sums' of such finger moves.* △

The connected sum

Consider now $M = I \times \Sigma$ for Σ a compact connected surface with possibly non-empty boundary. Then $\mathcal{K}(I\times\Sigma)$ has a structure of an H-space, by stacking in the I-direction, with $\mathrm{U} = I \times pt$. This makes $(\mathbb{K}(I\times\Sigma), \#)$ into a monoid.

PROPOSITION 10.11. *For each $n \geq 1$ $\mathbb{K}_n(I\times\Sigma;\mathrm{U})$ is a submonoid of $(\mathbb{K}(I\times\Sigma),\#)$. Moreover, the structure of an abelian group on $\mathbb{K}_n(I\times\Sigma;\mathrm{U})/\sim_{n+1}$ from the previous theorem coincides with the one induced from $\mathbb{K}_n(I\times\Sigma;\mathrm{U})$.*

Proof. If two knots are $(n-1)$-equivalent to the unknot then so is their connected sum, using the disjoint union of two collections of thick gropes for the respective knots as in Corollary 10.6.

For the second claim it is enough to check that $\mathcal{R}^T_n(F_1+F_2) = \mathcal{R}^T_n(F_1)\#\mathcal{R}^T_n(F_2)$. By Corollary 10.6 the knot $\mathcal{R}^T_n(F_1+F_2)$ is obtained from a collection of thick gropes, and we can ensure that those corresponding to trees in F_1 come first on U, and then those corresponding to F_2. Now push the grope collection for F_2 down along the I-direction of $I\times\Sigma$, using the move (3) from Theorem 10.5 to homotope edges of F_2 through those of F_1, not changing the $(n+1)$-equivalence class of $\partial^\perp(F_1+F_2)$. The resulting knot is the connected sum of $\mathcal{R}^T_n(F_1)$ and $\mathcal{R}^T_n(F_2)$. □

On the kernel of the realisation map

We now prove that $\mathcal{R}_n^T$ vanishes on AS and IHX relations, which were defined in (2.1), and also on the STU^2 relations from Definition 2.9.

Proof of Theorem G2. The fact that the relations $AS, IHX \subseteq \mathbb{Z}[\mathrm{Tree}_{\pi_1 M}(n)]$ are in the kernel of $\mathcal{R}_n^T$ is standard. For AS see [Gus00, Thm. 6.8] and [CT04a, Lem. 2.12]. For proofs of IHX see [Gus00, Thm. 6.7] and [CST07] (also for a 4-dimensional analogue). An argument is sketched in [Oht02, Lem. E.11]. These authors assume $M = I^3$, but both relation happen locally in a 3-ball.

Thus, the realisation map descends to a map $\mathcal{R}_n^T\colon \mathsf{Lie}_{\pi_1 M}(n) \to \mathbb{K}_n(M;\mathrm{U})/\!\sim_{n+1}$.

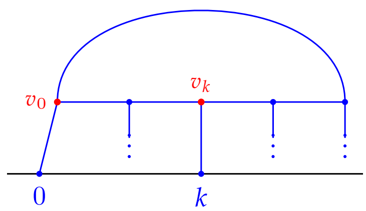
Let us now prove that for $n = 1$ this vanishes on $\overset{1}{\big|}{}^{1}$, the chord decorated with the trivial group element, so that

$$\mathcal{R}_1^T\colon \mathcal{A}_1^T(M) \to \mathbb{K}_1(M;\mathrm{U})/\!\sim_2$$

In Example 10.9 we saw that this is the case for $M = I^3$, since modulo 2-equivalence we can simplify a thick grope (clasper) of degree 1 to be just the simplest finger move, whose output knot is just the unknot. This argument extends to any M if the underlying decoration of the grope is the trivial group element $1 \in \pi_1 M$. Namely, we can simply shrink and slide the thick grope to a small 3-ball near J_0, and apply the argument for I^3.

Let us now show that the relation $STU_\pi^2 \subseteq \mathsf{Lie}_{\pi_1 M}(n)$ from (2.4) is in the kernel of $\mathcal{R}_n^T$ for $n \geq 2$. This has not yet appeared in literature; however, for $M = I^3$ and using Jacobi diagrams this follows from the STU relation, which was proven in [Gus00, Thm. 6.5] and [CT04a, Lem.2.12].

Firstly, consider a model 1-loop diagram



Replacing either the vertex v_k or v_0 by a leaf gives respectively the leftmost clasper C_{v_k} and the rightmost clasper C_{v_0} in Figure 40. Surgeries on these two claspers are equivalent modulo higher degree terms, because they can both be reduced to the clasper in the middle of Figure 40 as follows.

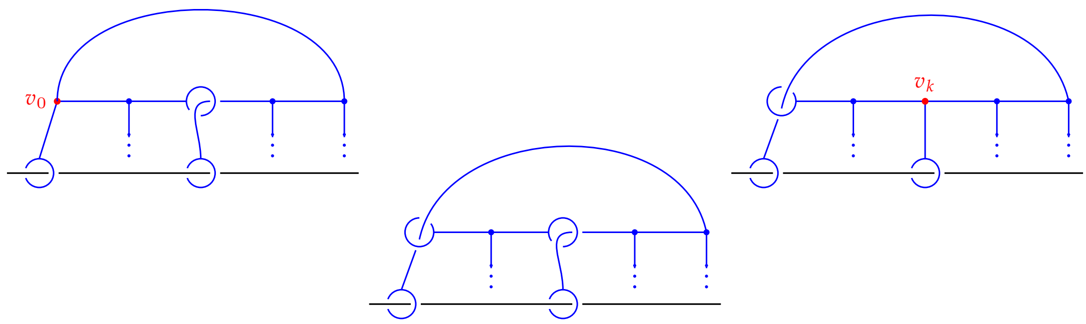


Figure 40. The claspers C_{v_0} and C_{v_k} and the middle clasper which relates them.

We first use Gusarov's identity from Figure 39 to replace the trivalent vertex v_0 by a leaf grabbing an edge. We then zip down thus obtained boxes, and prune all the leaves off modulo the higher degree. One of the resulting two claspers is precisely C_{v_0}, while the other one has a leaf grabbing an edge of C_{v_0} and nothing else. Modulo higher degree we can do the crossing change to unlink that leaf, so the clasper becomes trivial and can be removed.

Thus, C_{v_k} and C_{v_0} are non-simple tree claspers both with a unique non-simple leaf grabbing another leaf edge. More precisely, the leaf bounds a disk in M which does not intersect the unknot U or the clasper, except for exactly one transverse intersection with a leaf edge.

We now claim that such a clasper is equivalent to the one depicted in the middle of Figure 41. We simply pull the front part of the loop down and swing it to the back, and introduce two degree 1 claspers whose surgery will realise the crossing changes with the unknot U.

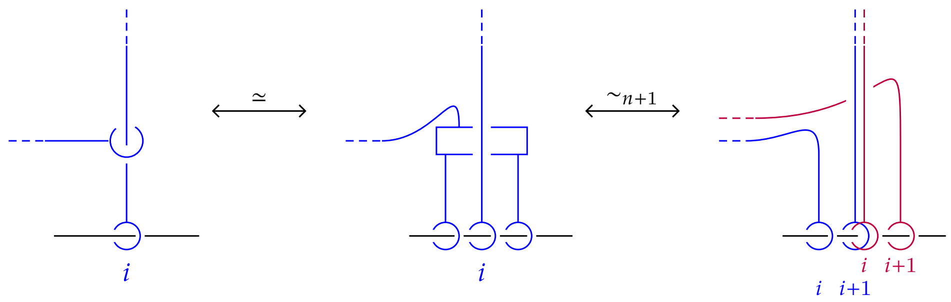


Figure 41. From a non-simple clasper to two simple tree claspers.

Finally, using the zip construction on the clasper in the middle and pruning the leaves off modulo higher degree, we obtain two claspers of degree n as on the right of Figure 41. They differ only by the order of the two consecutive leaves around the old leaf. Hence, the surgery on C_{v_i} for $i = 0, k$ is equivalent modulo higher degree to the surgery on the two claspers $STU(D, v_i)$. This precisely gives the $STU^2_{\pi_1 M}$ relation: $STU(D, v_0) = STU(D, v_k)$. □

A comparison of realisation maps

Proof of Theorem G3. We now consider $M = I^3$ and the diagram

$$\begin{tikzcd}
\mathcal{A}^T_n \arrow[r, hook, "P"] \arrow[d, two heads, "\mathcal{R}^T_n"'] & \mathfrak{pr}(\mathcal{A})_n \arrow[r, hook] & \mathcal{A}_n \arrow[r, two heads] \arrow[d, two heads, "\mathcal{R}_n"] & \mathcal{A}^I_n \arrow[d, two heads, "\mathcal{R}^I_n"] \\
\mathbb{K}_n(I^3)/\sim_{n+1} \arrow[rr, "K \mapsto K - U"] & & \mathcal{V}_n/\mathcal{V}_{n+1} \arrow[r, "cs_n"] & \mathbb{K}_n(I^3)/\sim_{n+1}
\end{tikzcd} \tag{10.2}$$

The left vertical map was defined in Theorem 10.5. Using the notation of Corollary 10.6, for trees $\Gamma_l \in \mathcal{A}^T_n$ and $\varepsilon_l \in \{\pm 1\}$ for $1 \leq l \leq N$ it is given by

$$\mathcal{R}^T_n\Big(\sum_l \varepsilon_l \Gamma_l\Big) = \mathop{\#}_{l=1}^{N} \mathbf{G}_l(a_0^{\pm}) \quad \in \mathbb{K}_n(I^3)/\sim_{n+1}$$

The middle vertical map is the classical one on the algebra of chord diagrams as defined in (7.2). Namely, given a chord diagram we take the alternating sum of knots obtained by doing a subset of crossing changes along chords.

However, Bar-Natan's isomorphism (7.1) identifies this algebra with the algebra of Jacobi diagrams, and in this description the map was provided by [CT04a] as follows (see there for details).

For a diagram $\varepsilon D \in \mathcal{A}_n$ let $\mathcal{D}$ be any embedding of D as a framed *graph* clasper on U with sign ε. Let $\mathcal{D}^i$, $1 \leq i \leq r$, denote its connected components (simple graph claspers), and let $\mathrm{U}^{\mathcal{D}^S}$ denote the knot obtained by performing surgeries along all claspers $\mathcal{D}^i$ for i in a set $S \subseteq \underline{r_l}$. Define

$$[\mathrm{U};\varepsilon D] := (-1)^{r_l} \sum_{S\subseteq \underline{r}} (-1)^{|S|} \mathrm{U}^{\mathcal{D}^S}.$$

This does not depend on the choice of the embedding $\mathcal{D}_l$ and we can let

$$\mathcal{R}_n\Big(\sum_{l=1}^{N} \varepsilon_l D_l\Big) = \sum_{l=1}^{N} [\mathrm{U}; D_l] \quad \in \mathcal{V}_n\!\big/\mathcal{V}_{n+1}$$

Lastly, Conant and Teichner define the vertical map on the right by $\mathcal{R}_n^I := cs_n \circ \mathcal{R}_n$, where cs_n takes a linear combination of knots to their connected sum (note that the target is a group so we have inverses $-K$). Thus, the square on the right hand side clearly commutes. More explicitly,

$$\mathcal{R}_n^I\Big(\sum_{l=1}^{N} \varepsilon_l D_l\Big) = \mathop{\#}_{l=1}^{N} \mathop{\#}_{S\subseteq \underline{r_l}} (-1)^{r_l+|S|} \mathrm{U}^{\mathcal{D}_l^S} \quad \in \mathbb{K}_n(I^3)\!\big/\!\sim_{n+1}$$

This is well-defined on $\mathcal{A}^I$, since any decomposable diagram $D_1 \cdot D_2$ can be written as a polynomial in connected diagrams T_i such that all monomials have degree at least 2 (see Lemma 2.15). In turn, for such monomials we have

$$\mathcal{R}_n^I(\varepsilon T_1 \cdots T_r) = (-1)^r \mathop{\#}_{\substack{S\subseteq \underline{r} \\ S=\{i_1,\dots,i_{|S|}\}}} (-1)^{|S|} \mathrm{U}^{\mathcal{T}_{i_1}} \# \cdots \# \mathrm{U}^{\mathcal{T}_{i_{|S|}}} = (-1)^r \mathop{\#}_{i\in \underline{r}} \Big(\sum_{S\subseteq \underline{r}\setminus\{i\}} (-1)^{|S\cup i|} \Big) \mathrm{U}^{\mathcal{T}_i} = 0$$

Outer square is clearly commutative since each Γ_l has a single component and $\mathrm{U}^{\mathbf{G}_l} = \mathbf{G}_l(a_0^{\perp})$, so

$$cs_n\Big(\mathcal{R}_n^T\Big(\sum_{l=1}^{N} \varepsilon_l \Gamma_l\Big) - \mathrm{U}\Big) = \mathop{\#}_{l=1}^{N} \mathrm{U}^{\mathbf{G}_l} = \mathcal{R}_n^I\Big(\sum_{l=1}^{N} \varepsilon_l \Gamma_l\Big)$$

Let us show that the left square commutes as well. One one hand, we get $\#_l K_l - \mathrm{U} \in \mathcal{V}_n\!\big/\mathcal{V}_{n+1}$ where $K_l = \mathrm{U}^{\mathbf{G}_l}$, and on the other, $\mathcal{R}_n(\sum_{l=1}^N \varepsilon_l \Gamma_l) = \sum_l [\mathrm{U};\Gamma_l] = \sum_l (K_l - \mathrm{U})$. It is enough to show

$$\sum_{l=1}^{N} (K_l - \mathrm{U}) = \mathop{\#}_{l=1}^{N} K_l - \mathrm{U} \quad \in \mathcal{V}_n\!\big/\mathcal{V}_{n+1} \tag{10.3}$$

We prove this by induction on $N \geq 2$. The induction base is the following claim.

Claim. $(K_1 - \mathrm{U}) \# (K_2 - \mathrm{U}) \in \mathcal{V}_{2n} \subseteq \mathcal{V}_{n+1}$, the quality (10.3) holds for $N = 2$.

This follows by letting $D := \Gamma_1 \cdot \Gamma_2 \in \mathcal{A}_{2n}$ and $\mathcal{D} = \mathbf{G}_1 \sqcup \mathbf{G}_2$, so by definition

$$[\mathrm{U}; D] = K_1 \# K_2 - K_1 - K_2 - \mathrm{U} \quad \in \mathcal{V}_{2n}$$

Now apply the induction base and induction hypothesis for $< N$ to get

$$\mathop{\#}_{l=1}^{N-1} K_l \# K_N - \mathrm{U} = \big(\mathop{\#}_{l=1}^{N-1} K_l - \mathrm{U}\big) + (K_N - \mathrm{U}) = \sum_{l=1}^{N-1} K_l - \mathrm{U} + (K_N - \mathrm{U})$$

implying (10.3). □

B Vassiliev invariants of pure braids

The main references for this brief survey are [Koh85], [CDM12], and [Fre17].

Let $\mathscr{P}(m)$ be the pure braid group on m strands. On the group ring $\mathbb{Z}[\mathscr{P}(m)]$ one can define the Vassiliev–Gusarov filtration $\mathcal{V}_n(\mathscr{P}(m))$ using resolutions of singular pure braids with at least n double points, cf. Section 7.1. This actually agrees with the filtration by the powers I^n of the augmentation ideal: $\mathcal{V}_1(\mathscr{P}(m)) = I$ is spanned by the set $\{\beta - \mathrm{U} : \beta \in \mathscr{P}(m)\}$, where U is the trivial braid, and each singular braid with n double points is a product of braids with exactly one double point. Hence, the corresponding linear combination of resolutions is precisely an element of I^n.

The associated graded of this filtration is simply

$$\operatorname{gr}\mathbb{Z}[\mathscr{P}(m)] := \bigoplus_{n\geq 1} I^n \big/ I^{n+1}$$

We again have a Hopf algebra $\widehat{\mathcal{A}}^h(m) := \prod \mathcal{A}^h(m)_n$, this time of horizontal chord diagrams, which consist of some number of horizontal chords attached to the (vertically drawn) trivial braid, modulo the $4T$ relation. There is also a corresponding realisation map, analogous to (7.2):

$$\mathcal{R}_n \colon \mathcal{A}^h(m)_n \to I^n \big/ I^{n+1}$$

A map of sets $v \colon \mathscr{P}(m) \to T$ is an invariant of type $\leq n-1$ if its $\mathbb{Z}$–linear extension vanishes on I^n.

Theorem B.1 (Dimension property of pure braid groups)**.** *A pure braid $\beta \in \mathscr{P}(m)$ is not distinguished from the trivial braid by invariants of type $\leq n-1$, i.e. $\beta - \mathrm{U} \in I^n$, if and only if β lies in the n-th lower central series subgroup $\gamma_n\mathscr{P}(m) \leqslant \mathscr{P}(m)$.*

In other words, the Gusarov–Habiro filtration on $\mathscr{P}(m)$ is simply the lower central series filtration, cf. (7.4). The theorem can be proven using that $\mathscr{P}(m) = \mathscr{P}(m-1) \ltimes \mathbb{F}_{m-1}$ is an almost-direct product[37] and that the dimension property holds for free groups, see [CDM12, Ch. 12].

Let $\operatorname{gr}\mathscr{P}(m) := \bigoplus_n \gamma_n\mathscr{P}(m) \big/ \gamma_{n+1}\mathscr{P}(m)$ be the associated graded Lie algebra. Note that this is not a graded Lie algebra (or, it is concentrated in degree 0), but it has an obvious weight grading by $n \geq 1$. As a corollary of the theorem, we have an isomorphism of weight-graded Lie algebras

$$\operatorname{gr}\mathscr{P}(m) \hookrightarrow\!\!\!\!\rightarrow \mathfrak{pr}\left(\operatorname{gr}\mathbb{Z}[\mathscr{P}(m)]\right), \quad [\beta] \mapsto [\beta - \mathrm{U}]. \tag{B.1}$$

where $\mathfrak{pr}$ are the primitives. If we let $\mathfrak{p}(m) := \mathfrak{pr}\,\mathcal{A}^h(m)$ then there is a commutative diagram

$$\begin{tikzcd}
\mathfrak{p}(m) \arrow[r, hook] \arrow[d, two heads, "\mathcal{R}^T"'] & \mathcal{A}^h(m) \arrow[d, two heads, "\mathcal{R}"] \\
\operatorname{gr}\mathscr{P}(m) \arrow[r, hook, "{[\beta] \mapsto [\beta - \mathrm{U}]}"] & \operatorname{gr}\mathbb{Z}[\mathscr{P}(m)]
\end{tikzcd} \tag{B.2}$$

where the horizontal maps are *inclusions onto primitives*, and the left vertical map sends a primitive chord diagram to the class of the braid obtained by doing crossing changes along all chords.

Lemma B.2. *$\mathfrak{p}(m)$ is the quotient of the free Lie algebra on $t_{ij} = t_{ji}$ for $1 \leq i \neq j \leq m$ by the infinitesimal braid relations (also called the Yang–Baxter relation)*

$$[t_{ij}, t_{kl}] = 0, \qquad [t_{ij}, t_{ik} + t_{jk}] = 0, \quad \textit{for distinct indices } i, j, k, l.$$

Proof. Indeed, there is an obvious map from this Lie algebra to $\mathcal{A}^h(m)$ sending t_{ij} to the horizontal chord between the i-th and j-th strand, and takes the Lie bracket to the algebra commutator.

[37] This is a semi-direct product and the induced action of $\mathscr{P}(m-1)$ on the abelianization $\mathbb{F}_{m-1}^{ab} \cong \mathbb{Z}^{m-1}$ is trivial.

This is well-defined because the $4T$ relation is precisely $[t_{ij}, t_{ik}] = -[t_{ij}, t_{jk}]$ written out as the commutator. Moreover, the induced map $\mathbb{U}\,\mathfrak{p}(m) \to \mathcal{A}^h(m)$ is an isomorphism. $\square$

One should compare this to the case of knots, where $\mathfrak{pr}\,\mathcal{A}$ remains mysterious, see Corollary 2.17.

Theorem B.3. *Both the map of Lie algebras $\mathcal{R}^T\colon \mathfrak{p}(m) \to \operatorname{gr}\mathscr{P}(m)$ and the map of algebras $\mathcal{R}\colon \mathcal{A}^h(m) \to \operatorname{gr}\mathbb{Z}[\mathscr{P}(m)]$ from (B.2) are isomorphisms.*

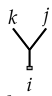
Proof. We show the first statement, and the second will follow by taking universal enveloping algebras and using (B.1). The proof is classical, but not easy to find in the literature. See for example [Fre17, Thm. 10.0.4], where it was attributed to [Koh85] and [Xic00]; we believe this should be more widely known.

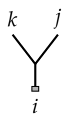
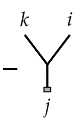
The functor of associated graded Lie algebra of the lower central series filtration passes through almost direct products (see [FR85, Section 3]), so $\operatorname{gr}\mathscr{P}(m) = \operatorname{gr}\mathscr{P}(m-1) \ltimes \mathbb{L}(m-1)$ as Lie algebras, since $\operatorname{gr}\mathbb{F}_{m-1}$ is precisely the free Lie algebra $\mathbb{L}(m-1)$.

Consider the map $\pi\colon \mathfrak{p}(m) \to \mathfrak{p}(m-1)$ which forgets the m-th strand (and all chords possibly connected to it). The kernel $\ker(\pi)$ is the free Lie algebra generated by $t_{im}, 1 \le i \le m-1$: it is generated by this set as an ideal, but then we can use the infinitesimal braid relations to rewrite $[t_{im}, t_{ik}] = -[t_{im}, t_{km}]$. Therefore, we have a commutative diagram

$$\begin{tikzcd}
\ker(\pi) \arrow[r, hook] \arrow[d, hook] & \mathfrak{p}(m) \arrow[r, two heads, "\pi"] \arrow[d, "\mathcal{R}^T"'] & \mathfrak{p}(m-1) \arrow[d] \\
\mathbb{L}(m-1) \arrow[r, hook] & \operatorname{gr}\mathscr{P}(m) \arrow[r, two heads] & \operatorname{gr}\mathscr{P}(m-1)
\end{tikzcd}$$

and the claim follows by induction. $\square$

Remark B.4. *We can think of the bracket $[t_{ij}, t_{ik}]$ as the rooted tree $T_i :=$*  *where the lower index denotes the label of the root (compare with Section 2.1, where 0 was always the root label). Now the relation $[t_{ij}, t_{ik}] = -[t_{ij}, t_{jk}] = -[t_{ji}, t_{jk}]$ says that exchanging the root i with the leaf j introduces the sign:*

$T_i =$  $= -$  $= -T_j^{i,j}$

Thus, we first act by the transposition $(i\,j) \in \mathcal{S}_m$ on the unrooted tree T to get $T^{i,j} = (i\,j)_* T$, and then take j for the root. Similarly, an iterated bracket in t_{ik} with a fixed index i and indices $k \in S$ each appearing exactly once, for some finite set $S \not\ni i$, corresponds to a tree $\Gamma \in \mathrm{Tree}(S)$ whose root is labelled by i instead of 0.

Remark B.5. *There are also Drinfeld–Kohno graded Lie algebras*

$$\mathfrak{p}_d(m) := \pi_*\mathsf{Conf}_n(\mathbb{R}^d) \cong \langle t_{ij} = (-1)^d t_{ji}, 1 \le i \ne j \le n \rangle \big/ [t_{ij}, t_{kl}] = 0, [t_{ij}, t_{ik} + t_{jk}] = 0$$

where $|t_{ij}| = d-2$. The cyclic operad structure mentioned in Section 2.1 precisely originates in the fact that $\mathfrak{p}_d(\bullet)$ is an operad and $\mathsf{Lie}_d(n-1) \subseteq \pi_{(n-1)(d-2)}\mathsf{Conf}_n(I^d) \subseteq \mathfrak{p}_d(n)$. See also Corollary 1.8.

Universal invariants

One can define universal Vassiliev invariants over a commutative ring R of any finitely generated group G, with $G = \mathscr{P}(m)$ as a special case. See [Qui68; Lin97; Bar16; SW19] for details.

Let $R[G]$ be the group ring filtered by the powers of the augmentation ideal and $\widehat{R[G]} := \lim R[G]/I^n$ its completion. Let $\operatorname{gr} R[G] = \bigoplus_{n\geq 1} I^n/I^{n+1}$ be the associated graded and $\widehat{\operatorname{gr}} R[G] = \prod_{n\geq 1} I^n/I^{n+1}$ its completion. Both $\widehat{R[G]}$ and $\widehat{\operatorname{gr}} R[G]$ are complete Hopf algebras over R, whose associated graded are canonically identified with $\operatorname{gr} R[G]$.

Definition B.6. *A universal Vassiliev invariant for G over R is a map $Z\colon G \to \widehat{\operatorname{gr}} R[G]$ whose linear extension $\overline{Z}\colon R[G] \to \widehat{\operatorname{gr}} R[G]$ is a filtration preserving R-linear map inducing identity on the associated graded $\operatorname{gr} R[G]$. Such Z is moreover a universal additive Vassiliev invariant if the induced map*

$$\widehat{Z}\colon \widehat{R[G]} \to \widehat{\operatorname{gr}} R[G]$$

is a filtration preserving isomorphism of Hopf algebras.

Lemma B.7 ([SW19])**.** *If R is a field of characteristic zero, then Z is a universal additive Vassiliev invariant for G over R if and only if $\overline{Z}$ is both an algebra and a coalgebra map.*

Hence, $\widehat{Z}$ restricts to an isomorphism of the grouplikes $\widehat{G}_R := \mathbb{G}(\widehat{R[G]}) \to \mathbb{G}(\widehat{\operatorname{gr}} R[G])$.

Here $\widehat{G}_R$ is the Malcev completion, see [Fre17]. Also compare with $\widehat{\mathbb{K}}_R$ from Remark 7.7.

Note that for the case of knots $\mathbb{K}(I^3)$ we were not in the convenient situation that $\operatorname{gr} \mathbb{Z}[\mathbb{K}]$ can be described by generators and relations as $\operatorname{gr} \mathbb{Z}[\mathscr{P}(m)] \cong \mathcal{A}^h$ was, see Theorem B.3. This is addressed in [BD17] (using a 'candidate' $\mathcal{A}$ and an '$\mathcal{A}$-expansion'), and also by the more flexible Definition 7.6 of an additive universal invariant. See the mentioned references for the study of these notion in general, and let us return to the case $G = \mathscr{P}(m)$.

Theorem B.8 ([Bar95b; Pap02; CDM12])**.** *Multiplying Magnus expansions of free groups gives a universal Vassiliev invariant over $\mathbb{Z}$*

$$\mathcal{M}\colon \mathscr{P}(m) \to \widehat{\mathcal{A}^h(m)}$$

which is injective, so Vassiliev invariants distinguish pure braids. However, $\mathcal{M}$ is not additive.

An element $\Phi \in \mathbb{G}(\widehat{\mathcal{A}^h}(3) \otimes R)$ is a Drinfeld associator if it satisfies certain pentagon and hexagon relations; Drinfeld showed existence of such an element for $R = \mathbb{Q}$. See [Fre17, Ch. 10.2].

Theorem B.9 ([Koh85])**.** *The Knizhnik–Zamolodchikov Drinfeld associator Φ over $\mathbb{C}$ gives a universal additive Vassiliev invariant for $\mathscr{P}(m)$ over $\mathbb{C}$, that is, an isomorphism*

$$\zeta_\Phi\colon \widehat{\mathscr{P}(m)}_{\mathbb{C}} \to \mathbb{G}(\widehat{\mathcal{A}^h(m) \otimes \mathbb{C}})$$

which induces the canonical isomorphism of associated graded from Theorem B.3.

Note that $\log\colon \mathbb{G}(\widehat{\mathcal{A}^h(m) \otimes \mathbb{C}}) \to \widehat{\mathfrak{p}(m) \otimes \mathbb{C}}$ is an isomorphism, so Theorem B.9 gives also an isomorphism of the Malcev Lie algebra of the pure braid group over $\mathbb{C}$ and the Drinfeld Kohno Lie algebra (which is its l.c.s. associated graded). This was generalised by Le and Murakami [LM96] who construct a combinatorial Kontsevich integral over R for tangles using any Drinfeld associator over R. In particular, there is a universal additive Vassiliev invariant of pure braids over $\mathbb{Q}$.

It is not known if such an invariant exists over $\mathbb{Z}$ [Pap02]. On the other hand, the first question in the list of open problems in the Vassiliev theory from Section 7.1 is answered affirmatively for pure braids by Theorem B.8: Vassiliev invariants separate braids. The answer to the second question is also positive: the pure braid groups are residually nilpotent, so Vassiliev invariants of pure braids with values in abelian groups detect the trivial braid.

C On the connecting maps

The classifying space of the layer is connected

We now prove Proposition 3.9, which says that $\mathsf{BF}_n(M) := \operatorname{holim}_{\emptyset\neq S\subseteq[n-1]} \mathscr{E}_{Sn}$ is a connected space. This was used to show that $p_n\colon \mathsf{P}_n(M) \to \mathsf{P}_{n-1}(M)$ are surjections.

Proof of Proposition 3.9. Using the iterative decomposition of homotopy limits over punctured cubes we get a homotopy pullback diagram

$$\begin{tikzcd} \mathscr{E}_{n-1n} \arrow[r, "c"] & \operatorname*{holim}_{\emptyset\neq S\subseteq[n-2]} \mathscr{E}_{Sn-1n} \\ \mathsf{BF}_n(M) \arrow[r] \arrow[u] & \operatorname*{holim}_{\emptyset\neq S\subseteq[n-2]} \mathscr{E}_{Sn} \arrow[u, "r_*^{n-1}"] \end{tikzcd}$$

By re-numerating J_n as J_{n-1} the space at the bottom is identified with $\mathsf{BF}_{n-1}(M)$, so we denote it by $\mathsf{BF}^n_{n-1}(M)$. As in Proposition 3.5, the diagram gives the fibre sequence

$$t^n_{n-1}(M) := \operatorname{hofib}(c) \to \mathsf{BF}_n(M) \to \mathsf{BF}^n_{n-1}(M).$$

Therefore, if we show that the connecting map $\delta\colon \Omega\mathsf{BF}^n_{n-1}(M) \to t^n_{n-1}(M)$ is surjective on π_0, we can prove that $\mathsf{BF}_n(M)$ is connected by induction on $n \geq 1$, using that $\mathsf{BF}_1(M) \simeq \mathbb{S}M$ is.

Observe that $t^n_{n-1}(M) \cong \operatorname{tofib}_{S\subseteq[n-2]} \mathscr{E}_{Sn-1n} \simeq \operatorname{tofib}_{S\subseteq\underline{n-2}} \mathscr{F}^n_{Sn-1}$ is the total fibre of the face of the cube $\operatorname{tofib}_{S\subseteq\underline{n-1}}(\mathscr{F}^n_S) \cong \mathsf{F}_n(M)$ corresponding to those sets which *contain the index* $n-1$. Moreover, the connecting map δ is equivalent to the map $r_*^{n-1}\colon \mathsf{F}^n_{n-1}(M) \to t^n_{n-1}(M)$ which introduces the puncture J_{n-1} (this is simply loops on the vertical map in the diagram above).

Note that r_*^{n-1} has a left homotopy inverse l_*^{n-1}, precisely the one we used to start delooping $\mathsf{F}_n(M)$ in Section 4.1. Using only the rest of our delooping maps we get equivalences

$$t^n_{n-1}(M) := \operatorname*{tofib}_{S\subseteq\underline{n-2}} \mathscr{F}^n_{Sn-1} \xrightarrow{\chi} \Omega^{n-2} \operatorname*{tofib}_{S\subseteq\underline{n-2}}(\mathscr{F}^n_{Sn-1}, l^k_{Sn-1}) \xrightarrow{\mathsf{retr}\mathscr{D}} \Omega^{n-2} \operatorname{tofib}\Omega(M \vee \mathbb{S}_{S\cup n-1}).$$

Now similarly as in Proposition 5.4 we find

$$t^n_{n-1}(M) \simeq \Omega^{n-2} \prod_w \Omega\Sigma^{1+(d-2)l_w}(\Omega M)^{\wedge l'_w}$$

where the product is over the subbasis of $\mathsf{B}(\underline{n-1} \cup \underline{n-1}')$ consisting of those words in letters $x^i, x^{i'}, i \in \underline{n-1}$, such that for each $i \in \underline{n-2}$ either x^i or $x^{i'}$ appears. Since x^{n-1} and $x^{n-1'}$ can but do not have to appear, this set can be written as the union $\mathsf{N}'\mathsf{B}(\underline{n-2}) \cup \mathsf{N}'\mathsf{B}(\underline{n-1})$.

Since $l_w \geq n-2$, the space $\Sigma^{1+(d-2)l_w}(\Omega M)^{\wedge l'_w}$ has non-trivial π_{n-1} if only if both $d = 3$ and $l_w = n-2$. Thus, δ is trivially surjective for $d \geq 4$. From now on assume $d = 3$, so

$$\pi_0 t^n_{n-1}(M) \cong \mathsf{Lie}_{\pi_1 M}(n-2)$$

using the letters x^g_i for $i \in \underline{n-2}$ (x_{n-1}, x'_{n-1} do not appear at all), by arguments as in Section 5.

Using the equivalence $\mathsf{retr}\mathscr{D}\chi$ as for $\mathsf{F}_{n-1}(M)$, but with the top index $n-1$ replaced by n, we get

$$\pi_0\mathsf{F}^n_{n-1}(M) \cong \pi_{n-1}(\operatorname{tofib}\Omega(M \vee \mathbb{S}_S \vee \mathbb{S}_{i_m n})) \cong \mathsf{Lie}_{\pi_1 M}(n-2)$$

in letters $x^g_1, \ldots, x^g_{n-3}$ and $x^g_{n-2,n}$. The map r_*^{n-1} corresponds to $\rho_S^{n-1} : M_{Sn-1} \to M_{Sn-1n}$, and after the retraction to the pinch map $\mathbb{S}_{i_m n} \to \mathbb{S}_{i_m n-1} \vee \mathbb{S}_{n-1n}$ (and Id on all other wedge factors). Under the equivalences above, we see that $\pi_0 r_*^{n-1}$ replaces each appearance of the letter $x^g_{n-2,n}$ in a word $w(x^g_i, x^g_{n-2,n}) \in \pi_0\mathsf{F}^n_{n-1}(M)$ by $x^g_{n-2} + x^g_{n-1}$. This is clearly surjective. $\square$

Observe that $\mathsf{F}_n(M) = \mathrm{hofib}(\mathsf{F}^n_{n-1}(M) \to t^n_{n-1}(M))$, and the first differential in the spectral sequence is induced from

$$\Omega\mathsf{F}_{n-1}(M) \xrightarrow{r^n_*} \Omega\mathsf{F}^n_{n-1}(M) \hookrightarrow \mathsf{F}_n(M).$$

On the image of the first differential

We now sketch the proof of our claims about the spectral sequence $E^1_{-n,t}(M) := \pi_{t-n}\mathsf{F}_n(M)$ from Section 2.3 – namely, that for $n \geq 2$ the $STU^2_{\pi_1 M}$ relation from (2.4) is contained in the image of

$$\begin{array}{ccc} E^1_{-n,n(d-2)+1}(M) & \xrightarrow{d^1_{-n,n(d-2)+1}} & E^1_{-(n+1),n(d-2)+1}(M) \\ \| & & \| \\ \pi_{n(d-3)+1}\mathsf{F}_n(M) & \longrightarrow & \pi_{n(d-3)}\mathsf{F}_{n+1}(M) \cong \mathsf{Lie}_{\pi_1 M}(n) \end{array}$$

Sketch of the proof. On the first line parallel to the vanishing, for $n \geq 2$ we have

$$E^1_{-n,n(d-2)+1} = \pi_{n(d-3)+1}\mathsf{F}_n(M) = \pi_{n(d-2)+1}\,\mathrm{tofib}(M \vee \mathbb{S}_S) \cong \bigoplus_{w \in \mathsf{N}'\mathsf{B}(\underline{n-1})} \pi_{1+n(d-2)}\Sigma^{1+l_w(d-2)}(\Omega M)^{\wedge l'_w}$$

$$\cong \bigoplus_{\substack{w \in \mathsf{N}'\mathsf{B}(\underline{n-1}),\\ l_w = n-1}} \pi_{1+n(d-2)}\Sigma^{1+(n-1)(d-2)}(\Omega M)^{\wedge l'_w} \oplus \bigoplus_{\substack{w \in \mathsf{N}'\mathsf{B}(\underline{n-1}),\\ l_w = n}} \pi_{1+n(d-2)}\Sigma^{1+n(d-2)}(\Omega M)^{\wedge l'_w}$$

using the computation of the homotopy type of $\mathrm{tofib}(M \vee \mathbb{S}_\bullet)$ from Theorem 5.4 and observing that $\Sigma^{1+l_w(d-2)}X$ is $1+n(d-2)$-connected for $l_w > n$, so the non-trivial terms have $l_w = n-1$ or $l_w = n$.

The terms in the first case can be quite complicated. We just note that for $M \simeq *$ they are given by $\pi_{1+n(d-2)}\mathbb{S}^{1+(n-1)(d-2)}$ which are torsion, so do not contribute to $\mathrm{im}(d^1) \subseteq \mathsf{Lie}_d(n) \cong \mathbb{Z}^{(n-1)!}$, except for $n = 2$ if d is odd, when they have a $\mathbb{Z}$ summand. But in that case one can show that $d^1 \colon \Omega\mathsf{F}_1(M) \simeq \Omega\mathsf{P}_1(M) \to \mathsf{F}_2(M)$ is an equivalence: both spaces have the homotopy type of $\Omega^2\mathbb{S}^{d-1}$ and one can use χ to check the equivalence, or try to generalise [BCSS05, Thm. 3.6].

The words in the second term have length $l_w = n$, so exactly one letter repeats, counting x^i and $x^{i'}$ as the same. By the same arguments as in Section 5.1 the corresponding generators in $\pi_{n(d-2)+1}\,\mathrm{tofib}(M \vee \mathbb{S}_S)$ are again Samelson products $w(x_i^{g_i}, x_k^{g_{k,1}}, x_k^{g_{k,2}})$ according to a word $w \in \mathbb{L}(n-1)$ in which, say, x^k repeats, and with $g_i, g_{k,1}, g_{k,2} \in \pi_1 M$.

Let us show that for such $w(x) := w(x_i^{g_i}, x_k^{g_{k,1}}, x_k^{g_{k,2}})$ the element $d^1(w(x)) \in \mathsf{Lie}_{\pi_1 M}(n)$ is precisely the $STU^2_{\pi_1 M}$ relation at v_k from (2.4).

We use Sinha's computation of the d^1 differential [Sin09, Thm. 7.1], and the comparison from Remark 4.16 of his cosimplicial space to our approach. To obtain a configuration in $\mathsf{Conf}_n\langle M\rangle$ we take the midpoint of J_0 as the 0-th point and the centre of the ball $\mathbb{B}_{ii+1}$ as the i-th configuration point – so we enumerate the configuration points by $0, 1, \ldots, n-1$, perhaps unorthodoxically.

For $0 \leq i \leq n-1$ the codegeneracy map $s^i \colon \mathsf{Conf}_n\langle M\rangle \to \mathsf{Conf}_{n-1}\langle M\rangle$ forgets the i-th point in the configuration, and for $-1 \leq i \leq n$ the coface map $d^i \colon \mathsf{Conf}_n\langle M\rangle \to \mathsf{Conf}_{n+1}\langle M\rangle$ doubles the i-th point, unless $i = -1$ or n for which it adds a point at $\partial\mathrm{U} \subseteq \partial M$.

Sinha defines the first page of the (reduced) spectral sequence for the Taylor tower for $\mathcal{K}(M)$ by

$$E^1_{-n,t}(M) := \bigcap_{i=0}^{n-1} \ker\left(s^i_* \colon \pi_{t-n}\mathsf{Conf}_n(M) \to \pi_{t-n}\mathsf{Conf}_{n-1}(M)\right)$$

and d_1 as the alternating sum $d_1 = \sum_{i=-1}^{n}(-1)^i d^i_*$, which indeed restricts on $\bigcap_{i=1}^{n} \ker\left(s^i\right)$.

Actually, we have $\pi_{t-n}\mathsf{F}_n(M) \cong \bigcap_{i=1}^n \ker(\mathscr{s}^i_*)$ by (5.1), keeping in mind that our x^i corresponds to the letter $x_{1,i}$) from [SS02, Thm. 4.4], where $M = I^d$ was considered. Moreover, Scannell and Sinha determine the maps $\mathscr{d}^i_*$ as induced from the maps on the letters

$$\mathscr{d}^0_* : \ x^i \mapsto x^{i+1} + x_{1,i+1}, \quad 1 \le i \le n-1$$
$$\mathscr{d}^k_* : \ x^i \mapsto x^i, \ x^k \mapsto x^k + x^{k+1}, \ x^j \mapsto x^{j+1}, \quad 1 \le i < k < j \le n-1$$

Note that we cannot rewrite $x_{1,i+1}$ as one of our letters x^j, as it describes the movement of the point 1 around $i+1$. Although the calculation in [SS02] is for $M = I^d$ only, it is straightforward to generalise, cf. Corollary 1.8.

We now proceed as in [Con08, Prop. 4.8], cf. also [Shi19]. Conant observes that it is enough to consider words $w = [w_1, w_2]$ such that the only repeating letter x^k appears both in w_1 and w_2. Moreover, the only possibly non-trivial terms in (2.14) are $-\mathscr{d}^1_*$ and $(-1)^k\mathscr{d}^k_*$, so

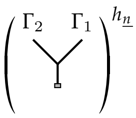
$$d^1(w(x)) = 0 \quad \Longleftrightarrow \quad (-1)^k\mathscr{d}^k_*(w(x)) = \mathscr{d}^0_*(w(x)). \tag{C.1}$$

He then shows that the left side gives the two terms of $STU(v_k)$, while the right side gives $STU(v_0)$. With our choice for $STU^2_{\pi_1 M}$ the exact same argument applies, as we now outline.

The left hand side is given by

$$\begin{aligned}\mathscr{d}^k_*(w(x)) &= w(x_i^{g_i},\, x_k^{g_{k,1}} + x_{k+1}^{g_{k,1}}, x_k^{g_{k,2}} + x_{k+1}^{g_{k,2}},\, x_{j+1}^{g_j})\\ &= \left[w_1(x_i^{g_i}, x_k^{g_{k,1}},\, x_{j+1}^{g_j}),\ w_2(x_i^{g_i}, x_{k+1}^{g_{k,2}},\, x_{j+1}^{g_j})\right] \ + \ \left[w_1(x_i^{g_i}, x_{k+1}^{g_{k,1}},\, x_{j+1}^{g_j}),\ w_2(x_i^{g_i}, x_k^{g_{k,2}},\, x_{j+1}^{g_j})\right]\end{aligned}$$

where $1 \le i < k < j \le n-1$. We now apply the map W^{-1} to see these words in $\mathsf{Lie}_{\pi_1 M}(n)$ (this map was defined in the proof of Theorem 5.5 and uses the isomorphism ω_d from Lemma 2.3). If we denote $\Gamma_1 := \omega_d^{-1}(w_1(x_i, x_k, x_{j+1}))$ and $\Gamma_2 := \omega_d^{-1}(w_2(x_i, x_{k+1}, x_{j+1}))$, then W^{-1} of the first term of $\mathscr{d}^k_*(w(x))$ is given as

$T :=$ 

$\in \mathsf{Lie}_{\pi_1 M}(n), \quad$ where $\quad h_i := \begin{cases} g_i\,, & 1 \le i < k, \\ g_{k,1}\,, & i = k, \\ g_{k,2}\,, & i = k+1, \\ g_{i-1}\,, & k+1 < i \le n. \end{cases}$

The second term in $\mathscr{d}^j_*(w(x))$ is then $-T^{k,k+1}$, where the sign appears since the number $(1|2)$ used by ω_d is changed by 1 as the result of the transposition $(k\,k+1)$.

The right hand side of (C.1) is given by

$$\mathscr{d}^1_*(w(x_i^{g_i})) = w(x_{i+1}^{g_i} + x_{1,i+1}^{g_i}) = \left[w_1(x_{1,i+1}^{g_i}),\, w_2(x_{i+1}^{g_i})\right] \ + \ \left[w_1(x_{i+1}^{g_i}),\, w_2(x_{1,i+1}^{g_i})\right]$$

where $i \in (\underline{n} \setminus k) \cup \{(k,1),(k,2)\}$. Namely, the mixed terms of the form $w_1(x_{i+1}^{g_i}, x_{1,j+1}^{g_j})$ vanish because, roughly speaking, they do not correspond to trees (see [Con08] for details).

Now for this final part of the argument we need to consider $w_1(x_{1,i+1}^{g_i})$ and show that it agrees with the k-replanting $T[k]$ from Definition 2.8. This requires considering the decorated tree $T \in \mathsf{Lie}_{\pi_1 M}(n)$ as living in the bigger group $\mathsf{Lie}_{\pi_1 M}(n) \subseteq \pi_{(n-1)(d-2)}\mathsf{Conf}_n(M)$ and showing that the analogue of the infinitesimal braid relation from Lemma B.2 and Remark B.4 holds there as well. See also Corollary 1.8 where we have determined homotopy groups of configuration spaces additively, and note that the infinitesimal braid relations will exhibit additional structure.

This is the part of the argument we omit, and will instead present elsewhere.

Note that the other term in $\mathscr{d}^1_*$ will then clearly be $T[k]^{0,1}$, so that (C.1) is indeed an $STU^2_{\pi_1 M}$ relation. To finish the proof one observes that all $STU^2_{\pi_1 M}$ relations can be realised this way. $\square$

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