EMBEDDING CALCULUS AND GROPE COBORDISM OF KNOTS

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Abstract. We show that the invariants \( cv_n \) of long knots in a 3-manifold, produced from embedding calculus, are surjective for all \( n \geq 1 \). On one hand, this solves some of the remaining open cases of the connectivity estimates of Goodwillie and Klein, and on the other hand, it confirms one half of the conjecture by Budney, Conant, Scannell and Sinha that for classical knots \( cv_n \) are universal additive Vassiliev invariants over the integers.

We actually study long knots in any manifold of dimension at least 3 and develop a geometric understanding of the layers in the embedding calculus tower and their first non-trivial homotopy groups, given as certain groups of decorated trees. Moreover, in dimension 3 we give an explicit interpretation of \( cv_3 \) using capped grope cobordisms and our joint work with Shi and Teichner.

The main theorem of the present paper says that the first possibly non-vanishing embedding calculus invariant \( cv_n \) 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.

As a corollary, we give a sufficient condition for the mentioned conjecture to hold over a coefficient group. By recent results of Boavida de Brito and Horel this is fulfilled for the rationals, and for the \( p \)-adic integers in a range, confirming that the embedding calculus invariants are universal rational additive Vassiliev invariants, factoring configuration space integrals.

In contrast to the study of spaces \( \text{Map}(P,M) \) of maps between topological spaces, which gave rise to numerous techniques of homotopy theory, spaces \( \mathcal{E}mb(P,M) \) of smooth embeddings of manifolds seem less tractable from the homotopy viewpoint. Already at the level of components (isotopy classes of embeddings), often purely geometric arguments are used.

In this paper we relate two well-known attempts to reconcile these viewpoints in the case of knots in a compact oriented 3-manifold, often purely geometric arguments are used.

The observation that having understood the space of smooth maps, we can try to describe its subspace of neat embeddings \( \mathcal{K}(M) := \mathcal{E}mb_\mathcal{N}(I,M) := \{ f : I = [0,1] \hookrightarrow M \ | \ f \equiv b \text{ near } \partial I \} \) (0.1)

The first approach, Vassiliev’s theory of finite type knot invariants [Vas90; Vas98], starts from the observation that having understood the space of smooth maps, we can try to describe its subspace of embeddings by studying homotopy types of the strata of the complement \( \text{Map}_\mathcal{P}(I,M) \setminus \mathcal{K}(M) \).

In its more geometric version [Gus00; Hab00; CT04b] this theory gives a sequence of equivalence relations \( \sim_n \) for \( n \geq 1 \) on the set \( \mathcal{K}(M) := \pi_0 \mathcal{K}(M) \), defined in terms of either claspers or gropes.

The second approach, the embedding calculus of Goodwillie and Weiss [Wei99; GW99], builds on the idea – having its roots in Hirsch–Smale immersion theory – that, since we understand embeddings of disjoint unions of disks, we could use them to approximate the space \( \mathcal{E}mb(P,M) \). The outcome is a tower of spaces \( \mathcal{P}_n(M) \) and maps \( \mathcal{E}v_n : \mathcal{K}(M) \to \mathcal{P}_n(M) \), for \( n \geq 1 \). See Introduction 1 for a brief survey of both approaches, and Sections 2.2 and 5 for more details.

It was suggested early on [GW99; GKW01] that these theories should be closely related for \( M = I^3 \), in which case \( \mathcal{K}(I^3) \cong \pi_0 \mathcal{E}mb(S^1, \mathbb{R}^3) \) is precisely the abelian monoid of classical knots. The study of the relationship was initiated in [BCSS05], where the following conjecture was stated, and proven in the first non-trivial degree \( n = 3 \) (see Example 2.25 below for another proof).
**Conjecture 0.1 ([BCSS05]).** For each $n \geq 1$ the map $\pi_0 \text{ev}_n : \mathbb{K}(I^3) \to \pi_0 \mathcal{P}_n(I^3)$ is a universal additive Vassiliev invariant of type $\leq n - 1$ over $\mathbb{Z}$, that is, it is a monoid homomorphism which factors as

\[
\begin{array}{c}
\mathbb{K}(I^3) \\
\downarrow_{\pi_0 \text{ev}_n} \\
\mathbb{K}(I^3)/\sim_n \\
\downarrow \\
\pi_0 \mathcal{P}_n(I^3)
\end{array}
\]

and the induced map on the right is an isomorphism of groups.

In other words, the paths in the space $\mathcal{P}_n(I^3)$ should precisely encode the $n$-equivalence relation. The work of [Vol06; Tou07; Con08] showed that, roughly speaking, graph complexes appearing in the two theories agree, while more recently a part of the conjecture was confirmed in [BCKS17]. They show that each $\pi_0 \text{ev}_n$ is an additive invariant of type $\leq n - 1$, namely, $\pi_0 \mathcal{P}_n(I^3)$ has a group structure so that $\pi_0 \text{ev}_n$ is homomorphism of monoids, and the mentioned factorisation exists. Our joint work [KST] reproves the latter claim from the perspective of gropes, see also Theorem C.

One of the main results of the present paper is the proof of the ‘surjectivity part’ of Conjecture 0.1.

**Theorem 0.2.** For each $n \geq 1$ the homomorphism $\pi_0 \text{ev}_n : \mathbb{K}(I^3) \to \pi_0 \mathcal{P}_n(I^3)$ is surjective.

This is just a special case of Theorem 0.5 which says that the same holds for an arbitrary 3-manifold. Starting from a geometric viewpoint, we use different models than the mentioned thread of work: capped gropes for finite type theory [CT04b] and Goodwillie’s punctured knots model for embedding calculus (see [Sin09]). Moreover, 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 which computes the homotopy groups of $\mathcal{P}_n(I^3)$ and our main Theorem A implies that (see Corollary 2.19 for the precise statement)

the evaluation map detects the underlying tree of a grope/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 $S^4$, shown by Watanabe [Wat18] to detect the underlying graph of a family constructed using similar claspers. However, a crucial difference is that while all these invariants use integrals over configuration spaces – and so can provide results only in characteristic zero – embedding calculus is a purely topological technique for studying homotopy types of embedding spaces themselves.

Indeed, Theorem A can be used both to confirm Conjecture 0.1 rationally and show that Kontsevich and Bott–Taubes integrals factor through the tower (see Remark 2.20), and also more generally:

**Corollary 0.3.** Let $A$ be a torsion-free abelian group. If the homotopy spectral sequence $E^c_{n,k}(I^3) \otimes A$ for the Taylor tower of $\mathcal{K}(I^3)$ collapses at the $E^2$-page along the diagonal, then $\pi_0 \text{ev}_n$ is a universal additive Vassiliev invariant of type $\leq n - 1$ over $A$, meaning that

\[
\pi_0 \text{ev}_n \otimes A : \mathbb{K}(I^3)/\sim_n \otimes A \xrightarrow{\text{ev}} \pi_0 \mathcal{P}_n(I^3) \otimes A.
\]

Here $E^c_{n,k}(I^3)$ is the usual spectral sequence for the homotopy groups of the tower of fibrations $p_{n+1} : \mathcal{P}_{n+1}(I^3) \to \mathcal{P}_n(I^3)$ and can be related to graph complexes: its $E^2$-page along the diagonal was identified by Conant [Con08] as the group of Jacobi trees $\mathcal{A}_n^T$ (see Definition 2.7 and Theorem 2.17).

Thus, the above collapse condition is equivalent to the claim that the canonical projection from the group $E^c_{2(n+1),n+1} \equiv \mathcal{A}_n^T$ of Jacobi trees to $E^c_{\infty,(n+1),n+1} = \ker(\pi_0 p_{n+1})$ is an isomorphism over $A$. 
Remarkably, Boavida de Brito and Horel [BH20] show vanishing of higher differentials in a range for this spectral sequence in positive characteristic, implying (2). Their results also imply that $E^r_{-n,d}(I^d)\otimes\mathbb{Q}$ collapses at the whole $E^2$-page (this could also be deduced from [FTW17]). Moreover, some existing low-degree computations show that the group $\mathcal{A}_d^T$ is torsion-free, giving (3). For proofs of both corollaries and further details see Section 2.3.2.

**Theorem 0.5.** For a compact oriented $3$-manifold $M$ the map of sets $\pi_0 ev_n : \mathcal{K}(M) \to \pi_0 P_n(M)$ is surjective for any $n \geq 1$.

This was expected to hold by analogy to the famous Goodwillie–Klein connectivity formula (see Theorem 1.1), which predicts that for a $1$-dimensional source manifold and a $3$-dimensional target the map $ev_n$ is $0$-connected. For a connected source this is precisely Theorem 0.5, and in future work we plan to investigate if our method can be extended to links.

**Remark 0.6.** The corollaries of Theorem A stated above apply to some extent also for knots in a general $3$-manifold $M$, using analogous groups $\mathcal{A}_d^T(M)$ as studied in [Kos20]; see also Remark 1.8.

Let us now introduce some notation, so that we can state Theorem A and deduce Theorem 0.5.

We will actually study the punctured knots model $P_n(M)$ even more generally: for $M$ any connected compact smooth manifold of dimension $d \geq 3$ with non-empty boundary. It is defined as a homotopy limit over a certain finite category and we will develop its properties in detail in Sections 3 and 4. We only restrict to oriented 3-manifolds when we later consider gropes.

Let us pick an arbitrary knot $U \in \mathcal{K}(M)$ as our basepoint and call it the unknot, and let $ev_n(U)$ be the basepoint of $P_n(M)$. There is a natural map $p_{n+1} : P_{n+1}(M) \to P_n(M)$ which is a surjective fibration and satisfies $p_{n+1} ev_{n+1} = ev_n$, so preserves basepoints. The fibres $F_{n+1}(M) := \text{hofib}_{ev_n U}(p_{n+1})$ are called the layers of the Taylor tower. Moreover, we also consider the homotopy fibre

$$H_n(M) := \text{hofib}_{ev_n U}(ev_n)$$

$$:= \{ (K, \gamma) \in \mathcal{K}(M) \times \text{Map}([0,1],P_n(M)) \mid \gamma(0) = ev_n(K), \gamma(1) = ev_n(U) \}.$$ 

and in Section 3.2 we construct a map $e_{n+1}$ making the following diagram commute:

\[
\begin{array}{ccc}
H_n(M) & \xrightarrow{e_{n+1}} & F_{n+1}(M) \\
\downarrow & & \downarrow \\
\mathcal{K}(M) & \xrightarrow{ev_{n+1}} & P_{n+1}(M) \\
\downarrow ev_n & & \downarrow \quad p_{n+1} \\
P_n(M) & \xrightarrow{\quad} & P_n(M)
\end{array}
\]

(0.2)

Remarkably, both $F_{n+1}(M)$ and $H_n(M)$ are related — for a priori different reasons — to the set $\text{Tree}_{\pi_1,M}(n)$ of $\pi_1 M$-decorated trees, where $\Gamma \in \text{Tree}_{\pi_1,M}(n)$ consists of a rooted planar binary tree $\Gamma$ with enumerated leaves which are also decorated by elements $g_i \in \pi_1(M)$, for $i \in \mathbb{N} := \{1, \ldots, n\}$.

See Section 2.1 for all definitions related to trees.
For example, \( \Gamma^S := \exists \in \text{Tree}_{n,1}(3) \).

Indeed, on one hand, the set \( \pi_0 F_{n+1}(M) \) is isomorphic to the group of Lie trees \( \text{Lie}_{n,1}(M) \), defined as the quotient of the \( \mathbb{Z} \)-span of \( \text{Tree}_{n,1}(M) \) by the antisymmetry (AS) and Jacobi relations (IHX). On the other hand, from the data of a capped grope cobordism \( G \) in a 3-manifold \( M \) we will construct a point \( \psi(G) \in \mathcal{H}_n(M) \), with the underlying combinatorics of \( G \) also described by \( t(G) \in \text{Tree}_{n,1}(M) \).

Let \( B(\pi) \) be a Hall basis for the free Lie algebra \( \mathcal{L}(x^i : i \in \pi) \), and \( \text{NB}(\pi) \subseteq B(\pi) \) the subset of words in which each letter \( x^i \) for \( i \in \pi \) appears at least once. Let \( l_w \) be the word length of \( w \in \text{NB}(\pi) \).

Further, for \( k \geq 1 \) denote by \( M^{\otimes k} \) the \( k \)-fold product of \( M \) with itself and by \( \Omega M^{\times k} \) the space of based loops in it; for a space \( X \) let \( X_+ := X \sqcup \{ \ast \} \) and \( \Sigma^k(X_+) \) its \( k \)-fold reduced suspension.

**Theorem A.** For any \( d \geq 3 \) there is an explicit homotopy equivalence

\[
F_{n+1}(M) \cong \Omega^n \prod_{w \in \text{NB}(\pi)} \Omega \Sigma^{1+l_w(d-2)}(\Omega \mathcal{M}^{\times l_w})_+.
\]

It follows that \( F_{n+1}(M) \) is \((n(d-3)-1)\)-connected and \( \pi_{n(d-3)} F_{n+1}(M) \cong \text{Lie}_{n,1}(M) \). Moreover, for \( d = 3 \) capped grope cobordisms give a map of sets

\[
\rho_n : \mathbb{Z}[\text{Tree}_{n,1}(M)] \to \pi_{n(d-3)} \mathcal{H}_n(M)
\]

such that \( \pi_{n(d-3)} e_{n+1} \circ \rho_n \) is the canonical quotient map by AS and IHX.

In other words, the two roles of trees, homotopy theoretic for \( F_{n+1}(M) \) and geometric for \( \mathcal{H}_n(M) \), are mutually compatible: we will define \( \rho_n(\Gamma^S) := [\psi(G)] \) for some grope \( G \) with \( t(G) = \Gamma^S \) and show that \( [\pi_{n+1}(\psi(G))] \in \pi_0 F_{n+1}(M) \cong \text{Lie}_{n,1}(M) \) is precisely the class of \( t(G) \) modulo AS and IHX.

**Remark 0.7.** There is an isomorphism \( \text{Lie}_{n,1}(M) \cong \left( \mathbb{Z}[\pi_1(M)] \right)^{(n-1)!} \). If \( M \) is simply connected, we obtain \( \text{Lie}(n) \cong \mathbb{Z}^{(n-1)!} \), the arity \( n \) of the Lie operad. Interestingly, in Goodwillie’s homotopy calculus the \( n \)-th Taylor layer for a functor \( F : \text{Top} \to \text{Top} \) is computed in terms of a spectrum \( \partial_n(\text{Id}) \) and these turn out to form an operad \( \partial_n(\text{Id}) \) whose homology is precisely the Lie operad.

The following is an immediate corollary of Theorem A, and implies Theorem 0.5.

**Corollary 0.8.** For \( d = 3 \) and \( n \geq 1 \) \( \pi_0 e_{n+1} : \pi_0 \mathcal{H}_n(M) \to \pi_0 F_{n+1}(M) \) is a surjection of sets.

**Proof of Theorem 0.5 assuming Theorem A.** It is a standard fact (see (3.0.1) below) that \( P_1(M) \) is homotopy equivalent to the loop space \( \Omega(\mathcal{M}) \) on the unit tangent bundle \( \mathcal{M} \) of \( M \). Thus, \( \pi_0 P_1(M) \cong \pi_1(M) \), and since each class here can be represented by an embedded loop (as \( d = 3 \)), the map \( \pi_0 e_{n+1} \) is surjective. Assume by induction that \( \pi_0 e_{n} \) is surjective for some \( n \geq 1 \).

Let us pick \( x \in P_{n+1}(M) \) and show it is in the image of \( \pi_0 e_{n+1} \). Denote \( y := p_{n+1}(x) \in P_n(M) \) and the corresponding fibres \( F_{p+1}^y(M) := \text{fib}_y(p_{n+1}) \) and \( H^y_n(M) := \text{hofib}_y(e_n) \). Since by definition \( x \in F^y_{n+1}(M) \) and \( e_{n+1} : H^y_n(M) \to F^y_{n+1}(M) \) similarly to (0.2), it suffices to prove \( \pi_0 e_{n+1} \) is surjective.

However, it is instead enough to check that \( \pi_0 e_{n+1} \) is surjective, where \( K \in \mathcal{K}(M) \) is any knot such that there is a path \( \gamma \) in \( P_n(M) \) from \( e_n(K) \) to \( y \) (this exists by the induction hypothesis).

Indeed, \( e_{n+1} \) is equivalent to the map induced on the homotopy fibres, and changing the basepoint on both sides using \( \gamma \) induces homotopy equivalences which commute with \( e_{n+1} \). As our choice of \( U \) was arbitrary, we can take \( U := K \), so \( e_{n+1} \) is surjective. Now apply Corollary 0.8. \( \square \)

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1 The weak product \( \Pi^* \) is defined as the filtered colimit of products over finite subsets.
In the next section, after giving a brief survey of the literature, we rephrase Theorem A as several intermediate results. Namely, Theorem B provides for any \( d \geq 3 \) an explicit description of the homotopy groups of \( Fr_{d+1}(M) \), and Theorem C constructs points \( \psi(G) \in H_d(M) \) for \( d = 3 \). The compatibility of the two roles of decorated trees is shown in Theorem D and Theorem E.

On the way, we point out crucial proof ingredients, which may be of independent interest, and give some corollaries. We end Section 1 with a proof of Theorem A and a detailed outline of the paper.

Finally, let us remark that similar results should hold more generally: invariants \( e_v \) are defined for any space of embeddings or diffeomorphisms and should detect analogous geometric constructions; see Remark 1.10 for \( \rho_n \) for \( d \geq 4 \). Moreover, we show in [KT] that the space of certain neatly embedded 2-disks in a 4-manifold is described by \( \Omega\mathcal{R}(M) \), so that such disks are classified up to isotopy by \( e_v2 \). This fully answers questions posed by Gabai in [Gab20a] (who used a map similar to \( \rho_1 : \mathbb{Z}[[\pi_1 M]] \to H_1(M) \)), and reproves the main result of [Gab20b] by completely new methods.

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1 Introduction

Finite type theory. Vassiliev’s study of the strata of the discriminant \( \text{Map}_\partial(I, I^3) \setminus \mathcal{K}(I^3) \) gave rise to the filtration \( V^*_n(A) \) by type \( n \geq 1 \) of the group \( H^n(\mathcal{K}(I^3); A) \) of knot invariants with values in an abelian group \( A \), as formulated by [BL93]. A new, very active field emerged: it was shown that quantum invariants give rise to invariants of finite type [Lin91] (for example, for the Jones polynomial \( J(q) \) the coefficient next to \( h^n \) in \( J(e^h) \) is of type \( \leq n \)); that for \( A = \mathbb{Q} \) there is a universal such invariant – the Kontsevich integral [Kon93; LM96]; and a comprehensive treatment of its target, the rational Hopf algebra of chord diagrams, was given in [Bar95].

A geometric approach to the field was introduced by Gusarov [Gus00] and Habiro [Hab00] independently, as a sequence of knot operations called surgeries on claspers (or variations) of degree \( n \geq 1 \). This gives a sequence of equivalence relations \( \sim_n \) on the monoid \( \mathbb{K}(I^3) := \pi_0 \mathcal{K}(I^3) \) and a decreasing filtration \( \mathbb{K}_n(I^3) := \{ K \in \mathbb{K}(I^3) : K \sim_n U \} \) by submonoids. The work of Stanford [Sta98] exhibits a close connection of this filtration with the lower central series of the pure braid group.

By the work of Conant and Teichner [CT04b; CT04a] one can instead of claspers equivalently use capped groove cobordisms, 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’ [Tei04]. See Section 5.1 for a background on grooves, and Remark 5.11 for an advantage of using them.

Notably, it has been shown that the map \( \mathbb{K}(I^3) \to \mathbb{Z}[\mathbb{K}(I^3)] = H_0(\mathcal{K}(I^3); \mathbb{Z}) \) defined by \( K \mapsto K - U \), takes \( \mathbb{K}_n(I^3) \) into \( V_n(\mathbb{Z}) \), the dual of the Vassiliev filtration for \( A = \mathbb{Z} \). Hence, this indeed gives a geometric version of the theory (or its primitive/additive part), since one works with knots instead of their linear combinations or invariants; see Section 2.2 for the comparison.

Additionally, the quotient of \( \mathbb{K}(I^3) \) by \( \sim_n \) is actually an abelian group and the projection

\[
v_n : \mathbb{K}(I^3) \to \mathbb{K}(I^3)/\sim_n
\]

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 \( v_n \). 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 chord diagrams or the group of Jacobi trees (see Section 2.1.2).

Embedding calculus. The pioneering approach of Goodwillie and Weiss [Wei99; GW99] for studying embedding spaces\(^2\) \( \text{emb}_{\partial}(P, M) \) produces a tower of spaces, called the Taylor tower,

\[
\cdots \to T_{n+1} \text{emb}_\partial(P, M) \to T_n \text{emb}_\partial(P, M) \to \cdots \to T_1 \text{emb}_\partial(P, M)
\]

and the evaluation maps \( \text{ev}_n : \text{emb}_\partial(P, M) \to T_n \text{emb}_\partial(P, M) \), starting from the space of immersions \( T_\partial \text{emb}_\partial(P, M) = \text{imm}_\partial(P, M) \). 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 \( \text{emb}_\partial(P, M) \), using a variety of tools. Indeed, a fundamental result in the field is the following theorem of Goodwillie and Klein (announced in [GW99]).

**Theorem 1.1** ([GK15]). The map \( \text{ev}_n \) is \( (1 - \dim P + n(\dim M - \dim P - 2))\)-connected\(^3\), except if \( \dim P = 1 \) and \( \dim M = 3 \). Hence, the induced map \( \text{ev}_{\infty} : \text{emb}_\partial(P, M) \to \lim T_n \text{emb}_\partial(P, M) \) is a weak homotopy equivalence if \( \dim M - \dim P > 2 \) (‘the tower converges to the embedding space’).

This result inspired a great deal of research on Taylor towers for various pairs \( (P, M) \).

---

\(^2\) One can 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 \( \pi_k \).
To mention just a few, in [LTV10; AT14] the rational homology of spaces $\mathbb{E}mb_0(\mathbb{D}^k, \mathbb{D}^{k+c})$ of disks of codimension $c > 2$ was expressed as the homology of certain graph complexes, and similarly for the rational homotopy groups [ALTVO8; AT15; FTW17]. The spaces $T_n \mathbb{E}mb_0(\mathbb{D}^k, \mathbb{D}^{k+c})$ were shown to be iterated loop spaces in [DH12; Tur14; BW18; DT19]. A different (cosimplicial) model for $T_n \mathbb{E}mb_0(I, M)$ was constructed in [Sin09] and studied in [Sin06; SS02; LT09] for $M = I^d, d \geq 4$.

Note that the excluded case in Theorem 1.1 is precisely the setting of knot theory. Moreover, by an argument of Goodwillie the tower for classical long knots $K(I^3) := \mathbb{E}mb_0(I, I^3)$ does not converge (see Proposition 2.22). 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.

Furthermore, the delooping results of [Tur14; BW18] apply in this case as well: for $n \geq 2$ each $T_n K(I^3)$ is weakly equivalent to a double loop space, so each $\pi_0 T_n K(I^3)$ is actually an abelian group (for $n = 1$ trivial as $T_1 K(I^3) \cong \Omega S^2$). Moreover, [Gr19] showed that $\mathbb{E}v^\text{BW}_n : K(I^3) \to T_n K(I^3)$, the model from [BW18], is a map of $H$-spaces. Thus, $\pi_0 \mathbb{E}v^\text{BW}_n$ is a monoid map (an additive invariant).

**Relating the two theories.** A different approach by [BCKS17] uses the model $AM_n$ for $T_n K(I^3)$ from [Sin09] to equip $\pi_0 T_n K(I^3)$ directly with an abelian group structure, so that the corresponding $\pi_0 \mathbb{E}v_n$ is also a monoid map, as predicted by Conjecture 0.1 of [BCSS05]. It has been an open problem whether the group structures of [BW18] and [BCKS17] on $\pi_0 T_n K(I^3)$ agree. We confirm this is indeed the case, see Corollary 2.23.

The authors of [BCKS17] also show that $\pi_0 \mathbb{E}v_n$ is of Vassiliev type $\leq n - 1$, and we reprove this below for any 3-manifold $M$. See Remark 1.8.

### 1.1 Intermediate results

**1.1.1 A careful study of the layers in the Taylor tower**

In the homotopy theoretic part we study the space $F_n(M)$ for $M$ any smooth manifold with non-empty boundary and dimension $\text{dim}(M) = d \geq 3$. The upshot is the following theorem, which reformulates the first part of Theorem A.

**Theorem B.** For $n \geq 1$ there is a weak equivalence $F_{n+1}(M) \simeq \Omega^n \bigwedge_{\mathbb{N} \cup \{0\}} \Omega^{1+\nu(d-2)}(\Omega M^{<\nu})_+^\ast$. Moreover, this space is $(n(d-3)-1)$-connected and there are explicit isomorphisms

$\text{Lie}_{n^2} M(n) \xrightarrow{W} \pi_{n(d-2)} \text{tofib}
\left(\Omega(M \vee S^1, \Omega \text{col})\right) \xrightarrow{(\text{retr} \circ \partial \circ \chi)^{-1}} \pi_{n(d-3)} F_{n+1}(M)$.

Let us give more details. Firstly, $F_{n+1}(M)$ in Section 3.2 is described as the total homotopy fibre

$F_{n+1}(M) = \text{tofib}\left(S^{n+1}_S, r\right)$

of the cube of spaces $\mathcal{S}^{n+1} := \mathbb{E}mb_0([0, 1], M_{0S})$, where $M_{0S} \subseteq M$ is obtained by removing $S+1$ $d$-dimensional balls from $M$. The map $r^S$ is induced from the inclusion $\rho^S_k : M_{0S} \hookrightarrow M_{0S^k}$, which adds the material between two balls (see Figure 8).

Secondly, in Section 3.3 we show that this is an $(n+1)$-fold loop space. Namely, $F_1(M) \simeq \Omega SM$ and for $n \geq 1$:

$F_{n+1}(M) \xrightarrow{\chi} \Omega^n \text{tofib}\left(S^{n+1}_S, l\right) \xrightarrow{\partial} \Omega^n \text{tofib}\left(\Omega M, \Omega \text{col}\right) \xrightarrow{\text{retr}} \Omega^n \text{tofib}\left(\Omega(M \vee S^1), \Omega \text{col}\right)$.

4 An $n$-cube $X_S$ consists of a space $X_S$ for each $S \subseteq n$ and a compatible collection of maps $x_k^S : X_S \to X_{S^k}$ for $k \not\in S$.

5 Of course, $\mathcal{S}^{n+1}_S$ depends on $M$, but we omit it from the notation.
These homotopy equivalences arise as follows.

- For $\chi$ and its inverse see Theorem 3.11: the map $l^2_5$ is defined using the left homotopy inverse $\Lambda^2_5: M_{05k} \to M_{05}$ for $p_5^2$ which adds back the $k$-th ball and then rescales (see Figure 9).

- In Theorem 3.19 taking unit derivatives is shown to give a homotopy equivalence of contravariant cubes $\mathcal{G}_c: (\mathcal{F}_d^{n+1}, I) \to (\Omega \Sigma M, \Omega \Sigma L)$, where $M_5 \supset M_{05}$ are obtained by gluing in a ball.

- Finally, for $S_d := \bigvee_{i \in S} S^d_i$ there are deformation retractions $\text{retr}_S: M_5 \to M \vee S_d$, such that $\Lambda^2_5$ commutes with the collapse map $\text{col}^2_5: M \vee S_d \to M \vee S_d/S$. Hence, $\text{retr}$ gives an equivalence of (contravariant) cubes $\text{retr}: (\Omega M, \Omega L) \to (\Omega (M \vee S_d), \Omega \text{col})$.

Thirdly, in Section 4 we describe the homotopy type of $\text{tofib}(\Omega (M \vee S_d), \Omega \text{col})$, using a generalisation of the Hilton–Milnor theorem due to Gray [Gra71] and Spencer [Spe71]. Namely, we find a weak equivalence (see Theorem 4.4):

$$
\prod_{w \in \text{NB}(l)} \Omega^{1 + \langle d-2 \rangle} (\Omega M)^{\times |w|} \xrightarrow{\mu \circ \text{hm}} \text{tofib}(\Omega (M \vee S_d), \Omega \text{col}).
$$

(1.1)

This formula differs slightly from the one we gave in [Kos20], but that one can be recovered using the James splitting $\Sigma \Sigma \Sigma Y \simeq \bigvee_{i=1}^{\infty} \Sigma Y^{\langle i \rangle}$. See also [Wei99] for other description of the layers, and [BCKS17] for $M = I^n$.

Remark 1.2. If $M \simeq \Sigma Y$ is homotopy equivalent to a suspension, the homotopy type of $F_{n+1}(M)$ was calculated in [GW99]; we can recover their result using the James splitting $\Sigma \Sigma \Sigma Y \simeq \bigvee_{i=1}^{\infty} \Sigma Y^{\langle i \rangle}$. See also [Wei99] for other description of the layers, and [BCKS17] for $M = I^n$.

However, in neither of those approaches could we understand the comparison map, which is crucial for the proof of Theorem D; we hope that our equivalence $\chi$ might be of independent interest.

For the second statement, in Section 4.1 we easily find that $\text{tofib}(M \vee S_d)$ is $(n(d-2) - 1)$-connected, and then construct an isomorphism $\nu$: it takes a decorated tree $F^\Sigma$ to a certain Samelson product $\Gamma(\chi^\Sigma_\Gamma): S^n(d-2) \to \Omega (M \vee S_d)$, according to the word described by $\Gamma$, and using classes $g_{\Sigma} \in (\pi_1 M)^n$.

However, to now find maps which generate $\pi_{n(d-3)} F_{n+1}(M) \cong \text{Lie}_{n+1}(M)$ we would need to invert the isomorphism $\text{retr} \circ \chi$. For $\text{retr}$ there is an obvious map $m_i: S^{d-2} \to \Omega (M \vee S_d) \to \Omega M_{n}$ satisfying $\text{retr} \circ m_i \simeq x_i$, which simply ‘swings a lasso’ around the missing $d$-ball, see Figure 12. In Section 4.2 we discuss the following corollary and why it will be enough for our purposes.

Corollary 1.3. The generators of $\pi_{n(d-2)} \text{tofib}(\Omega M, \Omega L)$ are given by the canonical extensions to the homotopy fibre of the Samelson products $\Gamma(m^{\Sigma \Sigma}_i): S^n(d-2) \to \Omega M_{n}$ of the maps $m^{\Sigma \Sigma}_i: S^{d-2} \to \Omega M_{n}$ given by $I \mapsto \gamma^i \cdot m_i(I) \cdot \gamma^{-1}_i$, where $\epsilon_i \in \{\pm 1\}$ and $\gamma_i \in \Omega M$.

About the convergence. Let us point out that we obtain our results from scratch, starting with the definition of the punctured knot model and assuming only the Hilton–Milnor–Gray–Spencer theorem (whose proof is briefly recalled in Appendix B). In particular, independently of the rest of the literature we have reproved the following.

Corollary 1.4. The Taylor tower for the space $\mathcal{K}(M)$ of long knots in a $d$-manifold $M$ converges if $d \geq 4$, i.e. the connectivity of $P_{n+1}: P_{n+1}(M) \to P_n(M)$ increases with $n \geq 1$.

Actually, by Goodwillie–Klein Theorem 1.1 the tower converges precisely to $\mathcal{K}(M)$ for $d \geq 4$: the homotopy groups of $H_n(M)$ in degrees below $(n+1)(d-3)$ agree with those of $F_{n+1}(M)$. We believe that our map $\rho_n$ will provide a geometric inverse to the isomorphism $\pi_{n(d-3)} \text{ev}_n$, see Remark 1.10.
For a tower of (surjective) pointed fibrations there is an associated (non-‘fringed’) spectral sequence built out of long exact sequences for the homotopy groups of a fibration [BK72]. The first page is given by
\[ E^1_{-n,t} := \pi_{t-n}F_n(M) \] and the differential is the composite
\[ d^1_{-n,t} : E^1_{-n,t}(M) = \pi_{t-n}F_n(M) \longrightarrow \pi_{t-n}P_n(M) \longrightarrow \pi_{t-n-1}F_{n+1}(M) = E^1_{-(n+1),t}(M). \]

of the fibre inclusion and the connecting map for \( p_{n+1} \). A vanishing slope for this spectral sequence was determined in [Sin09, Thm. 7.1]; see also [SS02] for \( M = I^d \). By Theorem 4.4 we have
\[ E^1_{-(n+1),t} := \pi_{t-n-1}F_{n+1}(M) \cong \bigoplus_{w \in \text{NB}(n)} \pi_1 \Sigma^{1+l_0(d-2)}(\Omega M^{\times l_0})_+. \]

**Corollary 1.5.** The group \( E^1_{-(n+1),t} \) vanishes for \( t \leq n(d-2) \), and for each \( l = n, n+1, \ldots \) 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
\[ E^1_{-(n+1),1+n(d-2)}(M) \cong \mathfrak{Lie}_{\pi_1 M}(n). \]

**About configuration spaces.** Taylor towers for embedding spaces are closely related to configuration spaces of manifolds \( \text{Conf}_S(M) := \text{emb}(S, M) \) for a finite set \( S \). See [Sin09; BW18; FTW17] to mention just a few. They are behind the scenes in our approach as well, and we record related corollaries. As usual, let \( M \) be a \( d \)-dimensional compact manifold with non-empty boundary.

**Corollary 1.6.** There is an additive isomorphism
\[ \pi_* \text{Conf}_S(M) \cong (\pi_* M)^n \oplus \bigoplus_{l=0}^{d-1} \pi_{l+1} \left( \Sigma^{1+l_0(d-2)}(\Omega M^{\times l_0})_+ \right). \]

**Proof.** Since \( \partial M \neq \emptyset \) there is an isomorphism \( \pi_* \text{Conf}_S(M) \cong \bigoplus_{l=0}^{d-1} \pi_l (M \setminus \partial M) \), where \( \partial M := \{1, \ldots, l\} \) is a set of \( l \) distinct points in \( M \) [Lev95]. By Lemma 4.1 there is a retraction \( r_M : SM \rightarrow M \cup S \) for any finite set \( S \) (recall that \( S := \bigvee S^d \) and \( \Omega(\Omega M \cup S) \cong \Omega M \times \prod_{w \in S} \Omega \Sigma^{1+l_0(d-2)}(\Omega M^{\times l_0})_+ \) by (4.2) and (4.4) from Section 4. \]

**Corollary 1.7.** If \( (\text{Conf}_S(M), \delta) \) is the contravariant \( n \)-cube with the maps for \( k \in S \subseteq [n] \) given by \( s^k_S : \text{Conf}_S(M) \rightarrow \text{Conf}_S(M) \) forgetting the \( k \)-th point in the configuration, then
\[ \Omega \text{ tolib} (\text{Conf}_S(M), \delta) \cong \prod_{w \in \text{NB}(s-1)} \Omega \Sigma^{1+l_0(d-2)}(\Omega M^{\times l_0})_+ . \]

Hence, the first non-trivial homotopy group\(^6\) is \( \pi_{(n-1)(d-2)+1} \text{ tolib} (\text{Conf}_S(M), \delta) \cong \mathfrak{Lie}_{\pi_1 S}(n-1). \)

**Proof.** Each map \( s^k_S \) for \( S \subseteq [n-1] \) is a fibre bundle whose fibre is homeomorphic to \( M \setminus S \approxeq M \cup S \). By taking fibres first in the direction of \( s^k \)-maps, the total fibre of the \( n \)-cube \( (\Omega \text{Conf}_S(M), \Omega \delta) \) is equivalent to that of the \( (n-1) \)-cube tolib \( (\Omega(M \cup S), \Omega \delta) \), and this was computed in (1.1). \]

Sinha [Sin09] uses certain compactifications of configuration spaces to construct the mentioned model \( A\text{M}_n(M) \) for \( T_n \mathcal{K}(M) \), then employed in [BCKS17]. See Remark 3.21 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.

---

\(^6\) That this cube is \((n-1)(d-2)+1\)-cartesian can also be calculated using the Blakers–Massey theorem, but we could not find a computation of the homotopy type in the literature.
1.1.2 Gropes give points in the layers of the Taylor tower

In this geometric part we specialise to $d = 3$ (but this restriction is not essential, see Remark 1.10). We build on our joint work [KST], where we constructed points in $H_n(I^3)$ from (simple capped genus one) grope cobordisms of degree $n$ of [CT04b]; here we extend this to any oriented 3-manifold $M$.

**Gropes.** In Section 5.1 we discuss grope cobordisms, which are certain 2-complexes in $M$ modelled on trees, that ‘witness’ $n$-equivalence of the two knots on ‘the boundary of a cobordism’.

More precisely, one first defines (see Definition 5.1) the abstract (capped) grope $G_\Gamma$ modelled on an undecorated tree $\Gamma \in \text{Tree}(n)$ as a 2-complex with circle boundary built by inductively attaching surface stages according to $\Gamma$ as on the left of Figure 1: each leaf contributes a disk (called a cap), and each trivalent vertex a torus with one boundary component; we also fix an oriented subarc $a_0 \subseteq \partial G_\Gamma = S^1$. There is a canonical embedding $\Gamma \hookrightarrow G_\Gamma$ of the tree into this 2-complex.

A (capped) grope cobordism (of genus one) on a knot $K \in \mathcal{N}(M)$ modelled on $\Gamma$ is a map $G : G_\Gamma \to M$ which embeds all stages mutually disjointly and disjointly from $K$ except that $G(a_0) \subsetneq K$ and for $i \in \mathbb{N}$ the $i$-th cap intersects $K$ transversely in a point $p_i$, so that $G(a_0) < p_1 < \cdots < p_n$ in $K$. The degree of $G$ is $n$, the number of its caps. See Definition 5.2 for details and orientation conventions.

A simple example of a grope cobordism of degree 2 is shown on the right of Figure 1. Note how the two caps or ‘arms’ could instead be twisted and tied into knots, producing non-isotopic grope cobordisms on $K$ which are all modelled on the same tree $\Gamma$.

Moreover, we denote $a_0^\perp := \partial G_\Gamma \setminus a_0$ and define the output knot of $G$ by

$$\partial^+ G := (K \setminus G(a_0)) \cup G(a_0^\perp).$$

Thus, a grope describes a modification of the knot $K$ by replacing its arc $G(a_0) \subsetneq K$ by $G(a_0^\perp)$. We say that $K \sim_n \partial^+ G$ are $n$-equivalent. More generally, two knots are $n$-equivalent if there is a finite sequence of grope cobordisms of degree $n$ from one knot to the other. This gives the variant due to [CT04b] of the Gusarov–Habiro filtration $\mathcal{K}_n(M; U) := \{K \in \mathcal{K}(M) : K \sim_n U\}$ mentioned above.

Another important notion related to a grope cobordism $G$ modelled on $\Gamma \in \text{Tree}(n)$ is its signed decoration $G = (\varepsilon_i, \gamma_i)_{i \in \mathbb{N}}$, where $\varepsilon_i \in \{\pm 1\}$ is the sign of the intersection point $p_i$ in $K$ and the $i$-th cap of $G$, and $\gamma_i \in \partial M$ is the loop from $K(0)$ to $p_0$ first following the unique path in the tree $G(\Gamma)$, then going back along $K$ (see Definition 5.4).

Finally, let $\varepsilon := \bigcap_i \varepsilon_i$ and $G_\varepsilon = [\gamma_i] \in \pi_1 M$ and define the underlying decorated tree

$$t(G) := \varepsilon^\mathcal{K}_\varepsilon \in \{\pm 1\} \times \text{Tree}_{n_1 M}(n).$$

---

\(^7\) Although our pictures sometimes seem not smooth, the corners are present only for convenience.
Note that each corresponding paths in (1.2) the factorisation is an open problem (see Remark 2.16) if such an equivalence holds for any oriented Remark 1.8. This equivalence to Vassiliev’s theory is discussed in Section 2.2. In contrast, it is invariant of type indeed, if \( g \) gropes of genus see Definition 5.5 for details. Finally, in Definition 5.7 we define the space \( \text{Grop}^\text{b}(M; K) \) of thick gropes of genus 1 and degree \( n \) in \( M \) on \( K \), so that taking the output knot gives a continuous map \( \partial^+: \text{Grop}^\text{b}(M; K) \to \mathcal{K}(M) \). This is extended below to any genus.

**Theorem C.** If \( G \) is a thick grope of degree \( n \geq 1 \) in \( M \) on a knot \( K \), then there is a path \( \Psi^G : I \to \mathcal{P}_n(M) \) from \( \text{ev}_n(\partial^+ G) \) to \( \text{ev}_n(K) \). Moreover, for \( K = \mathbb{U} \) this gives a continuous map

\[
\psi : \text{Grop}^\text{b}_n(M; \mathbb{U}) \to \mathcal{H}_n(M), \quad \psi(G) := (\partial^+ G, \Psi^G).
\]

We give the proof in Section 5.2, using the crucial isotopy between the two surgeries on a capped torus (Lemma 5.10). Namely, combining these isotopies for each stage of \( G \) gives an \((n-1)\)-parameter family of disks \( D_u \) contained in the model ball \( B_r \) and with \( \partial D_u = \partial G_R \). Moreover, the interior of each disk \( G(D_u) \) intersects the knot \( K \) only inside of certain subarcs of \( K \), and so that the homotopy of \( G(a_0) \) back to \( G(0) \) across \( G(D_u) \) precisely defines a path in \( \mathcal{P}_n(M) \).

The theorem immediately implies that there is a factorisation

\[
\mathbb{K}(M) \xrightarrow{\pi_0 \text{ev}_n} \pi_0 \mathcal{P}_n(M) \xrightarrow{\sim_n} \mathbb{K}(M) \tag{1.2}
\]

Indeed, if \( K \sim_n K' \), there is a sequence of thick gropes witnessing it, so concatenation of the corresponding paths in \( \mathcal{P}_n(M) \) is a path from \( \text{ev}_n K \) to \( \text{ev}_n K' \). In particular, as mentioned in the discussion after Conjecture 0.1, for \( M = I^3 \) this is equivalent to the claim that \( \pi_0 \text{ev}_n \) is a Vassiliev invariant of type \( \leq n-1 \) (this was first shown by [BCKS17]).

**Remark 1.8.** This equivalence to Vassiliev’s theory is discussed in Section 2.2. In contrast, it is an open problem (see Remark 2.16) if such an equivalence holds for any oriented 3-manifold \( M \): the factorisation (1.2) just says that \( \pi_0 \text{ev}_n \) is an invariant of \( n \)-equivalence of knots in \( M \).

**Remark 1.9.** The remaining part of Conjecture 0.1 says that if \( \text{ev}_n K \) is in the path component of \( \text{ev}_n \mathbb{U} \), then there exists a path between them induced from a grope forest.

In [KST] we reformulate this in terms of a map \( \mathcal{R}_n(I^3) \to \mathcal{P}_n(I^3) \) extending \( \text{ev}_n \), where we construct the simplicial space \( \mathcal{R}_n(I^3) \) using \( \mathcal{K}(I^3) \) and \( \text{Grop}_n(I^3) \) for spaces of 0- and 1-simplices, respectively. We hope to prove it is a homotopy equivalence, giving a very geometric description of \( \mathcal{P}_n(I^3) \).

**Grope forests.** We will also need to realise arbitrary linear combinations of decorated trees. The corresponding geometric notion which is standardly used is a grope cobordism of ‘higher genus’, but we instead define a slightly different notion, called a grope forest. This is an embedding

\[
F : \bigsqcup_{1 \leq l \leq N} B_{r_l} \to M
\]

such that \( F|_{B_{r_l}} \) for \( 1 \leq l \leq N \) are mutually disjoint thick gropes on \( K \) whose arcs \( F|_{B_{r_l}}(a_0) \subseteq K \) appear in the order of their label \( l \) (see Definition 5.6).

---

8 The first statement for \( M = I^3 \) is part of the joint work [KST], and appeared first in [Shi19].
Let $\text{Grop}_n(M; U) := \bigsqcup_{N \geq 1} \text{Grop}_{n}^N(M; U)$ denote the space of grope forests of any cardinality (the component $N = 1$ is exactly the space of thick gropes). Taking underlying trees of all the thick gropes in a grope forest gives the underlying decorated tree map

$$t: \pi_0\text{Grop}_n(M; U) \rightarrow \mathbb{Z}[\text{Tree}_{n,M}(n)].$$

This is a surjection of sets: any linear combination of $\pi_1M$-decorated trees is realised by a grope forest on $U$ (see Proposition 5.8). Furthermore, in Proposition 5.13 we extend the map $\psi$ from Theorem C to grope forests $\psi: \text{Grop}_n(M; U) \rightarrow \text{H}_n(M)$.

**Remark 1.10.** One can generalise gropes to any $d \geq 3$ by simply replacing the model 3-ball $B_3$ by a $d$-dimensional ball obtained as a $(d - 2)$-thickening of the 2-complex $G_3$. Then a thick grope in $M$ is again an embedding $B_3 \hookrightarrow M$ so that for each $1 \leq i \leq n$ the neighbourhood of the $i$-th cap ($\cong \mathbb{D}^2 \times \mathbb{D}^{d-2}$) intersects $K$ in a neighbourhood of a single point $p_i \in K$.

One can similarly construct maps $\psi(G): S^{n(d-3)} \rightarrow \text{H}_n(M)$, using that $(d - 1)$-dimensional normal disks to $K$ at $p_i$’s give an $n(d-2)$-family of arcs. This gives points $e_{n+1}\psi(G) \in \Omega^{n(d-3)}\text{F}_{n+1}(M)$ and we believe the proofs of our main theorems below readily extend to show that $e_{n+1}$ is a surjection onto the first non-trivial group $\pi_{n(d-3)}\text{F}_{n+1}(M)$ for any $d \geq 3$. We will explore this in future work.

### 1.1.3 The underlying tree is detected in the Taylor tower

The first step on the journey relating the homotopy theory of punctured knots and the geometry of gropes was to connect them both to the language of decorated trees: they generate the group of components of the layers and also underlie gropes. It remains to show their compatibility via

$$\text{Grop}_n(M; U) \xrightarrow{\psi} \text{H}_n(M) \xrightarrow{e_{n+1}} \text{F}_{n+1}(M).$$

**Theorem D** (Main Theorem). For $G \in \text{Grop}_n^1(M; U)$ the connected component of the point $e_{n+1}\psi(G) \in \text{F}_{n+1}(M)$ is given by the class of its underlying tree $[t(G)] \in \text{Lie}_{n,1M}(n)$.

More explicitly, for a thick grope $G: B_3 \rightarrow M$ on $U$ with the underlying tree $\epsilon\Gamma_{\mathbb{R}^2}$, we claim

$$e_{n+1}\psi(G) = [\epsilon\Gamma_{\mathbb{R}^2}] \in \pi_0\text{F}_{n+1}(M) \cong \text{Lie}_{n,1M}(n).$$

We prove this in Section 6 using the above Corollary 1.3: it is enough to show that the Samelson product $\Gamma(m_i^{\mathbb{R}^2}) \colon S^n \rightarrow \Omega M_{\mathbb{R}^2}$ is homotopic to the map (the initial coordinate of $D(\chi e_n\psi(G))$):

$$D(\chi e_n\psi(G))_{\mathbb{R}^2} : S^n \rightarrow \Omega M_{\mathbb{R}^2}.$$

The maps $D$ and $\chi$ were constructed in Theorem B. The idea of the proof is to use inductive descriptions of both Samelson products (see Lemma B.5) and thick gropes, to reduce to checking that $D(\chi e_n\psi(G))_{\mathbb{R}^2}$ is homotopic to a certain pointwise commutator map.

A crucial step for this reduction is our description of the map $\chi$ in Appendix A as

$$(\chi f)^{\mathbb{R}^2} = \bigboxplus_{S \subset \mathbb{R}^2} (f_{S})^{h_{\mathbb{R}^2}}.$$

This is a map on $S^n$ obtained by gluing together along faces $2^n$ different maps $(f_{S})^{h_{\mathbb{R}^2}}$, each defined on $I^n$ as a certain ‘$h_{\mathbb{R}^2}$-reflection’ of the original map $f_{S}$ across a face of $I^n$.

Hence, every generator of $\pi_0\text{F}_{n+1}(M)$ is in the image of $\pi_0 e_{n+1}$. However, to prove that this map of sets is surjective we must also realise linear combinations. Recall that they arise as underlying trees of grope forests, so the following is all we need (for a proof see the end of Section 6).

**Theorem E.** We have $[e_{n+1}\psi(F)] = [t(F)] \in \text{Lie}_{n,1M}(n)$ for any grope forest $F \in \text{Grop}_n(M; U)$. 
Proof of Theorem A. The statements about $F_{n+1}$ are contained in Theorem B.

It remains to construct the map $\rho_n$ making the lower triangle in the following diagram commute:

$$
\begin{array}{c}
\pi_0 \text{Grop}_n(M; U) \\
\downarrow \pi_0 \psi \\
\pi_0 \text{H}_n(M)
\end{array} \quad \xrightarrow{\rho_n} \quad 
\begin{array}{c}
\mathbb{Z}[\text{Tree}_{n+1}(M)] \\
\downarrow \text{mod} (AS, IHX) \\
\pi_0 \text{F}_{n+1}(M)
\end{array}
$$

Observe that Theorem E is equivalent to the commutativity of the outer square. Thus, it is enough to pick any set-theoretic section of $t$, or in other words, let $\rho_n(f) := [\psi(F)]$ for any grope forest $F \in \text{Grop}_n(M; U)$ with the underlying tree $t(F) = f$. □

1.1.4 The outline

In the preliminary Section 2 we define several variants of trees and survey finite type theory, and in Section 2.3 prove the corollaries of Theorem A announced at the beginning.

In Section 3 we study the punctured knots model $P_n(M)$ for $M$ any $d$-manifold with boundary, $d \geq 3$. In Section 3.3 we show the layers are iterated loop spaces, while in Section 4 we determine their homotopy type, and describe geometrically the generators of the first non-trivial homotopy group, proving Theorem B. In Section 4.2 we outline the proof strategy for Theorem D.

In Section 5 we are concerned with 3-manifolds. Firstly, Section 5.1 presents a self-contained account of gropes. Then in Section 5.2 we prove Theorem C and its extension for grope forests, and in Section 5.3 describe points $e_{n+1}\psi(G)$ and $e_{n+1}\psi(F)$ explicitly. Finally, main Theorems D and E are proven in Section 6; the proof of Theorem D is by induction, using two auxiliary lemmas.

The construction of an explicit homotopy equivalences $\chi$ (from total fibres of certain cubes to iterated loop spaces) is deferred to Appendix A, while Appendix B provides background on Samelson products and contains two important lemmas about their inductive behaviour.

Throughout the paper we aim to make both homotopy theory and geometry accessible without assuming much background. The mutually related Examples 3.1, 4.7, 4.8, 5.15, and Figure 27 all describe the lowest degree computation for a 3-manifold $M$, which is also the induction base in the proof of Theorem D. The induction step is outlined in Example 4.9.

2 Preliminaries

2.1 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 $\Gamma \in \text{Tree}(S)$ is a tree with one distinguished univalent vertex (the root) and all other univalent vertices (the leaves) labelled in bijective manner by the set $S$. The grafting of two rooted trees $\Gamma_j \in \text{Tree}(S_j)$ for $j = 1, 2$ is the rooted tree

$$
\begin{array}{c}
\Gamma_2 \\
\Gamma_1
\end{array} \in \text{Tree}(S_1 \sqcup S_2)
$$

obtained by gluing the two roots together and ‘sprouting’ a new edge with a new root.
Define the group of Lie trees \( \text{Lie}(S) := \mathbb{Z}[\text{Tree}(S)]/\text{AS, IHX} \) as the quotient of the free abelian group on the set of rooted trees by the following relations (dots represent the remaining unchanged part of an arbitrary tree):

\[
\begin{align*}
\text{AS} : & \quad \gamma_2 \gamma_1 \gamma_1 \gamma_2 = 0, \\
\text{IHX} : & \quad \gamma_3 \gamma_2 \gamma_1 \gamma_1 \gamma_2 + \gamma_1 \gamma_3 \gamma_1 \gamma_2 \gamma_3 = 0. \\
\end{align*}
\]

We now 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 \( \mathbb{N}_0 \)-graded Lie algebra over \( \mathbb{Z} \), with each \( x^k \) having degree \( |x^k| = d - 2 \). Thus, the degree of a word \( w \in \mathbb{L}_d(S) \) is \( |w| = l_w(d - 2) \) where \( l_w \) is the length of \( w \), that is, the total number of letters in \( w \).

The normalised Lie algebra \( \mathbb{N}_d(S) \) is the Lie subalgebra of \( \mathbb{L}_d(S) \) generated by the words in which every letter appears at least once.\(^9\) Let \( \text{Lie}_d(S) \subseteq \mathbb{N}_d(S) \) be its subgroup generated by the words in which each letter appears exactly once. This is precisely the part of degree \( |S|(d - 2) \) of \( \mathbb{N}_d(S) \).

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

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

\[
[w_1, w_2] + (-1)^{|w_1||w_2|} [w_2, w_1] = 0,
[w_1, [w_2, w_3]] - [[w_1, w_2], w_3] - (-1)^{|w_1||w_2|} [w_2, [w_1, w_3]] = 0,
\]

while the relations (2.1), which are inspired by applications in geometric topology (see [CST07] for example), never involve graded signs. Nevertheless, as we learned from [Con08] and [Rob04] a correspondence can be obtained as follows. Let us denote \( (1|2)_d := (d-2)! \left\{ (i_1, i_2) \in S_1 \times S_2 : i_1 > i_2 \right\} \).

**Lemma 2.3.** If \( S \) is ordered, there is an isomorphism of abelian groups \( \omega_d : \text{Lie}(S) \cong \text{Lie}_d(S) \) defined inductively on \( |S| \) by \( \Gamma_2 \Gamma_1 \mapsto x_i \) and for \( S = S_1 \cup S_2 \) and \( \Gamma_j \in \text{Tree}(S_j) \) by \( \Gamma_2 \Gamma_1 \Gamma_j \mapsto (-1)^{|(1|2)_d|} \omega_d(\Gamma_1), \omega_d(\Gamma_2) \).

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

For \( n := \{1, \ldots, n\} \) we write \( \text{Tree}(n) := \text{Tree}(n) \) and \( \text{Lie}(n) := \text{Lie}(n) \). 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 edges might intersecting, but this is not part of the data). The vertex orientation is still induced from the plane.

**Figure 2.** Trees \( \omega : \Gamma_i \mapsto x^i \), \( \Gamma_1 \mapsto [x^1, x^2] \), \( \Gamma_2 \mapsto (-1)^{d-2}[x^2, (-1)^{d-2}[x^1, x^3]] \) drawn in the plane.

\(^9\) That is, \( \mathbb{N}_d(S) := \bigcap_{k \in S} \ker(s^k : \mathbb{L}_d(S) \to \mathbb{L}_d(S \setminus k)) \), where \( s^k \) replaces each appearance of \( x^k \) by zero.
Using the AS and IHX relations repeatedly one can show that $\text{Lie}(n) \cong \mathbb{Z}^{(n-1)!}$, with a basis given by trees from Figure 3 (ignoring red decorations for now) for various permutations $\sigma \in \Delta_{n-1}$, corresponding to left-normed Lie words $[x^{\sigma(1)}, [x^{\sigma(2)}, [\ldots [x^{\sigma(n-1)}, x^n] \ldots]]]$. However, $\text{Lie}(n)$ is also an interesting $\Delta_n$-representation, by permuting the leaf labels, giving the arity $n$ of the Lie operad.

![Figure 3. A left-normed tree $\Gamma^n \in \text{Tree}_n$](image)

**Definition 2.4.** Define the abelian group $\text{Lie}_n(S)$ of $\pi$-decorated Lie trees by $\text{Lie}(S) \otimes \mathbb{Z}[\pi^5]$.

If we let $\text{Tree}_n(S) := \text{Tree}(S) \times \pi^5$, then $\text{Lie}_n(S)$ is the quotient of $\mathbb{Z}[\text{Tree}_n(S)]$ by the relations analogous to $AS, IHX$ from (2.1), which respect decorations in the natural way. We denote elements of $\text{Tree}_n(S)$ by $\Gamma^S$, where $\Gamma \in \text{Tree}(S)$ and $g_S := (g_i)_{i \in S} \in \pi^5$, and call them $\pi$-decorated trees. Namely, these are 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.

When $\pi = \pi_1 M$ we view a $\pi_1 M$-decorated tree $\Gamma^S$ as a homotopy class of a map $x : \Gamma \to M$ 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 $\gamma_i$, 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 $\gamma_i$ should be conjugated by the piece of $K$ between $p_0$ and $x(i)$.

**Remark 2.5.** The group $\text{Lie}_n(n)$ is equal to $\Lambda_{n-1}(\pi, n+1)$ from the work of Schneiderman and Teichner [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.

### 2.1.2 Jacobi diagrams and Jacobi trees

In the theory of finite type invariants for $M = I^3$ one considers more general uni-trivalent graphs, with univalent vertices $0, \ldots, |u| - 1$ (the leaves) and vertex-oriented trivalent vertices (as in Definition 2.1). The degree of such a graph is half of the total number of vertices.

**Definition 2.6.** For $n \geq 0$ define the abelian group $\mathcal{A}_n$ of Jacobi diagrams as the quotient of the $\mathbb{Z}$-linear span of the set of degree $n$ graphs by the linear combinations which locally look like

$$STU : \quad = 0, \quad 1T : \quad = 0. \quad (2.3)$$

Here we use the convention from Figure 2 to draw graphs in the plane (now without roots). However, in geometric finite type theory one can reduce to considering trees only, see Section 2.2.
**Definition 2.7** ([Con08]). Define the abelian group of Jacobi trees by

\[
\mathcal{A}_1^j(I^3) := \text{Lie}(1)/i = 0 \quad \text{and for } n \geq 2 \text{ by } \mathcal{A}_n^j(I^3) := \text{Lie}(n)/\text{STU}^2
\]

where the STU\(^2\) relation is given by applying STU in two different ways:

\[
\text{STU}^2 : \quad \text{STU}(D, v_k) = \text{STU}(D, v_0).
\] (2.4)

Here a Jacobi diagram D has degree n and exactly one loop (i.e. the first Betti number \(\beta_1(D) = 1\)) and \(v_0\) and \(v_k\) lie on the loop of D and are neighbours of the leaf 0 or k respectively (see Figure 4).

![Figure 4](#)

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

**Remark 2.8.** Actually, Conant more generally has \(\text{STU}(D, v_j) = \text{STU}(D, v_i)\) for vertices \(v_i, v_k\) which lie on the loop of \(D\) and are neighbours of the leaves \(j, k \in \{0, 1, \ldots, n\}\) respectively.

But this follows from (2.4) via \(\text{STU}(D, v_j) = \text{STU}(D, v_i) = \text{STU}(D, v_k)\), since we can assume that the distance of the root to the unique loop of \(D\) is one. Indeed, in the IHX relation (2.1) let \(v_0\) be the vertex joining \(\Gamma_2\) and \(\Gamma_3\), with the root 0 in \(\Gamma_1\). Then two of the terms have distance from 0 to the loop smaller than the third, so we can proceed by induction.

The natural inclusion \(\mathcal{A}_n^j \hookrightarrow \mathcal{A}_n\) sends a Jacobi tree to itself viewed as a Jacobi diagram modulo STU, and lands in the primitives of the Hopf algebra \(\mathcal{A} := \oplus_{n \geq 0} \mathcal{A}_n\), see [Con08; Kos20].

### 2.2 Geometric finite type theory

Let us briefly review classical and geometric approaches to finite type theory; for book treatments see [Oht02; CDM12]. We restrict to the case of classical (long) knots \(\mathbb{K}(I^3) := \pi_0 \mathcal{H}(I^3)\) (monoid under the connected sum \#), with unit the unknot \(U\); for general 3-manifolds, see [Kos20].

A singular knot is an immersion \(\sigma : I \hookrightarrow I^3\) with finitely many transverse double points, which agrees with \(U\) near boundary. Each double point can be resolved by pushing the two strands off each other in two different ways, and all possible resolutions of \(\sigma\) give \(K_\sigma \in \mathbb{Z}[\mathbb{K}(I^3)]\), a linear combination of knots. Now depending on the minimal number \(n \geq 1\) of double points this defines a decreasing filtration \(V_n \subseteq \mathbb{Z}[\mathbb{K}(I^3)]\) of the monoid ring, with \(V_1\) precisely the augmentation ideal.

The associated graded of this filtration is related to the Hopf algebra of chord diagrams: those Jacobi diagrams from Definition 2.6 in Section 2.1.2 which have no trivalent vertices. Namely, for a singular knot \(\sigma\) with \(n\) double points one has \(n\) pairs of points on the source interval \(I\) which are identified by \(\sigma\); we record each pair by a chord to get a chord diagram \(D_\sigma\) on \(I\) of deg\((D_\sigma)\) = \(n\).
This assignment is surjective, but far from being injective. However, there is a well-defined map $R_n$ which takes a chord diagram $D$ to the class $[K_{\sigma(D)}] \in \mathcal{V}_{n+1}$, 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 (2.3) (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 2.6, so there is a linear map

$$\mathbb{Z}[\text{chord diagrams of deg } n]_{\mathcal{A}_n}/4T, 1T \to \mathbb{Z}[\text{Jacobi diagrams of deg } n]_{\mathcal{A}_n}/STU, 1T =: \mathcal{A}_n$$

(2.5)

Moreover, by Bar-Natan this is an isomorphism [Bar95] (the proof was given over $\mathbb{Q}$, but it actually applies integrally). Combining this with the previous paragraph gives a surjection of finitely generated abelian groups

$$R_n : \mathcal{A}_n \longrightarrow \mathcal{V}_{n+1}/\mathcal{V}_{n+1} \quad D \mapsto [K_{\sigma(D)}].$$

(2.6)

called the realisation map. It is an open problem if its kernel is non-trivial, and a potential inverse is classically called a universal Vassiliev knot invariant of type $\leq n$ over $\mathbb{Z}$.

Namely, a knot invariant $\nu : \mathbb{Z}(I^3) \to T$ is of type $\leq n$ if its linear extension $\nabla : \mathbb{Z}[\mathbb{Z}(I^3)] \to T$ vanishes on $\mathcal{V}_{n+1}$. Here $T$ is an abelian group and $\nabla$ is just a map of sets.

**Definition 2.9.** Let $R$ be a ring, $A$ a graded $R$-module and $\hat{A} := \prod_{n \geq 1} A_n$ its completion. A map $\zeta : \mathbb{Z}(I^3) \to \hat{A}$ is a universal Vassiliev invariant over $R$ if the linear extension $\zeta : R[\mathbb{Z}(I^3)] \to \hat{A}$ 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 $\zeta_n$ is an invariant of type $\leq n$,
2. the restriction $\zeta_n|_{\mathcal{V}_n} : \mathcal{V}_n/\mathcal{V}_{n+1} \otimes R \to A_n$ is an isomorphism.

We say that $\zeta$ is classical if the composite $\zeta_n|_{\mathcal{V}_n} \circ (R_n \otimes R)$ is the identity (so $\mathcal{A}_n \otimes R = A_n$).

**Lemma 2.10** (justifying the ‘universality’). If $\zeta$ is a universal Vassiliev invariant over $R$, then any invariant $\nabla : \mathbb{Z}(I^3) \to T$ of type $\leq n$ with values in an $R$-module $T$ can be written as a sum $\sum_{k=1}^n v_k \circ \zeta_k$, where $v_k := \nabla|_{\mathcal{V}_k} \circ (\zeta_k|_{\mathcal{V}_k})^{-1} : A_k \to T$, called the $k$-th symbol of $\nabla$.

*Proof.* Indeed, $\nabla - R_n \circ \zeta_n$ 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. \(\square\)

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 [Les02] (note that there may be several universal invariants over the same coefficient ring since only the ‘bottom part’ $\zeta_n|_{\mathcal{V}_n}$ is determined). As a consequence,

$$R_n \otimes \mathbb{Q} : \mathcal{A}_n \otimes \mathbb{Q} \longrightarrow \mathcal{V}_{n+1}/\mathcal{V}_{n+1} \otimes \mathbb{Q}.$$ 

(2.7)

Therefore, the kernel of $R_n$ consists of torsion elements, but it is unknown if $\mathcal{A}_n$ has any.

The Bar-Natan’s isomorphism (2.5) gives more power to the theory as it is relatively easy to construct interesting invariants of Jacobi diagrams, called weight systems. For example, invariants are obtained by interpreting each trivalent vertex as the Lie bracket in a fixed semisimple Lie algebra and the horizontal line as its representation. Actually, symbols of quantum invariants of knots are precisely these weight systems, but by [Vog11] this is a strict subset of all of them.

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 2.11. For \( K, K' \in \mathbb{K}(I^3) \) and \( n \geq 1 \) the following are equivalent:

1. \( K \sim K' \in V_n \) 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 \((1) \Leftrightarrow (2)\) is due to [Sta98], \((1) \Leftrightarrow (3)\) are independently by [Gus00] and [Hab00, Thm. 3.17 & 6.18] and \((3) \Leftrightarrow (4)\) 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 Section 5.1 using the last approach of the theorem (see Remark 5.3).

Let us define the Gusarov–Habiro filtration by sumbonomoids \( \mathbb{K}_n(I^3) := \{ K \in \mathbb{K}(I^3) : K \sim_n U \} \subseteq \mathbb{K}(I^3) \). Then the theorem implies that it maps to the Vassiliev–Gusarov filtration:

\[
\begin{array}{ccc}
\mathbb{K}_n(I^3) & \xrightarrow{\pi_0 \mathbb{R}(I^3)} & V_n \\
\downarrow & & \downarrow \\
\mathbb{K}(I^3) & \xrightarrow{K \mapsto K-U} & \mathbb{Z}[\mathbb{K}(I^3)] \\
\end{array}
\]

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 \( H^0(\mathbb{R}(I^3); T) \). 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 \( \mathbb{K}(I^3) \) to abelian groups.

Lemma 2.12. An additive invariant has type \( \leq n \) if and only if it vanishes on \( \mathbb{K}_{n+1}(I^3) \). That is, \( \nu : \mathbb{K}(I^3) \to A \) is a monoid map vanishing on \( \mathbb{K}_{n+1}(I^3) \) if and only if the linear extension \( \overline{\nu} : \mathbb{Z}[\mathbb{K}(I^3)] \to A \) vanishes on \( V_1 \cdot V_1 + V_{n+1} \).

Proof. Since \( \nu(K_1 \# K_2) - \nu(K_1) - \nu(K_2) = \overline{\nu}((K_1 - U) \# (K_2 - U)) \), \( \nu \) is a monoid map if and only if its linear extension \( \overline{\nu} \) vanishes on \( V_1 \cdot V_1 \subseteq \mathbb{Z}[\mathbb{K}(I^3)] \). On one hand, by Theorem 2.11 we have \( \{ K - U : K \in \mathbb{K}_{n+1}(I^3) \} \subseteq V_{n+1} \) and on the other, \( V_{n+1} \subseteq V_1 \cdot V_1 + \{ K - U : K \in \mathbb{K}_{n+1}(I^3) \} \) by a result of Habiro [Hab00, Thm. 6.17]. Since \( \nu(K) = \overline{\nu}(K - U) \), the claim follows.

In this setting we pass from Jacobi diagrams \( \mathcal{A}_n \) to its subgroup \( \mathcal{A}_n^T \subseteq \mathcal{A}_n \) of Jacobi trees, and from the realisation map \( \mathbb{R}_n \) to its ‘tree part’ \( \mathbb{R}_n^T \), defined as the unique map completing the diagram:

\[
\begin{array}{ccc}
\mathbb{K}_n(I^3) & \xrightarrow{\pi_0 \text{Grop}_n(I^3; U)} & \mathbb{Z}\{\text{Tree}(n)\} \\
\downarrow & & \downarrow \\
\mathbb{K}(I^3) & \xrightarrow{\partial} & \mathbb{Z}\{\text{Tree}(n)\}/\sim_{n+1} \\
\end{array}
\]

Recall from Section 1.1.2 that \( \text{Grop}_n(I^3; U) \) is the space of degree \( n \) grope forests, \( \partial^T \) is the output knot map and \( t \) the underlying tree map. The following describes the exact relation between the two realisation maps.
This is equivalent to the claim that the previous discussion largely generalises to long knots in any oriented 3-manifold. According to Remark 2.16, the equivalence of the definitions of the $n$-equivalence relation analogous to (2, 3, 4) of Theorem 2.11 still hold. However, their equivalence to (1) remains open, see [Hab00, Sec. 6].
2.3 Proofs of corollaries

As mentioned in the introduction, an important result is the identification due to Conant of the diagonal of the second page of spectral sequence for the tower $P_n(M)$.

**Theorem 2.17** ([Con08]). There is an isomorphism $E^2_{-(n+1),n+1}(I^3) \cong \mathcal{A}_n^T := \text{Lie}(n)/\text{STU}^2$.

We saw in Corollary 1.5 that the first page has $\text{Lie}(n)$ on the diagonal, so Conant identifies the image of the first differential as $\text{STU}^2 \subseteq \text{Lie}(n)$. See also [Shi19].

2.3.1 The diagram

We now summarise the preceding discussion in the diagram

$$
\begin{array}{ccc}
\pi_0 \text{Grop}_n(I^3; U) & \xrightarrow{\partial} & \mathbb{Z}[\text{Tree}(n)] \\
\uparrow \pi_0 \psi & & \downarrow \text{mod (AS, IHX)} \\
\pi_0 H_n(I^3) & \xrightarrow{\rho_n} & \text{Lie}(n) = \pi_0 F_{n+1}(I^3) \\
\downarrow \mathcal{A}_n^T & & \downarrow \text{mod im } \pi_0 \delta \\
\mathbb{K}_n(I^3)/_{\sim_{n+1}} & \rightarrow & \ker(\pi_0 P_{n+1}) \subseteq \pi_0 P_{n+1}(I^3) \\
\end{array}
$$

(2.9)

All objects here are abelian groups except that $\pi_0 \text{Grop}_n(I^3; U)$ and $\pi_0 H_n(I^3)$ are only sets. The vertical dashed map on the right takes the quotient by the image on $\pi_0$ of the connecting map $\delta : \Omega P_n(I^3) \to F_{n+1}(I^3)$ for fibration $p_{n+1}$. This factors through $\mathcal{A}_n^T \cong E^2_{-(n+1),n+1}$ by Theorem 2.17, since $\text{Lie}(n) \cong E^1_{-(n+1),n+1}$ and the quotient by higher differentials is $\ker(\pi_0 p_{n+1}) = E^\infty_{-(n+1),n+1}(I^3)$.

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

$$
\begin{array}{cccc}
\mathbb{K}_n(I^3)/_{\sim_{n+1}} & \rightarrow & \mathbb{K}(I^3)/_{\sim_{n+1}} & \rightarrow & \mathbb{K}(I^3)/_{\sim_{n}} \\
\bar{e}_{n+1} & & \downarrow \pi_0 \psi & & \downarrow \pi_0 \psi \\
\ker(\pi_0 P_{n+1}) & \rightarrow & \pi_0 P_{n+1}(I^3) & \rightarrow & \pi_0 P_n(I^3) \\
\end{array}
$$

(2.10)

using that $\pi_0 \psi$ factors though the quotient by $\sim_{n}$, which is a corollary of Theorem C, see (1.2).

**Remark 2.18.** By Corollary (1.2) $\pi_0 \psi$ vanishes on $\mathbb{K}_n(I^3)$, so $\mathbb{K}_n(I^3) \subseteq \text{im } (\pi_0 H_n(I^3) \to \mathbb{K}(I^3))$, and Conjecture 0.1 precisely claims that this inclusion is an equality. Thus, on the left side of (2.9) there is a priori no vertical map.

**Corollary 2.19.** The diagram (2.9) commutes.

**Proof.** The subdiagram comprised of solid arrows commutes by Theorem 2.13. The upper rectangle commutes by Theorem E, see (1.3). It remains to check that the triangle on the right commutes.

To this end, let $F \in \mathbb{Z}[\text{Tree}(n)]$ and $[F] \in \mathcal{A}_n^T$ its class. By the surjectivity of $\tau$ we can find $F \in \text{Grop}_n(I^3; U)$ with $\tau(F) = F$. Let $K = \partial^2(F)$ and note that $[K] = R_n^T[F]$ by the solid diagram. Then

$$
\bar{e}_{n+1}(R_n^T[F]) = [\psi_{n+1}(K)] = [\psi(F)] = [F] \pmod{\text{im } \delta_n}.
$$

Here the second equality holds since $\psi_{n+1}(K) = i \circ e_{n+1} \circ \psi(F)$, where $i : F_{n+1}(I^3) \to P_{n+1}(I^3)$, by definition, see (0.2). The last equality follows from the commutativity of the upper rectangle. \qed
2.3.2 The spectral sequence and the universality

From the bottom triangle in the diagram (2.9) we deduce Corollary 0.3: if for some \( n \geq 1 \) the map (mod \( d^{>1} \)) 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 (mod \( d^{>1} \)): \( \mathcal{A}^T_d \otimes A \to \ker(\pi_0 p_{n+1}) \otimes A \) is an isomorphism, then both \( \mathcal{R}_d \otimes A \) and \( \mathcal{T}_{n+1} \otimes A \) are isomorphisms.

If for some \( A \) this is the case for all degrees below a fixed degree \( n \), then \( \pi_0 \text{ev}_n \) is a universal additive Vassiliev invariant of type \( \leq -1 \) over \( A \), meaning that there is an isomorphism

\[
\pi_0 \text{ev}_n \otimes A : \frac{\mathbb{K}(I^3)}{\sim_n} \otimes A \xrightarrow{\cong} \pi_0 P_n(I^3) \otimes A.
\]  

(2.11)

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

From this we concluded in Corollary 0.4 that the isomorphism (2.11) holds for \( A = \mathbb{Q} \) for all \( n \geq 1 \), and the \( p \)-adics \( A = \mathbb{Z}_p \) in the range \( n \leq p + 2 \), using the results of [BH20] (see also Remark 2.21). Furthermore, they also show that for \( n \leq p + 2 \) there is a splitting

\[
\pi_0 P_n(I^3) \otimes \mathbb{Z}_p \cong \bigoplus_{1 \leq k \leq n-1} \mathcal{A}_k \otimes \mathbb{Z}_p.
\]

To deduce the integral result, we use that the kernels of both \( \mathcal{R}_d \otimes A \) and \( \mathcal{T}_{n+1} \otimes A \) can be injective.

Remark 2.20. There exists an inverse \( z_n \) to \( \mathcal{R}_d \otimes \mathbb{Q} \) obtained as the logarithm of either the Kontsevich integral [Kon93] or the Bott–Taubes integrals [BT94; AF97] (see the end of Section 2.2). Hence, \( \mathcal{T}_n \otimes \mathbb{Q} \) agrees with these invariants, implying that the configuration space integrals factor through the embedding calculus tower:

\[
\frac{\mathbb{K}(I^3)}{\sim_n} \otimes \mathbb{Q} \xrightarrow{\pi_0 \text{ev}_n} \pi_0 P_n(I^3) \otimes \mathbb{Q}
\]

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

Remark 2.21. Let us remark that the collapse of the spectral sequence \( E^*_{n,d}(I^3) \otimes \mathbb{Q} \) which converges to the rational homotopy groups of \( \mathbb{K}(I^3) \) was shown earlier by [ALTV08] but only for \( d \geq 4 \).

The collapse of the corresponding homology spectral sequences for the Taylor tower of \( \mathbb{K}(I^3) \) 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 collapse for \( d = 3 \). This follows from the results of [FTW17], and more directly from [BH20].

2.3.3 Further consequences and examples

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

Proposition 2.22 (Goodwillie). The set \( \pi_0 P_n(I^3) \) is uncountable, so the Taylor tower does not converge to \( \mathbb{K}(I^3) \), i.e. the map \( \text{ev}_n : \mathbb{K}(I^3) \to P_n(I^3) := \lim_{d \to n} \pi_0 P_d(I^3) \) is not a weak equivalence.
Proof. We claim that \( \pi_0 P_\infty(I^3) \) is uncountable, while \( \pi_0 \mathcal{H}(I^3) \) is countable. We have a surjection of sets \( \pi_0 P_\infty(I^3) \twoheadrightarrow \lim \pi_0 P_n(I^3) \), so it is enough to show that \( \lim \pi_0 P_n(I^3) \) is uncountable.

Indeed, \( \pi_0 P_{n+1} : \pi_0 P_n(I^3) \twoheadrightarrow \pi_0 P_n(I^3) \) is surjective for every \( n \geq 1 \), but not injective since we saw that \( \ker(\pi_0 P_{n+1}) \otimes \mathbb{Q} \cong A_n^7 \otimes \mathbb{Q} \), and these groups are non-trivial for all \( n \geq 2 \). \( \square \)

Nevertheless, recalling that we denote the Gusarov-Habiro completion by \( \mathbb{K}(I^3)_\sim = \lim \mathbb{K}(I^3)/\sim_n \), we have an exact sequence

\[
\lim \left( \ker \pi_0 \text{ev}_n \right) \xrightarrow{\mathbb{K}(I^3)_\sim} \mathbb{K}(I^3)_\sim \xrightarrow{\mathbb{K}(I^3)_\sim} \lim \pi_0 P_n(I^3) \xrightarrow{\lim} \left( \ker \pi_0 \text{ev}_n \right)
\]

(2.12)

This is obtained by taking limits in (2.10), using Milnor’s \( \lim^1 \)-sequence and \( \lim^1 (\mathbb{K}(I^3)/\sim_n) = 0 \), as the maps in that tower are surjective. Thus, if Conjecture 0.1 is true then \( \mathbb{K}(I^3)_\sim \) is an isomorphism.

Group structures.

**Corollary 2.23.** Two group structures on the \( n \)-components of Taylor stages constructed by [BW18] and [BCKS17] are equivalent, i.e. \( \pi_0 T_n^{\text{BW}} \cong \pi_0 \text{AM}_n \) as abelian groups. More generally, any two group structures on \( \pi_0 \mathcal{T}_{\text{K}}(I^3) \) respecting the connected sum of knots must agree.

Proof. The models are weakly equivalent, so there is a bijection of sets \( f : \pi_0 \text{AM}_n \to \pi_0 T_n^{\text{BW}} \) so that \( f \circ \pi_0 \text{ev}_n = \pi_0 \text{ev}_n^{\text{BW}} \). Since \( \pi_0 \text{ev}_n \) is a \( \ker \) surjective monoid map, for \( x_1 \in \pi_0 \text{AM}_n \) we find \( K_1 \in \mathbb{K}(I^3) \) with \( \pi_0 \text{ev}_n(K_1) = x_1 \); then \( x_1 + x_2 = \pi_0 \text{ev}_n(K_1 \# K_2) \). Using that \( \pi_0 \text{ev}_n^{\text{BW}} \) is also a monoid homomorphism we have

\[
f(x_1 + x_2) = \pi_0 \text{ev}_n^{\text{BW}}(K_1 \# K_2) = \pi_0 \text{ev}_n^{\text{BW}}(K_1) + \pi_0 \text{ev}_n^{\text{BW}}(K_2) = f(x_1) + f(x_2). \quad \square
\]

Examples.

**Example 2.24.** Let \( n = 2 \). The grope cobordism \( G^2 \) on the unknot \( U \) from Figure 1 is modelled on the unique tree of degree 2, and has \( K = \partial^2 G \) the right handed trefoil (RHT):

Thus, \( \text{RHT} \sim \text{U} \). Actually, every knot is 2-equivalent to the unknot (see e.g. [MN89]), so

\[
\mathbb{K}(I^3)/\sim_2 = \left\{ [U] \right\}.
\]

Moreover, [BCSS05] show that \( P_3(I^3) \cong \ast \), confirming Conjecture 0.1 in degree \( n = 2 \).

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

\[
\pi_0 \text{ev}_3 : \mathbb{K}(I^3) \to \pi_0 P_3(I^3) \cong \pi_0 \text{AM}_3(I^3) \cong \text{Lie}(2) \cong \mathbb{Z}.
\]

Using the linking of certain ‘colinearity submanifolds’ of configuration spaces, [BCSS05] show that \( \pi_0 \text{ev}_3 \) agrees with the unique Vassiliev invariant \( v_2 \) of type \( \leq 2 \) taking value \( 1 \) on RHT. Classically, \( v_2 \) is given as the second coefficient of the Conway polynomial (lifting the Arf invariant) and induces

\[
v_2 : \mathbb{K}(I^3)/\sim_3 \xrightarrow{\mathbb{Z}} \mathbb{Z}.
\]

Our approach not only recovers \( \pi_0 \text{ev}_3 = v_2 \) but also lifts this computation to the fibres via the map \( \varepsilon_3 : H_2(I^3) \to \text{F}_3(I^3) \). Namely, by the previous example for any \( K \in \mathbb{K}(I^3) \) there exists a grope
forest \( F \) of degree 2 from \( K \) to \( U \). By the extension of Theorem C for grope forests we get a point \( \psi(F) \in H_2(I^3) \) and by definition \( \pi_0ev_3(K) = [e_3\psi(F)] \in \text{Lie}(2) \). Now, our main Theorem E says that this element is the class of the underlying trees of \( F \). Actually, in Example 4.8 we do this computation for the case \( K = \text{RHT} \), as a warm-up problem for the proof of that theorem.

We get precisely \( \pi_0ev_3(\text{RHT}) = \sum \binom{1}{2} \), implying \( \pi_0ev_3(K) = \nu_2(K) \cdot \sum \binom{1}{2} \) by the uniqueness of \( \nu_2 \). If we then for computing the coefficient \( \nu_2(K) \) use the Hopf invariant \( \text{Lie}(2) \subseteq \pi_0(S^2 \vee S^2) \to \mathbb{Z} \) given as the linking number \( \text{lk}(f^{-1}(p_1), f^{-1}(p_2)) \) for a suitable representative \( f : S^3 \to S^2 \vee S^2 \) of the desired homotopy class, then we are in the colinearity story of \([BCSS05]\).

### 2.4 Homotopy limits and the notation

A diagram over a small category \( C \) is a functor \( X : C \to \text{Top} \) to the category of topological spaces. Let \( \text{Top}^C \) denote the category of diagrams over \( C \). The categories we will be using are the cube \( C = \mathcal{O}(n) \), which is the poset of all subsets of \( n := \{1, 2, \ldots, n\} \), and the punctured cube category \( C = \mathcal{O}_n \), the poset of all non-empty subsets of \( [n] = \{0, 1, 2, \ldots, n\} \).

We will need the notion of a homotopy limit of a diagram \( X \in \text{Top}^C \); for an introduction see \([BK72]\) or \([MV15]\). This is the space \( \text{holim}(X) \in \text{Top} \), also written \( \text{holim} X_c \), defined as the mapping space

\[
\text{holim}(X) := \text{Map}_{\text{Top}^C} (|C| \downarrow \bullet, X).
\]

Firstly, \( |C| \downarrow \bullet \in \text{Top}^C \) is the diagram which sends \( c \in C \) to the classifying space of the category \( (C \downarrow c) \), called the overcategory, whose objects are morphisms \( c' \to c \in C \), and arrows are triangles over \( c \in C \). Recall that the classifying space \( [D] \) of a category \( D \) is the geometric realisation of the nerve of \( D \) – the simplicial set whose \( k \)-simplices are sets of \( k \)-composable arrows in \( D \).

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

The crucial property of a homotopy limit is its homotopy invariance: if \( X_c \to Y_c \) is a map of diagrams such that each \( X_c \to Y_c \) is a weak equivalence, then the induced map \( \text{holim} X \to \text{holim} Y \) is a weak equivalence as well.

\[
\begin{array}{ccc}
2 & 23 & 3 \\
12 & 123 & 13
\end{array}
\]

**Figure 5.** Examples of \( \Delta^S \) for \( S = \{2, 3\} \) and \( S = \frac{3}{2} \).

In particular, a punctured \((n + 1)\)-cube \( X_n : \mathcal{O}_n \to \text{Top} \) consists of spaces \( X_S \) for \( \emptyset \neq S \subseteq [n] \) and mutually compatible maps \( x^k_S : X_S \to X_{S \cup k} \) for \( k \in [n] \setminus S \). If \( \Delta^S \) denotes the simplex on the vertex set \( S \), observe that there is a levelwise homeomorphism of punctured cubes

\[
[\mathcal{O}_n] \downarrow \bullet \cong \Delta^S
\]

Namely, \( [\mathcal{O}_n] \downarrow S \) is the simplicial set obtained by barycentric subdivision of the standard \((|S| - 1)\)-simplex, see Figure 5. The maps precisely correspond to inclusions \( \iota^{SR}_k : \Delta^R \hookrightarrow \Delta^S \) for \( R \subseteq S \) of the face whose barycentric coordinates in \( S \setminus R \) are zero. Therefore, in this case we have

\[
\text{holim}(X) = \text{Map}_{\text{Top}^C \mathcal{O}_n} (\Delta^S, X).
\]
and a point $f \in \text{holim}(X_\cdot)$ consists of maps $f^S : \Delta^S \to X_S$ such that for all $k \neq S \subseteq [n]$ the following diagram commutes

\[
\begin{array}{ccc}
\Delta^S & \xrightarrow{f^S} & \Delta^{S \cup k} \\
\downarrow i^S_k & & \downarrow i^S_{S \cup k} \\
X_S & \xrightarrow{f^S_k} & X_{S \cup k}
\end{array}
\]

Similarly, there is a levelwise homeomorphism of cubes $|\mathcal{P}_n| \downarrow \cdot | \equiv \Gamma$, since $|\mathcal{P}_n \downarrow S| \equiv I^S$ is a cube whose coordinates are indexed by $S$, and the map $i^S_{R} : I^R \hookrightarrow I^S$ for $R \subseteq S \subseteq n$ is the inclusion of the face whose coordinates in $S \setminus R$ are zero. But now for $Y_\cdot \in \text{Top}^{\mathcal{P}_2}$ we have $\text{holim}(Y_\cdot) \cong Y_\emptyset$, since $\emptyset \in \mathcal{P}_n$ is the initial object.

However, we can instead take the homotopy limit of the punctured $n$-cube with $Y_\emptyset$ omitted, and compare it to $Y_\emptyset$. More precisely, for $Y_\cdot \in \text{Top}^{\mathcal{P}_2}$ define the total homotopy fibre by

\[\text{tofib}(Y_\cdot) := \text{hofib}(c : Y_\emptyset \longrightarrow \text{holim}(Y_\emptyset)),\]

the homotopy fibre of the natural map $c$ (see Definition 3.5). We will show in Lemma 3.6 that $f \in \text{tofib}(Y_\cdot)$ can also be given as a suitable collection $f^S : I^S \to Y_S$, using the following lemma.

**Lemma 2.26.** There is a levelwise homeomorphism of cubes

\[h^* : \Gamma' \to (C^{\bar{\Delta}})^*,\]

(2.13)

where $(C^{\bar{\Delta}})^S$ is the cone on the barycentric subdivision of $\Delta^S$.

**Sketch of the proof.** Each $h^S$ should map the initial vertex of the cube $I^S$ (i.e. the one with coordinates $0^S$) to the cone point of $\Delta^S$, and the 1-faces to the barycentrically subdivided simplex. This will clearly respect maps in the diagrams. We omit writing out explicit formulae. \[\square\]

**Notation 1** (Spaces). Let $I := [0,1]$ denote the unit interval, $\mathcal{P}X$ the space of free paths $[0,1] \to X$ in a space $X$, and $\mathcal{P}X$ the subspace of paths that start at the basepoint $\ast \in X$. Further, $\Sigma X$ is the reduced suspension of $X$ and $\Omega X$ is its based loop space.

For $\gamma \in \mathcal{P}X$ we write $\gamma : \gamma(0) \sim \gamma(1) \subseteq X$. The use $\gamma^{-1}$ or $\gamma_{1-}$ to denote the inverse path. The concatenation of loops will be denoted by $\gamma \cdot \eta$, and the commutator by $[\gamma, \eta] := \gamma \cdot \eta \cdot \gamma^{-1} \cdot \eta^{-1}$. All manifolds $M$ have non-empty boundary and $\mathbb{S}M \subseteq TM$ is the unit tangent bundle.

**Notation 2** (Main objects).

\[
\begin{array}{ll}
\mathcal{K}(M) & - \text{the space of knots in } M, \text{ see (0.1)} \\
\mathcal{A}_n^\Gamma & - \text{the group of Jacobi trees, Def. 2.7} \\
U & - \text{an arbitrarily chosen basepoint in } \mathcal{K}(M) \\
\mathcal{G}_\Gamma & - \text{an abstract grope modelled on } \Gamma, \text{ Def. 5.1} \\
\mathcal{P}_n(M), \text{ also } \mathcal{F}_n(M), \mathcal{H}_n(M) & - \text{maps } p_n, ev_n, e_n \\
\text{the punctured knots model, see (0.2)} \\
\mathcal{G}, \mathcal{F} & - \text{a thick grope, grope forest, Def. 5.5, 5.6} \\
\mathcal{F}_S, \mathcal{F}_S^{n+1} & - \text{Def. 3.9} \\
\text{Grop}_n(M; U) & - \text{the space of grope forests, Def. 5.7} \\
M_{05}, M_S & - \text{Cor. 3.10} \\
\mathbb{B}, \mathbb{S}, \mathbb{D} & - \text{a d-ball, a } (d - 1)\text{-sphere, a 2-disk} \\
\Gamma, \Gamma^\mathbb{R} & - \text{a tree, a } \pi\text{-decorated tree, Sec. 2.1} \\
\mathcal{R}_n^\Gamma & - \text{the realisation map, Thm. 2.13} \\
\end{array}
\]

See also Notation 3 for the notation related to the punctured knots model, Notation 4 for manifolds $M_{05}$, and the beginning of Section 4 for $M \lor S_5$. 
3 The punctured knots model

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

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

whose elements we simply call knots. We equip it with the Whitney $C^\infty$ topology, and choose an arbitrary knot $U \in \mathcal{H}(M)$ for the basepoint. The $n$-th Taylor approximation of $\mathcal{H}(M)$, for $n \geq 0$, is defined as the homotopy limit

$$T_n \mathcal{H}(M) := \underset{U \in \mathcal{E}\text{mb}_b(U, M)}{\text{holim}} \mathcal{E}\text{mb}_b(U, M).$$

Here the category $\mathcal{E}\text{mb}_b(I)$ 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 $\partial I$. Equivalently, $U$ is of the shape $I \setminus V$, where $V \subseteq I \setminus \partial I$ consists of at most $n + 1$ closed subintervals. The space $\mathcal{E}\text{mb}_b(U, M)$ similarly consists of embeddings $U \hookrightarrow M$, which near $\partial I$ agree with $b$, and 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 $P_n(M)$ which we define next; see [MV15, Example 10.2.18] for a proof. Namely, the desired subposet contains only sets $I \setminus J_S$ for $\emptyset \neq S \subseteq [n] := \{0, 1, \ldots, n\}$, where $J_S := \bigcup_{i \in S} J_i$ 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 (and its opposite) is equivalent to the punctured cube category $\mathcal{E}\text{mb}_b([n])$. Thus, we have a punctured cubical diagram (\mathcal{E}\text{mb}_b(I \setminus J_i, M), r), where for $k \notin S \subseteq [n]$ the restriction map $r^k_S : \mathcal{E}\text{mb}_b(I \setminus J_S, M) \to \mathcal{E}\text{mb}_b(I \setminus J_{S \cup \{k\}}, M)$ introduces a ‘puncture’ at $J_k$. The space

$$P_n(M) := \underset{S \subseteq [n]}{\text{holim}} \mathcal{E}\text{mb}_b(I \setminus J_S, M)$$

is called the punctured knots model for $T_n \mathcal{H}(M)$. Indeed, by the definition of homotopy limits from Section 2.4, a point $f := \{ f_S \}_{S \subseteq [n]} \in P_n(M)$ consists of a compatible collection of maps $f^S : \Delta^S \to \mathcal{E}\text{mb}_b(I \setminus J_S, M)$. That is, each $f^S$ is a $\Delta^S$-family of knots punctured at $J_k$, for $k \in S$.

**Example 3.1.** In degree $n = 2$ the space $P_2(M)$ is the homotopy limit of the punctured 3-cube

Thus, $f \in P_2(M)$ consists of three once-punctured knots, for each two of them an isotopy between their restrictions to twice-punctured knots, and three two-parameter isotopies of thrice-punctured knots connecting restrictions of respective isotopies of twice-punctured knots.

**Remark 3.2.** The condition $f \equiv b$ near $\partial I$ for $f \in \mathcal{E}\text{mb}_b(I \setminus J_S, M)$ (also for $\mathcal{H}(M)$) can be replaced by the requirement that $f$ is ‘flat’ outside of $[L_0, R_{\infty}]$, that is, it agrees with $U \in \mathcal{H}(M)$ on $I \setminus [L_0, R_{\infty}]$. This clearly gives equivalent spaces.

**Notation 3.** To save space we shall denote $\mathcal{E}\text{mb}_b(I \setminus J_S, M)$ by $\mathcal{E}_S$ and write $\mathcal{E}_S^S = \{ \mathcal{E}_S \}_{S \subseteq [n]}$, where the ambient manifold $M$ will be clear from the context. We also simply write $\mathcal{E}_{S_k} := \mathcal{E}_{S \cup \{k\}}$ and equip each $\mathcal{E}_S$ with the basepoint $U_S$, so $r^k_S : \mathcal{E}_S \to \mathcal{E}_{S_k}$ with $k \notin S \subseteq [n]$ is a based map.
Using \([n] \subseteq [n+1]\) we consider two inclusions \(\mathcal{P}_0[n] \hookrightarrow \mathcal{P}_0[n+1]\) given by \(\text{Id}: S \hookrightarrow S\) and \(\text{Id} \cup n+1: S \hookrightarrow S \cup \{n+1\}\). The punctured \((n+1)\)-cube \(\varepsilon_{n+1}^* \circ \text{Id}\) is precisely \(\varepsilon^n\). Let us denote the other cube \(\varepsilon_{n+1}^* \circ (\text{Id} \cup n+1): S \hookrightarrow \\text{emb}_0(I \setminus J_{n+1}, M)\) by \(\varepsilon_{n+1}^*\). Hence, the punctured \((n+2)\)-cube \(\varepsilon_{n+1}^*\) decomposes as

\[
\varepsilon_{n+1}^* = \lim_{\to} \varepsilon_{n+1}^* \\
\varepsilon_{n+1}^* \\
\varepsilon_{n+1}^*
\]

The upper row forms an \((n+1)\)-cube also denoted by \(\varepsilon_{n+1}^*\), but with the index now in \(\mathcal{P}_0[n]\). For \(K \in \mathcal{K}(M)\) and \(S \in \mathcal{P}_0[n]\) we denote by \(K_S := K \mid_{I^S} \in \varepsilon_S\) 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 \(U_S = W_{\infty} \cup W_{01} \cup W_{12} \cup \cdots \cup W_{j,i} \cup W_{\infty}\). Here by abuse of notation \(W_{ij}\) is both in the source \(I\) and in the image \(U \subseteq M\). By Remark 3.2 we assume \(f(W_{\infty}) = W_{\infty}\) for any \(f \in \varepsilon_S\). Lastly, denote by \(\hat{w}_i\) the midpoint of the interval \(W_{i,i+1}\).

\[
U_{023} = \begin{array}{cccc}
W_{-\infty} & W_{02} & W_{23} & W_{\infty} \\
-\infty & \hat{w}_0 & \hat{w}_1 & \hat{w}_2 & \hat{w}_3 & \infty \\
\end{array}
\]

\[
\begin{array}{cc}
r_{023}^1 \\
\end{array}
\]

\[
U_{0123} = \begin{array}{cccc}
W_{-\infty} & W_{01} & W_{12} & W_{23} & W_{\infty} \\
-\infty & \hat{w}_0 & \hat{w}_1 & \hat{w}_2 & \hat{w}_3 & \infty \\
\end{array}
\]

Figure 6. Examples of \(U_S\) and the restriction map \(r_S^j\) for \(n = 3, S = \{0,2,3\}, j = 1\).

Given \(K \in \mathcal{K}(M)\) various restrictions \(K_S\) are mutually compatible, so assemble to give a map \(\mathcal{K}(M) \to \lim_{\to} \varepsilon_S\). Composing it with the canonical map from the limit to the homotopy limit gives the evaluation map

\[
\mathcal{K}(M) \xrightarrow{\text{ev}_n} \lim_{\to} \varepsilon^n_S \xrightarrow{\text{const}} \text{holim} \varepsilon^n_S = P_n(M).
\]

More explicitly, for \(S \in \mathcal{P}_0[n]\) this is given as the constant family

\[
\text{ev}_n(K)^S: \Delta^S \to \varepsilon_S, \quad t \mapsto K_S.
\]

Actually, for \(n \geq 2\) there is a homeomorphism \(\mathcal{K}(M) \cong \lim \varepsilon^n_S\). This follows since having at least three different punctures ensures that all \(f^S \in \varepsilon_S\) are pairwise disjoint, apart from agreeing on intersections. However, for \(n = 1\) this does not hold, since \(f^{(0)}|_{I_1}\) and \(f^{(1)}|_{I_0}\) potentially intersect. Instead, we shall see below that \(\text{holim} \varepsilon^n_S \cong P_1(M)\).

Remark 3.3. By a family version of the isotopy extension theorem, \(r_S^j\) is a locally trivial 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 \(U_{S_k}\), namely \(\text{fib}(r_S^j) = \text{emb}_0(J_k, M \setminus U_{S_k})\).

3.0.1 The zeroth and first Taylor stages

Given \(K \in \varepsilon_i\) for some \(i \geq 0\) we can start ‘shortening’ its both ends until only the flat parts \(W_{-\infty}\) and \(W_{\infty}\) remain. In other words, there is a deformation retraction of \(\varepsilon_i = \text{emb}_0(I \setminus J_i, M)\) onto the point \(U_{-1} \in \varepsilon_i\). Hence, \(P_0(M) = \varepsilon_0\) is contractible as well.

\[10\] In [BCKS17] this is denoted as restriction to subdiagram \(\mathcal{P}_* \subseteq \mathcal{P}_0[n]\).
Next, as we mentioned above, the limit of the diagram
\[
\varepsilon^1_{\mathfrak{mb}}(I \setminus I_1, M) \longrightarrow \varepsilon^1_{\mathfrak{mb}}(I \setminus I_{01}, M)
\]
\[
\varepsilon^1_{\mathfrak{mb}}(I \setminus I_0, M)
\]
is not homeomorphic to the space of knots. Instead, it is given as
\[
\lim \varepsilon^1_{\mathfrak{mb}} = \{(f^0, f^1) \mid f^1_{|I_{01}} = f^1_{|I_{01}} \} = \{ K \in \mathfrak{mm}_d(I, M) \mid K_0, K_1 \text{ are embeddings} \}
\]
the space of those immersions which are embeddings when restricted to $I \setminus I_0$ or $I \setminus I_1$. Actually, since both maps in the diagram $\varepsilon^1_{\mathfrak{mb}}$ are fibrations (see Remark 3.3), the limit is equivalent to the homotopy limit.\(^\dagger\)

Hence we have the upper row in the commutative diagram
\[
\begin{array}{ccc}
E \cong \lim \varepsilon^1_{\mathfrak{mb}} & \xrightarrow{\text{const}} & \text{holim} \varepsilon^1_{\mathfrak{mb}} =: P_1(M) \\
\xrightarrow{\text{ev}_1} & \xrightarrow{\sim} & \xrightarrow{\sim} \\
\mathcal{K}(M) & \xrightarrow{\mathfrak{mm}_d(I, M)} & \text{holim} \mathfrak{mm}_d(I, M) \\
\mathfrak{mm}_d(I, M) & \xrightarrow{\text{ev}_1} & \text{holim} \mathfrak{mm}_d(I, M) \\
\end{array}
\]

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:
\[
\begin{array}{ccc}
\mathfrak{mm}_d(I \setminus I_1, M) & \longrightarrow & \mathfrak{mm}_d(I \setminus I_{01}, M) \\
\longrightarrow & \longrightarrow & \xrightarrow{\sim} \\
\mathfrak{mm}_d(I \setminus I_{0}, M) & \xrightarrow{\mathfrak{mm}_d(I, M)} & \mathfrak{mm}_d(I \setminus I_{01}, M) \\
\xrightarrow{\mathfrak{mm}_d(I, M)} & \xrightarrow{\sim} & \mathcal{P}(\mathfrak{mm}_d(I, M)) \\
\mathcal{P}(\mathfrak{mm}_d(I, M)) & \xrightarrow{\mathfrak{mm}_d(I, M)} & \mathcal{P}(\mathfrak{mm}_d(I, M)) \\
\xrightarrow{\text{ev}_1} & \xrightarrow{\sim} & \mathcal{P}(\mathfrak{mm}_d(I, M)) \\
\end{array}
\]

The first equivalence is induced from the weak equivalences $\mathfrak{mm}_d(V, M) \rightarrow \mathfrak{mm}_d(V, M)$ for $V$ a disjoint union of disks, see for example [Cer61]. The second equivalence is induced from the unit derivative maps, giving paths in the unit tangent bundle $\mathfrak{S}M$, with $\mathcal{P}\mathfrak{S}M \simeq \mathfrak{S}M$ (both endpoints free) and $\mathcal{P}\mathfrak{S}M \simeq \ast$ (one endpoint fixed). One can check that the homotopy limit of the rightmost diagram is $\Omega(\mathfrak{S}M)$, so one has the triangle in (3.4).

On the other hand, the strict limit in the middle diagram is clearly $\lim \mathfrak{mm}_d = \mathfrak{mm}_d(I, M)$. 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, $T_n \mathfrak{mm}_d(I, M) \simeq \mathfrak{mm}_d(I, M)$ for all $n \geq 1$. Here we similarly define $T_n \mathfrak{mm}_d(I, M) := \text{holim} \mathfrak{mm}_d$, using $\mathfrak{mm}_d := \mathfrak{mm}_d(I \setminus I_0, M)$. See [Wei05; GW99].

However, to obtain $P_1(M) = \Omega(\mathfrak{S}M)$ we did not need Smale’s result. Finally, observe that as a consequence of this discussion the inclusion $i : \lim \varepsilon^1_{\mathfrak{mb}} \hookrightarrow \lim \mathfrak{mm}_d$ of ‘special’ immersions into all immersions is – maybe surprisingly – a weak equivalence.

### 3.1 The projection maps

Fix $n \geq 1$. Let $p_{n+1} : P_{n+1}(M) \rightarrow P_n(M)$ be the map induced by forgetting the last puncture $I_{n+1}$, i.e. the map induced on homotopy limits from the inclusion of diagrams $\varepsilon^n_d \subseteq \varepsilon^{n+1}_d$ (see Notation 3). We clearly have $p_{n+1} \circ \text{ev}_{n+1} = \text{ev}_n$, so $p_{n+1}$ respects the basepoints $p_{n+1}(\text{ev}_{n+1}) = \text{ev}_n$.

**Proposition 3.4.** The map $p_{n+1} : P_{n+1}(M) \rightarrow P_n(M)$ is a fibration. Furthermore, its fibre $F_{n+1}(M) := \text{fib}_{\text{ev}_{n+1}}(p_{n+1})$ is homeomorphic to the total homotopy fibre of the $(n + 1)$-cube $\varepsilon^{n,n+1}$.

\(\dagger\)  Warning: although all maps in cubes for higher $n$ are also fibrations, one cannot conclude that $\text{holim} \varepsilon^n_d = \lim \varepsilon^n_d$, as is the case for $n = 1$. Namely, for $n \geq 2$ this is not enough to make an $n$-cube ‘fibrant’. 
Before proving this, we recall the notion of a total homotopy fibre and its properties.

**Definition 3.5.** The total homotopy fibre of an \((n + 1)\)-cube \((C, r): \mathcal{P}[n] \to \text{Top}\) is the space

\[
\text{tofib}(C, r) := \text{hofib}_{c(U)} \left( C_0 \xrightarrow{c} \text{holim}(C|_{\mathcal{P}[n]}) \right).
\]

Here \(U_5 \subset C_5\) are the basepoints and \(c\) is the natural map sending \(x \in C_0\) to the collection of constant maps \(c(x)^S\), each equal to the image \(x\) under \(r_0^5: C_0 \to C_5\). This factors as

\[
\begin{array}{c}
C_0 = \lim C \xrightarrow{c} \text{holim}(C|_{\mathcal{P}[n]}) \\
\text{const} \xrightarrow{=} \text{holim} C \xrightarrow{\tau} \text{tofib}(\mathcal{P}[n])
\end{array}
\]

where \(\tau\) is the restriction map to the homotopy limit of a subdiagram and \(\text{const}\) is the canonical map from the limit to the homotopy limit. Since \(C\) has the initial object, \(\text{const}\) is a weak equivalence. Hence, \(\text{hofib}(c)\) and \(\text{hofib}(\tau)\) are weakly equivalent.

Even something stronger is true.

**Lemma 3.6.** The map \(\tau\) is a fibration and its fibre \(\text{fib}_{c(U)}(\tau)\) is homeomorphic to \(\text{tofib}(C, r)\).

**Proof.** See \cite{Goo92} for several descriptions of total homotopy fibres and inspiration for this proof. Consider the mapping path space of \(c\). The natural projection \(p: E_c \to \text{holim}(C|_{\mathcal{P}[n]})\) is a fibration and \(\text{fib}_{c(U)}(p) = \text{hofib}_{c(U)}(c)\), and the latter is our definition of \(\text{tofib}(C, r)\).

We will construct a homeomorphism \(\tilde{q}: E_c \to \text{holim} C\) and a commutative diagram:

\[
\begin{array}{ccc}
E_c & \xrightarrow{\tilde{q}} & \text{holim} C \\
\downarrow{\sim} & & \downarrow{\sim} \\
\text{holim} C & \xrightarrow{\tau} & \text{tofib}(\mathcal{P}[n])
\end{array}
\]

It will immediately follow that \(\tau\) is a fibration as well (as the composition of a fibration and a homeomorphism) with the fibre homeomorphic to \(\text{tofib}(C, r)\).

Let \((x, y) \in E_c\), so \(x \in C_0\) and \(y: I \to \text{holim}(C|_{\mathcal{P}[n]})\) with \(y(0) = c(x)\). Equivalently, \(y\) is a collection of maps \(y(-)^S: I \times \Delta^S \to C_S\) for \(S \neq 0\), which is on \([0] \times \Delta^S\) constantly equal to \(r_0^5(x)\).

Hence, \(y(-)^S\) factors through the quotient by \([0] \times \Delta^S\), so is a map on the cone \(\mathcal{C}\Delta^S\). Let us define \(\mathcal{C}\Delta^S := I^0\) and \(\gamma(-)^S = x: \mathcal{C}\Delta^S \to C_0\). Then our point gives a map of cubical diagrams

\[
\gamma(-)^S: \mathcal{C}\Delta^S \to C,
\]

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

Recall the homeomorphism \(\tilde{h}^*: I^* \to (\mathcal{C}\Delta^S)^S\) of cubes from Section 2.4 and define \(\tilde{q}: E_c \to \text{holim} C\) by

\[
\tilde{q}(x, y) := \gamma(-)^S \circ \tilde{h}^*.
\]

This is also a homeomorphism, and makes the diagram above commute. \(\square\)

Therefore, a point \(f \in \text{tofib}(c) \equiv \text{fib}_{c(U)}(\tau)\) consists of maps \(f^S: I^S \to C_S\) for \(S \in [n]\) compatible on the 0-faces \(f^S_0 \equiv f^S|_{t_0=0}\), and sending the 1-faces \(\partial_1 I^S \subseteq I^S\) to the basepoint \(U_5 \subset C_5\).

---

\(^{12}\) Aka mapping cocylinder: for a map \(f: X \to Y\) this is \(E_f := \text{holim}(X \to Y - \mathcal{P}) = \{ (x, y) \in X \times \mathcal{P} Y | y(0) = f(x) \}\), and is a usual way of turning \(f\) into a fibration \(p: E_f \to Y\). Actually \(\text{hofib}(f)\) is precisely defined as \(\text{fib}(p)\).

\(^{13}\) If we do not subdivide, we get \((\mathcal{C}\Delta)^S \equiv \Delta^{S+1}\), where \(S + 1\) is a new index labelling the cone point.
Proof of Proposition 3.4. Using the decomposition of $\xi^m_{n+1}$ into subcubes from (3.2) and the fact that the homotopy limits can be computed ‘iteratively’, we obtain\(^{14}\) a homeomorphism:

\[
P_{n+1}(M) = \text{holim}
\begin{pmatrix}
\xi_{\text{ev}_{n+1}} \\
\xi^m_{\text{ev}_{n+1}}
\end{pmatrix}
\cong \text{holim}
\begin{pmatrix}
\xi_{\text{ev}_{n+1}} \\
\xi^m_{\text{ev}_{n+1}}
\end{pmatrix}
\cong \text{holim}(\xi^m_{\text{ev}_{n+1}})
\]

Thus, $P_{n+1}(M)$ 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 $\text{ev}_n$ but for $\text{ev}_{n+1}$-punctured knots $\xi_{\text{ev}_{n+1}} := \xi_{\text{mb}}(I \setminus J_{n+1}, M)$, while $r^m_{n+1} : P_n(M) \to \text{holim}_{\text{ev}_{n+1}}(\xi^m_{\text{ev}_{n+1}})$ is the induced map on the homotopy limits from the maps $r^m_{n+1}$, so it punctures at $J_{n+1}$ 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 3.6, the path fibration $E_c \to \text{holim}_{\text{ev}_{n+1}}(\xi^m_{\text{ev}_{n+1}})$ is equivalent to the fibration $\overline{c}$, so we have a (strict) pullback square:

\[
\begin{array}{ccc}
\text{holim}(\xi^m_{\text{ev}_{n+1}}) & \xrightarrow{\overline{c}} & \text{holim}(\xi^m_{\text{ev}_{n+1}}) \\
\text{ev}_{\text{ev}_{n+1}} & \downarrow & \text{ev}_{\text{ev}_{n+1}} \\
\text{p}_{n+1}(M) & \xrightarrow{\text{ev}_{\text{ev}_{n+1}}} & \text{p}_{n+1}(M)
\end{array}
\]

Since $\overline{c}$ is a fibration, $p_{n+1}$ is also (‘pullbacks preserve fibrations’) and the fibres are homeomorphic:

$F_{n+1}(M) := \text{fib}_{\overline{c}}(p_{n+1}) \cong \text{fib}_{\text{ev}_{\text{ev}_{n+1}}}(\overline{c}) \cong \text{tofib}(\xi^m_{\text{ev}_{n+1}})$.\(\Box\)

The diagram (3.5) from the proof can be seen as an inductive definition of the Taylor tower. Moreover, if we denote $BF_{n+1}(M) := \text{holim}_{\text{ev}_{n+1}}(\xi^m_{\text{ev}_{n+1}})$, and use $\xi_{\text{ev}_{n+1}} \cong *$ from Section 3.0.1, we get $P_{n+1}(M) \cong \text{holim}(\xi_{\text{ev}_{n+1}})$ and $F_{n+1}(M) \cong \text{hobib}(\xi_{\text{ev}_{n+1}})$. Thus, $BF_{n+1}(M)$ is indeed a delooping of $F_{n+1}(M)$, explaining the notation. Moreover, $BF_{n+1}(M)$ is connected, so $p_{n+1}$ is surjective, see [Kos20].

Remark 3.7. In Section 3.3 we will see that $BF_{n+1}(I^3)$ is an $n$-fold loop space, so one can try to show that $P_{n+1}(I^3) = \text{hobib}(P_n(I^3) \to BF_{n+1}(I^3))$ is a double loop space by induction on $n \geq 1$ and showing that $r^m_{n+1}$ is a map of double loop spaces. Such deloopings were shown in other models by [Tur14] and [BW18], but in this approach one could check if they also exist for some other $M$.

3.2 The layers and homotopy fibres of evaluation maps

Recall that $H_n(M)$ was defined in (0.2) as the homotopy fibre of the map $\text{ev}_n : \mathcal{R}(M) \to P_n(M)$ over the basepoint $U$. Since $\mathcal{R}(M) = \xi_{\text{mb}}(I, M) = \xi_0$ and $P_n(M) := \text{holim}_{\text{ev}_{n+1}}(\xi^m_\text{ev}_{n+1})$, the homotopy fibre $\text{hobib}(\text{ev}_n)$ is by definition the total homotopy fibre $H_n(M) \cong \text{tofib}_{\text{ev}_{n+1}}(\xi^m_\text{ev}_{n+1})$ (see Definition 3.5).

\(^{14}\)To prove this one uses homeomorphisms $\Delta^m_{\text{ev}_{n+1}} \cong \mathbb{C} \Delta^3$ which assemble into a map $(\mathbb{C} \Delta^1)^* \to \Delta^*$ (see Footnote 13); for details see [Goo92] or [MV15, Lemma 5.3.6].
Since in Proposition 3.4 we found $F_{n+1}(M) \cong \text{tofib}_{\mathbb{P}[n]}(\mathcal{E}_{n, n+1})$, let us define

$$e_{n+1}: H_n(M) \to F_{n+1}(M)$$

as the map induced on total homotopy fibres from the map $r^{n+1}_*: \mathcal{E}_n^* \to \mathcal{E}_{n,n+1}$ of $(n+1)$-cubes. This again 'punctures at zero', that is, we take homotopy fibres of total homotopy fibres from the proof of Lemma 3.6 we immediately have the following.

**Lemma 3.8.** The composition $H_n(M) \xrightarrow{e_{n+1}} F_{n+1}(M) \xrightarrow{\text{hofib}(p_{n+1})} \text{hofib}(p_{n+1})$ agrees with the canonically induced map $I_{n+1}: H_n(M) := \text{hofib}(e_n) \to \text{hofib}(p_{n+1})$ given by $I_{n+1}(K, \eta) = (e_n(K), \eta)$.

This completes the diagram (0.2) from the introduction.

The total homotopy fibre of an $(n+1)$-cube can also be computed 'iteratively', by first taking homotopy fibres in one arbitrary direction and then finding the total fibre of the resulting $n$-cube. This is similar to Footnote 14, and uses $F_{n+1} = I \times F^n$; see [Goo92] or [MV15] for a proof. For the first direction we 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 3.9.** For each $S \subseteq \mathbb{N} := \{1, 2, \ldots, n\}$ define

$$\mathcal{F}_S := \text{fib}(r^0_S: \mathcal{E}_S \to \mathcal{E}_{0S})$$

and

$$\mathcal{F}^{n+1}_S := \text{fib}(r^{n+1}_S: \mathcal{E}_{n,n+1} \to \mathcal{E}_{0S,n+1}).$$

The map $r^{n+1}_S: \mathcal{F}_S \to \mathcal{F}^{n+1}_S$ gives the right vertical map in the commutative diagram

$$\begin{array}{ccc}
H_n(M) \cong \text{tofib}(\mathcal{E}_S) & \to & \text{tofib}(\mathcal{F}_S) \\
\downarrow e_{n+1} & & \downarrow \\
F_{n+1}(M) \cong \text{tofib}(\mathcal{E}_{n,n+1}) & \cong & \text{tofib}(\mathcal{F}^{n+1}_S)
\end{array}$$

(3.7)

The basepoint of $\mathcal{E}_S$ is $U^0_S := U_{1J_S}$, so writing the first fibre out, we get

$$\mathcal{F}_S = \text{fib}_{U^0_S}(r^0_S: \mathcal{E}_{0S} \to \mathcal{E}_{0S})$$

$$= (r^0_S)^{-1}(U^0_S) = \{ K : I \backslash J_S \hookrightarrow M \mid K_{I\backslash J_S} = U_{0S} \} \cong \mathcal{E}_{0S}(J_0, M \backslash U_{0S}).$$

Thus, $\mathcal{F}_S$ is the space of embeddings of the arc $J_0$ into the complement in $M$ of the punctured unknot $U^0_S$ with condition that they agree near the boundary $\partial J_0$ with $U_{I_0}$ (see Figure 7). The maps in the $n$-cube $(\mathcal{F}_r, r)$ are restriction maps as before $r^k_S: \mathcal{F}_{S} \to \mathcal{F}_{S^k}$, with $k \notin S \subseteq \mathbb{N}$.

Similarly, the $n$-cube $(\mathcal{F}^{n+1}_r, r)$ can be given by $\mathcal{F}^{n+1}_S \cong \mathcal{E}_{0S}(J_0, M \backslash U_{0S,n+1})$ with the restriction maps $r^{n+1}_{S,n+1}: \mathcal{F}^{n+1}_S \to \mathcal{F}^{n+1}_{S^k}$. However, note that one of the vertices of the cube computing $H_n(M)$ is the space of knots itself. This is in contrast to the cube for $F_{n+1}(M)$, in which the piece $I_{n+1}$ is always absent – precisely this will allow us to compute its homotopy type in the next two sections.
Namely, the space $\mathcal{F}^{n+1}_S$ can equivalently be described as the space of embeddings of the arc $f_0$ in the complement in $M$ of the $d$-dimensional balls $B_{i,p+1} \subseteq M$ obtained as neighbourhoods of the pieces $W_{i,p+1}$ of the punctured unknot $U_{0S_{n+1}}$ (recalling Notation 3). For example, the lower picture in Figure 8 corresponds to the point in $\mathcal{F}^{n+1}_S$ from the bottom of Figure 7 for $n = 6$ and $S = \{2, 3, 5\}$. Let us introduce notation for these complements.

**Notation 4.** Write $S = \{i_1 < \cdots < i_m\}$ for $m \geq 1$ and by convention $i_0 := 0, i_{m+1} := n + 1$. Firstly, let $S_i := S_{i-1} \subseteq M$ be the sphere with the diameter $W_{i,i+1}$ for $0 \leq i \leq n$ and centre $w_i \in W_{i,i+1}$.

Then for $1 \leq p \leq m$ let $S_{i,p+1} \subseteq M$ be the ellipsoid consisting of the cylinder $[w_{i,p}, w_{i,p+1}] \times S^{d-2}$ together with the west hemisphere of $S_i$ and the east of $S_{i-1}$.

Let $B_{i,p+1}$ to be the region interior to this ellipsoid (so it contains $W_{i,p+1}$). Finally, remove from $M$ small neighbourhoods of $W_{\infty}$ (shrunken to a collar of $\partial M$) to get $M' \cong M$ and define

$$M_{0S} := M' \setminus \big( B_{01} \cup B_{12} \cup \cdots \cup B_{in,n+1} \big).$$

Figure 8. For $n + 1 = 6$ the manifold $M_{0S}$ (resp. $M_{0235}$) is the complement of the three (four) balls.

Thus, for $S \subseteq \pi$ there is a homeomorphism $\mathcal{F}^{n+1}_S \cong \text{Emb}_0(f_0, M_{0S})$ and $r_S^k$ is the composition with

$$\rho_S^k : M_{0S} \hookrightarrow M_{0Sk} = M_{0S} \cup \big( B_{k-1,k+1} \setminus (B_{k-1,k} \cup B_{k,k+1}) \big).$$

**Corollary 3.10.** The $n$-cube $(\mathcal{F}^{n+1}_S, \rho_S^k)$ is levelwise homeomorphic to the one obtained from the $n$-cube $(M_{0S}, \rho_S^k)$ by applying the functor $\text{Emb}_0(f_0, -)$.

### 3.3 Delooping the layers

In this section we make a crucial step for the description of the homotopy type of $F_{n+1}(M)$ by constructing a homotopy equivalence $\chi$ from $F_{n+1}(M)$ to an $n$-fold loop space (Section 3.3.2), and then deloop once more (Section 3.3.3).

#### 3.3.1 The initial delooping

**Theorem 3.11.** For the $(n+1)$-st layer $F_{n+1}(M) \simeq \text{tofib}(\mathcal{F}^{n+1}_S, r)$ of the Taylor tower for $\mathcal{H}(M)$, $n \geq 0$, there is a contravariant $n$-cube $(\mathcal{F}^{n+1}_S, l)$ and an explicit homotopy equivalence

$$\chi : \text{tofib}(\mathcal{F}^{n+1}_S, r) \xrightarrow{\rho_{(n)}^0} \Omega^n \text{tofib}(\mathcal{F}^{n+1}_S, l).$$

We prove this using Proposition 3.16, which says that such a homotopy equivalence exists for any cube which has an $n$-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 $(\mathcal{F}^{n+1}_S, l)$ for our cube $(\mathcal{F}^{n+1}_S, r)$. All proofs about left homotopy inverses are deferred to Section A.
A left homotopy inverse (a retraction up to homotopy) for a map \( r : X \to Y \) is a map \( l : Y \to X \) such that \( l \circ r \simeq \text{Id}_X \). For our purposes it is crucial to specify a homotopy \( h \) from \( \text{Id} \) to \( l \circ r 
olimits \):

\[
\begin{array}{ccc}
X & \xrightarrow{l} & Y \\
\downarrow & & \downarrow \\
X & \xrightarrow{l} & Y \\
\end{array}
\]

Moreover, we have \( \pi_{-1} \text{hofib}(r) \cong \pi_{-1} \text{hofib}(l) \) and split short exact sequences

\[
0 \to \pi_* X \xrightarrow{r_*} \pi_* Y \to \pi_{-1} \text{hofib}(r) \to 0
\]

since \( l \) is a section in the long exact sequence of homotopy groups for \( r \). Actually, more is true.

**Lemma 3.12.** Given the data of (3.8) there are explicit inverse homotopy equivalences

\[
\chi : \text{hofib}(r) \cong \Omega \text{hofib}(l) : \chi^{-1}
\]

One can generalise this from 1-cubes (maps), to diagrams over \( \mathfrak{D}_m \) for \( m \geq 1 \) as follows.

**Definition 3.13.** Let \( R_* = C_{\ast m} \xrightarrow{r^m} C_{\ast m} \) be an \( m \)-cube with \( m \geq 1 \), seen as a 1-cube of \( (m-1) \)-cubes. A left homotopy inverse for \( R_* \) is the data of a diagram:

\[
\begin{array}{ccc}
C_{\ast m} & \xrightarrow{Id} & C_{\ast m} \\
\downarrow & & \downarrow \\
C_{\ast m} & \xrightarrow{r^m} & C_{\ast m} \\
\end{array}
\]

In more detail, it consists of

1. an \( m \)-cube \( L_* = C_{\ast m} \xrightarrow{l^m} C_{\ast m} \)
2. for each \( S \subseteq m-1 \) a homotopy \( h^m_S : \text{Id}_{C_S} \rightarrow l^m_S \circ r^m_S \), that are mutually compatible in the sense that \( h^m_t(l) : C_{\ast m} \to C_{\ast m} \) is an \( m \)-cube for each fixed \( 0 \leq t \leq 1 \).

**Lemma 3.14.** Given the data of (3.10), there are inverse homotopy equivalences

\[
\chi_m : \text{tofib}(R_*) \cong \Omega \text{tofib}(L_*) : (\chi_m)^{-1}
\]

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

1. For each \( S \subseteq m \) and \( k \in m \setminus S \) a map \( l^k_S : C_{S^k} \to C_S \) is given such that
   \[
   \begin{align}
   l^k_S \circ l^i_{S^i} &= l^k_S \circ l^i_{S^i}, & \forall i \notin S, \ i \neq k \\
   l^k_S \circ r^k_{S^k} &= r^k_S \circ l^k_S, \quad \forall i \notin S, \ k > Si := S \cup \{i\}.
   \end{align}
   \]
   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 \( r^k_S \) by \( l^k_S \) for \( k + 1 \leq i \leq m \). In particular, \( D^0 = (C_*, l) \).
2. For each \( 0 \leq k \leq m \) and \( t \in [0,1] \) a map of diagrams \( h^k_t(t) : D^k_{S^k} \to D^k_{S^k} \)
   is given, such that \( h^k_t(0) = \text{Id} \) and \( h^k_t(1) = l^k_t \circ r^k_t \).

\( ^{15} \) 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.
d\chi = \Omega \to \Omega^m \text{tofib}(D^m). 

Moreover, the homotopy inverse is given by \( \chi^{-1} : \Omega^m \text{tofib}(D^0) \xrightarrow{\Omega^m \text{forg}} C_m \hookrightarrow \text{tofib}(D^m) \), where \( \text{forg} : \text{tofib}(D^0) \to C_m \), \( \{f \in H(S^1) : f \to C_m \} \to f^m \).

The entrywise homotopy groups of such \( D^0 = (C, \ell) \) form a contravariant \( m \)-cube \( \pi_r D^0 = (\pi_r C, \pi_r \ell) \) in graded groups (with \( * > 0 \)), which has a right \( m \)-fold inverse. Thus, there is an injection

\[
\pi_r(\text{tofib}(D^0)) \cong \bigcap_{k \in m} \ker (\pi_r I^{k}_{\mathbb{Z}^{m}}) \xrightarrow{\text{forg}} \pi_r C_m,
\]

analogously to (3.9). For proofs of all these results see Section A.

Let us now turn to applying them in our situation: Theorem 3.11 will follow from Proposition 3.16 once we construct an \( n \)-fold left homotopy inverse \((\mathcal{P}^n, I^n)\) for \((\mathcal{F}^n, I^n)\). Recall that by Corollary 3.10 the latter is obtained by applying \( \mathcal{E} \text{Camb}(f_0, -) \) to the \( n \)-cube \((M_{0S}, \rho_S^k)\).

**Theorem 3.17.** The \( n \)-cube \((M_{0S}, \rho_S^k)\) has an \( n \)-fold left homotopy inverse \((M_{0S}, \lambda_S^k)\).

From this we get the desired \((\mathcal{P}^n, I^n)\) by applying \( \mathcal{E} \text{Camb}(f_0, -) \) to \((M_{0S}, \lambda_S^k)\), i.e. letting \( I^n = \lambda_S^k \) and \( \rho_S^k \circ \) gives a cube satisfying conditions of Definition 3.15, and proving Theorem 3.11.

Now to prove Theorem 3.17 we first define a left homotopy inverse \( \lambda_S^k \) for each \( \rho_S^k \) in the sense of (3.8), and then revisit the construction to ensure that all mentioned conditions are satisfied.

**Lemma 3.18.** For \( k \in S \subseteq \mathbb{N} \) the map \( \rho_S^k \) has a left homotopy inverse \( \lambda_S^k : M_{0S} \to M_{0S} \).

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

\[
e_{k_{p+1}} : M_{0S} \hookrightarrow M_{0S} \cup \mathbb{B}_{k_{p+1}}
\]

which adds back the ball \( \mathbb{B}_{k_{p+1}} \). We visualise this by erasing \( \mathbb{B}_{k_{p+1}} \) as in Figure 9.

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

\[
\text{drag}_{k_{p+1}}(t) : M \to M, \quad \text{drag}_{k_{i_{p+1}}}^k(0) = \text{Id}_M, \quad \text{drag}_{k_{p+1}}^k(1)(M_{0S} \cup \mathbb{B}_{k_{p+1}}) = M_{0S},
\]

which, loosely speaking, elongates \( \mathbb{B}_{k_{p+1}} \) by gradually dragging the right hemisphere of \( S_{k-1} \) to the right, until it equals the right hemisphere of \( S_{i_{p+1}} \). We will define a specific parametrisation in the proof of Theorem 3.17 below (it will indeed depend on \( S > k \) and not only on \( i_{p+1} \)).

Now let \( d_{i_{p+1}}^k(t) = \text{drag}_{k_{i_{p+1}}}^k(t)|_{M_{0S} \cup \mathbb{B}_{k_{i_{p+1}}}} \) and \( \lambda_{i_{p+1}}^k := d_{i_{p+1}}^k(1) \circ e_{k_{p+1}} : M_{0S} \to M_{0S} \).
It remains to provide a homotopy $h^k_S$ between $\text{Id}_{M_{0S}}$ and the composite

$$
\lambda^k_S \circ \rho^k_S : M_{0S} \xrightarrow{\rho^k_S} M_{0Sk} \xrightarrow{\epsilon_{kp+1}} M_{0Sk} \cup \BB_{kp+1} \xrightarrow{d^k_{kp+1}(t)} M_{0S}
$$

The composition of the first two maps adds to $M_{0S}$ the material $\BB_{kp+1} \setminus \BB_{kp}$, which is diffeomorphic to a ball (note that $\BB_{k-1,k+1} \setminus (\BB_{k-1} \cup \BB_k) = \BB_{kp+1} \setminus (\BB_{kp} \cup \BB_{kp+1})$). Now adding this material gradually gives an isotopy $\text{add}_t : M_{0S} \hookrightarrow M$ such that $\text{im}(\text{add}_0) = M_{0S}$ and $\text{im}(\text{add}_1) = M_{0Sk} \cup \BB_{kp+1}$.

We can parametrise this so that $\text{im}(\text{add}_t) = \text{im}(d^k_{kp+1}(t))$ for each $t \in [0,1]$, so the two isotopies can be composed into the desired homotopy

$$
h^k_S(t) : M_{0S} \xrightarrow{\text{add}_t} \text{im}(\text{add}_t) \xrightarrow{d^k_{kp+1}(t)} M_{0S}.
$$

**Proof of Theorem 3.17.** We now ensure that the maps $\lambda^k_S$ and $h^k_S$ constructed in the previous proof satisfy conditions of Definition 3.15. We are still free to specify a particular parametrisation of the ambient isotopy $\text{drag}^k_{S \to k}(t) : M \to M$, which we roughly described as a ‘dragging move’, acting non-trivially only in a tubular neighbourhood of $W_{kp+1}$.

Firstly, for $S \subseteq \underline{n} \setminus \{i,k\}$ the conditions (3.12) and (3.11) are respectively equivalent to having that the following left diagram commute for $k > Si$ and the right diagram for, say, $i < k$:

$$
\begin{array}{ccc}
M_{0Si} \xrightarrow{\lambda^k_S} & M_{0Sk} \\
\Uparrow \rho^k_S & & \Uparrow \rho^k_S \\
M_{0S} & \xrightarrow{\lambda^k_S} & M_{0Sk}
\end{array}
\quad
\begin{array}{ccc}
M_{0Si} \xleftarrow{\lambda^k_S} & M_{0Sk} \\
\Downarrow \rho^k_S & & \Downarrow \rho^k_S \\
M_{0S} & \xleftarrow{\lambda^k_S} & M_{0Sk}
\end{array}
$$

For the left diagram this is clear. Indeed, $\rho^k_S$ and $\rho^k_S$ both add the same material $\BB_{i-1,i+1} \setminus (\BB_{i-1} \cup \BB_i)$ independently of the location of the other punctures, and as $k > Si$, both $\lambda^k_S$ and $\lambda^k_S$ erase the ball $\BB_{kn}$ and then use the same flow $\text{drag}^k_{S \to k} = \text{drag}^k_{S \to k} = \text{drag}^k_{S \to k}$. On the other hand, the commutativity of the right diagram will follow if we ensure that

$$
\text{drag}^i_{S \to i}(1) \circ \text{drag}^k_{S \to k}(1) = \text{drag}^k_{S \to k}(1) \circ \text{drag}^i_{S \to i}(1).
$$

(3.16)
Lastly, the condition (3.13) is equivalent to having that for each \( t \in [0, 1] \) the following left square commute if \( i > k \) and the right square if \( i < k \):

\[
\begin{array}{c}
M_{0S} \xrightarrow{\rho^i_0} M_{0k} \\
\downarrow h^i_0(t) & \downarrow h^i_0(t)
\end{array}
\quad \begin{array}{c}
M_{0S} \xleftarrow{\lambda^i_0} M_{0k} \\
\downarrow h^i_0(t) & \downarrow h^i_0(t)
\end{array}
\]

Again, the case on the left is clear since \( \text{drag}_{S_{k+1}^e}(t) = \text{drag}_{S_{k+1}^e}(t) \), and for the right one we should ensure that

\[
\text{drag}_{S_{k+1}^e}(t) \circ \text{drag}_{S_{k+1}^e}(1) = \text{drag}_{S_{k+1}^e}(1) \circ \text{drag}_{S_{k+1}^e}(t) \quad \forall t \in [0, 1].
\]  

(3.17)

Note that (3.16) follows from (3.17) by putting \( t = 1 \) and using \( \{S> k\} = \{S> k\} \), since \( i < k \).

We now define parametrisations of \( \text{drag}_{S_{k+1}^e} \) inductively on \( |S| \geq 0 \) for \( i \in \mathbb{N} \) and \( S \subseteq \mathbb{N} \setminus \{i\} \). Pick each \( \text{drag}_i \) freely and assume for some \( s \geq 0 \) we chose \( \text{drag}_{S_{k+1}^e} \) for all \( |S| > i \) \( < s \). Let now \( |S| > i = s \) for some \( S = Sk \) with \( k = \min\{(S > i) \cup \{n\}\} \). Then let

\[
\text{drag}_{S_{k+1}^e}(t) := \text{drag}_{S_{k+1}^e}(1)^{-1} \circ \text{drag}_{S_{k+1}^e}(t) \circ \text{drag}_{S_{k+1}^e}(1).
\]  

(3.18)

This finishes the definition. Let us check that (3.17) holds for any fixed \( i < k \) and \( S \subseteq \mathbb{N} \setminus \{i, k\} \) by induction on \( |i < S < k| \geq 0 \). Firstly, if there is no \( i_p \in S \) with \( i < i_p < k \), then (3.18) becomes precisely (3.17). Otherwise, take the smallest such \( i_p \); write \( S = R_{i_p} \). Applying (3.18) for \( S' = (Rk)p \) and the induction hypothesis for \( \text{drag}_{S_{k+1}^e}(t) \) gives

\[
\text{drag}_{S_{k+1}^e}(t) = \text{drag}_{S_{k+1}^e}(R_{i_p}k)(1)^{-1} \circ \text{drag}_{S_{k+1}^e}(R_{i_p}k)(1) \circ \text{drag}_{S_{k+1}^e}(R_{i_p}k)(1) = \text{drag}_{S_{k+1}^e}(R_{i_p}k)(1) \circ \text{drag}_{S_{k+1}^e}(R_{i_p}k)(1).
\]

For the second equality we used \( \text{drag}_{S_{k+1}^e}(1) \circ \text{drag}_{S_{k+1}^e}(1) = \text{drag}_{S_{k+1}^e}(1) \circ \text{drag}_{S_{k+1}^e}(1) \) again by the induction hypothesis (3.17). Now observe that \( \{R_{i_p} > k\} = \{R > k\} \), so the last expression equals \( \text{drag}_{S_{k+1}^e}(1)^{-1} \circ \text{drag}_{S_{k+1}^e}(t) \circ \text{drag}_{S_{k+1}^e}(1) \), finishing the induction step.

\[
\square
\]

### 3.3.2 The final delooping

Our approach is motivated by the following observation about the diagram as in Section 3.0.1:

\[
\begin{array}{c}
\varepsilon \mathbb{m}_\beta(I \setminus J_1, M) \xrightarrow{r^0_\beta} \varepsilon \mathbb{m}_\beta(I \setminus J_{01}, M) \\
\downarrow \varepsilon \mathbb{m}_\beta(I \setminus J_1, M) \downarrow r^0_\beta
\end{array}
\]

\[
P_1(M) := \lim \varepsilon^1 \xrightarrow{p} \cdots \xrightarrow{p} P_0(M)
\]

We can use the weak equivalences of fibrations given there to find the homotopy type of the layer

\[
F_1(M) := \text{fib}(p) = \text{fib}(r^0_\beta) \cong \varepsilon \mathbb{m}_\beta(J_0, M \setminus U^0_{\beta}) =: \mathfrak{F}_\beta^1,
\]

namely:

\[
\begin{array}{c}
F_1(M) \xrightarrow{\varepsilon \mathbb{m}_\beta(I \setminus J_1, M)} \xrightarrow{r^0_\beta} \varepsilon \mathbb{m}_\beta(I \setminus J_{01}, M) \\
\downarrow \varepsilon \mathbb{m}_\beta(I \setminus J_1, M) \downarrow r^0_\beta \varepsilon \mathbb{m}_\beta(I \setminus J_{01}, M) = \Omega SM \xrightarrow{\varepsilon \mathbb{m}_\beta(I \setminus J_1, M)} \xrightarrow{r^0_\beta} \varepsilon \mathbb{m}_\beta(I \setminus J_{01}, M)
\end{array}
\]

\[
\varepsilon \mathbb{m}_\beta(I \setminus J_1, M) \xrightarrow{r^0_\beta} \varepsilon \mathbb{m}_\beta(I \setminus J_{01}, M) \xrightarrow{r^0_\beta} \varepsilon \mathbb{m}_\beta(I \setminus J_{01}, M)
\]

(3.19)

Note how the disjointness condition with \( U^0_{\beta} \) is lost in \( \text{fib}(r^0_\beta) \) in the case of immersions. The equivalence \( F_1(M) \cong \varepsilon \mathbb{m}_\beta(J_0, M) \equiv \Omega SM \) takes the unit derivative \( \partial f : I \to SM \) of \( f : J_0 \to M \).
and makes it into a closed loop based at \((R_0, \tilde{e})\), by concatenating it with the unit derivative of any arc \(\tilde{U}_{f_0}\), which agrees with \(U_{f_0}\) except near endpoints, at which its derivative is \(-\tilde{e}\) instead.

Namely, the endpoints of \(\mathcal{D} f\) are \((L_0, \tilde{e})\) and \((R_0, \tilde{e})\) (see Figure 10).

Figure 10. The manifold \(M_{i_1 i_2} := M \setminus (B_{i_1 i_2} \cup B_{i_2 n+1})\). An example of \(\tilde{U}_{f_0}\) is in orange.

We now analogously determine the homotopy type of each \(\mathcal{F}^n_{i_i} := \text{fib}(r^0_S) = \text{emb}_d(f_0, M_{05})\) for possibly empty \(S = \{i_1, \ldots, i_m\} \subseteq \mathbb{n}\). Namely, recall that \(M_{05} := M' \setminus (B_{0i_1} \cup B_{i_1 i_2} \cup \cdots \cup B_{i_m n+1})\) from Notation 4, and consider the space

\[
M_5 := M' \setminus (B_{i_1 i_2} \cup \cdots \cup B_{i_m n+1}) = M_{05} \cup B_{0i_1}.
\]

We analogously have the composite

\[
\mathcal{D}_5 : \mathcal{F}^n_{i_i} = \text{emb}_d(f_0, M_{05}) \longrightarrow \text{imm}_d(f_0, M_5) \longrightarrow \Omega(SM_5) \quad (3.21)
\]

of the inclusions which forget embeddedness and the disjointness between \(f_0\) and \(U_{0m+1}\), and a similar derivative map \(f \mapsto (\mathcal{D} \tilde{U}_{f_0}) \circ (\mathcal{D} f)_{1-1}\). To see that \(\mathcal{D}_5\) is a weak equivalence we can simply replace \(M\) by \(M_5\) in the diagram (3.19). This is actually a homotopy equivalence since the spaces are of the homotopy type of CW complexes; for an alternative proof see [Kos20], where \(\mathcal{D}_5\) is shown to arise also as a homotopy equivalence \(\chi\) for a certain left homotopy inverse of \(r^0_S\).

Now observe that we also have maps \(\lambda^k_S : M_{S^k} \to M_5\) for \(k \not\in S\) as in the proof of Lemma 3.18, since the presence of the index 0 was irrelevant there (note that \(\lambda^k : M' \setminus B_{kn+1} \to M'\) not only adds the ball \(B_{kn+1}\), but also deforms \(M'\) by dragging). Similarly as before, this forms an \(n\)-cube \((M_\lambda, \lambda)\) and we let \((\Omega SM_5, \Omega S\lambda)\) be the corresponding cube of loops on the unit tangent bundles. Furthermore, the maps \(\mathcal{D}_5\) are clearly compatible with the \(\lambda\)-maps, \(\mathcal{D}_5 \circ \lambda^k_S = \lambda^k_S \circ \mathcal{D}_5\).

Theorem 3.19. The map \(\mathcal{D}_5 : \mathcal{F}^n_{i_i} \longrightarrow \Omega(SM_5, \Omega S\lambda)\) is a homotopy equivalence of cubes. Moreover, this gives a homotopy equivalence

\[
\mathcal{D} : \text{tofib}(\mathcal{F}^n_{i_i}) \longrightarrow \text{tofib}(\Omega(M_\lambda, \Omega\lambda)).
\]

Proof. It remains to show that for any \(n \geq 1\) the map of cubes \(\mathcal{S}(M_\lambda) \to M_5\), forgetting the tangent data is a homotopy equivalence on total homotopy fibres. The rows in the commutative diagram

\[
\begin{array}{ccc}
\mathcal{S}^{d-1} & \longrightarrow & \mathcal{S}(M_{S^k}) \\
\downarrow & & \downarrow \\
\mathcal{S}^{d-1} & \longrightarrow & \mathcal{S}(M_5)
\end{array}
\]

are fibre bundles, so comparing the vertical homotopy fibres gives \(\text{hofib}(\mathcal{S}^{d-1}) \cong \text{hofib}(\lambda^k_S)^d\).

Remark 3.20. With tangent data now gone, define \(\mathcal{D}_5 : \mathcal{F}^n_{i_i} \to \Omega M_5\) using simply \(\tilde{U}_{f_0} = U_{f_0}\).

Remark 3.21. As mentioned in the introduction, the authors of [BCKS17] use Sinha’s cosimplicial model \(AM_n(I^3) = \text{holim} \text{Conf}_n'(I^3, \partial)\), where \(\text{Conf}_n'(I^3)\) is a compactified configuration space of \(n\) points in \(I^3\) together with tangent vectors [Sim09]. To compute \(F_n(I^3)\) they use the cosimplicial identity \(S^k \circ d^k = \text{Id}\), which precisely says that the codegeneracy \(S^k\) (forgetting the \(k\)-th point in the configuration) is a strict left inverse for \(d^k\) (doubling the \(k\)-th point).
Remark 3.22. Actually, the maps $D_S$ factor through spaces $\Omega M_{0S}$, giving the following diagram

\[
\begin{array}{cccc}
\mathcal{F}^{n+1} & \xrightarrow{D_S} & \Omega M_{0S} & \xrightarrow{\rho^0} & \Omega M_{Sk} \\
\mathcal{F}^{n+1}_S & \downarrow \Delta^S & \Omega^k & \downarrow \rho^k_S & \Omega^k_S \\
\mathcal{F}^{n+1}_S & \xrightarrow{D_S} & \Omega M_{0S} & \xrightarrow{\rho^0} & \Omega M_S \\
\end{array}
\]

in which if either all upward or all downward arrows are omitted, the resulting diagram commutes. By Theorem 3.19 the first and last dashed maps form cubes with homotopy equivalent total fibres. By Theorem 3.17 there are the cubes $(\mathcal{F}^{n+1}, r^k_S)$. The reason lies in the fact that the information about the disjointness of $J_0$ with $B_{0S}$ is lost when we pass from $M_{0S}$ to $M_S$. More precisely, there are no maps $M_S \rightarrow M_{Sk}$ when $k$ is smaller than all indices in $S$, but otherwise we do have $\rho^k_S$ (and the homotopies $h^k(\ell)$ do restrict to $M_S$ and also commute with $D_S$ by construction).

4 Homotopy Type of the Layers

We now express the homotopy type of $F_{n+1}(M)$ in terms of suspensions of the space of loops on the iterated product of $M$ with itself. Such computations go back to [GW99, Section 5] for the case when $M$ has the homotopy type of a suspension, and also [BCKS17] for $M = F^3$. However, as mentioned in the introduction, even then, those results do not suffice for our purposes as we need a geometric interpretation of the homotopy classes (see Section 4.2 below): for the discussion in Section 6 it will be crucial to determine the class in $\pi_0 F_{n+1}(M)$ of a geometrically described point $x \in F_{n+1}(M)$, for $d = 3$.

For $S = \{i_1, \ldots, i_m\} \subseteq \Xi$ let us denote the wedge of $(d-1)$-dimensional spheres $S_{l_1p+1} := \partial B_{l_1p+1}$ (cf. Notation 4 and Figure 8) by $S_S := S_{i_1i_2} \vee \cdots \vee S_{i_m}$. Further, let $M \vee S$ be the $n$-cube with spaces $M \vee S_S$ and maps

\[
\text{col}^k : M \vee S_{Sk} \rightarrow M \vee S_S
\]

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

Lemma 4.1. For $n \geq 1$ there is a homotopy equivalence $\text{retr}_r : (M, \lambda) \rightarrow (M \vee S_S, \col)$.

Proof. Recall that $M_S := M \setminus B_S$ for $B_S := B_{i_1i_2} \cup \cdots \cup B_{i_m}$. Take a thin enough neighbourhood $V := U_{\{i_1, i_2\}} \times D^{d-1} \subseteq M$ of $U$ containing all balls $B_{ij}$. Then $V \setminus B_S$ is diffeomorphic to $(I^d)_S$, and this clearly retracts onto $S_S$: first project vertically onto the ‘collection of beads’ on $U$ (see Figure 10) and then contract $U_S$ 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 $\text{retr}_r : M_S = M' \cup (V \setminus B_S) \rightarrow M' \vee S_S$ by applying the above retraction on $V \setminus B_S$ 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 $\lambda^k_S$ commutes with $\text{col}^k_S$. \[\Box\]

The assumption $\partial M \neq \emptyset$ is essential as the lemma does not hold for closed manifolds. For another proof see [GW99, Cor. 5.3]. Together with Theorems 3.11 and 3.19 we obtain the following.

Corollary 4.2. There are homotopy equivalences $F_1(M) = \Omega(SM)$ and for $n \geq 1$

\[
F_{n+1}(M) \xrightarrow{\lambda} \Omega^n \xrightarrow{T} \Omega^{n+1} \xrightarrow{\text{retr}} \Omega^{n+1} \xrightarrow{T} \Omega \xrightarrow{\text{col}}
\]


Assume $n \geq 1$ and let us determine the homotopy type of $\text{tolib}(M \vee S_\ast, \text{col})$ using some classical results which we now recall, referring the reader to Appendix B for more details.

Figure 11. Several values $\eta_{B1}(t)$ of the canonical map $\eta_{B1} : S^1 \to \Omega S^2$.

Let $t_X : X \hookrightarrow X \vee YA$ be the natural inclusion and $\eta_A : A \to \Omega \Sigma A$ the unit of the loop-suspension adjunction, taking $a \in A$ to the loop $\theta \mapsto \theta \land a := [(\theta, a)]$. See Figure 11. Consider the composite

$$x_A : A \xrightarrow{\eta_A} \Omega \Sigma A \xrightarrow{\Omega \Sigma \eta_A} \Omega(M \vee \Sigma A).$$

(4.1)

and the map $\Omega_{IM} : \Omega M \to \Omega(M \vee \Sigma A)$. We form their Samelson product (defined in Appendix B) $[x_A, \Omega_{IM}] : A \land \Omega M \to \Omega(M \vee \Sigma A)$, and the wedge sum

$$x_A \lor [x_A, \Omega_{IM}] : A \lor (A \land \Omega M) \to \Omega(M \vee \Sigma A).$$

This is a map to a loop space, so has a unique multiplicative extension $\mu_{M, \Sigma A} = x_A \lor [x_A, \Omega_{IM}]$ to $\Omega \Sigma(A \lor (A \land \Omega M))$. It maps the loop $\theta \mapsto t_\theta \land y_\theta$ to $\theta \mapsto (x_A \lor [x_A, \Omega_{IM}](y_\theta)t_\theta$, see (B.6).

**Lemma 4.3 ([Gra71; Spe71]).** For well-pointed spaces $M$ and $A$ there is a fibration sequence

$$\Omega \Sigma(A \lor (A \land \Omega M)) \xrightarrow{\mu_{M, \Sigma A}} \Omega(M \lor \Sigma A) \xrightarrow{\Omega \text{col}_{lA}} \Omega_{IM} \to \Omega M$$

(4.2)

Moreover, this fibration of $H$-spaces has a section $\Omega_{IM}$, so it is trivial.

Now, if we have $A = \Sigma A' \equiv A' \land S^1$ for some space $A'$, and if $(\Omega M)_+$ denotes the space $\Omega M$ with a disjoint basepoint added, then there is a homeomorphism

$$A \land (\Omega M)_+ \equiv A' \land S^1 \land (\Omega M)_+ \equiv A' \land (S^1 \lor \Sigma \Omega M) \equiv A \lor (A \land \Omega M)$$

(4.3)

using the associativity and distributivity of the smash product. For $a \in A$ and $\gamma_t \in \Omega M$ this map is the sum (under the comultiplication $A \to A \lor A$) of the maps $a \land \gamma_t \mapsto a$ and $a \land \gamma_t \land a \land \gamma_t$.

Therefore, for $A := \vee_{i \in S} S_{i}^{d-2}$ with $S \subseteq \mathbb{N}$, we have $\Omega(M \lor \Sigma S) \equiv (\Omega \Sigma Z_S) \times \Omega M$ where

$$Z_S := \left( \bigvee_{i \in S} S_{i}^{d-2} \right) \land (\Omega M)_+ \equiv \bigvee_{i \in S} (S_{i}^{d-2} \land (\Omega M)_+) \equiv \bigvee_{i \in S} \Sigma_{i}^{d-2}(\Omega M)_+.$$  

In particular, $Z_i = \Sigma_{i}^{d-2}(\Omega M)_+$. Now, since $\Omega \Sigma Z_S$ is a loop space on a wedge of suspensions, the Hilton–Milnor Theorem B.2 (a generalisation of Lemma 4.3) applies: there is a weak equivalence

$$hm_S : \prod_{w \in B(S)} \Omega \Sigma \omega(Z_i) \longrightarrow \Omega \Sigma Z_S$$

(4.4)

where $B(S)$ is a *Hall basis* (see Remark B.3) for the free Lie algebra $L(x^i : i \in S)$ and the space $\omega(Z_i)$ is the iterated smash product of spaces $Z_i = \Sigma_{i}^{d-2}(\Omega M)_+$. Using the associativity again, and the identity $X_\ast \land Y_\ast = (X \times Y)_\ast$, for a Lie word $w \in B(S)$ of length $l_w$ we have

$$\omega(\Sigma_{i}^{d-2}(\Omega M)_+) \equiv \Sigma_{l_w(d-2)}((\Omega M)_+)^{l_w} \equiv \Sigma_{l_w(d-2)}((\Omega M)^{l_w})_+ \equiv \Sigma_{l_w(d-2)}(\Omega M)^{l_w}.$$  

Moreover, the Hilton–Milnor map $hm_S$ in (4.4) is analogous to $\mu_{M, \Sigma A}$ (see (B.7)): it is the pointwise product of the multiplicative extensions $\bar{w}(z_i)$ of the Samelson products according to $w \in B(S)$ of the maps $z_i := \Omega t \circ \eta : Z_i \to \Omega \Sigma Z_i \to \Omega \Sigma Z_S$ similarly to the notation (4.1).
Theorem 4.4. For each \( n \geq 1 \) there is a weak equivalence
\[
\prod_{w \in \text{NB}(n)} \Omega^{1 + l_w(d-2)}(\Omega M^{x_{l_w}})_+ \xrightarrow{\mu \circ h_m} \text{tofib} (\Omega(M \vee S_n), \Omega \text{col}),
\]
(4.5)

where \( \text{NB}(n) \subseteq \text{B}(n) \) consists of those words in which every \( x^i \) for \( i \in \mathbb{n} \) appears at least once. Therefore,
\[
F_{n+1}(M) \cong \prod_{w \in \text{NB}(n)} \Omega^{n+1 + l_w(d-2)}(\Omega M^{x_{l_w}})_+.
\]

Proof. By the naturality of equivalences \( \Omega(M \vee S) \cong (\Omega \Sigma Z_S) \times \Omega M \) from (4.2) and \( hms \) from (4.4) there is an equivalence of contravariant \( n \)-cubes
\[
\left( \Omega M \times \prod_{w \in \text{B}(S)} \Omega^{1 + l_w(d-2)}(\Omega M^{x_{l_w}})_+, \text{proj}^k \right) \xrightarrow{\Omega_{M} \times \mu \circ h_m} \left( \Omega(M \vee S), \Omega \text{col}^k \right).
\]

We will show that the total homotopy fibre of the first cube is the desired product over \( \text{NB}(n) \).

The map \( \text{proj}^k \) for \( k \in S \) is a projection onto the factors corresponding to those words \( w \in \text{B}(S) \) which also belong to \( \text{B}(S \setminus k) \). These are precisely the words in which \( x^k \) does not appear.

For \( T \subseteq S \) let \( A_T \) be the product of factors \( w \in \text{B}(S) \) in which for each \( i \in T \) the letters \( x^i \) appears at least once. Now, one clearly has \( \text{tofib}(\text{proj}^k_{01}) \colon A_0 \times A_{01} \to A_0 \approx A_{01} \) and more generally:
\[
\text{tofib}(\text{proj}^k_{\Sigma S}) \left( A_0 \times \prod_{T \subseteq S} A_T, \text{proj} \right) \cong A_{\Sigma S}.
\]

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

In Section 4.1 we compute the first non-trivial homotopy group of \( F_{n+1}(M) \) and describe its generators as maps to \( \text{tofib} \Omega(M \vee S_n) \). Then in Section 4.2 we discuss how to transform this into direct maps to \( F_{n+1}(M) \), along with a strategy for the main proofs in Section 6, and some examples.

4.1 The First Non-trivial Homotopy Group

We will now restate Theorem B as two propositions. Recall from Section 2.1 that the group \( \text{Lie}_{\pi_n(M)}(n) \cong \mathbb{Z}[(\pi_1 M)^n]^{n-1} \) is generated by decorated trees \( \Gamma \in \text{Tree}_{\pi_1 M} \) consisting of a tree \( \Gamma \in \text{Tree}(n) \) together with decorations \( g_i \in \pi_1 M \) for \( i \in \mathbb{n} \).

Proposition 4.5. For each \( n \geq 1 \) the space \( \text{tofib} \Omega(M \vee S_n) \) is \((n(d-2) - 1)\)-connected and the first non-trivial homotopy group admits an isomorphism
\[
\text{Lie}_{\pi_{n}(M)}(n) \cong \pi_{n(d-2)} \text{tofib} \Omega(M \vee S_n),
\]

Proof. Since \( \Sigma^k X \) is \((k-1)\)-connected for any \( X \), the group \( \pi_k(\Sigma^{1 + l_w(d-2)}X) \) is trivial for \( k < n(d-2) \), since \( l_w \geq n \). Hence, by Theorem 4.4 we immediately have that \( \text{tofib} \Omega(M \vee S_n) \) is \((n(d-2) - 1)\)-connected and the first non-trivial homotopy group is \( \pi_{n(d-2)} \text{tofib} \Omega(M \vee S_n) \). Note that this has precisely \((n-1)! \) summands. For \( k := 1 + n(d-2) \geq 2 \) we have
\[
\pi_k(\Sigma^k(\Omega M^{x_{l_w}})_+) \cong H_k(\Sigma^k(\Omega M^{x_{l_w}})_+) \cong \widetilde{H}_0((\Omega M^{x_{l_w}})_+) = H_0(\Omega M^{x_{l_w}}) = \mathbb{Z}[(\pi_1 M)^n],
\]
by the Hurewicz theorem and a basic homology computation, finishing the proof.\( \square \)
Therefore, the desired generating maps are of the shape $\mathcal{G}$ where we use the adjoint map forgetting homotopies induces an injection $\text{forg.}_*: \pi_{n(d-2)} \Omega(M \vee S^n) \hookrightarrow \pi_{n(d-2)} \Omega(M \vee S^n)$. Recalling from (3.15) that the map forgetting homotopies are the homotopy classes of the canonical extensions (by null-homotoping its image in all other vertices) to the total fibre of the generating maps of the group on the right.

Let us determine those. Unraveling the definitions, the composite

$$
\prod_{w \in B(S)} \Omega \Sigma w(Z_i) \xrightarrow{\eta Z_i} \Omega \Sigma Z_i \cong \Omega \Sigma (S_i^{d-2} \vee (S_i^{d-2} \wedge \Omega M)) \xrightarrow{\mu M, \beta_i} \Omega (M \vee S^n)
$$

is the pointwise product of the multiplicative extensions of the Samelson products according to $w \in B(S)$ of the maps $\mu M, \beta_i \circ Z_i$ which can be equivalently written as the composites

$$
\prod_{w \in B(S)} \eta Z_i \quad \xrightarrow{\eta Z_i} \quad \Omega \Sigma Z_i \cong \Omega \Sigma (S_i^{d-2} \vee (S_i^{d-2} \wedge \Omega M)) \quad \xrightarrow{\mu M, \beta_i} \quad \Omega (M \vee S^n)
$$

Under the identification $Z_i \cong S_i^{d-2} \vee (S_i^{d-2} \wedge (\Omega M))$ from (4.3) this is equal to $x_i \vee [x_i, \Omega_M]$, where we use the canonical map (cf. (4.1))

$$x_i: S_i^{d-2} \rightarrow \Omega (M \vee S^n)
$$

and the Samelson product $[x_i, \Omega_M]$. The value of $x_i$ at $\tilde{t} \in S^{d-2}$ is the loop $\eta_{S^n}(\tilde{t}) \subset S_i \subset M \vee S^n$ (as in Figure 11 for $d = 3$), while $[x_i, \Omega_M]$ sends $\tilde{t} \wedge \gamma \in S_i^{d-2} \wedge \Omega M$ to the commutator of the loops $x_i(\tilde{t})$ and $t_M \gamma: S^1 \rightarrow M \hookrightarrow M \vee S^n$ which we simply denote by $\gamma$.

Therefore, the desired generating maps are of the shape

$$
\Sigma^{n(d-2)} \xrightarrow{\tilde{q}_\gamma} \Omega \Sigma w(Z_i) = \Omega \Sigma w(S_i^{d-2} \vee (S_i^{d-2} \wedge \Omega M)) \xrightarrow{\tilde{\omega}(x_i \vee [x_i, \Omega_M])} \Omega (M \vee S^n)
$$

where we use the adjoint $\tilde{q}_\gamma$ of $\Sigma^{1+n(d-2)}(\Pi \gamma_i)$ which is for $\theta \in S^1$ and $\tilde{t} \in S_i^{d-2}$ given by $\Sigma^{1+n(d-2)}(\Pi \gamma_i): S_1^{1+n(d-2)}(\Omega M^{\infty}) \cong S_1^{1+n(d-2)}((\Omega M)_1)^{\infty} \cong \Sigma w(Z_i)$

$$
\theta \wedge \bigwedge_{1 \leq i \leq n} \tilde{t}_i \mapsto \theta \wedge \bigwedge_{1 \leq i \leq n} \tilde{t}_i \wedge (\gamma_1 \times \cdots \times \gamma_n) \equiv \theta \wedge \bigwedge_{1 \leq i \leq n} \tilde{t}_i \wedge \bigwedge_{1 \leq i \leq n} \gamma_i \equiv \theta \wedge \bigwedge_{1 \leq i \leq n} \gamma_i
$$

Thus, we have $\tilde{q}_\gamma(\lambda \tilde{t}_i) := \theta \mapsto \theta \wedge \bigwedge_{1 \leq i \leq n} \tilde{t}_i \wedge \gamma_i$, where the wedge is according to the permutation given by the word $\omega$. Now, by the definition $\tilde{\omega}(\theta \mapsto t_{\theta} \wedge y_{\theta}) := \omega(y_{\theta})_{\theta}$ of a multiplicative extension in (B.6), the composite (4.7) is given by

$$
\tilde{\omega}(x_i \vee [x_i, \Omega_M])(\tilde{q}_\gamma(\lambda \tilde{t}_i)) = \theta \mapsto \omega(x_i \vee [x_i, \Omega_M])(\bigwedge_{1 \leq i \leq n} \tilde{t}_i \wedge \gamma_i)_{\theta}
$$

$$
\quad = \theta \mapsto \omega(x_i(\tilde{t}_i) + [x_i(\tilde{t}_i), \gamma_i])_{\theta}
$$

Let us now simplify these generating maps.

For a decorated tree $\Gamma \in \text{Tree}_{n}(M)$ we define in (B.8) the corresponding Samelson product

$$
\Gamma(x_\gamma): \Sigma^{n(d-2)} \rightarrow \Omega (M \vee S^n)
$$

where $x_\gamma: S_i^{d-2} \rightarrow \Omega (M \vee S^n)$ is defined as the pointwise conjugate $\tilde{t} \mapsto x_\gamma(\tilde{t}) := \gamma \cdot x_i(\tilde{t}) \cdot \gamma^{-1}$. 


Proposition 4.6. The map $W: \text{Lie}_{\pi, M}(n) \rightarrow \pi_{n(d-2)} \text{tolfib} \Omega(M \vee S_n)$ which takes $\Gamma^8$ to the canonical extension to the total fibre of the Samelson product $\Gamma(x_1^8)$ is an isomorphism.

Proof. We define $W$ on decorated trees as the canonical extensions of (4.8) and then linearly extend to $\mathbb{Z}[\text{Tree}_{\pi, M}(n)]$. 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 – so $W$ is well-defined. We now show it is surjective.

It is enough to check that any $\omega(x_i + [x_i, y_i])$ is in the image of $W$. Using the linearity of Samelson products (see Appendix B), this is equal to the sum $\sum_{\sigma \subseteq \sigma'} \omega^{\sigma}$ of Samelson products $\omega^{\sigma}$ according to the word $\omega$ of the maps $[x_i, y_i]$ for $i \in \sigma$, and $x_i$ for $i \notin \sigma$. Using the homotopy equivalence $[x_i, y_i] \simeq x_i - x_i^{\gamma_i}: \mathbb{S}^{n(d-2)} \rightarrow \Omega(M \vee S_{\mathbb{S}})$ from (B.3) and the linearity of the Samelson bracket once more, each $\omega^{\sigma}$ expands as

$$\omega^{\sigma} \simeq \sum_{\sigma' \subseteq \sigma}(\pm 1)^{|\sigma'|} \omega(x_i^{\gamma_i})$$

where $\gamma_i' = \gamma_i$ for $i \in \sigma'$, and $\gamma_i = 1$ for $i \notin \sigma'$. Now by Lemma B.4 the map $\omega(x_i^{\gamma_i})$ is homotopic to $\Gamma(x_i^{\gamma_i})$ for $\Gamma = \omega_{\gamma}^{-1}(\omega)$ (see Lemma 2.3), so all generators are in the image of $W$.

The inverse $W^{-1}$ is obtained similarly, by defining $[\omega(x_i^{\gamma_i})] \mapsto \Gamma^8$, extending linearly and projecting to $\text{Lie}_{\pi, M}(n)$. We then immediately have $W \circ W^{-1} = \text{Id}$ and $W^{-1} \circ W = \text{Id}$. \hfill $\Box$

4.2 The generating maps

At this point it is not yet clear what the generating maps $\mathbb{S}^{n(d-3)} \rightarrow F_{n+1}(M)$ are. It remains to find an explicit inverse of the isomorphism $(\text{retr} \circ D \circ \chi)_*: \pi_{n(d-2)} F_{n+1}(M) \rightarrow \pi_{n(d-2)} \text{tolfib} \Omega(M \vee S_{\mathbb{S}})$, for the equivalences $\text{retr}$, $D$ and $\chi$ from Corollary 4.2.

The retraction. At least for $\text{retr}$: tolfib $\Omega M \rightarrow \text{tolfib} \Omega(M \vee S_{\mathbb{S}})$ this is not hard to do.

Firstly, we can pick an explicit lift $m_1: \mathbb{S}^{d-2} \rightarrow \Omega M$ of the map $x_i: \mathbb{S}^{d-2} \rightarrow \Omega(M \vee S_{\mathbb{S}})$: namely, the $(d-2)$-parameter ‘swing of a lasso’ around the $d$-ball $S_1 \subseteq M$, as in Figure 12 for $d = 3$. Indeed, using the definition of $\text{retr}$ in Lemma 4.1 this family of loops covers the $(d-1)$-sphere $S_1$ exactly once, so $\text{retr} \circ m_1 \simeq x_i$ (cf. Figure 11).

![Figure 12](image-url)
Further, \( m_i^{-1} : S^{d-2} \to \Omega M_0 \) can be obtained by reversing orientations of all loops in the family or, equivalently, by performing a twist as in Figure 13. Moreover, any \( \gamma_i \in \pi_1 M \) can be realised by a loop \( \gamma_i \) in \( M \) that misses all \( B_1, \ldots, B_n \), so defines \( \gamma_i : S^0 \to \Omega M_0 \). Thus, we can define \( m_i^{\gamma_i} : S^{d-2} \to \Omega M_0 \), the pointwise conjugate of \( m_i^{-1} \) by \( \gamma_i \), see the same figure.

**Figure 13.** The family \( m_i^{\gamma_i} : S^1 \to \Omega M_1 \).

Finally, as the target is a loop space, we have their Samelson products (see Figure 14 for \( n = 2 \)):

\[
\Gamma(m_i^{\gamma_i\gamma_j}) : S^{n(d-2)} \to \Omega M_n
\]

(4.9)

Now, since \( \text{forg} : \pi_{n(d-2)} \to \Omega M_n \) is injective in this setting as well, the generators of the source group are represented by the extensions of the maps (4.9) to the total fibre using the canonical null-homotopies of \( \gamma_i \) by ‘pulling up’ through the ball \( B_i \).

**Figure 14.** The value of \( \bigwedge_1^2 (m_1^{\gamma_1}, m_2^{\gamma_2}) = [m_1^{\gamma_1}, m_2^{\gamma_2}] : S^2 \to \Omega M_{12} \) at \( (t_1, t_2) \in S^1 \land S^1 = S^2 \) is the commutator of the depicted loops \( m_1^{\gamma_1}(t_1) \) and \( m_2^{\gamma_2}(t_2) \).

**The derivative.** Consider now \( D_n : \mathcal{F}_n^{n+1} \to \Omega M_n \) which closes up \( f_0 \leftrightarrow M_n \) into a loop based at \( L_0 \) (the tangent vectors are forgotten, see Remark 3.20). There is an obvious lift \( \varphi_i : S^{d-2} \to \mathcal{F}_n^{n+1} \) of \( m_i \) by ensuring that each \( m_i(t) \in \Omega M_n \) is embedded and changing it to an arc from \( L_0 \) to \( R_0 \). We can also ensure that different \( \varphi_i \) for \( i \in \mathbb{N} \) are mutually disjoint.

Furthermore, \( \gamma_i \) can be chosen to be embedded in \( M_n \), so we may define \( \varphi_i^{\gamma_i} : S^{d-2} \to \mathcal{F}_n^{n+1} \) as an *embedded conjugate*, by slightly pushing copies of \( \gamma_i \) off of each other. See Figure 15 for \( d = 3 \).
Similarly, we would need to define Samelson products $\Gamma(\psi^i_G)$ using some embedded analogue of commutators. However, this is not immediate: $\mathcal{F}^{n+1}$ is not an $H$-space in an obvious way, as concatenation of arcs $f_0 \leftrightarrow M_n$ might result in a non-embedded arc. If this has been done, the generators of $\pi_{\delta(n-2)}\text{tofib}(\mathcal{F}_n^{n+1}, l)$ would be canonical extensions of $\Gamma(\psi^i_G)$, again by (3.15).

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

We do not, however, pursue defining such embedded commutators directly, as we will not need them. Namely, for $d = 3$ we will in Section 5 directly construct points $\psi(G) \in H_\delta(M)$ using gropes – which can indeed be seen as embedded commutators, see Remark 5.3 – and then prove that $\chi_{\delta+1}(\psi(G)): \mathbb{S}^{n(d-2)} \to \text{tofib}(\mathcal{F}_n^{n+1}, l)$ are precisely the generators, using the following strategy.

**The strategy.** Suppose that we want to check whether the homotopy class of a given map $f: \mathbb{S}^{n(d-3)} \to F_{\delta+1}(M)$ corresponds to some class $\varepsilon \Gamma e^i \in \text{Lie}_{\delta+1}(M)$ under the isomorphism $W^{-1}(\text{retr}D\chi): \pi_{\delta(n-3)}F_n(M) \to \text{Lie}_{\delta+1}(M)$ from Theorem B, with $\varepsilon \in \{\pm 1\}$. By the preceding discussion, this is equivalent to considering $D\chi(f): \mathbb{S}^{n(d-3)} \to \Omega^n\text{tofib}\Omega M$, and checking that the homotopy class of its adjoint $\mathbb{S}^{n(d-2)} \to \text{tofib}\Omega(M)$ is the class of the canonical extension of $\varepsilon \Gamma(m_i^G)$. Actually, we saw that is instead enough to simply check this for the initial vertex (recall that $\text{forg}D\chi(f) = (D\chi f)^2 = D_\mathbb{S}((\chi f)^2)$)

$$D_\mathbb{S}(\chi f)^2 \simeq \varepsilon \Gamma(m_i^G): \mathbb{S}^{n(d-2)} \to \Omega M_\mathbb{S}$$

We now claim $\varepsilon \Gamma(m_i^G) \simeq \Gamma(m_i^G)$, for any tuple $\varepsilon_i \in \{\pm 1\}$ such that $\prod_{i=1}^n \varepsilon_i = \varepsilon$. Namely, define $m_i^{G\gamma_i}(\bar{t}) := \gamma_i \cdot m_i(\bar{t})^{\varepsilon_i} \cdot \gamma_i^{-1}$, where $m_i(\bar{t})^{-1}$ is the inverse of the loop $m_i(\bar{t}) \in \Omega M_\mathbb{S}$. Then $m_i^{G\gamma_i} \simeq \varepsilon_i m_i^G$ are homotopic maps by the Eckmann–Hilton argument, and $\Gamma(m_i^G)$ is the bilinearity of Samelson products.

To prove Theorem D in Section 6 we will show that for $d = 3$ and $f_G = e_{\delta+1}(\psi(G)) \in F_{\delta+1}(M)$, the point coming from a thick grope $G: \mathcal{B}_G \to M$ on $U$, we have

$$D_\mathbb{S}(\varepsilon f_G)^2 \simeq \Gamma(m_i^G): \mathbb{S}^{n(d-2)} \to \Omega M_\mathbb{S}$$

where $(\varepsilon_i, \gamma_i)_\mathbb{S}$ is the signed decoration of $G$.
The proof will be based on the fact that both $\psi(G)$ and Samelson products are constructed inductively. For the former see Section 5 and for the latter see Lemma B.5.

Furthermore, for the proof of Theorem E we will use that $\sum_{i=1}^{N} e_iG^{N}_{i,2}$ is represented by the following pointwise product—again by the Eckmann–Hilton argument:

$$\prod_{1 \leq i \leq N} \Gamma_i(m_i^{\eta_i};) : S^{m_i^{\eta_i}} \to \Omega \Omega M_{2i} \quad \bar{t} \mapsto \Gamma_i(m_i^{\eta_i}(\bar{t})) \cdots \Gamma_N(m_N^{\eta_N}(\bar{t})).$$

We note that the same strategy should work for appropriate notion of gropes for any $d \geq 4$, as mentioned in Remark 1.10. Let us now illustrate our discussion so far on several examples.

**Example 4.7** $(n = 2)$. The punctured cube $\mathcal{E}_{d}^2$ computing $F_2(M)$ was displayed in Example 3.1. On one hand, $F_2(M) \simeq \text{hofib}(\mathcal{F}_{2}^1)$ is the total homotopy fibre of the top square:

$$\begin{array}{ccc}
\mathcal{F}_{1} & \xrightarrow{r_1^0} & \mathcal{E}_{\text{mb}}(I \setminus J_{12}, M) \\
\mathcal{F}_{2} & \xrightarrow{r_2^0} & \mathcal{E}_{\text{mb}}(I \setminus J_{01}, M)
\end{array}$$

On the other hand, if we complete $\mathcal{E}_{d}^2$ with the initial vertex $R(M) := \mathcal{E}_{\text{mb}}(I, M)$, then the space $H_1 \simeq \text{hofib}(\mathcal{F}_{2})$ is the total fibre of the bottom square:

$$\begin{array}{ccc}
\mathcal{F}_{1} & \xrightarrow{r_1^0} & \mathcal{E}_{\text{mb}}(I \setminus J_{1}, M) \\
\mathcal{F}_{2} & \xrightarrow{r_2^0} & \mathcal{E}_{\text{mb}}(I \setminus J_{0}, M)
\end{array}$$

and $e_2 : H_1(M) \to F_2(M)$ is the obvious upward map (see Section 3.2).

Now by Theorem 3.11, we have

$$F_2(M) \simeq \text{hofib}(r_1^0 : \mathcal{F}_{2} \to \mathcal{F}_{2}^1) \xrightarrow{\chi} \Omega \text{hofib}(l_2^1 : \mathcal{F}_{2} \to \mathcal{F}_{2}^1)$$

The map $l_2^1$ corresponds to $\lambda^1 : M_1 = M \setminus B_{12} \to M_0 \simeq M$ which adds back the ball $B_{12}$ and rescales using the map $\text{drag}$, see the proof of Lemma 3.18. Next, by Theorem 3.19 the derivative and by Lemma 4.1 the retraction induce equivalences

$$\begin{array}{c}
\Omega \text{hofib}(\Omega M_1 \smallsetminus \Omega B_{12}) \xrightarrow{\text{retr}} \Omega \text{hofib}(\Omega (M \cup \{x \}) \to \Omega M_1)
\end{array}$$

Finally, $\text{hofib}((\Omega col)^{(1)}_{B_1}) \simeq \Omega (S_1 \cup (S_1 \cup \Omega M))$ by the Grey- Spencer Lemma 4.3, so we have

$$\begin{array}{c}
\pi_{d-3}F_2(M) \equiv \pi_{d-2} \text{hofib}(l_2^1) \equiv \pi_{d-2} \text{hofib}(\Omega \lambda_2^{(1)}) \equiv \pi_{d-2} \text{hofib}((\Omega col)^{(1)}_{B_1}) \\
\equiv \pi_{d-2} \Omega (S_1 \cup (S_1 \cup \Omega M)) \\
\equiv \pi_{d-2} \Omega (S_1 \cup (S_1 \cup \Omega M)) \\
\equiv \mathbb{Z} \{x_1 \} \oplus \bigoplus_{x \neq x_1 \in \pi_{d-1} M} \mathbb{Z} \{x_1, x_1 \} \xrightarrow{W^{-1}} \text{Lie}_{\pi_{d-1} M}(1) \cong \mathbb{Z} \{x_1 \}
\end{array}$$

using the isomorphism $W^{-1}x_1 = 1$, $W^{-1}[x, x_1, g_1] = W^{-1}x_1 - W^{-1}x_1 x_1 = 1 - 1 = 0$.

The generators for $\text{hofib}((\Omega col)^{(1)}_{B_1})$ are the canonical extensions of $x_1$ and $x_1^3$, while for $\text{hofib}(\Omega \lambda_2^{(1)})$ they are the extensions of $m_1$ and $m_1^3$. See Figure 12. The generators for $\text{hofib}(l_2^1)$ are the extensions of $\varphi_1$ and $\varphi_1^3$ (Figure 15). For example, the extension of $\varphi_1^3 : S^{d-2} \to \mathcal{F}_{2}^1$ to $\text{hofib}(l_2^1)$ uses the family of obvious null-homotopies of $l_2^1(\varphi_1^3)$ across the $d$-ball $B_1$. 
Example 4.8 \((n = 3)\). For the punctured 4-cube \(E^3_{3,3}\), we can draw its top subcube \(E^3_{3,3}\):

\[
\begin{align*}
\mathcal{F}_2 & \quad \longrightarrow \quad \varepsilon_{mb}(I \setminus J_{23}, M) \\
\mathcal{F}_1 & \quad \longrightarrow \quad \varepsilon_{mb}(I \setminus J_{21}, M) \\
\mathcal{F}_0 & \quad \longrightarrow \quad \varepsilon_{mb}(I \setminus J_{3}, M)
\end{align*}
\]

where the dashed arrows are fibres.

We apply Theorems 3.11 and 3.19 to get homotopy equivalences

\[
F_3(M) = \text{tofib} \left( \begin{array}{ccc}
\mathcal{F}_1 & \longrightarrow & \mathcal{F}_1 \\
\downarrow & & \downarrow \\
\mathcal{F}_2 & \rightarrow & \mathcal{F}_2
\end{array} \right) \overset{\Omega^2}{\longrightarrow} \text{tofib} \left( \begin{array}{ccc}
\mathcal{F}_1 & \leftarrow & \mathcal{F}_1 \\
\downarrow & & \downarrow \\
\mathcal{F}_2 & \rightarrow & \mathcal{F}_2
\end{array} \right) \overset{\Omega^2}{\longrightarrow} \text{tofib} \left( \begin{array}{ccc}
\Omega^{M_1} & \leftarrow & \Omega^{M_1} \\
\downarrow & & \downarrow \\
\Omega & \leftarrow & \Omega
\end{array} \right)
\]

Hence, the first non-trivial homotopy group is \(\text{Lie}_{p_1,M}(2)\) 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

\[
\text{forg(retr)}^{-1}W \left( \begin{array}{ccc}
2 & 1 \\
\downarrow & \downarrow \\
2 & 1
\end{array} \right) = \left( \begin{array}{ccc}
m_1^{\xi_1} & m_2^{\xi_2} \\
\downarrow & \downarrow \\
m_1^{\xi_1} & m_2^{\xi_2}
\end{array} \right) \in \pi_2 \Omega M_{12}. \quad (4.11)
\]

Example 4.9 (Sketch of the proof of Theorem D for \(n = 3\)). Assume \(t_2(G) = \left( \begin{array}{ccc}
2 & 1 \\
\downarrow & \downarrow \\
2 & 1
\end{array} \right) \) for a thick grope \(G\) in a 3-manifold \(M\), using the underlying forest map from Proposition 5.8. The construction in Section 5.3 produces the point

\[
e_{3,3}(G) = \left( \begin{array}{ccc}
\psi^G(-)^{[1]}_{J_0} & \psi^G(-)^{[12]}_{J_0} \\
G(a_0^{\xi}) & \psi^G(-)^{[2]}_{J_0}
\end{array} \right) \in F_3(M)
\]

and so we obtain a class \(\text{forg}(D\chi e_{3,3}(G)) \in \pi_2 \Omega M_{12}\). Then Theorem D asserts that this class agrees with (4.11). One can visualise this by comparing Figure 14 with Figure 21.

A close look at the definition of \(\chi\) implies that \((\chi e_{3,3}(G))^{[12]}\) is obtained from the square-family of loops \(\psi^G(-)^{[12]}_{J_0}\) by ‘reflections relative to the balls \(B_1\) and \(B_2\)’, see Proposition A.6.

In Lemma 6.2 we will show that \(D_{12} \psi^G(-)^{[12]}_{J_0} : F^3_{12} \rightarrow \Omega M_{12}\) is homotopic to the commutator of certain loops corresponding to degree 1 gropees out of which \(G\) is built (the two caps of \(G\)). On the other hand, the Samelson product \([m_1^{\xi_1}, m_2^{\xi_2}] : S^2 \rightarrow \Omega M_{12}\) is also defined inductively in terms of commutators. Hence, we will be able finish the proof by induction.
5 Gropes and punctured knots

Throughout this section $M$ is an oriented 3-manifold with non-empty boundary. In 5.1 we define grope cobordisms and their modifications, and in 5.2 we prove Theorem C.

5.1 Grope cobordisms, thick gropes and grope forests

5.1.1 Abstract gropes

For a finite non-empty set $S$ we defined the set of (rooted vertex-oriented uni-trivalent) trees $\text{Tree}(S)$ in Definition 2.1. Now we define certain 2-complexes modelled on such trees.

Definition 5.1. A punctured torus $T$ is a genus one compact oriented surface with one boundary component $\partial T$, see Figure 16. 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 component of $\partial b_j$ which contains a part of $a_0$ (so $\partial T \cong [\beta_1, \beta_2] = \beta_1 \beta_2^{-1} \beta_2^{-1}$).

An abstract (capped) grope $G_\Gamma$ modelled on $\Gamma \in \text{Tree}(S)$ is a 2-complex with boundary $\partial G_\Gamma = a_0 \cup a_0^\perp$ built inductively on $|\Gamma|$ as follows.

- For $S = \{i\}$ the only tree is $\Gamma = \{i\}$ and we let $G_\Gamma$ 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 $\Gamma \in \text{Tree}(S)$ is obtained by grafting two trees of lower degrees

$$\Gamma = \Gamma_2 \sqcup \Gamma_1,$$

$\Gamma_j \in \text{Tree}(S_j), \ S_1 \sqcup S_2 = S.$

Thus, abstract gropes $G_{\Gamma_1}$ and $G_{\Gamma_2}$ are defined by the induction hypothesis. Let $G_\Gamma$ be the result of attaching both of them to a single punctured torus $T$, called the bottom stage of $G_\Gamma$, 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 $\partial T$.

![Figure 16. The model of a punctured torus as the plumbing of two bands.](image)

Note that $G_\Gamma$ 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 $G_\Gamma$, that is, the union of products of all stages with an interval, is homeomorphic to $\mathbb{R}^3$ (see also Figures 22 and 24).

Abstract gropes are just combinatorial objects: there is a 1–1 correspondence between them and rooted trees. In fact, the tree $\Gamma$ on which $G_\Gamma$ was modelled can be seen as its subset $\Gamma \subseteq G_\Gamma$, called the underlying tree of $G_\Gamma$, using the following construction (equivalent [CST07, Def. 16 & Sec. 3.4]).

The root of $\Gamma$ is the initial point $*$ of $a_0 \subseteq \partial G_\Gamma$, and each trivalent vertex of $\Gamma$ is the intersection point $\beta_1 \cap \beta_2$ in the corresponding grope stage. The leaves of $\Gamma$ are the centres of caps. Finally,
the edges are obtained at each stage as in Figure 17, and are cyclically ordered using the order \((\beta_1, \beta_2)\), which agrees with the corresponding vertex orientation in \(\Gamma\).

### 5.1.2 Grope cobordisms

GROKE COBORDISMS ARE PARTICULAR EMBEDDINGS OF ABSTRACT GROPE INTO A 3-MANIFOLD \(M\).

**Definition 5.2.** Let \(K \in \mathcal{K}(M)\) and \(\Gamma \in \text{Tree}(S)\) for a finite nonempty set \(S \subseteq \mathbb{N}\). A \textit{(simple capped genus one) grope cobordism} \(^{16}\) on \(K\) modelled on \(\Gamma\) is an embedding \(\mathcal{G} : \Gamma \to M\) 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 \(K_0 := K(I \setminus j_0)\) transversely in exactly one point \(p_i \in K_0\), which is the centre of the cap and which belongs to \(K(j_i) \subseteq K_0\).

We see \(\mathcal{G}\) as a cobordism between \(K\) and the output knot \(\partial^+\mathcal{G} := K_0 \cup \mathcal{G}(a_0^+)\), smoothened at the corners and oriented compatibly with the orientation of \(K_0\). For examples see Figures 18, 19 and 21.

**Remark 5.3.** Note that the arc \(\mathcal{G}(a_0^+)\) is oriented oppositely in \(\partial^+\mathcal{G}\) than as a subset of \(\mathcal{G}\), as usual for oriented cobordisms. The crucial observation is that \(\mathcal{G}(a_0^+)\) is an ‘embedded commutator’ of the curves \(\mathcal{G}(\beta_1)\) and \(\mathcal{G}(\beta_2)\), as for the Borromean link, see Figure 19 and [Tei02; Tei04].

### 5.1.3 The underlying decorated tree

We now extend the underlying tree \(\Gamma \in \text{Tree}(S)\) of a grope cobordism \(\mathcal{G} : \Gamma \to M\) on a knot \(K\) to a \(\pi_1(M)\)-decorated tree (such trees were defined in Definition 2.4).

**Definition 5.4.** Let \(\gamma_i^+: I \to M\) be the path from \(K(L_0)\) to \(p_i\) obtained as the image under \(\mathcal{G}\) of the unique path in the tree \(\Gamma \subseteq \mathcal{G}(\Gamma)\) from the root to its \(i\)-th leaf. Let \([p_i, K(L_0)]\) be the image of \(K\) between \(p_i \in K(j_i) \cap \mathcal{G}(\Gamma)\) and \(K(L_0)\) (see Figures 18, 19, 21).

Then we have a loop in \(M\) given by

\[\gamma_i := \gamma_i^+ \cup [p_i, K(L_0)]\]

Let \(\varepsilon_i := \text{sgn}(p_i) \in \{\pm\}\) 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 \textit{signed decoration} of \(\mathcal{G}\).

Lastly, the underlying \textit{decorated tree} of \(\mathcal{G}\) is \(\varepsilon\Gamma^S \in \mathbb{Z}[\text{Tree}_{\pi_1(M)}(S)]\), where \(\varepsilon := \prod_{i=1}^S \varepsilon_i\) and \(g_S(\mathcal{G}) \in (\pi_1 M)^S\), the tuple of classes \(g_i = [\gamma_i] \in \pi_1 M\).

In other words, \(\gamma_i\) 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 \(\mathcal{G}(\Gamma) \subseteq \mathcal{G}(\Gamma) \subseteq M\).

\(^{16}\) 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 5.6 are related to higher genus grope cobordisms.
Two grope cobordisms of degree 1 on $K: I \hookrightarrow M$ (the horizontal line). In both cases $\partial^1 G$ is the union of black and red arcs; the left one is contained in $I^3 \subseteq M$ and is isotopic to the trefoil. The signed decorations are respectively $\varepsilon(G) = 1 = -1$ and $+1 \gamma_1 = [\gamma_1] \in \pi_1 M$.

A grope cobordism $G: G_\Gamma \to I^3$ on $K = U$ with the underlying tree $G(\Upsilon)$ depicted in light blue. The knot $\partial^2 G$ is the union of $U_\Gamma$ and the long black arc $G(a^0_0)$, which is the commutator of $G(b_0)$, the meridian of the arc $K(\gamma_i)$ for $i = 1, 2$. The signs are $\varepsilon_1 = +1, \varepsilon_2 = -1$.

The knot $\partial^1 G$ from Figure 19. 'Swinging' the bands of $\partial^1 G$ is an isotopy which introduces twists into the bands giving a projection of the right-handed trefoil, cf. Example 2.25.

A grope cobordism $G$ in a manifold $M$ whose underlying decorated tree is $G(\Upsilon)$, since $\varepsilon_1 = \varepsilon_2 = +1$. If $M = I^3$ and $K$ is the unknot, then $\partial^2 G$ is the figure eight knot.
5.1.4 Thick gropes

Let us observe that a regular neighbourhood of a grope cobordism $G$ is diffeomorphic to a 3-ball $B^3 \hookrightarrow M$, since inductively we are just thickening the punctured torus and attaching cancelling 2-dimensional 2-handles, see Figure 22. This 3-ball $G$ intersects the knot $K$ in the neighbourhood $G(a_i) \subseteq I_i$ of the intersection points $p_i \in K(I_i)$, for some arcs $a_i \subseteq B^3$ with $a_i \cap \partial B^3 = \partial a_i$, $1 \leq i \leq n$. It is convenient to fix a choice of such a neighbourhood $G$ as follows; we pick some $\varepsilon > 0$.

![Figure 22. The plumbing of the blue ball $B_{r_1}$ and the orange ball $B_{r_2}$.](image)

**Definition 5.5.** A thick grope on $K \in \mathcal{K}(M)$ modelled on a tree $\Gamma \in \text{Tree}(S)$ is an embedding

$$G : B_{\Gamma} \hookrightarrow M$$

which does not intersect $K$ except that $G(a_i) \subseteq K(I_j)$ for certain arcs $a_i \subseteq B_{\Gamma_i}$, $i \in \{0\} \cup S$. Here the model ball $B_{\Gamma} \cong B^3$, its set of arcs and a subset $G_{\Gamma} \subseteq B_{\Gamma}$ are defined inductively on $|S|$ as follows.

For the induction base, we have $c = \emptyset$ and we define $B_c := G_c \times I \cong D^2 \times I$ 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 $\partial G_c$.

For $\Gamma = \bigcup_{\Gamma_1, \Gamma_2}$ define $B_{\Gamma}$ as the plumbing of the already defined model balls $B_{\Gamma_1}$ and $B_{\Gamma_2}$ along the respective squares $a_0 \times [-\varepsilon, \varepsilon] \subseteq \partial B_{\Gamma_1}$ (by first swapping the two coordinates, as usual). Let $\{a_i\}_{i \in S}$ be the disjoint union of the sets of arcs for $B_{\Gamma_{1}}$ and $B_{\Gamma_{2}}$.

Define the abstract grope $G_{\Gamma} \subseteq B_{\Gamma}$ as the plumbing of the bands $\partial G_{\Gamma_i} \times [-\varepsilon, \varepsilon] \subseteq \partial B_{\Gamma_i}$ along the squares $a_0 \times [-\varepsilon, \varepsilon]$. Finally, let $a_0$ for $B_{\Gamma}$ be the distinguished arc in $\partial G_{\Gamma}$ as in Definition 5.1.

Note that $G := G|_{\bar{G}}$ is a grope cobordism on $K$ in the sense of Definition 5.2. We can thus also define an underlying decorated tree $\varepsilon(G)\Gamma_{\varepsilon(G)}$ of a thick grope as in Definition 5.4. Moreover, we define the output of $G$ as the knot $\partial^2 G := \partial^2 (G) = K_G \cup G(a_0^+)$, see Definition 5.1 and 5.2. Conversely, for a given grope cobordism $G$ and a choice of its regular neighbourhood, there is a unique thick grope $G$ whose image is precisely that neighbourhood and $G|_{\bar{G}} = G$.

5.1.5 Grope forests

Recall from Theorem 2.11 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.

**Definition 5.6.** A grope forest of degree $n$ and cardinality $N \geq 1$ on a knot $K$ is a map

$$F := \bigcup_{i=1}^{N} G_i : \bigcup_{i=1}^{N} B_{\Gamma_i} \hookrightarrow M$$

such that $G_i : B_{\Gamma_i} \hookrightarrow M$ are mutually disjoint thick gropes on $K$ modelled on $\Gamma_i \in \text{Tree}(n)$, and whose arcs $G_i(a_0) \subseteq K(I_0)$ appear in $K(I_0)$ in the decreasing order of their indices $N \geq i \geq 1$.

The output knot $\partial^2 F$ is obtained from $K$ by replacing each interval $G_i(a_0)$ by the arc $G(a_0^+)$ (the order in which replacements are done is irrelevant by the disjointness assumption).
Note that for a fixed \( i \in \mathbb{Z} \) we allow an arbitrary order of intersections of \( K(\varepsilon_i) \) with the \( i \)-th caps of different gropes, see Figure 23 for an example with \( \text{cap}_1(G_1) < \text{cap}_1(G_2) \), but \( \text{cap}_2(G_2) < \text{cap}_2(G_1) \).

![Figure 23. A grope forest \( F = G_1 \cup G_2 \) of degree 2 is a thickening of the depicted 2-complex.](image)

Grobe forests are suitable for defining ‘spaces of gropes’ in a straightforward manner.

**Definition 5.7.** Fix \( K \in \mathcal{K}(M) \). The space of thick gropes on \( K \) modelled on \( \Gamma \in \text{Tree}(n) \) is the subspace \( \mathfrak{emb}_K(\mathcal{B}_\Gamma, M) \subseteq \mathfrak{emb}(\mathbb{B}^3, M) \) of those embeddings satisfying conditions of Definition 5.5. Similarly, for \( N \geq 1 \) define \( \mathfrak{emb}_K(\bigcup_{\Gamma_i \in \text{Tree}(n)^N} \mathcal{B}_{\Gamma_i}, M) \subseteq \mathfrak{emb}(\bigcup_{\Gamma} \mathbb{B}^3, M) \) to be the space of grope forests of cardinality \( N \) on \( K \) modelled on \( (\Gamma_1, \ldots, \Gamma_N) \) and let

\[
\text{Grop}_N^N(M; K) := \bigcup_{(\Gamma_1, \ldots, \Gamma_N) \in \text{Tree}(n)^N} \mathfrak{emb}_K \left( \bigcup_{\Gamma_i = 1}^N \mathcal{B}_{\Gamma_i}, M \right).
\]

In particular, \( \text{Grop}_1^N(M; K) \) is the space of thick gropes on \( K \). Finally, define the space of all grope forests on \( K \) as the disjoint union

\[
\text{Grop}_n(M; K) := \bigsqcup_{N \geq 1} \text{Grop}_N^N(M; K).
\]

**Proposition 5.8.** There is a surjection of sets

\[
t : \pi_0 \text{Grop}_n(M; K) \longrightarrow \mathbb{Z}[\text{Tree}_{\pi_1}(M)],[n],
\]

which sends a grope forest \( \bigcup_{i=1}^N G_i : \bigcup_{i=1}^N \mathcal{B}_{\Gamma_i} \hookrightarrow M \) to the linear combination \( \sum_{i=1}^N \varepsilon(G_i) \cdot \Gamma_i^{g_i(G_i)} \).

**Proof.** To prove that this map is well-defined, first consider \( N = 1 \). For a fixed tree \( \Gamma \) the only allowed isotopies of thick gropes modelled on \( \Gamma \) – that is, paths in the space \( \mathfrak{emb}_K(\mathcal{B}_\Gamma, M) \) – are those isotopies of the 3-ball \( \mathcal{B}_\Gamma \) which preserve the property that each special arc \( a_i \subseteq \mathcal{B}_\Gamma \) is mapped into \( K(\varepsilon_i) \). Such an isotopy cannot change the homotopy classes \( g_i(G_i) \), so \( \Gamma_i^{g_i(G_i)} \) is an invariant. Similarly, the sign \( \varepsilon_i(G_i) \) as defined in Section 5.1.3 is positive if and only if the orientation \( G_i(a_i) \) agrees with the orientation of \( K \). This is preserved during an isotopy.

An analogous argument applies to grope forests \( N \geq 1 \), considering one thick grope at a time.

For the surjectivity, let \( \sum_{i=1}^N \varepsilon_i \Gamma_i^{g_i} \) be a linear combination of decorated trees, \( \varepsilon_i \in \{\pm 1\} \). Any \( g_i \in (\pi_1 M)^n \) can be represented by a tuple of disjointly embedded loops \( \gamma_i \subseteq M \). Thus, there is a map \( \Gamma_i \rightarrow M \) which embeds the edges mutually disjointly, maps the \( i \)-th leaf to a point \( p_i \in K(\varepsilon_i) \) and has the associated path (from \( K(L_0) \) to \( p_i \) along \( \Gamma \) and then back along \( K \) isotopic to \( \gamma_i \)). Thicken this to a ball to get a thick grope \( G_i \), introducing a twist to one cap if \( \varepsilon_i = -1 \).

This can be done so that \( G_i \) are mutually disjoint (as they are neighbourhoods of 1-complexes), and that the order \( G_i(a_0) \) is decreasing with \( i \), so this defines a desired grope forest. \( \square \)
5.2 Gropes give paths in the Taylor tower

Let $G$ be a thick grope in $M$ on a knot $K$ modelled on $\Gamma \in \text{Tree}(n)$. According to Theorem C there is a path in $P_n(M)$ between the evaluation of the output knot and of the original knot

$$\Psi^G : ev_G(\partial^G G) \rightsquigarrow ev_G(K).$$

In this section we prove this based on ideas from [KST], and also show there is a continuous map

$$\psi : \text{Grop}_n^0(M; U) \to H_n(M), \quad \psi(G) = (\partial^G G, \Psi^G).$$ (5.1)

We reformulate the theorem as the following proposition.

Recall that $f \in P_n(M) := \operatorname{holim}_k \mathcal{E}_k$ is given as a collection $f^S : \Delta^S \to \mathcal{E}_k^{|I| \setminus \bar{J}_S, M}$ for $S \subseteq [n]$, which is compatible under inclusions $i_S : \Delta^S \to \Delta^2$, see Section 2.4. Recall also that $K_{f_0}$ denotes the restriction of an arc $K$ to $f_0 \subseteq I$, while $K_{\delta}$ denotes the restriction to $I \setminus \bar{J}_S$.

**Proposition 5.9.** For $G$ as above there is a continuous map

$$\mathcal{P}^G : \Delta^2 \longrightarrow \text{Map}_\partial([0,1], \mathcal{E}_k^{|I| \setminus \bar{J}_S, M})$$

which gives a well-defined map $\Psi^G : [0,1] \to P_n(M)$ taking $\theta \in [0,1]$ to

$$\Psi^G(\theta)^S : \Delta^S \to \mathcal{E}_k^{|I| \setminus \bar{J}_S, M}, \quad \iota \mapsto \begin{cases} K_{f_0} & \text{if } 0 \in S, \\ K_{f_0} \cup \mathcal{P}^G_{i_0}(\theta) & \text{if } 0 \notin S. \end{cases}$$ (5.2)

Let us outline the proof. Let $\mathcal{E}_k^{|D^2, B_T|}$ denote the space of embeddings of disks in the model ball with the boundary condition $\partial D^2 = \partial G_T$. Firstly, in Proposition 5.12 we construct a family of disks $\phi_T : \Delta^2 \longrightarrow \mathcal{E}_k^{|D^2, B_T|}$ satisfying certain condition (5.4). Then we choose a homeomorphism $[0,1] \times f_0 \to D^2$. This gives an isotopy $j_\theta : f_0 \to D^2$, $\theta \in [0,1]$, relative to the endpoints from one half of the boundary circle to the other across $D^2$. Finally, for $u \in \Delta^2, \theta \in [0,1]$ we define

$$\mathcal{P}^G_u(\theta) \colon J_0 \longrightarrow D^2 \overset{\phi_T(\theta)}{\longrightarrow} B_T \overset{G}{\longrightarrow} M.$$ (5.3)

We will finish the proof by checking that $\Psi^G$ is well-defined thanks to conditions (5.4). The continuity of (5.1) follows as well, since the space $\text{Grop}_n^0(M; U)$ of thick gropes of degree $n$ on $U$ from Definition 5.7 was given the subspace topology $\text{Grop}_n^0(M; U) \subseteq \mathcal{E}_k^{|B^3, M|}$.

5.2.1 The symmetric surgery

Let us first construct a 1-parameter family of disks $D_u \subseteq B_T, u \in \Delta^1$, for $\Gamma$ an abstract grope modelled on the unique tree of degree $n = 2$ (Figure 24). This consists of a punctured torus (yellow) and two caps bounded by its core curves $\beta_1$ (blue) and $\beta_2$ (orange).

![Figure 24. The abstract grope modelled on \(\Delta\).](Image)

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 25. Note that the thick grope specifies concrete push-offs of caps.

In addition, one can do both surgeries at once, called the symmetric surgery (or contraction), as depicted in the middle part of Figure 25. The following lemma says that there actually exists a whole 1-parameter family of disks containing the three disks we have described.

**Lemma 5.10** (Symmetric Isotopy). For $\Gamma = \bigcup_{i=1}^2$ there is an isotopy $\phi_T : [0,1] \to \text{Emb}(D^2, B_T)$ such that $D_t$ for $t \in \{0,1\}$ is the surgery on $G_T$ using the cap labelled by $1+t$.

**Proof.** Recall that $B_T$ is the model ball obtained by plumbing together $B_1$ and $B_2$. We now specify an isotopy from $D_1 \subseteq B_T$ to $D_2 \subseteq B_T$, which passes through the symmetric surgery, using Figure 25 as an accurate model of these disks.

First isotope the interior of the blue band of $D_1$ by pushing it across the interior of the ball $B_T$, 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 26, 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 $j_0 : I_0 \to D^2$ which we fixed at the beginning of this section (also, smoothen the corners).

Symmetrically, for increasing $t \in [\frac{1}{2},1]$ the isotopy uses the ball $B_T$ 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 $t = 1$. □

**Remark 5.11.** 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 $P_0(M)$ 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. Instead, gropes precisely keep track of all necessary homotopies in a canonical way, missing in the clasper picture. Moreover, we will use our exact choice of the isotopy in the crucial Lemma 6.2.

5.2.2 Families of disks

We now generalise the Symmetric Isotopy Lemma 5.10 to trees of any degree \( n \geq 2 \). We view \( \Delta^S \) as the simplicial set obtained by barycentric subdivision from the standard simplex with the vertex set \( S \) (see Figure 5).

**Proposition 5.12.** Let a finite set \( S \neq \emptyset \) and a tree \( \Gamma \in \text{Tree}(S) \) there is a continuous map

\[
\phi_T: \Delta^S \rightarrow \text{emb}_3(D^2, B_T)
\]

describing a family \( D_u := \text{im} \phi_T(u) \subseteq B_T \) of neatly embedded disks in the model ball such that

\[
(V_i \in S) \quad \text{int}(D_u) \cap a_i \neq \emptyset \implies i \in |\zeta_u|
\]

(5.4)

where \( \zeta_u \subseteq \Delta^S \) denotes the top dimensional simplex to which \( u \) belongs and \( |\zeta_u| \) its set of vertices.

**Proof.** We prove this by induction on \( |S| \). For \( |S| = 1 \) we have \( \Gamma = \frac{1}{1} \) and \( |\Delta^S| = \Delta^0 = \{i\} \), so we need to construct only one disk \( D_i \subseteq B \) whose boundary is the boundary of the grope and such that \( \text{int}(D_i) \cap a_i \neq \emptyset \). Clearly, we can just let \( D_i := G_\Gamma \), 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 \( \Gamma \in \text{Tree}(S) \) such that

\[
\Gamma = \Gamma_0 \cup \cdots \cup \Gamma_j, \quad \Gamma_i \in \text{Tree}(S_j), \quad S = S_1 \cup S_2.
\]

Pick \( u \in \Delta^S \) and let us define \( D_u \subseteq B_T \), using the identification \( \Delta^S \cong \Delta^S_1 \star \Delta^S_2 \), the join of two simplices. Thus, \( u \) is given as a linear combination

\[
u = (1-t)u_1 + tu_2, \quad t \in [0,1], \quad u_j \in \Delta^S_j.
\]

The ball \( B_T \) is by definition the plumbing of the balls \( B_{\Gamma_j} \) for \( j = 1,2 \), and since \( 1 \leq |S_j| \leq |S| - 1 \), by induction hypothesis we have maps \( \phi_{\Gamma_j} \) satisfying (5.4). In particular, we have disks \( D_{u_j} \subseteq B_{\Gamma_j} \).

Let us pick some neat tubular neighbourhoods \( vD_{u_j} \subseteq B_{\Gamma_j} \), so that \( \partial(vD_{u_j}) \cap \partial B_T = \partial G_{\Gamma_j} \times [-\varepsilon, \varepsilon] \). Then we can plumb \( vD_{u_1} \) and \( vD_{u_2} \) together along \( a_0 \times [-\varepsilon, \varepsilon] \) and get a ball \( B \subseteq B_T \) such that \( G_T \subseteq B \). Now by Lemma 5.10 there is an isotopy inside of \( B \) from the disk obtained by surgery on \( G_T \) along \( D_{u_1} \) to the disk obtained by surgery on \( G_T \) along \( D_{u_2} \).

Let \( D_u \) be the time \( t \) of that isotopy. Clearly \( \partial D_u = \partial G_T \). Let us show that the property (5.4) holds. Since \( D_u \) is contained in \( B \), which is a sufficiently small neighbourhood of the disks \( D_{u_1} \) and \( D_{u_2} \), it will intersect an arc \( a_T \) only if one of those disks did. Hence, by the induction hypothesis \( i \) belongs either to \( |\zeta_{u_1}| \) or \( |\zeta_{u_2}| \), but \( |\zeta_u| = |\zeta_{u_1}| \cup |\zeta_{u_2}| \) by the definition of the join.

In particular, for \( n = 2 \) we have \( u = (1-t) + 2t = 1 + t \) and so \( D_u = D_{1+t} \) is precisely the isotopy from Lemma 5.10. 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 \( |\Delta^2| = \Delta^{n-1} \)).
5.2.3 The end of the proof: isotopies across disks

Proof of Proposition 5.9. As announced in (5.3) at the beginning of the section, we use the isotopy of the previous proposition for $S = \mathfrak{n}$ and the given thick grope to define for $u \in \Delta^2$ and $\theta \in [0,1]$

$$\mathcal{P}_u^G(\theta) : I_0 \xrightarrow{\theta} D \xrightarrow{\phi(u)} B \xrightarrow{G} M.$$ We clearly have $\mathcal{P}_u^G(0) = (\partial^3 G)_0 = G(a_0)$ and $\mathcal{P}_u^G(1) = K_{f_0} = G(a_0)$ for all $u \in \Delta^2$. We claim that thanks to the condition (5.4), the map $\Psi^G$ as defined in (5.2) is well-defined, that is

$$\Psi^G(\theta) \tilde{t} \in \mathfrak{mb}(I \setminus f_0, M).$$

This is clear for $S \subseteq [n]$ such that $0 \in S$, since we then constantly have the punctured unknot $U^{\mathfrak{n}}_S$. On the other hand, for $0 \notin S$ we need to check that for each $\tilde{t} \in \Delta^S$ and $\theta \in [0,1]$ we have

$$\mathcal{P}_u^G(\theta) \cap K_{\mathfrak{n}} = \emptyset$$

where $u := t_3(\tilde{t})$. Equivalently, if the interior of $G(D_u)$ intersects some $K(j)$, then $i \in S$. Indeed, if $\text{int}G(D_u) \cap K(j) \neq \emptyset$, then we must have $\text{int}D_u \cap a_i \neq \emptyset$, since $G$ is an embedding. But then (5.4) implies that $i \in |z_u|$. As $u$ is obtained by inclusion from the face $\Delta^S$, the maximal simplex that contains it must be contained in $\Delta^S$. Hence, $i \in |z_u| \subseteq S$. 

5.3 Grope forests give points in the layers

5.3.1 The extension of Theorem C to grope forests

Proposition 5.13. For a grope forest $F$ of degree $n$ on $K$ there exists a path $\Psi^F : [0,1] \to P_n(M)$ from $\mathcal{E}(\partial^3 F)$ to $\mathcal{E}_n K$. Moreover, this defines a map on the space of all grope forests

$$\psi : \text{Grop}_n(M; U) \to H_n(M)$$

which extends the map $\psi$ from the space of thick gropes $\text{Grop}_n^1(M; U) \subseteq \text{Grop}_n(M; U)$.

Proof. If $F = \bigsqcup_{i=1}^N G_i : \bigsqcup_{i=1}^N B_{G_i} \hookrightarrow M$, then each $G_i$ can be viewed as a thick grope on $K$. Indeed, it has $G_i(a_0) \subseteq K_{f_0}$ and the conditions for all the arcs $a_i$, $i \in \mathfrak{n}$, are satisfied.

Therefore, by Theorem C we have a path $\Psi^G_i : P_n(M)$ from $\mathcal{E}_n(\partial^3 G_i)$ to $\mathcal{E}_n K$, which was constructed in Proposition 5.9 using the arcs $\mathcal{P}^G_i(\theta) : I_0 \hookrightarrow M \setminus K_{\mathfrak{n}}$. For a fixed $\theta \in [0,1]$ and $S \subseteq \mathfrak{n}$ these arcs are pairwise disjoint for varying $l = 1, \ldots, N$, because of the mutual disjointness of $G_i$. Hence, we can concatenate them to get an arc

$$\Psi^F(\theta) \tilde{t} := \Psi^G_1(\theta) \tilde{t}_1 \cdots \Psi^G_N(\theta) \tilde{t}_N \in \mathfrak{mb}(I \setminus f_0, M \setminus K_{\mathfrak{n}}).$$

We then define $\Psi^F$ analogously to the definition of $\Psi^G$ in (5.2), by letting

$$\Psi^F(\theta) \tilde{t} : \Delta^S \to \mathfrak{mb}(I \setminus f_0, M), \quad \tilde{t} \mapsto K_{\mathfrak{n}} \cup \Psi^F(\theta) \tilde{t} \in H_n(M),$$

for $\theta \in [0,1]$ and $S \subseteq [n]$. As in the proof of Proposition 5.9, this is indeed a path $\mathcal{E}_n(\partial^3 F) \sim \mathcal{E}_n K$.

Finally, for $K := U$ we let $\psi(F) := (U, \Psi^F) \in H_n(M)$.

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 $\mathfrak{mb}(\bigsqcup_{i=1}^N B^3, M)$, small deformations of grope forests lead to small deformations of each of the arcs, keeping them disjoint. 

\qed
Remark 5.14. A perhaps more obvious choice for $Ψ^F$ would simply be
\[ Ψ^G_1 : Ψ^G_2 : \ldots : Ψ^G_N : I → P_n(M), \]
the concatenation of the paths in $P_n(M)$.
This will actually give an equivalent point $e_n(Ψ^F) ∈ F_n(M)$, essentially because $F_n(M)$ is an iterated loop space and – while our definition was concatenation in the $I_0$ direction, this definition corresponds to the concatenation in the ‘diagonal’ $Ω^n$ direction. However, our choice will make the proof of Theorem E straightforward.

We omit the proof, only indicating that the two choices $Dχe_n(Ψ^F) ∈ Ω^n$ tofib$(M, ρ)$ can be compared using the description of $χe_n(Ψ^F)$ in terms of the $h$-reflections of Proposition A.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 $H_n(M)$.

Example 5.15 (degree 1). We now demonstrate the map $Ψ$ on an example in the lowest degree.
A grope cobordism $G$ on $K$ modelled on $Γ = \frac{1}{4}$ is simply a disk (see Figure 18 for examples) guiding a crossing change homotopy $K_0$ from $K_0 = \partial^2 G$ to $K_1 = K$. The corresponding thick grope $G$ is a tubular neighbourhood of this disk.

Its underlying decorated tree is $\frac{1}{4}$ for some element $g ∈ \pi_1(M)$. The disk family in this case consists of a single disk $D ⊆ B$ and $G(D) = G ⊆ M$. The map $\mathcal{P}G : \Lambda^0 → Map_2([0, 1], \text{emb}_b(I_0, M))$ swings the arc $G(a_i^\perp)$ across $G(D)$ to $K_0$. Note that the path through immersions $K_0 ∪ \mathcal{P}G(θ)$ is precisely $K_θ$, $θ ∈ [0, 1]$. The path $Ψ^G : [0, 1] → P_1(M) = \text{holim}_{θ∈[1]} ε_1^1$ is hence given by
\[
Ψ^G(θ)^{(0)} : \Lambda^0 → \text{emb}(I \setminus I_0, M), \quad pt → K_0
\]
\[
Ψ^G(θ)^{(1)} : \Lambda^0 → \text{emb}(I \setminus I_1, M), \quad pt → (K_θ)^1
\]
\[
Ψ^G(θ)^{(01)} : Λ^1 → \text{emb}(I \setminus I_{01}, M), \quad t → K_{01}, \quad ∀t ∈ Λ^1
\]

Only $Ψ^G(−)^{(1)} : Λ^0 → \text{emb}_b(I \setminus I_1, M)$ is not constant with $θ ∈ [0, 1]$. It is the isotopy between $(∂^2 G)^1_1$ and $K_1$ – the crossing change homotopy, now unobstructed since $I_1$ is gone. See also Figure 27 below for the corresponding points $Ψ(G) ∈ H_1(M)$ and $e_2Ψ(G) ∈ F_2(M)$.

5.3.2 Grope forests give points in the layers

Given a thick grope $G ∈ \text{Grop}_n(M; U)$ we obtain a point $Ψ(G) := (∂^2 G, Ψ^G) ∈ H_n(M)$.
Since $H_n(M) := \text{tofib}(ev_n) ∋ \text{tofib}_{SU[1]}(ε_S)$, in the latter coordinates this is given by
\[
Ψ(G)^S = \begin{cases} 
I^0 \xrightarrow{∂^+ G} ε_0, & S = ∅ \\
I^S \xrightarrow{h^S} C^\text{bar}(Λ^S) \xrightarrow{Ψ^G(−)^S} ε_S, & ∅ ≠ S ⊆ n
\end{cases}
\]
where $h^S$ is the homeomorphism of cubes from (2.13), 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 $\text{tofib}_{SU[1]}(ε_S)$ is homotopy equivalent to its subspace $\text{tofib}_{SU[2]} F_S$.

Lemma 5.16. $Ψ(G)$ lies in the subspace $\text{tofib}(F_S)$ and in the coordinates $F_S ∋ \text{emb}_b(I_0, M \setminus U_{02})$ it is given simply by restricting $Ψ(G)^S$ to $I_0 ⊆ I$. 
Proof. It is enough to check that for $S \subseteq \{n - 1\}$ with $S \ni 0$ the map $\psi(G)^S : I^S \to \delta_S$ is constantly equal to $U_\delta$ (since then the only non trivial part of $\psi(G)^S$ for $S \not\ni 0$ is $\psi(G)^S|_{I_0}$). However, this is clear from $\psi(G)^S := \psi(G)^S \circ h^S$ and the very definition $\psi(G)^S = U_\delta$ in (5.2). \hfill $\Box$

Recall that $F_{n+1}(M)$ is also homotopy equivalent to its subspace $\operatorname{tobil}(\mathcal{F}_S^{n+1})$ (which we studied in Sections 3.3 and 4) and in (3.7) we saw that $e_{n+1} : H_n(M) \to F_n(M)$ corresponds to the map $r^*_n : \operatorname{tobil}(\mathcal{F}_S) \to \operatorname{tobil}(\mathcal{F}_S^{n+1})$ induced by postcomposition with

$$\rho^*_n : M \setminus U_\delta \hookrightarrow M \setminus U_\delta^{n+1},$$

which is the obvious inclusion map, adding the appropriate neighbourhood of $J_{n+1}$.

Hence, the image under the evaluation map of our grope point is (recalling that $(\partial^+G)|_0 = G(a^+_0)$)

$$f_G := e_n\psi(G) = \begin{cases} I^0 \xrightarrow{G(a^+_0)} \mathcal{F}_0^{n+1}, & S = \emptyset, \\ I^S \xrightarrow{h^S} C^{\bar{\text{bar}}}((\Delta^S) \xrightarrow{\psi(G)^S|_{I_0}} \mathcal{F}_S^{n+1}, & \emptyset \neq S \subseteq \mathbb{N}. \end{cases} \tag{5.6}$$

Similarly, for $F \in \text{Grop}_n(M; U)$ the corresponding point in $F_{n+1}(M)$ is given by

$$f_F := e_n\psi(F) = \begin{cases} I^0 \xrightarrow{(\partial^+F)|_0} \mathcal{F}_0^{n+1}, & S = \emptyset, \\ I^S \xrightarrow{h^S} C^{\bar{\text{bar}}}((\Delta^S) \xrightarrow{\psi(G^1(-)|_{I_0}) \cdots \psi(G^N(-)|_{I_0})} \mathcal{F}_S^{n+1}, & \emptyset \neq S \subseteq \mathbb{N}. \end{cases} \tag{5.7}$$

where $\psi(G^i(-)|_{I_0}) : C^{\bar{\text{bar}}}((\Delta^S) \to \mathcal{F}_S^{n+1}$ are concatenated pointwise, along their $I_0$ direction.
Let $G: B_I \to M$ be a thick grope on $U$ with the underlying decorated tree $\varepsilon \Gamma U \in \text{Tree}(n)$. In the previous section we have constructed $\psi(G) \in H_n(M)$ and in (5.6) we described the point

$$f_G := e_{n+1} \psi(G) \in F_{n+1}(M).$$

In this section we prove Theorem D – namely, that

$$[f_G] = [\varepsilon \Gamma U] \in \pi_0 F_{n+1}(M) \cong \text{Lie}_{n+1}(n).$$

In Section 4.2 we have reduced this to checking (4.10), that is

$$D_n(\chi f_G)^\# = \Gamma(m_{i}^{(\gamma_{i})}) : S^n \to \Omega M_\#.$$

where $\varepsilon_{i} \in \{\pm 1\}$ and $\gamma_{i} \in \Omega M$ with $i \in \pi$ are signed decorations of $G$, and $g_{i} = [\gamma_{i}]$.

**Remark 6.1 (A reminder).**

- The map $\chi: F_{n+1}(M) \to \Omega^n \text{tolib} (\mathcal{F}_{n+1}^{\#}, I)$ was defined in Proposition 3.16 using left homotopy inverses $l_5^\# = (d_5^\#(1) \circ e_5^\#) \circ -$ and homotopies $h_5^\# = (d_5^\#(s) \circ \text{add}_{s}) \circ -$ constructed in Section 3.3.1.

- For $S \subseteq \pi$ the map $D_S: \mathcal{F}_S^{n+1} \to \Omega M_S := \Omega(M \setminus B_S)$ which takes a punctured knot $\kappa: I_0 \to M_S$ to the loop obtained by concatenating $U_{\kappa}$ and the arc $\kappa$ in reverse (see Remark 3.20).

- The map $\Gamma(m_{i}^{(\gamma_{i})})$ on the right hand side of (6.1) is the Samelson product according to the word $\omega_{2}(\Gamma)$ of the maps $m_{i}^{(\gamma_{i})} : S^1 \to \Omega M_\#$. These are given by $m_{i}^{(\gamma_{i})}(\theta) := \gamma_{i} \cdot m_{i}(\theta)^{\varepsilon_{i}} \cdot \gamma_{i}^{-1}$, where $m_{i} : S^1 \to \Omega M_\#$ is the ‘swing of a lasso’ around $B_{i}$. See Section 4.2 for details.

**Proof of Theorem D.** We prove (6.1) by induction on $n \geq 1$ (for a proof sketch see Example 4.9).

**The induction base.** In this case $R = \{1\}$, $\Gamma = \overline{1}$ and $G$ a thickening of a disk $G$. We need to check that $D_{\{1\}}(\chi f_G)^{(1)} : S^1 \to \Omega M_1$ is homotopic to $m_{1}^{(\gamma_{1})} : S^1 \to \Omega M_1$.

![Figure 28](image-url)

**Figure 28.** Merging Figures 18 and 12 together: a grope cobordism $G$ and the family $m_{1}$.

Firstly, the loop $(\chi f_G)^{(1)} : (f_G^{(1)})^{h_{1}^{(1)}} \cdot f_G^{(1)}$ is the concatenation of the path $f_G^{(1)} := \Psi G(t)^{1}_{0}$ which is the isotopy across the disk $G$ (see Example 5.15), and the path

$$\left( f_G^{(1)} \right)^{h_{1}^{(1)}} := r_{\emptyset}^{1} \left( h_{1}^{(1)}(G(a_{0}^{\emptyset})) \cdot l_{1}^{(1)}(\Psi G(s))^{1}_{0} \right)_{t=1-s}$$

This is obtained by concatenating $h_{1}^{(1)}(-)(G(a_{0}^{\emptyset}))$ with $l_{1}^{(1)}(\Psi G(-))^{1}_{0}$ in $\mathcal{F}_{\emptyset}^{2} := \emptyset \text{mb}_{0}(f_{0}, M_{0})$, then reverse this path and include it into $M_{01} = M_{0} \cup B_{01}$. Recall from Lemma 3.18 that maps $l_{0}^{1}$ and $h_{0}^{1}$ act non-trivially only in the region $[L_{1}, R_{2}] \times D_{2} \subseteq M$. Also recall that $h_{1}^{(1)}(s)(G(a_{0}^{\emptyset})) := d_{2}^{(1)}(s) \circ \text{add}_{s}(G(a_{0}^{\emptyset}))$ and that the isotopy $d_{2}^{(s)}$ drags the east hemisphere of $B_{01}$ to that of $S_{1}$. 

Therefore, \( h_\Theta^D (s) (G(a_\Theta^D)) \) gradually ‘drags to the right’ the part of \( G(a_\Theta^D) \) inside of this region, and the disk \( F(s) G \) agrees with \( G \) except having the tip shifted into \( F_2 \). So \( F(s) G \) moves the shifted arc \( h_\Theta^D (s) (G(a_\Theta^D)) = h_\Theta^D (1) (G(a_\Theta^D)) \) back to \( U_\Gamma \) across the shifted disk \( F(s) G \). In other words, we use the puncture \( F_2 \) instead of \( F_1 \) to isotope \( G(a_\Theta^D) \) back in similar manner.

Applying \( D_1 \) to this loop \( (\chi f_G)^{(1)} \) allows us to homotope the part of the disk \( G \) which is in \( M \setminus \{ L_1, R_2 \} \times D^2 \) (equal to the part of \( F(s) G \) onto its core arc (its underlying chord). Hence, we conclude that \( D_1 (\chi f_G)^{(1)} \) is indeed homotopic to \( \theta \mapsto \gamma_1 \cdot m_1 (\theta) \gamma_1^{-1} \).

**Preliminaries for the induction step**

It will be convenient to consider trees labelled by a finite set \( R \).

Let \( G \) be a thick grope on \( U \) modelled on a tree \( \Gamma \in \text{Tree}(R) \) obtained by grafting together \( \Gamma_1 \in \text{Tree}(R_1) \) and \( \Gamma_2 \in \text{Tree}(R_2) \) 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 \( G \).

In order to prove (6.1) for \( R = \Omega \) we first simplify the map \( D_R (\chi f_G)^{\Omega} : \Omega M_R \to \Omega M_R \) as follows. By Proposition A.6 we have

\[
(\chi f_G)^{\Omega} = \bigoplus_{S \subseteq R} (f_G^S)^{h_S}.
\]

In words, \( (\chi f_G)^{\Omega} : \Omega M \to \Omega M \) is obtained by gluing all \( h \)-reflections \( (f_G^S)^{h_S} : \Omega M \to \Omega M \) along their 0-faces. These maps were defined inductively in Definition A.5 by (for \( k = \min S \))

\[
(f_G^S)^{h_S} = (f_G^{S_k})^{h_S^{k}} \bigoplus_k (f_G^{S_{k-1}})^{h_S^{k-1}}.
\]

Since \( D_R \) is applied pointwise, we obtain

\[
D_R (\chi f_G)^{\Omega} = \bigoplus_{S \subseteq R} D_R ((f_G^S)^{h_S}).
\]

In the **Commutator Lemma 6.2** we will show that \( D_R (f_G^S) \) is homotopic to a certain commutator map and in the **Reflections Lemma 6.3** generalise this to all \( h_S \)-reflections \( D_R (f_G^S)^{h_S} \). Having these homotopies collected in Corollary 6.4, we will be able to finish the proof of Theorem D.

**The Commutator Lemma.** For each \( S \subseteq R \) we now study the map

\[
D_S f_G^S : I^S \to \bigoplus_{\Sigma} \| \nabla \|^{\Sigma | R |} \to \Omega M_S
\]

given by \( D_S f_G^S (\theta) = (U_{\Theta_0} \cdot (f_G^S (\theta)))_{1-\theta} \) where \( f_G^S (\theta) := \Psi^G (\theta)_\Theta (u) \) for \( h_S (\theta) = (\theta, u) \in C^{b/a} (\Lambda S) \).

Using the inductive nature of Definition 5.5 we can write the thick grope \( G \) as the plumbing (see Figures 16 and 22) of two thick gropes \( G_j := G|_{B_{\Gamma_j}} \) modelled on trees \( \Gamma_j \) for \( j = 1, 2 \).

More precisely, the boundary of the abstract grope \( \partial G_{\Gamma_j} = \beta_j \) has its corresponding distinguished subarc \( \beta_j^+ \subseteq \beta_j \). Thus, the map \( G_j : B_{\Gamma_j} \to M \) can be seen as a thick grope modelled on \( \Gamma_j \) on the knot obtained from \( U \) as follows: replace \( G(a_\Theta) \subseteq U_{\Theta_0} \) by the arc \( G(\beta_j^+) \), together with some arcs connecting their endpoints (the dotted arcs in the model \( G \subseteq B_F \) 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 \( G_j \), 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 \( \partial^2 G_j := (U \setminus G(\beta_j^+)) \cup G(\beta_j^-) \). Actually, for \( G_j \) to be a grope on \( U \) we also need to reparametrise \( U \) so that punctures indeed have labels \( 1 \leq i \leq |R_j| \). Also, \( G_2 \) should have the orientation of all stages reversed.
By the following result each loop recalling from Remark 3.22 that the last map is well-defined on the image of between the viewpoints. Moreover, we define immediately reparametrise back to get the analogous maps Thanks to these modifications we have points $\psi(G_i) \in H_{|R_j|}(M)$ for $j = 1, 2$. However, we now immediately reparametrise back to get the analogous maps $f^j_G : I^i_j \rightarrow \mathscr{P}^{|R_j|+1}$ with $S_j := S \cap R_j$. In other words, although formally $G_j$ are not thick gropes on $U$, we can easily switch back and forth between the viewpoints. Moreover, we define

$$D_{S_j}^{|R_j|} : I^i_j \xrightarrow{f^j_G} \mathscr{P}^{|R_j|+1} \xrightarrow{D_{S_j}} \Omega M_{S_j} \xrightarrow{\Omega \partial^j \theta} \Omega M_S,$$

recalling from Remark 3.22 that the last map is well-defined on the image of $D_{S_j}$.

By the following result each loop $D_{R_j}f^j_G(\bar{t})$ is either the commutator of loops $D_{R_j}f^j_G(\bar{t}_1)$ or some time of a canonical null-homotopy. We use the convention $[0, \frac{1}{2}]^0 = I^0$ and $[\frac{1}{2}, 1]^0 = \emptyset$.

**Lemma 6.2.** Assume $|R| \geq 2$. The map $D_{R_j}f^j_G$ is homotopic to the composition of the map $g_1^{(R_1, R_2)} : I^R \rightarrow I^{R_1} \times I^{R_2}$ which permutes the coordinates, and the map $C_R^G : I^{R_1} \times I^{R_2} \rightarrow \Omega M_R$ given by

$$C_R^G(\bar{t}_1, \bar{t}_2) := \left\{ \begin{array}{ll}
D_{R_1}f^j_G(\bar{t}_1), & (\bar{t}_1, \bar{t}_2) \in [0, \frac{1}{2}]^{R_1} \times [0, \frac{1}{2}]^{R_2} \\
D_{R_2}f^j_G(\bar{t}_2), & (\bar{t}_1, \bar{t}_2) \in [\frac{1}{2}, 1]^{R_1} \times [0, \frac{1}{2}]^{R_2} \\
v_1|\bar{t}_1|D_{R_1}f^j_G(\bar{t}_1), & (\bar{t}_1, \bar{t}_2) \in [0, \frac{1}{2}]^{R_1} \times [\frac{1}{2}, 1]^{R_2} \\
v_2|\bar{t}_2|D_{R_2}f^j_G(\bar{t}_2), & (\bar{t}_1, \bar{t}_2) \in [\frac{1}{2}, 1]^{R_1} \times [\frac{1}{2}, 1]^{R_2} \\
const|\bar{t}_0, & (\bar{t}_1, \bar{t}_2) \in [0, \frac{1}{2}]^{R_1} \times [\frac{1}{2}, 1]^{R_2} \\
\end{array} \right.$$ (6.5)

where $\nu_0(x)$ is the time $\theta$ of the canonical null-homotopy $x \cdot x^{-1} \sim const_{\bar{t}_0}$ for a loop $x \in \Omega M_R$. In Figure 30 these are shown as blue lines, and the subspace on which $C_R^G$ is constant is contracted.

**Proof.** Assume $R = \emptyset$. We have $f^0_G(pt) = (\partial^2 G)_0 = G(a^+_0)$ and $D_{\partial G}f^0_G(pt) = (U_0)_1 : G(a^+_0)_{1-1}$ is exactly the loop $G(\partial G_T)$, 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 $[G(\beta_1), G(\beta_2)] \in \Omega M_R$. 

Figure 29. Modifying the bottom stage of a thick grope.

Figure 30. Schematic depiction of the map $C_R^G : I^{R_1} \times I^{R_2} \rightarrow \Omega M_R$, with $F_i := D_{R_j}G_i$ for short.
Now each $G(\beta_j) = G(\beta_j^+ \cdot G(\beta_j \setminus \beta_j^+)$ is precisely the loop $\partial_\theta f_{Gj}^R(\theta) := (U_{\theta})_0 \cdot \Gamma_j(a_j^{h_0}))_1$, so we conclude that $\partial_\theta f_{Gj}^R(\theta)$ is homotopic to $C_j^R(\theta)$ as claimed.

Assume now $R \neq 0$ and recall that for $h^R(\theta) = (\theta, u) \in C^R(\Delta^R)$ the arc $f_{Gj}^R(\theta) := \Psi_j^G(\theta)^{h_0}(u)$ is the time $\theta$ of an isotopy across the disk $G(\Delta^R)$ (see Proposition 5.9): as $\theta \in [0, 1]$ increases, the arc $a_j^{h_0}$ is being homotoped to $a_j$ across $\partial_\Delta G$ using a foliation which we are still free to specify.

The disk $D_u \subseteq B_1$ was in turn defined as the time $t \in [0, 1]$ of the symmetric isotopy (Lemma 5.10) between the two disks obtained by surgery on the bottom stage along $\Delta_u \subseteq B_{1}$ or $\Delta_u \subseteq B_{2}$ (see Proposition 5.12), where $u = (1 - t)u_0 + tu_2 \in \Delta^R = \Delta^{R_1} \star \Delta^{R_2}$, with $u_j \in \Delta^{R_j}$. Without loss of generality, assume $t < \frac{1}{2}$, so $D_u$ looks like in the left of Figure 31.

Here $\overline{t} \in I^R \equiv C^R(\Delta^R) \equiv C^R(\Delta^{R_1} \star \Delta^{R_2}) = C^R(\Delta^{R_1}) \times C^R(\Delta^{R_2})$ precisely gives $h^R(\overline{t}) = (\theta, u_1)$.

The loop $\partial_\theta f_{Gj}^R(\theta)$ is obtained by closing up the arc $\Psi_j^G(\theta)^{h_0}(u)$ using for all $\overline{t}$ the same arc $U_{\theta}$.

Thus, we can collapse this $U_{\theta}$ to the basepoint $p_0$ throughout the whole family, so that $\partial_\theta f_{Gj}^R(\theta)$ becomes, for a fixed $u$, a basepoint preserving homotopy of the loop $G(\partial \Delta^R)$ to $\text{const}_{p_0}$.

We now specify the foliation of $D_u$ in such manner that this homotopy is first done across the two parallel copies of $D_u$ (vertical disks in Figure 31) and the two pieces of $\Delta_u$ (two regions lying flat), until for $\theta = \frac{1}{2}$ we have completely exhausted the parts of $D_u$ 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 $D_u$ onto its skeleton. So ‘parallel copies of curves’ get identified similarly as for $R = 0$. The final result is as on the left of Figure 32: for any $u \in \Delta^R$, $\theta \geq \frac{1}{2}$ our $\partial_\theta f_{Gj}^R(\overline{t})$ became the commutator of the loops $\partial_\theta f_{Gj}^R(\theta_1) = \partial_\theta(b_j^R(\theta_1))$, with $\theta_1 \in [0, 1]$ and $\theta_2 \in [0, c]$.

The left of Figure 32: Disk $\Delta_u$ 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 $\partial_\theta f_{Gj}^R(\theta_1) = \text{const}_{p_0}$, while $\partial_\theta f_{Gj}^R(\theta_2)$ is the curve $x$ on the right of Figure 32. Hence, for $\theta = \frac{1}{2}$ and a fixed $u$ we have $\partial_\theta f_{Gj}^R(\overline{t}) = [\text{const}_{p_0}, x]$ and our null-homotopy across $b(u)$ for $\theta \geq \frac{1}{2}$ indeed becomes the canonical null-homotopy $t \mapsto x_3|_{[0,1]} \cdot x_{1-3}|_{[1-t,1]}$ after the collapse. \qed
The Reflections Lemma. We now extend the previous result to describe each $h^S$-reflection

$$\mathcal{D}_R(f^R_G)^h^S : I^R \xrightarrow{(f^R_G)^h^S} \mathcal{F}_R^{[R]+1} \xrightarrow{\mathcal{D}_R} \Omega M_R.$$ 

**Lemma 6.3.** Assume $|R| \geq 2$ and $S \subseteq R$. The map $\mathcal{D}_R(f^R_G)^h^S$ is homotopic to the composition of the map $\delta_{(R_1, R_2)}$ as before with the map $(C^R_G)^h^S : I^{R_1} \times I^{R_2} \rightarrow \Omega M_R$ given by

$$(C^R_G)^h^S(\vec{t}_1, \vec{t}_2) := \begin{cases}
\mathcal{D}_R(f^R_G)^{h^S : (\vec{t}_1), \mathcal{D}_R(f^R_G)^{h^S : (\vec{t}_2)}}, & (\vec{t}_1, \vec{t}_2) \in [0, \frac{1}{2}]^{R_1} \times [0, \frac{1}{2}]^{R_2} \\
\mathcal{D}_R(f^R_G)^{h^S : (\vec{t}_2)}, & (\vec{t}_1, \vec{t}_2) \in \left[\frac{1}{2}, 1\right]^{R_1} \times [0, \frac{1}{2}]^{R_2} \\
\mathcal{D}_R(f^R_G)^{h^S : (\vec{t}_1)}, & (\vec{t}_1, \vec{t}_2) \in [0, \frac{1}{2}]^{R_1} \times \left[\frac{1}{2}, 1\right]^{R_2} \\
\text{const}_{p_0}, & (\vec{t}_1, \vec{t}_2) \in \left[\frac{1}{2}, 1\right]^{R_1} \times \left[\frac{1}{2}, 1\right]^{R_2}
\end{cases}$$

**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 $\hat{R}$ of cardinality $|\hat{R}| < |R|$ and any $\hat{S} \subseteq R$ of cardinality $|\hat{S}| < |S|$. Thus, letting $k := \min S$ and $R' := R \setminus k$ and $S' := S \setminus k$, the statement is true for the pairs $(R', S')$ and $(R, S')$.

Using the defining formula for an $h^S$-reflection from (6.2), we compute

$$\mathcal{D}_R((f^R_G)^h^S) = \mathcal{D}_R \rho^k \left(h^k(f^R_G)^{h^S : \mathcal{D}_R((f^R_G)^h^S)}\right)
= \Omega \rho^k \circ \mathcal{D}_R \left(h^k(f^R_G)^{h^S : \mathcal{D}_R((f^R_G)^h^S)}\right)
= \Omega \rho^k \circ \mathcal{D}_R \left(h^k(f^R_G)^{h^S : \mathcal{D}_R((f^R_G)^h^S)}\right)
= \Omega \rho^k \circ \mathcal{D}_R \left(h^k(f^R_G)^{h^S : \mathcal{D}_R((f^R_G)^h^S)}\right).$$

(6.6) For the second equality we have used that $\rho^0 \circ \mathcal{D}_R \circ \rho^k = \rho^0 \circ \Omega \rho^k \circ \mathcal{D}_R$ by Remark 3.22 (recall that we omit $\rho^0$ from notation), the third equality holds since $\mathcal{D}_R$ is applied pointwise, and for the last see again Remark 3.22. The induction hypothesis now implies

$$\mathcal{D}_R((f^R_G)^h^S) = \Omega \rho^k \left(h^k((C^R_G)^{h^S : \mathcal{D}_R((f^R_G)^h^S)})\right)$$

(6.7) and it remains to show that the last expression is equal to $(C^R_G)^{h^S : \delta_{(R_1, R_2)}}$.

To this end, assume without loss of generality that $k \in S \cap R_1$, and denote $R'_1 = R_1 \setminus k$ and $R'_2 = R_2$. Then (6.7) at $t \in I'$ equals

$$\Omega \rho^k \left(h^k(C^R_G)^{h^S : (\vec{t}_1, \vec{t}_2)}\right) \mathcal{D}_R((f^R_G)^h^S).$$

Let us plug in the formulae for $(C^R_G)^{h^S}$ and $(C^R_G)^{h^S}$ into this. Observe that $h^k$ and $\Omega \rho^k$ act trivially on the maps involving the grope $G_2$, as those maps interact only with the punctures indexed by $S_2 \setminus k$. On the other hand, for $t_1 \in [0, \frac{1}{2}]^{R_1}$ we will get maps

$$h^k \circ \mathcal{D}_R((f^R_G)^{h^S : (\vec{t}_1)}) \mathcal{D}_R((f^R_G)^{h^S : (\vec{t}_1)}) \mathcal{D}_R((f^R_G)^{h^S : (\vec{t}_1)})$$

and

$$h^k \circ v_{[t_2]}(\mathcal{D}_R((f^R_G)^{h^S : (\vec{t}_1)})) \mathcal{D}_R((f^R_G)^{h^S : (\vec{t}_1)}).$$

The second expression is just $v_{[t_2]}$ applied to the first, which is in turn equal to $\mathcal{D}_R((f^R_G)^{h^S : (\vec{t}_1)})$, by running the equalities from (6.6) in reverse.

Therefore, we indeed have with $\mathcal{D}_R((f^R_G)^h^S) = (C^R_G)^{h^S : \delta_{(R_1, R_2)}}$ as claimed. $\square$
Corollary 6.4. The homotopies from the last lemma glue to a homotopy
\[ D_R(\chi f_G)^R = \coprod_{S \subseteq R} D_R(f_G^S)^{h_S} = \left( \coprod_{S \subseteq R} (C_G^S)^{h_S} \right) \circ \delta_{(R_1, R_2)}. \]

The end of the proof

Assume inductively that (6.1) is true for all \( G \) as in (setup) with \(|R| < n\). Let \(|R| = n\) and let us prove that \( \Gamma(m_i^{\nu_i}) \) and \( D_R(\chi f_G)^R \approx \left( \coprod_{S \subseteq R} (C_G^S)^{h_S} \right) \circ \delta_{(R_1, R_2)} \) are homotopic.

Firstly, \( G \) is the plumbing of thick gropes \( G_1 \) and \( G_2 \) modelled respectively on \( \Gamma_1 \in \text{Tree}(R_1) \) and with signed decorations \((\epsilon_i, \gamma_i)\)\(_{i \in R_1}\). Since both \(|R_1| < n\) the induction hypothesis implies that
\[ D_R(\chi f_G)^{R_1} \simeq \Gamma_1(m_i^{\nu_i}) \colon (I^{R_1}, \partial) \to (\Omega M_{R_1}, \text{const.}). \]  

Secondly, in (B.8) we have defined \( \Gamma(m_i^{\nu_i}) \) inductively by
\[ \Gamma(m_i^{\nu_i}) := \left[ \Gamma_1(m_i^{\nu_i}), \Gamma_2(m_i^{\nu_i}) \right] \circ \delta_{(R_1, R_2)}. \]

The first map in the formula is the Samelson product which was shown in Lemma B.5 to be obtained by canonically trivialising all the faces of the map\(^{17}\)
\[ I^{R_1} \times I^{R_2} \xrightarrow{\Gamma_1(m_i^{\nu_i}) \times \Gamma_2(m_i^{\nu_i})} \Omega M_{R_1} \times \Omega M_{R_2} \xrightarrow{[\partial_{R}(\chi f_{G_1})^{R_1}, \partial_{R}(\chi f_{G_2})^{R_2}]} \Omega M_R. \]

Plugging in (6.8) we get \( \Gamma(m_i^{\nu_i}) \simeq w^{ind} \circ \delta_{(R_1, R_2)} \) for the map \( w^{ind} \) obtained by trivialising the faces of the map\(^{18}\)
\[ I^{R_1} \times I^{R_2} \xrightarrow{[\partial_{R}(\chi f_{G_1})^{R_1}, \partial_{R}(\chi f_{G_2})^{R_2}]} \Omega M_R. \]  

The map \( w^{ind} \) is depicted in Figure 33, with the map (6.9) given as the green square with the two coordinate axes \( I_i \in I^{R_i} \) (so it is an \( n \)-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 \( x \cdot x^{-1} \simeq * \) along straight blue lines. Here \( x \in \Omega M_R \) is some value of (6.9) on the boundary of the inner \( n \)-cube, and so \( w^{ind} \) is indeed constant on the boundary of the outer \( n \)-cube.

We now show that \( w^{ind} \) agrees with the map \( \coprod_{S \subseteq R} (C_G^S)^{h_S} \), so Corollary 6.4 will finish the proof.

Figure 33. Schematic depiction of the map \( w^{ind} \), where \( I_i := D_R(\chi f_{G_i})^{R_i} \) for short.

---

\(^{17}\) More precisely, in that lemma we had \( m_i^{\nu_i} := \Omega^{R_i}\_{\nu_i} \circ m_i^{\nu_i} \) if \( i \in R_1 \), but we have already abused the notation when we decided to write \( m_i := \Omega^{R_i}\_{\nu_i} \circ f_{G_1} \) (cf. (4.6)).

\(^{18}\) Here we denote \( D_R = \Omega^{R}\_{R_1} \circ D_{R_1} \) as in (6.4).
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
\[
\begin{align*}
\psi_{\text{ind}} &:= \left[ \mathcal{D}_R(\varepsilon G_1)^{R_1}, \mathcal{D}_R(\varepsilon G_2)^{R_2} \right] \\
&= \left[ \bigoplus_{S \subseteq R_1} \mathcal{D}_R(f_{G_1}^{R_1})^{h_S}, \bigoplus_{S \subseteq R_2} \mathcal{D}_R(f_{G_2}^{R_2})^{h_S} \right] \\
&= \bigoplus_{S \subseteq R} \mathcal{D}_R(f_{G_1}^{R_1})^{h_{SC^1}} \mathcal{D}_R(f_{G_2}^{R_2})^{h_{SC^2}} \bigoplus_{S \subseteq R} (C_G^R)^{h_S}
\end{align*}
\]
where the second equality is by (6.3), the third holds because the commutator bracket is applied pointwise and the last equality is by definition of \((C_G^R)^{h_S}\) in Lemma 6.3.

Similarly, for \(\tilde{t}_1 \in [0, \frac{1}{2}]^{R_1}\) we have a blue line null-homotopy, where \(\tilde{t}_2\) runs in \([\frac{1}{2}, 1]^{R_2}\), so
\[
\psi_{\text{ind}}(\tilde{t}_1, \tilde{t}_2) := \psi_{\tilde{t}_1} \left( \bigoplus_{S \subseteq R_1} \mathcal{D}_R(f_{G_1}^{R_1})^{h_S}(\tilde{t}_1) \right) \\
= \bigoplus_{S \subseteq R} \psi_{\tilde{t}_1} \left( \mathcal{D}_R(f_{G_1}^{R_1})^{h_{SC^1}}(\tilde{t}_1) \right) = \bigoplus_{S \subseteq R} (C_G^R)^{h_S}(\tilde{t}_1, \tilde{t}_2).
\]
\(\square\)

**The proof of Theorem E**

**Proof.** In Section 5.2 we have defined the extension \(\psi: \text{Grop}_n(M; U) \to H_n(M)\) and in Proposition 5.8 the underlying tree map \(t: \pi_0 \text{Grop}_n(M; U) \to \mathbb{Z}[\text{Tree}_{n,1}(M)]\). We now show that for a grope forest \(F \in \text{Grop}_n(M; U)\) we have \([e_{n+1}\psi(F)] = [t(F)] \in \text{Lie}_{n,1}(M)\).

In other words, for \(F = \bigsqcup_{i=1}^N G_i\): \(\bigsqcup_{i=1}^N \mathbb{B}_{R_i} \hookrightarrow M\) with \(t(G_i) = \varepsilon^i \Gamma_i\) and, denoting \(f_F := e_{n+1}\psi(F)\), we need to show
\[
[f_F] = \sum_{i=1}^N [\varepsilon^i \Gamma_i] \in \pi_0 F_{n+1}(M) \cong \text{Lie}_{n,1}(M).
\]
This was reduced in Section 4.2 to proving that \(\mathcal{D}_R(\chi f_F)^R: \mathbb{S}^n \to \Omega M_R\) is homotopic to a map realising the class on the right, namely, the pointwise product \(\prod_{i=1}^N \Gamma_i(m^{\varepsilon^i \Gamma_i})\) which takes \(\tilde{t} \in \mathbb{S}^n\) to the concatenation of the loops
\[
\Gamma_i(m^{\varepsilon^i \Gamma_i}(\tilde{t})) \in \Omega M_R, \quad 1 \leq l \leq N.
\]
Since each \(G_i\) is a thick grope on \(U\) with the underlying decorated tree \(t(G_i) = \varepsilon^i \Gamma_i\), the maps \(\Gamma_i(m^{\varepsilon^i \Gamma_i}) \approx \mathcal{D}_R(\chi f_G)^R\) are homotopic by Theorem D. Hence, it remains to prove that \(\mathcal{D}_R(\chi f_F)^R\) is homotopic to the pointwise product \(\prod_{i=1}^N \mathcal{D}_R(\chi f_{G_i})^R\).

Recall the definition of \(F_F\) in (5.7). Similarly as in the proof of the Commutator Lemma 6.2, there is a homotopy between \(\mathcal{D}_R(f_F^R)\) and the pointwise product of \(\mathcal{D}_R(f_{G_i}^R)\) – since we can collapse \(U_{G_i}\) for all loops in the family. This extends to all \(h\)-reflections as in the Reflections Lemma 6.3 – there we had commutators of loops and here just their pointwise concatenations.

Therefore, using the same arguments as in the proof of Theorem D we can conclude
\[
\mathcal{D}_R(\chi f_F)^R = \mathcal{D}_R \left( \bigoplus_{S \subseteq R} (f_{G_1}^R)^{h_S} \bigoplus_{S \subseteq R} (f_{G_2}^R)^{h_S} \right) = \bigoplus_{S \subseteq R} \mathcal{D}_R(f_{G_1}^R)^{h_S} = \prod_{i=1}^N \mathcal{D}_R(f_{G_i}^R)^{h_S} = \prod_{i=1}^N \mathcal{D}_R(\chi f_{G_i})^R. \quad \square
\]
A \hspace{1em} ON LEFT HOMOTOPY INVERSES

In this section we prove Lemmas 3.12 and 3.14, and Propositions 3.16 and A.6.

Proof of Lemma 3.12. Consider the commutative square

\[
\begin{array}{ccc}
X & \xrightarrow{I \circ r} & X \\
\downarrow & & \downarrow \\
X & \xrightarrow{r} & Y
\end{array}
\]

\hspace{1em} (A.1)

Its total homotopy fibre \( Z \) is according to Lemma 3.6 given by

\[
\{(x_0, x_s, y_t, x_s, t) \in X \times \mathcal{P}X \times \mathcal{P}X \times X^I \mid x_s : x_0 \to *, y_t : r(x_0) \to *, x_s, t : lr(x_s) \cdot l(y_t) \to const.\}
\]

where \(-\) is path concatenation and the square \( f^* \) is contractible, so \( p_1 \) is a weak equivalence.

On the other hand, the path space \( \mathcal{P}X = \text{hofib}(\Id_X) \) is also contractible, so we immediately have

\[
\chi^{-1} : \Omega \text{hofib}(l) \xrightarrow{\delta_2} Z \xrightarrow{p_1} \text{hofib}(r).
\]

However, we now determine an explicit homotopy inverse \( \chi \) by finding inverses \( p_1^{-1} \) and \( \delta_2^{-1} \).

To define \( p_1^{-1} : \text{hofib}(r) \to Z \) first recall there is a chosen homotopy \( h : X \times I \to X \) from \( \Id \) to \( lr \).

Thus, for \((x_0, y_l) \in \text{hofib}(r)\) we have a path \( h_l(x_0) : x_0 \to lr(x_0) \), and since \( y_l = r(x_0) \), this can be concatenated with \( l(y_l) \).

We let

\[
p_1^{-1}(x_0, y_l) = \begin{cases} x_0, & h_s(x_0) \cdot l(y_s), & y_t, & h_s(h_l(x_0)) \cdot l(y_t) \end{cases} \in Z.
\]

The square \( h_s(h_l(x_0)) \cdot l(h_l(y_l)) \in X \) is obtained by identifying the two edges \( h_l(x_0) \equiv h_s(x_0) \) of the square \((s, t) \mapsto h_s(h_l(x_0)) \) to get a bigon, to which \((s, t) \mapsto h_s(l(y_l)) \) is glued along the common edge \( h_s(lr(x_0)). \)

We reshape this to a square and see it as a path from \( lr(h_s(h_l(x_0)) \cdot l(y_l)) \) to \( const. \).

Since clearly \( p_1 \circ p_1^{-1} = \Id \) and \( p_1 \) is a weak equivalence, \( p_1^{-1} \) is a homotopy inverse for \( p_1 \) (alternatively, there is a homotopy \( p_1^{-1} \circ p_1 \equiv \Id \) by gradually introducing back the coordinate \( x_s \).

The map \( \delta_2^{-1} : Z \to \Omega \text{hofib}(l) \) comes from comparing the bottom raw in the diagram (A.2) to the fibre sequence \( \Omega \text{hofib}(l) \to \mathcal{P}, \text{hofib}(l) \to \text{hofib}(l). \) We define it by

\[
\delta_2^{-1}(x_0, x_s, y_t, x_s, t) = \{ t \mapsto (r(x_{s\leftarrow}) \cdot y_t, lr(x_{s\leftarrow}) \cdot x_s, t) \}
\]

where \( x_{s\leftarrow} \) is the inverse of the path \( x_s \) and \( x_{s\rightarrow} \) is the square \((s, t) \mapsto x_{s\leftarrow} \mid t \in [0,1] \). Since \( \delta_2^{-1} \circ \delta_2((y_t, x_s, t) = (r(const.) \cdot y_t, lr(const.) \cdot x_s, t) = (y_t, x_s, t) \), the map \( \delta_2^{-1} \) is indeed a homotopy inverse for \( \delta_2 \), by the same argument as above.
Hence, the map \( \chi := \delta_Z^{-1} \circ p_1^{-1} : \hofib(r) \to \Omega \hofib(I) \) is given by
\[
\chi(x_0, y_t) = \left\{ t \mapsto \left( r \left( h_t(x_0) \cdot l(y_t) \right) \right)_{s=1-t} \cdot y_t, \quad lr \left( h_t(x_0) \cdot l(y_t) \right) \right\}
\]
and is the desired homotopy inverse to \( \chi^{-1} \).

**Remark A.1.** All triangles in the following diagram commute
\[
\begin{array}{ccc}
\{ t \mapsto y_t \} \in \Omega Y & \xrightarrow{\delta} & \hofib(r) \\
\begin{array}{c}
\Downarrow \chi^{-1} \\
\Downarrow p_1^{-1}
\end{array} & & \begin{array}{c}
\Downarrow \chi \\
\Downarrow \delta_Z^{-1}
\end{array} \\
\{ t \mapsto (y_t, x_{s,t}) \} \in \Omega \hofib(I) & \xrightarrow{\Delta_Z} & Z \\
\end{array}
\tag{A.3}
\]

We simplify the expression for \( \chi \) using the following notation.

**Definition A.2.** In the situation of the previous proof let us define the \( h \)-reflection of \( y \) by
\[
y_t^h := r(h_t(x_0) \cdot l(y_t))_{s=1-t}
\]
Note that this is a path from \( \ast \) to \( rx_0 \in Y \). We now rewrite \( \chi \) as
\[
\chi(x_0, y_t) = \left( y_t^h \cdot y_t, l y_t^h \oplus (h_t x_0 \overline{h_x} l y_t) \right).
\tag{A.4}
\]
and represent it pictorially by (note how the path \( y_t \) gets ‘reflected’ across its starting point)
\[
\begin{array}{c}
x_0 \xrightarrow{r x_0} y_t \xrightarrow{\chi} \bullet \xrightarrow{y_t^h} \xrightarrow{r x_0} y_t \xrightarrow{l y_t^h} \xrightarrow{\Delta_Z} \square
\end{array}
\tag{A.5}
\]

As a word of caution, note that the composite map \( \Omega Y \leftarrow \hofib(r) \xrightarrow{\chi} \Omega \hofib(I) \) is not a loop map: \( \chi(\ast, y_t) = (ry_{1-t} \cdot y_t, lry_{1-t} \oplus h_x l y_t) \). When attempting to prove Proposition 3.16 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 \( \mathcal{P}_S^{n+1} \) for example), we need to start delooping from ‘above’, using the following lemma.

**Proof of Lemma 3.14.** We have two 1-cubes of \((m - 1)\)-cubes, namely the original cube \( R_* \), which uses maps \( r^m_2 \) and the cube \( L_* \), which uses \( l^m_2 \) instead, so we can write
\[
R_* : \quad C_{s^m} \xrightarrow{r^m_2} C_{s^m} \quad : \quad L_*
\]
Their total fibres can be computed as the homotopy fibres of the induced maps
\[
\hofib(R_\ast) \xrightarrow{r^m_2} \hofib(C_{s^m}) \xleftarrow{l^m_2} \hofib(C_{s^m}) \xrightarrow{r^m_2} \hofib(L_\ast)
\]
We claim that \( l^m_2 \circ r^m_2 = (l^m_2 \circ r^m_2) \), is homotopic to \( \text{Id} \). Indeed, by the condition (2) of Definition 3.13 for each \( t \in [0, 1] \) the homotopies \( h^m_S(t) : l^m_2 \circ r^m_2 \rightarrow \text{Id} \) assemble into a map of cubes
\[
h^m_S(t) : C_{s^m} \to C_{s^m}
\]
Hence, the induced map \( h^m_*(t) \) on the total fibres is precisely a homotopy \( (I^m \circ r^m)_* \sim \Id \).

Therefore, we can simply apply the preceding Lemma 3.12 to the left homotopy inverse \( l^m_\ast \) and the homotopy \( h^m_* \) to obtain the desired homotopy equivalence

\[
\chi_m : \text{tofib}(R, \ast) \equiv \text{hofib}(r^m_\ast) \xrightarrow{\sim} \Omega \text{hofib}(l^m_\ast) \equiv \Omega \text{tofib}(L, \ast). \quad \square
\]

**Proof of Proposition 3.16.** We will construct for each \( 0 \leq k \leq m - 1 \) a homotopy equivalence \( \chi_{m-k} : \text{tofib}(D^{m-k}) \rightarrow \Omega \text{tofib}(D^{m-k-1}) \), with the case \( k = 0 \) covered in the previous lemma. The argument is actually the same: conditions (3.11) and (3.12) in Definition 3.15 of an \( m \)-fold homotopy inverse ensure that for each \( k \) we have two 1-cubes of \((m-1)\)-cubes:

\[
D^{m-k} : D^{m-k}_{c,m-k} \xrightarrow{r_{c,m-k}} D^{m-k}_{s,m-k} \xrightarrow{l_{c,m-k}} D^{m-k-1}
\]

Moreover, the condition (3.13) ensures that \( h^{m-k}_*(t) \) is for each \( t \in [0,1] \) a map of cubes, so \( h^{m-k}_*: l^{m-k}_* \circ r^{m-k}_* \sim \Id_{D^{m-k}} \) witnesses that \( l^{m-k}_\ast \) is a left homotopy inverse. Therefore, by Lemma 3.12

\[
\chi_{m-k} : \text{tofib}(D^{m-k}) \equiv \text{hofib}(r^{m-k}_\ast) \xrightarrow{\sim} \Omega \text{hofib}(l^{m-k}_\ast) \equiv \Omega \text{tofib}(D^{m-k-1})
\]

and the composite \( \chi := \chi_1 \circ \cdots \circ \chi_m : \text{tofib}(C, \ast) \xrightarrow{\sim} \Omega^m \text{tofib}(C, l) \) is the desired equivalence. \( \square \)

**A DESCRIPTION OF \( \chi \) IN TERMS OF REFLECTIONS OF CUBES**

**The first delooping.** Let us first describe \( \chi_m : f \in \Omega \text{tofib}(D^{m-1}) \) for a point \( f \in \text{tofib}(R, \ast) \subseteq \mathbb{R}^m \).

The case \( m = 1 \) is Lemma 3.12 and picture (A.5). For \( m = 2 \) we have

\[
R_* = D^2_{y_2} \xrightarrow{r^2} D^2_{y_2} := l_1 \xrightarrow{r_1} C^1 \xrightarrow{r^2} C^{12} \quad L_* = D^2_{y_2} \leftarrow D^2_{y_2} := l_1 \leftarrow r_1 \xrightarrow{l^2} C^1 \xrightarrow{l^2} C^{12} \quad (\text{A.6})
\]

and \( \chi_2 : \text{hofib}(r^2) \rightarrow \Omega \text{hofib}(l^2) \) is depicted in (A.7), with the colours indicating the ambient spaces from (A.6). Note that \( f^1 \) is itself discarded, but used in the rest of the diagram. For example, \( (f^{12})^b := r^2(h^2_2(f^1) \boxplus_2 l^2 f^{12}) \), where \( \boxplus_2 \) denotes the concatenation \( \cdot \) along the second coordinate.
Remark A.3. Observe that $\chi_2(f)$ is a well-defined point in $\Omega \operatorname{hofib}(L)$ thanks to the conditions of Definition 3.13. For example, the orange line is indeed mapped to the bottom green line:

$$r^1(f^2)^{h^2} = r^1r^2(h_2^2(f^2)) = r^2r^1(h_2^2(f^2)) = r^2(r^1f^2) = (r^1f^2)^{h^2}$$

since $r^1$ commutes with $l^2$ by condition (1) and with $h_2^2$ by condition (2) of the definition.

For a general $m \geq 1$, let us denote $f_{l^m}(t_{p \in P}) := f_{l^m}(t_{p \in P}, t_m) \in C_{P_m}$ and rewrite $f$ as

$$\left( \{ f^P \}_{P \subseteq m-1}, \{ f_{l^m} \}_{P \subseteq m-1} \right) \in \operatorname{hofib}(r^P_p).$$

Then $\chi_m(f) \in \Omega \operatorname{hofib}(l^P)$ is given by

$$\chi_m(f^P, f_{l^m}) = \left( (f^P)_{l^m} \otimes_m f_{l^m}, \, l^m(f^P)_{l^m} \otimes_m h^m f_{l^m} \otimes_m h^m l^m f_{l^m} \right),$$

where $\otimes_m$ denotes concatenation in the $t_m$-direction and $(f^P)_{l^m}$ is the $h^m$-reflection as in Definition A.2, namely reflection of $f^P$ across the wall $l^P \times \{0\}$ in $l^m$. Explicitly,

$$(f^P)_{l^m} := r^m \left( h^m f^P \otimes_m l^m f_{l^m} \right)_{s=1}^{t_m} = (A.9)$$

Therefore, we see that $\chi_m$ discards $f^P$ for $P \subseteq m-1$ but incorporates it into its first coordinate. The second coordinate of $\chi$ is another ‘higher’ layer of loops, in the spaces $C^P$.

The second delooping. Consider again $D^2 = \mathbb{R}$, from (A.6) and $\chi_1\chi_2(f) \in \Omega^2 \operatorname{hofib}(D^0)$. The right part of (A.10) depicts its coordinates $S = \{1\}$ and $S = \{1, 2\}$ (omitting $S = \emptyset, \{2\}$). Note that the large green square $\operatorname{for} \circ \chi(f) = \chi_1\chi_2(f)^{(12)} \in \Omega^2 C_2$ is obtained by gluing reflections of $f^{(12)}$.

In order to generalise this observation we consider $m \geq 2$ and

$$\chi_{m-1}\chi_m(f) = \chi_{m-1} \left( (f^P)_{l^m} \otimes_m f_{l^m}, \, x^P \right)_{P \subseteq m-1}$$

$$= \left( (f^{Rm-1m})_{l^m} \otimes_m f^{Rm-1m}_{l^m} \right)_{l^m} \otimes_m -1 \left( (f^{Rm-1m})_{l^m} \otimes_m f^{Rm-1m}_{l^m} \right)_{l^m-1},$$

$$(x^{Rm-1m})_{l^m} \otimes_m -1 x^{Rm-1m}, \, y^{Rm} \right)_{R \subseteq m-2} \tag{A.11}$$

For a general $m \geq 1$, let us denote $f_{l^m}(t_{p \in P}) := f_{l^m}(t_{p \in P}, t_m) \in C_{P_m}$ and rewrite $f$ as

$$\left( \{ f^P \}_{P \subseteq m-1}, \{ f_{l^m} \}_{P \subseteq m-1} \right) \in \operatorname{hofib}(r^P_p).$$

Then $\chi_m(f) \in \Omega \operatorname{hofib}(l^P)$ is given by

$$\chi_m(f^P, f_{l^m}) = \left( (f^P)_{l^m} \otimes_m f_{l^m}, \, l^m(f^P)_{l^m} \otimes_m h^m f_{l^m} \otimes_m h^m l^m f_{l^m} \right),$$

where $\otimes_m$ denotes concatenation in the $t_m$-direction and $(f^P)_{l^m}$ is the $h^m$-reflection as in Definition A.2, namely reflection of $f^P$ across the wall $l^P \times \{0\}$ in $l^m$. Explicitly,

$$(f^P)_{l^m} := r^m \left( h^m f^P \otimes_m l^m f_{l^m} \right)_{s=1}^{t_m} = (A.9)$$

Therefore, we see that $\chi_m$ discards $f^P$ for $P \subseteq m-1$ but incorporates it into its first coordinate. The second coordinate of $\chi$ is another ‘higher’ layer of loops, in the spaces $C^P$.

The second delooping. Consider again $D^2 = \mathbb{R}$, from (A.6) and $\chi_1\chi_2(f) \in \Omega^2 \operatorname{hofib}(D^0)$. The right part of (A.10) depicts its coordinates $S = \{1\}$ and $S = \{1, 2\}$ (omitting $S = \emptyset, \{2\}$). Note that the large green square $\operatorname{for} \circ \chi(f) = \chi_1\chi_2(f)^{(12)} \in \Omega^2 C_2$ is obtained by gluing reflections of $f^{(12)}$.

In order to generalise this observation we consider $m \geq 2$ and

$$\chi_{m-1}\chi_m(f) = \chi_{m-1} \left( (f^P)_{l^m} \otimes_m f_{l^m}, \, x^P \right)_{P \subseteq m-1}$$

$$= \left( (f^{Rm-1m})_{l^m} \otimes_m f^{Rm-1m}_{l^m} \right)_{l^m} \otimes_m -1 \left( (f^{Rm-1m})_{l^m} \otimes_m f^{Rm-1m}_{l^m} \right)_{l^m-1},$$

$$(x^{Rm-1m})_{l^m} \otimes_m -1 x^{Rm-1m}, \, y^{Rm} \right)_{R \subseteq m-2} \tag{A.11}$$
Here we have applied (A.8) twice and denoted by \( x \) and \( y \) the remaining irrelevant coordinates. The first coordinate is \( (\chi_{m-1}\chi_m(f))^{Rm-1m} \in \Omega^2C_{Rm-1m} \) where \( R \) runs through subsets of \( m-2 \).

**Lemma A.4.** \( (f_{Rm-1m}^{Rm-1m})^h_m \otimes_m f_{Rm-1m}^{Rm-1m})^{h_m-1} = (f_{Rm-1m}^{Rm-1m})^{h_m-1} \otimes_m (f_{Rm-1m}^{Rm-1m})^{h_m-1} \).

**Proof.** The left hand side is by (A.9) equal to \( f^{m-1} \) applied to the map (denoting \( s := t_{m-1} \))

\[
= h_s^{m-1} \left( (f_{Rm}^{Rm})^h_m \otimes_m f_{Rm}^{Rm} \right) \otimes_m (f_{Rm-1m}^{Rm-1m})^{h_{m-1}}
\]

\[
= h_s^{m-1} \left( (f_{Rm}^{Rm})^h_m \otimes_m h_{m-1}^{Rm} \otimes_m (f_{Rm-1m}^{Rm-1m})^{h_{m-1}} \right) \otimes_m (f_{Rm-1m}^{Rm-1m})^{h_{m-1}}
\]

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

\[
= \left( h_s^{m-1} \left( (f_{Rm}^{Rm})^h_m \otimes_m h_{m-1}^{Rm} \otimes_m (f_{Rm-1m}^{Rm-1m})^{h_{m-1}} \right) \right) \otimes_m (h_s^{Rm} \otimes_m (f_{Rm-1m}^{Rm-1m})^{h_{m-1}}) \otimes_m (f_{Rm-1m}^{Rm-1m})^{h_{m-1}}
\]

Finally, applying \( f^{m-1} \) gives the desired right hand side in the statement of the lemma. \( \square \)

Therefore, we make the following definition.

**Definition A.5.** Fix \( P \subseteq \mathbb{M} \) and let \( f^P : I^P \to C_P \) for an \( m \)-cube \( C \). 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

\[
(f^P)^{h_S} := \left( (f^P)^{h^S_k} \right)^{h^S_k}
\]

using the definition of \( h^S \)-reflection from (A.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 A.6.** For \( D^m \) as above, for \( \varphi \in \chi : \text{tofib}(D^m) \to \Omega^m C_{\mathbb{M}} \) maps \( f \in \text{tofib}(D^m) \) to

\[
(\chi f)^{\mathbb{M}} = \bigoplus_{S \subseteq \mathbb{M}} (f^S)^{h_S}
\]

obtained by gluing together all \( h \)-reflections \( (f^S)^{h_S} \) of \( f^S : I^m \to C_{\mathbb{M}} \) along the 0-faces of \( I^m \).

**Proof of Proposition A.6.** From (A.11) and Lemma A.4 we conclude

\[
\chi_{m-1}\chi_m(f)^{Rm-1m} = \left( (f_{Rm-1m}^{Rm-1m})^{h_{m-1}} \otimes_m (f_{Rm-1m}^{Rm-1m})^{h_{m-1}} \right) \otimes_m (f_{Rm-1m}^{Rm-1m})^{h_{m-1}}
\]

\[
= (f_{Rm-1m}^{Rm-1m})^{h_{m-1}} \otimes_m (f_{Rm-1m}^{Rm-1m})^{h_{m-1}} \otimes_m (f_{Rm-1m}^{Rm-1m})^{h_{m-1}}
\]

In the second line we simply omitted the brackets and used the symbol \( \otimes \) instead, since the operation \( \otimes \) glues unambiguously any two maps which have matching 0- and 1-faces indexed by \( k \). Continuing in the manner of (A.11), we find

\[
\chi_k \circ \cdots \circ \chi_{m-1}\chi_m(f)^{Rk-\cdots-m-1m} = \bigoplus_{S \subseteq \{k,\ldots,m-1,m\}} (f^{Rk-\cdots-m-1m})^{h_S}
\]

so the coordinate of \( \chi_1 \circ \cdots \circ \chi_m(f) \) corresponding to \( \mathbb{M} \) is given as claimed by

\[
(\chi f)^{\mathbb{M}} = \bigoplus_{S \subseteq \mathbb{M}} (f^S)^{h_S}. \quad \square
\]
B 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 $G := \Omega(M \vee_5 S^d)$ with an inverse for $\gamma \in G$ given as the inverse loop $(\gamma^{-1})_t = \gamma_{-t}$ and the canonical homotopy $\gamma \cdot \gamma^{-1} \rightsquigarrow \text{const}$, given by $t \mapsto \gamma|_{[0,1-t]} \cdot \gamma^{-1}|_{[t,1]}$.

The homotopy groups $\pi_\ast G$ 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 $f_1 \cdot f_2 : X_1 \times X_2 \to G \times G \to G$ of maps $f_j : X_j \to G$, and then if $X_1 = X_2 = S^n$, precompose with the diagonal $S^n \to S^n \times S^n$.

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 $f : X \to G$ 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 $\pi_\ast G$. When $G$ is a loop space this corresponds to the standard action of the fundamental group on the higher homotopy groups.

The Samelson product is a non-associative product of maps $f_j : X_j \to G$ for $j = 1, 2$, given by

$$[f_1, f_2] : X_1 \times X_2 \xrightarrow{f_1 \vee f_2} G \vee G \xrightarrow{[\cdot, \cdot]} G.$$  \hfill (B.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 $X_j = S^n$ is a sphere, and using homeomorphisms

$$\delta_{(n_1, n_2)} : S^{n_1 + n_2} \to S^{n_1} \wedge S^{n_2}$$  \hfill (B.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\footnote{To see (B.3), plug $f_1 = f$ and $f_2 : S^0 \to G$ into (B.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.}

$$[f, \gamma] \simeq f \cdot f^\gamma, \quad f \in \pi_{>0} G, \quad \gamma \in \pi_0 G.$$  \hfill (B.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 $\theta : S^{n_1} \wedge S^{n_2} \to S^{n_2} \wedge S^{n_1}$ induces the self-map $\delta_{(n_2, n_1)} \circ \theta = \delta_{(n_1, n_2)}$ of $S^{n_1 + n_2}$ 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

$$[f, g]^\gamma = [f^\gamma, g^\gamma], \quad f, g \in \pi_{>0} G, \quad \gamma \in \pi_0 G,$$

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 $h : \pi_\ast G \to H_\ast(G; \mathbb{Z})$ takes the Samelson bracket to the graded commutator in the Pontrjagin Hopf algebra $H_\ast(G; \mathbb{Z})$. 

19 To see (B.3), plug $f_1 = f$ and $f_2 : S^0 \to G$ into (B.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 $f_i : X_i \to G$ for $i \in S = \{i_1 < i_2 < \cdots < i_m\}$ according to a Lie word (a non-associative bracketing) on the letters $x^i$, $i \in S$. To spell out this explicitly, we recursively define the space $w(X_i)$ and the map $w(f_i) : w(X_i) \to G$.

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 $w(X_i) = w_1(X_i) \wedge w_2(X_i)$ and define

$$w(f_i) : w(X_i) \xrightarrow{w_1(f_i) \wedge w_2(f_i)} G \wedge G \xrightarrow{[,]_1} G.$$ (B.4)

In particular, if $X_i = S^{d-2}$ for all $i \in S$, to get a map from a sphere we need to precompose with some homeomorphism $\phi_i : S^{l_w} \to S^{d-2}$ similarly as in (B.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 4 we have the inclusion $\iota_{\Sigma X} : \Sigma X_i \hookrightarrow \bigvee_{i \in S} \Sigma X_i$ and the canonical map $\eta_{\Sigma} : X_i \to \Omega \Sigma X_i$. Plugging into (B.4) the composite maps

$$x_i : X_i \xrightarrow{\eta_{\Sigma}} \Omega \Sigma X_i \xrightarrow{\Omega i_j} \Omega \bigvee_{i \in S} \Sigma X_i$$

gives the Samelson product

$$w(x_i) : w(X_i) \to \Omega \bigvee_{i \in S} \Sigma X_i.$$ (B.5)

**Remark B.1.** For $G = \Omega Y$ the Samelson bracket on $\pi_*(\Omega Y) \cong \pi_{n+1}(Y)$ is adjoint to the Whitehead bracket on the latter group. The (generalised) Whitehead product of $f_i : \Sigma X_i \to Y$ is defined via

$$[f_1, f_2]w : \Sigma X_1 \vee \Sigma X_2 \to \Sigma X_1 \vee \Sigma X_2 \xrightarrow{f_1 \vee f_2} Y \vee Y \to Y,$$

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 $[x_1, x_2] : X_1 \wedge X_2 \to \Omega (\Sigma X_1 \wedge \Sigma X_2)$ from (B.5). If $X_i = S^{n-1}$ are spheres, this is the attaching map $S^{n_1+n_2-1} \to S^{n_1} \wedge S^{n_2}$ of the top cell in $S^{n_1} \times S^{n_2}$.

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 (B.5) is a map into a loop space, there is a unique multiplicative extension

$$\tilde{w}(x_i) : \Omega \Sigma w(X_i) \to \Omega \bigvee_{i \in S} \Sigma X_i.$$ (B.6)

Namely, for any space $X$ the map $\eta_X : X \to \Omega \Sigma X$ is initial among all maps from $X$ to a loop space, so any $f : X \to \Omega X$ factors as the composition of $\eta_X$ with $\tilde{f}$ := $\Omega (\nu \ast f) : \Omega \Sigma X \to \Omega \Sigma \Omega Z \to \Omega Z$. Explicitly, $\tilde{f}(\theta \equiv t_0 \wedge a_0) = \theta \equiv f(a_0)^{t_0}$ for $t_0 \in S^1$ and $a_0 \in X$, when $\theta$ ranges $S^1$.

Moreover, given Lie words $w_1$ and $w_2$ we can take the pointwise product $\tilde{w}(x_i) \cdot \tilde{w}(x_i)$ (pointwise concatenate loops) as we saw above. Therefore, if $\mathcal{B}(S)$ denotes a Hall basis for the free Lie algebra $L(x^i : i \in S)$, we can define the map

$$hm := \prod_{w} \tilde{w} : \prod_{w \in \mathcal{B}(S)} \Omega \Sigma w(X_i) \to \Omega \bigvee_{i \in S} \Sigma X_i.$$ (B.7)

where the source is the weak product, defined as the filtered colimit of products over the finite subsets of $\mathcal{B}(S)$. Thus, points in it have all but finitely many coordinates equal to the basepoint.

**Theorem B.2** ([Hil55; Mil72; Gra71; Spe71]). If for each $i \in S$ the space $X_i$ is well-pointed and path-connected, then the map (B.7) is a weak homotopy equivalence.
This can be proven by first iterating Gray–Spencer Lemma 4.3 to get a weak homotopy equivalence
\[ \Omega A \times \bigvee_{i \geq 0} [x_A, [x_A, \ldots, [x_A, x_B] \ldots]] : \Omega A \times \Omega \bigvee_{i \geq 0} (A^i \wedge B) \longrightarrow \Omega (\Sigma A \vee \Sigma B), \]
and then using an inductive argument on the word length. See [Mil72, Thm. 4].

**Remark B.3.** The set \( \mathcal{B}(S) \) 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 \( \pi_*(\Omega \vee_{S} \mathbb{S}^{n_i+1}) \otimes \mathbb{Q} \cong \mathbb{L}(x_i : i \in S) \otimes \mathbb{Q} \) is the free graded Lie algebra, with \( x_i \) having degree \( n_i \).

### 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 \( \omega_2 : \text{Lie}(R) \to \text{Lie}_2(R) \) (see also next subsection).

As mentioned above, given maps \( f_i : \mathbb{S}^{d-2} \to G \) one obtains a map from a sphere by precomposing the Samelson product \( \omega(f) : \mathbb{S}^{d-2} \to G \) with \( \delta_{\sigma_\nu} : \mathbb{S}^{d-2} \to \mathbb{L}(X_i) \), which permutes the factors according to the permutation \( \sigma_\nu \) corresponding to the word \( \nu \). However, in the case when letters do not repeat we can instead define this map directly by induction. This was used in Section 4.1.

**Lemma B.4.** The map \( \omega(f) \circ \delta_{\sigma_\nu} \) for \( \omega = \omega_2(\Gamma) \) is homotopic to the map \( \Gamma(f) \) defined inductively by \( \Gamma(f) = f_1 \) and for \( \Gamma_j \in \text{Tree}(R_j) \) with \( R_1 \cup R_2 = R \) by
\[ \Gamma_2 \circ \Gamma_1 : (\mathbb{S}^{d-2})^{\wedge} R \longrightarrow (\mathbb{S}^{d-2})^{\wedge} R_1 \wedge (\mathbb{S}^{d-2})^{\wedge} R_2 \]
\[ \longrightarrow G \]
where \( (R_1, R_2) \) permutes the ordered set \( R \) into \( R_1 \cup R_2 := \text{first all indices of } R_1, \text{then of } R_2 \).

**Proof.** For \( \nu = [\nu_1, \nu_2] \) with \( \nu_i \) on letters in \( R_j \) we have homotopies
\[ \omega(f_1) \circ \delta_{\sigma_\nu} \simeq (\text{sgn } \sigma_\nu)^{d-2} \omega(f_1), \quad \Gamma(f_1) \simeq (-1)^{|\nu|}[\Gamma_1(f_1), \Gamma_2(f_1)] \]

since \( \deg \delta_{(R_1, R_2)} = (-1)^{|\nu|} \nu_1 \) where \( (1/2) := (d-2) \cdot (1/2) \) for \( (1/2) := |\{(i_1, i_2) \in R_1 \times R_2 : i_1 > i_2\}| \) as in Lemma 2.3 from Section 2.1 (see below for its proof). The proof now follows by induction using that the sign of permutation satisfies the recursive formula
\[ \text{sgn } \sigma_\nu = (-1)^{|\nu|} \text{sgn } \sigma_{\nu_1} \cdot \text{sgn } \sigma_{\nu_2}. \]

In the proof of Theorem D in Section 6 we will need the following observation. Let \( (M_S, \rho)_{S \subseteq R} \) be a cube with maps \( \rho^i_S : M_S \to M_{S^i} \) and assume we are given maps \( f_i : \mathbb{S}^{d-2} \to \Omega M_i \) for \( i \in R \). For \( S \subseteq R \) with \( i \in S \) let us denote
\[ f_{i,S} := \Omega \rho^i_S \circ f_i : \mathbb{S}^{d-2} \longrightarrow \Omega M_i \longrightarrow \Omega M_S. \]

**Lemma B.5.** The map \( [\Gamma_1(f_{i,R}), \Gamma_2(f_{i,R})] \) as in (B.8) is obtained by canonically trivialising on the boundary the map
\[ x : (I^{d-2})^{R_1} \times (I^{d-2})^{R_2} \longrightarrow \Omega M_{R_1} \times \Omega M_{R_2} \]
\[ \longrightarrow \Omega M_R \]
More precisely, for each \( \tilde{t} \in \partial(I^{d-2}) \) we glue in the standard null-homotopy \( x(\tilde{t}) \cdot x(\tilde{t})^{-1} \simeq * \) of loops in \( \Omega M_R \) to extend \( x \) to a bigger cube on whose boundary it is constant.
Here we defined a map on $(S^{d-2})^R \cong (I^{d-2})^R / \partial$ by giving it on the cube so that it is constant on the boundary. The proof of the lemma is clear from definitions. See Section 4.2 for how it is used.

**Proof of Lemma 2.3**

We now prove Lemma 2.3, which says that the map $\omega_d : \text{Lie}(n) \to \text{Lie}_d(n)$ given by $\omega_d(\Gamma) = x^i$, $\omega_d(\Gamma) = \omega_T := (-1)^{(1|2)d}[x_1(\Gamma_1), x_2(\Gamma_2)]$ is an isomorphism. Here $(1|2)_d := (d - 2) \cdot (1|2)$ and $(1|2) := \{ (i_1, i_2) \in R_1 \times R_2 : i_1 > i_2 \}$. Note that $\text{Lie}(n)$ extends to an $\delta_{n+1}$-representation by permuting all the labels $\{0, 1, \ldots, n\}$; this is related to the cyclic operad structure on $\text{Lie}(\bullet)$. Then Lemma 2.3 precisely gives $\text{Lie}_d(n) \cong \text{Lie}(n) \otimes \text{sgn}_{n+1}$ as representations of $\delta_{n+1}$; see [Rob04, Prop. 3.4] for details.

**Proof of Lemma 2.3.** We define $\omega_d$ by linearly extending the definition in the lemma and check it descends to the quotient by (2.1). We write $\omega_T := \omega_d(\Gamma)$ for short.

To this end, let $\omega_{AS}$ and $\omega_{IHX}$ be the images under $\omega_d$ of the linear combinations as in (2.1), but with roots instead of dots. It suffices to show that these are trivial, since then $\omega_d$ will also vanish on any tree in which $AS$ or $IHX$ appears as a subtree.

Firstly, using $[\omega_{\Gamma_1}] = [S_1](d - 2)$ and the obvious identity $(1|2)_d + (2|1)_d = [S_1][S_2](d - 2)$ we obtain:

$$
\omega_{AS} = (-1)^{(1|2)}[\omega_{\Gamma_1}, \omega_{\Gamma_2}] + (-1)^{(2|1)}[\omega_{\Gamma_2}, \omega_{\Gamma_1}]
$$

$$
= (-1)^{(1|2)}[\omega_{\Gamma_1}, \omega_{\Gamma_2}] + (-1)^{(2|1)}\omega_{\Gamma_1}(d - 2)[\omega_{\Gamma_2}, \omega_{\Gamma_1}]
$$

$$
= (-1)^{(1|2)}[\omega_{\Gamma_1}, \omega_{\Gamma_2}] + (-1)^{(2|1)}[\omega_{\Gamma_2}, \omega_{\Gamma_1}]
$$

which vanishes by the graded antisymmetry in $\text{Lie}_d(S)$. Secondly, recall that

$$
\text{IHX} : \Gamma_3 \Gamma_2 \Gamma_1 - \Gamma_3 \Gamma_2 \Gamma_1 + \Gamma_3 \Gamma_1 \Gamma_2 = 0.
$$

and note that by $AS$ the last tree is equal to

$$
\text{IHX} : \Gamma_3 \Gamma_2 \Gamma_1 - \Gamma_3 \Gamma_1 \Gamma_2 = 0.
$$

Therefore, $\omega_{IHX}$ is equal to

$$
(-1)^{(1|2)}[\omega_{\Gamma_1}, [\omega_{\Gamma_2}, \omega_{\Gamma_3}]] - (-1)^{(1|2)}[\omega_{\Gamma_2}, [\omega_{\Gamma_1}, \omega_{\Gamma_3}]] - (-1)^{(1|2)}[\omega_{\Gamma_3}, [\omega_{\Gamma_1}, \omega_{\Gamma_2}]]
$$

$$
= (-1)^{(1|2)}[\omega_{\Gamma_1}, [\omega_{\Gamma_2}, \omega_{\Gamma_3}]] - [\omega_{\Gamma_2}, [\omega_{\Gamma_1}, \omega_{\Gamma_3}]] - (-1)^{(1|2)}[\omega_{\Gamma_3}, [\omega_{\Gamma_1}, \omega_{\Gamma_2}]]
$$

where we have used the identities

$$
(1|2) + (2|3) = (1|2) + (1|3) + (2|3) = (1|2) + (1|3) + (2|3) = (1|2) + (1|3) + (2|3),
$$

$$
(2|3) + (1|3) = (2|1) + (2|3) + (1|3).
$$

Now again plugging in $(2|1|3)_d + (1|3)_d = [\omega_{\Gamma_1}][\omega_{\Gamma_2}]$ we get that the terms in the parenthesis are precisely those of the graded Jacobi relation (2.2), which holds in $\text{Lie}_d(S)$.

Finally, $\omega_d$ is clearly a surjection and an inverse $\omega_d^{-1}$ can be constructed in an analogous way – $AS$ and $IHX$ will imply it is well-defined modulo graded antisymmetry and Jacobi relations. □
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