MILNOR INVARIANTS OF STRING LINKS, TRIVALENT TREES, AND CONFIGURATION SPACE INTEGRALS

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Abstract. We exhibit a correspondence, given by configuration space integrals, between Milnor's homotopy link invariants and trivalent trees. Two main ingredients in the proof are the fact that Milnor invariants are finite type invariants and that there is a certain space of trivalent "homotopy link diagrams" that corresponds to all finite type homotopy link invariants via configuration space integrals. The third main ingredient is that configuration space integrals take the shuffle product of diagrams to the product of invariants. Motivated by the problem of determining explicit integral formulas for Milnor invariants, we provide an analysis, in purely combinatorial terms, of the space of these homotopy link diagrams in terms of Milnor invariants. The main result giving a correspondence between Milnor invariants and trivalent trees in terms of configuration space integrals follows as a corollary. As another consequence, we get cohomology classes in a spaces of link maps from Milnor invariants and products thereof.

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1. Introduction

This article studies the relationship between two concepts. The first is the link invariants defined by Milnor in his senior thesis in 1954 [20]. Some of these are invariant under not just isotopy but also *link homotopy*, which esentially means that they detect linking of different strands but ignore knotting of individual strands. Milnor considered closed links, for which these invariants are only defined modulo greatest common divisors of lower-order invariants. In 1990, Habegger and Lin [10] succeeded in classifying links up to link homotopy (i.e., homotopy links) by using string links, for which the Milnor invariants are well defined integer invariants. (See Section 2 for the precise definitions of string links and link homotopy.) Furthermore, Milnor invariants are *finite type* (or *Vassiliev*) invariants (see Section 2.2), and these invariants are known [2] to distinguish string links up to link homotopy.

The second side of the story is configuration space integrals (a brief overview of which is given in Section 2.5). They were first used by Gauss to define the linking number of two closed curves and were generalized by Bott and Taubes [3] in the 1990s. (This is why they are sometimes called *Bott-Taubes integrals.*) D. Thurston [24] used them to construct finite type knot and link invariants, and Cattaneo, Cotta-Ramusino, and Longoni extended them to knots in higher dimensions to obtain information about the cohomology of spaces of knots [5]. A further development was undertaken in [16] where the authors extended configuration space integrals to string links and used them to construct all finite type invariants of this space. The motivation for the results in this paper in fact comes from the work in [16]. In short, as mentioned above, Milnor invariants are in particular of finite type, so some of the integrals (or combinations thereof) constructed in [16] are thus Milnor invariants. It is our goal here to elucidate that relationship.

An important auxiliary ingredient for configuration space integrals are trivalent diagrams (or graphs), which are combinatorial objects and which form a part of a cochain complex (see Section 2.3). More specifically, each finite type invariant is given by a sum of integrals, and this linear combination of integrals corresponds to a linear combination of diagrams (see Section 2.5 for an overview). The subspace of diagrams which correspond to *link homotopy* invariants of string links was first found by Bar-Natan [2] and further developed (in terms of the cochain complex and configuration space integrals) in [16]. It is these diagrams that will ultimately provide the connection between Milnor invariants of string links and configuration space integrals.

Combinatorial formulas for Milnor invariants were studied before by Mellor [18] who describes them recursively in terms of *chord diagrams* (which are a special kind of trivalent diagrams). This by itself does not give a clear conceptual picture of the situation, in part because Mellor's construction involves only the space of chord diagrams while configuration space integrals require enlarging this space to include all trivalent diagrams. Our results not only provide the diagram combinatorics for Milnor invariants, but in addition give an explicit way to construct them, up to lower order invariants, from certain trivalent trees using configuration space integrals.

Earlier related results are those of Bar-Natan [2, Theorem 3] and Habegger and Masbaum [11, Theorem 6.1, Proposition 10.6], who in fact established a more conceptual relationship between Milnor invariants and a space of trivalent trees modulo the IHX relation. (This relationship was perhaps expected, given that trivalent trees with $n+1$ leaves can be viewed as iterated commutators of n elements and the fact that Milnor invariants of type n are related to the n-th term in the lower central series of the link group.) The work of Habegger and Masbaum allows one to compute a formula [11, Figures 7, 8] in terms of the Kontsevich integral [6, 1, 12], at least for the first nonvanishing Milnor invariant of a string link. However, this formula does not appear to correspond in an obvious way to the one in terms of configuration space integrals. Our purpose is to show how to organize the conceptual relationship between Milnor invariants and trivalent trees into configuration space integral formulas for Milnor invariants. The advantage of working with configuration space integrals is that they are fairly well understood and geometrically motivated.

The main content of this paper is a definition of certain filtrations of the space of homotopy link diagrams (or their dual) and finite type invariants of homotopy string links as well as a proof that these correspond to each other. As a result, we recover Habegger and Masbaum's correspondence between Milnor invariants and trivalent trees and the fact that products of Milnor invariants span finite type invariants of any given type. Our approach, following the work of Cattaneo–Cotta-Ramusino–Longoni, has the advantage that the shuffle product of diagrams corresponds to the product of invariants. In the setting used by Habegger and Masbaum, as well as by Bar-Natan, the product of invariants corresponds to a *coproduct* of diagrams. Thus our approach facilitates a combinatorial analysis which would be awkward in the latter approach (even if it were possible by ubiquitous dualizing).

In summary, our refined combinatorial analysis of the space of trivalent diagrams in terms of Milnor invariants has two main consequences. The first is to provide alternative proofs of certain facts about Milnor invariants, proofs which are more combinatorial in nature than the existing ones in the literature. The second is to give configuration space integral formulas for Milnor invariants, up to products of lower order invariants.

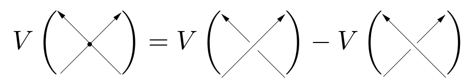
The paper is organized as follows. In Section 2, we review some background material on finite type invariants, Milnor invariants, trivalent diagrams, and configuration space integrals. In Section 3, we express the simplest few Milnor invariants in terms of configuration space integrals. This illustrates the main result of this paper. It also shows that the formulas become quite complicated even for type 3 Milnor invariants of 4-component links. In Section 4, we state and prove the main result of this paper, Theorem 4.10. This involves defining filtrations on spaces of diagrams and on spaces of finite type link homotopy invariants. Finally, in Section 4.4, we consider spaces of link maps of 1-manifolds in $\mathbb{R}^d$, $d \geq 4$, and observe that the graph cocycles which yield Milnor invariants in the case $d = 3$ yield nontrivial cohomology classes in these spaces. This uses our previous work in [16].

1.1. **Acknowledgments.** The first author thanks Ben Williams for a discussion about linear algebra.

2. Background

2.1. **Homotopy string links.** A *string link* L on m *components* or *strands* is a smooth embedding of m disjoint copies of $\mathbb{R}$ into $\mathbb{R}^d$, $d \geq 3$, which outside of $\coprod_{i=1}^m [-1,1]$ is given by a fixed affine-linear embedding on each component. For technical reasons, we require the directions of the m affine-linear embeddings to be distinct (see [16, Section 2.1]). A *homotopy string link* is defined similarly, except that we no longer require L to be an embedding on $\coprod_{i=1}^m [-1,1]$; instead we only require it to be a smooth map such that the images of any pair of components are disjoint. (Such a map is often also called a *link map* of $\coprod_{i=1}^m \mathbb{R}$ into $\mathbb{R}^d$.) We denote the set of all homotopy string links $\mathrm{Link}(\coprod_{i=1}^m \mathbb{R}, \mathbb{R}^d)$, and give it a topology as in [16, Section 2.2]. A path in this space is called a *link homotopy*. By abuse of terminology, we also use "homotopy string link" to refer to a path component (i.e., link homotopy class), rather than an element, of this space (just as a "knot" may refer to either an embedding or its isotopy class). We abbreviate $\pi_0(\mathrm{Link}(\coprod_{i=1}^m \mathbb{R}, \mathbb{R}^3))$ as $\mathcal{H}_m$.

2.2. **Finite type invariants of homotopy string links.** An invariant of m-component homotopy string links is a map from $\mathcal{H}_m$ to a set (often an abelian group), which we will take to be $\mathbb{R}$ in this paper. Any such invariant extends to *singular homotopy string links*, that is, homotopy string links with finitely many intersection points of distinct strands; the extension is determined by inductively using the Vassiliev skein relation:



The arrows denote the orientation of the link components.

An invariant is said to be *finite type of* type n (or of *order* n) if it vanishes on all links with more than n such intersection points. Let $\mathcal{HV}_n$ denote the $\mathbb{R}$-vector space of type n finite type invariants of homotopy string links in $\mathcal{H}_m$. Milnor's homotopy invariants of links (which we will review in Section 2.6) are of finite type. In particular, an invariant involving $n+1$ strands of the link is of type n.

Bar-Natan [2] showed, using work of Habegger and Lin [10], that finite type invariants classify homotopy string links.

The product of two finite type invariants V_1 and V_2 is given simply by $V_1 V_2(L) := V_1(L) V_2(L)$. The proof of the following can be found, for example, in [7, p. 75].

Lemma 2.1. *The product of two finite type link invariants of types r and s is a finite type invariant of type $r+s$.* □

2.3. **Chord diagrams, trivalent diagrams, and unitrivalent diagrams.**

2.3.1. *Chord diagrams.* The main result regarding finite type invariants $\mathcal{H}_m$ is that they can be described completely in terms of certain combinatorial diagrams.

Definition 2.2. A *homotopy link chord diagram* consists of m disjoint intervals called *segments*, labeled by $\{1, ..., m\}$, together with n pairs of vertices on these segments, with each pair joined by a *chord*. We require that the vertices in each pair lie on distinct segments. (We do not however require that every segment has a vertex on it.) We call n the *order* of the diagram. We consider these diagrams up homeomorphisms which preserve the orientation and label of each segment, so that there are finitely many such diagrams for each n. Let $\mathcal{HC}_n$ be the $\mathbb{R}$-vector space generated by homotopy link chord diagrams of order n.

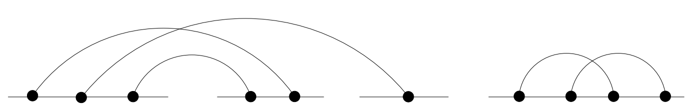
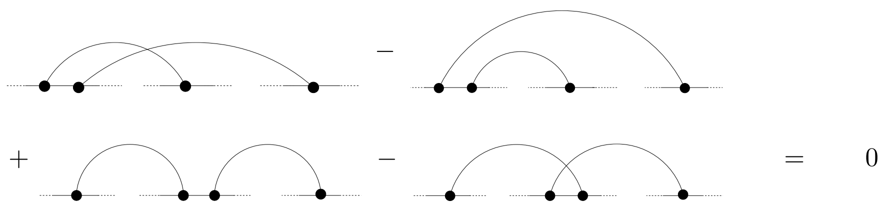


Figure 1. A chord diagram in $\mathcal{HC}_5$, where the number of segments is $m = 4$.

Let $\mathcal{HC}_n^*$ denote the linear dual to $\mathcal{HC}_n$. Given a diagram $\Gamma \in \mathcal{HC}_n$, we can find a singular link L_Γ with n intersection points prescribed by the n chords (see [16, Section 5.2]). A type n invariant $V \in \mathcal{HV}_n$ then gives rise to an element of $W(V) \in \mathcal{HC}_n^*$ via the formula

$$\begin{aligned} W\colon \mathcal{HV}_n &\longrightarrow \mathcal{HC}_n^* \\ V &\longmapsto (W(V)\colon \mathcal{HC}_n \to \mathbb{R},\ \Gamma \mapsto V(L_\Gamma)). \end{aligned}$$

In fact, since V is of type n, all choices of L_Γ yield the same value for $V(L_\Gamma)$. Moreover, $W(V)$ lies in the subspace $(\mathcal{HC}_n/(4T, 1T))^*$. The symbol $1T$ stands for all diagrams which contain a chord joining points on the same strand that is not crossed by any other chord. (This relation comes from the fact that we are considering *unframed* links.) The symbol $4T$ stands for all elements of the form on the left side of the equation below:



The pictured strands have the same labels in all four diagrams, but there are no other restrictions on these labels. For example, they may or may not be distinct. We call $(\mathcal{HC}_n/(4T, 1T))^*$ the space of *(homotopy link) weight systems* and often abbreviate it as $\mathcal{HW}_n$. It is not difficult to check that the kernel of W is $\mathcal{HV}_{n-1}$, and we thus have an injection

$$\mathcal{HV}_n/\mathcal{HV}_{n-1} \hookrightarrow (\mathcal{HC}_n/(1T, 4T))^* \tag{1}$$

which we will call the *canonical map* from finite type invariants to weight systems.

2.3.2. *Trivalent diagrams.* To express link invariants in terms of configuration space integrals, one must enlarge the space of chord diagrams to a space of trivalent diagrams (a.k.a. trivalent graphs). We review their definition briefly; for more detail, see [16, Sections 3.1 and 3.3].

Definition 2.3. A *(homotopy link) trivalent diagram* of order n consists of m segments, $2n$ vertices, some of which lie on the segments, and some *edges* between vertices. The vertices which lie on segments are called *segment vertices*, while the others are called *free vertices*. For a diagram Γ, we denote the set of these by $V_{seg}(\Gamma)$ and $V_{free}(\Gamma)$ respectively, and let $V(\Gamma) = V_{seg}(\Gamma) \cup V_{free}(\Gamma)$. We require

- each vertex to be trivalent, where both the edges and segments contribute to the valence of a vertex;
- every vertex to be connected by a path of edges to some segment;
- that no two vertices on the same segment are joined by a path of edges; and
- that the diagram have no closed loops (or equivalently, that the diagram has trivial first homology).

As in the case of chord diagrams, we consider trivalent diagrams up to homeomorphisms which preserve the orientations and labels of the segments.

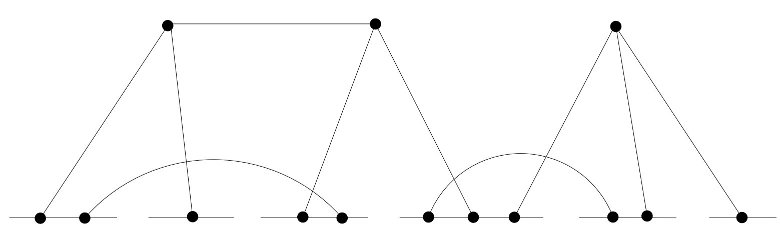
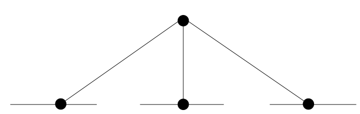


FIGURE 2. A trivalent diagram of order $n = 7$, where the number of segments is $m = 6$.

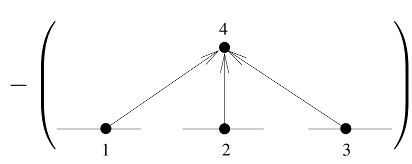
A trivalent diagram Γ as defined above is enough to determine an integral associated to Γ up to sign. To consistently determine signs, we need to add orientations to our diagrams. This means that we add certain decorations to diagrams, but diagrams which differ only in these decorations are set equal, up to sign (see for example [16, Definition 3.11]). Thus the vector space of oriented diagrams is isomorphic to the vector space of the unoriented diagrams defined above (though the isomorphism is canonical only up to signs). Furtheremore, there are multiple equivalent ways of orienting trivalent diagrams, with each way having its own advantage. We chose to define unoriented diagrams first for these reasons. We will use three types of orientations. The first two are used in our constructions and proofs while the third one is only used to translate between the first two:

- One way to orient diagrams is to order the vertices and orient each edge. If Γ and Γ' differ by a permutation σ of the vertices, then Γ is declared to be equal to $(-1)^{\mathrm{sign}(\sigma)}\Gamma'$. If Γ and Γ' differ by the orientation of one edge, then $\Gamma = -\Gamma'$. The advantage of this orientation is that it is most directly related to configuration space integrals. We thus call this an *integration orientation*.
- A second way, often called a *Lie orientation* [17], is to order the half-edges emanating from each vertex. Typically, one specifies such an orientation using a planar embedding of Γ, ordering the half-edges at each vertex counter-clockwise. If Γ and Γ' differ by a permutation σ of half-edges at one vertex, then Γ is declared to be equal to $(-1)^{\mathrm{sign}(\sigma)}\Gamma'$. Note that if Γ is a chord diagram, such an orientation consits of no data at all. The Lie orientation has the advantage that it requires only a planar embedding of a diagram and no labels or arrows. It is equivalent to an integration orientation by considering another orientation as follows.
- A third type of orientation is given by an ordering of the vertices and an ordering of all the half-edges in the diagram. We call this a *half-edge orientation*. If two diagrams Γ, Γ' differ by a permutation σ of either the vertices of the half-edges, then Γ is set equal to $(-1)^{\mathrm{sign}(\sigma)}\Gamma'$. An integration orientation canonically determines such an orientation, as explained in [17, p. 4]. Similarly, a Lie orientation canonically determines such an orientation. The composition of these canonical isomorphisms associates to a Lie orientation a canonical integration orientation.

Example 1. Consider the diagram T which we will refer to as the *tripod*:



Its planar embedding specifies an ordering of the three half-edges emanating from the free vertex and thus a Lie orientation. The canonical corresponding half-edge orientation is given by choosing any labeling of the vertices, say 1, 2, 3 on the segment vertices from left to right, and 4 on the free vertex; this orders the six half-edges (up to an even permutation) by taking the half-edges at vertex 1, 2, and 3 in order and then the three half-edges at 4 in the order given by the planar embedding, say from left to right. To obtain a half-edge orientation coming from an integration orientation, we regroup the half-edges so that they are grouped by edge (in any order) rather than by vertex. This involves 2+1 transpositions in the order of the half-edges. We arrive at the following "integration-oriented" diagram



where each edge's orientation is determined by the order of its half-edges and where the minus sign comes from $(-1)^{2+1}$, i.e., the fact that we performed an odd permutation of half-edges.

Definition 2.4. Let $\mathcal{HT}_n$ denote the vector space generated by trivalent diagrams on $2n$ vertices, oriented as above, modulo the relation that any diagram with multiple edges between a pair of vertices is set to zero. Set $\mathcal{HT} := \bigoplus_{n=0}^{\infty} \mathcal{HT}_n$.

In view of the above discussion, any two types of orientations above yield *canonically* isomorphic vector spaces $\mathcal{HT}_n$. So when we draw diagrams, we will omit labels and arrows and consider them equipped with a Lie orientation. When needed, we will write down the corresponding integration orientation.

One then considers a relation on $\mathcal{HT}_n$, called the *STU relation*, given in Figure 3, where the diagrams are identical outside of the pictured portions.

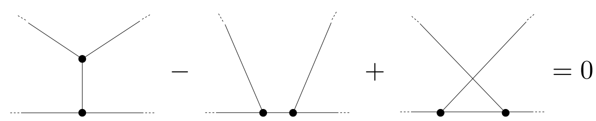


FIGURE 3. The STU relation.

The orientations on the diagrams are the Lie orientations given by the planar embeddings. Modulo the STU relation, one can reduce any trivalent diagram to a sum of chord diagrams, and in fact there is an isomorphism

$$\mathcal{HT}_n/\mathrm{STU} \cong \mathcal{HC}_n/4\mathrm{T}.$$

(See [1, Theorem 6] for the analogous statement for knots; the proof is the same for homotopy links.) Thus we can rewrite the canonical map (1) from finite type invariants to weight systems as

$$\mathcal{HV}_n/\mathcal{HV}_{n-1} \hookrightarrow (\mathcal{HT}_n/(1T, STU))^*. \tag{2}$$

The following theorem may be thought of as the "Fundamental Theorem of Finite Type Invariants" for homotopy links. It is an analogue of a theorem for finite type (isotopy) invariants of knots, first established via the Kontsevich integral [6]. The original theorem for knot invariants can also be proven via configuration space integrals [24], and this is the approach taken in proving the theorem for homotopy links in [16]:

Theorem 2.5 ([16], Theorem 5.8)**.** *The canonical map* (2) *is an isomorphism. Its inverse is given by configuration space integrals (described below in Section 2.5).*

2.3.3. *Unitrivalent diagrams.* By removing each segment i from a trivalent diagram and replacing it by labels i on the vertices which lie on it, one obtains a diagram which is now unitrivalent with each leaf labeled by an element of $\{1, ..., m\}$. Bar-Natan denotes the space of trivalent diagrams $\mathcal{A}$ and the space of unitrivalent diagrams by $\mathcal{B}$. He established an isomorphism ([1, Theorem 8]) between unitrivalent diagrams and trivalent diagrams where the map from the former is given by averaging over all the possible ways of attaching the leaves to their corresponding segments. In Section 4, we will sometimes find it useful to consider these unitrivalent diagrams.

2.4. **The cochain complex of diagrams.** The vector spaces $\mathcal{HT}_n$ are part of a certain cochain complex $\mathcal{HD}$ of homotopy link diagrams, which are not necessarily trivalent.[1] This complex will be used in Section 4.4.

[1]We note however that $\mathcal{HT}$ is *not* a *subcomplex* of $\mathcal{HD}$.

Definition 2.6. Elements of $\mathcal{HD}$ are defined exactly as the elements of $\mathcal{HT}_n$, except that instead of requiring every vertex to have valence three, one requires that every vertex has valence *at least* three. Rather than just counting the number of vertices in a diagram, we define

- the *defect* of a diagram Γ to be $2|E(\Gamma)| - |V_{seg}(\Gamma)| - 3|V_{free}(\Gamma)|$, and
- the *order* of a diagram Γ to be $|E(\Gamma)| - |V_{free}(\Gamma)|)$.

Then let $\mathcal{HD}_n^k$ be the vector space of diagrams of defect k and order n, and let $\mathcal{HD} = \bigoplus_{k,n} \mathcal{HD}_n^k$.

Note that $\mathcal{HT}_n = \mathcal{HD}_n^0$ since trivalence is equivalent to having defect zero. We equip $\mathcal{HD}$ with a differential d which takes Γ to a signed sum of graphs $\sum_i \Gamma_i$ where each Γ_i is obtained by contracting either an edge or an *arc* of Γ. An arc is defined as part of a segment between two vertices. The signs of the Γ_i are determined using integration orientations on diagrams. The differential is a map $\mathcal{HD}_n^k \to \mathcal{HD}_n^{k+1}$. See [16, Definition 3.19] for details.

The importance of the diagram complex $\mathcal{HD}$ is due to the fact that there is a (co)chain map [16, Theorem 4.33]

$$\mathcal{I} : \mathcal{HD}_n^k \longrightarrow \Omega_{dR}^{n(d-3)+k}\mathrm{Link}(\coprod_{i=1}^{m} \mathbb{R}, \mathbb{R}^d) \tag{3}$$

where $\Omega_{dR}^{n(d-3)+k}$ stands for de Rham cochains (i.e. differential forms) of degree $n(d-3)+k$. This induces a map in cohomology. The map is given by associating to each diagram a configuration space integral. These integrals will be reviewed in Section 2.5.

2.4.1. *Describing the cocycles in defect zero.* The space $\mathcal{HW}_n = (\mathcal{HT}_n/(1T, STU))^* \subset \mathcal{HT}_n^*$ of weight systems can be viewed as the dual to the space of cocycles $Z(\mathcal{HD}_n^0) \subset \mathcal{HT}_n$, as follows. Consider the pairing of diagrams, given by

$$\langle \Gamma, \Gamma' \rangle = \begin{cases} |\mathrm{Aut}(\Gamma)|, & \text{if } \Gamma \cong \Gamma'; \\ 0, & \text{otherwise.} \end{cases} \tag{4}$$

Then as in [16, Proposition 3.29], the cocycles in $\mathcal{HD}_n^0$ are precisely the elements α which give 0 when paired with every diagram with a closed loop of edges and which satisfy $\langle S - T + U, \alpha \rangle = 0$ for all S,T,U as in Figure 3. Thus the isomorphism of $\mathcal{HT}^*$ with $\mathcal{HT}_n$ induced by this pairing restricts to an isomorphism of $\mathcal{HW}_n$ with $Z(\mathcal{HD}_n^0)$.[2]

Proposition 2.7. *For any homotopy link diagram* Γ*,* $\mathrm{Aut}(\Gamma) = 1$.

Proof. An automorphism of diagrams must fix all the segment vertices. Now recall that homotopy link diagrams have no cycles. Thus every remaining vertex appears on some path (possibly many) that is the unique path between two segment vertices. □

Remarks 2.8.

(1) As a consequence of this proposition, the pairing above reduces to the Kronecker pairing on diagrams Γ. Then via the identification of the space cocycles $Z(\mathcal{HD}_n^0) = \mathcal{HW}_n^*$ with the space of weight systems $\mathcal{HW}_n$, we can view a cocycle as a linear combination of diagrams such that for every triple of diagrams S, T, U as in Figure 3, the coefficients of these three diagrams sum to zero. We will mostly work in terms of such cocycles rather than the

[2] In [16] we defined the space of weight systems $\mathcal{HW}_n$ as a space of functionals on $\mathcal{HT}_n^*$, rather than on $\mathcal{HT}_n$, to make this isomorphism canonical. Here we have chosen to define $\mathcal{HW}_n$ as a space of functionals on $\mathcal{HT}_n$ to match the early literature on finite-type invariants, such as [1].

associated weight systems from now on. While the relations in the *quotient* $\mathcal{HT}_n/STU$ are often referred to as the *STU relation*, we will use the term *STU condition* to describe the restriction that determines the *subspace* of cocycles in $\mathcal{HT}_n$.

(2) The above proposition does not hold for diagrams in the more general diagram complex $\mathcal{LD}$ in [16].

Considering the cochain map (3) in the special case of defect $k = 0$ and ambient dimension $d = 3$, we then get a map

$$\mathcal{I} : \mathcal{HW}_n^* = Z(\mathcal{HD}_n^0) \longrightarrow \mathrm{H}^0(\mathrm{Link}(\coprod_{i=1}^m \mathbb{R}, \mathbb{R}^3)).$$

Elements in the image lie in $\mathcal{HV}_n$, and the composition of this map followed by the quotient by $\mathcal{HV}_{n-1}$ is essentially the "inverse map" in Theorem 2.5. More precisely, the composite

$$\mathcal{HW}_n^* \xrightarrow{\mathcal{I}} \mathcal{HV}_n \longrightarrow \mathcal{HV}_n/\mathcal{HV}_{n-1} \tag{5}$$

is inverse to the composite

$$\mathcal{HV}_n/\mathcal{HV}_{n-1} \longrightarrow \mathcal{HW}_n \longrightarrow \mathcal{HW}_n^* \tag{6}$$

of the canonical map followed by the isomorphism induced by choosing the basis of diagrams (up to signs). We prefer to use diagrams rather than weight systems (i.e. functionals on diagrams), so it will be convenient for us to view the "canonical map" from link invariants as the composite (6).

Remark 2.9. In [16], two other relations (or dually, conditions) were considered, namely the IHX relation, given in Figure 4, and the H1T relation, which sets diagrams containing closed paths of edges to zero. However, IHX follows from the STU relation [1, Theorem 6, part (2)], while H1T follows from the STU relation and the fact that diagrams with chords joining vertices on the same segment are set to zero [2, p. 7]. Thus we do not need these conditions to characterize cocycles. However, both the H1T and IHX relations/conditions will be important in proving our main result. As mentioned above for the STU relation/condition in Remark 2.8, we do not need to introduce factors of Aut(Γ) when converting between the IHX relation and IHX condition because homotopy link diagrams have no nontrivial automorphisms.

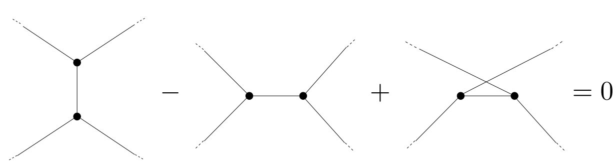


FIGURE 4. The IHX relation.

2.4.2. *The shuffle product.* There is also a product on $\mathcal{HD}$ called the *shuffle product*, defined as follows. Given two diagrams Γ_1 and Γ_2 with q_i and r_i vertices on the i-th segment for $i = 1, ..., m$, let σ be an m-tuple of shuffles, that is, orderings of the $q_i + r_i$ vertices which respect the orderings in Γ_1 and Γ_2. Such a σ specifies a way of attaching the "legs" of Γ_1 and Γ_2 to the m segments to form a new diagram $\Gamma_1 \bullet_\sigma \Gamma_2$. The shuffle product is then defined as

$$\Gamma_1 \bullet \Gamma_2 := \varepsilon(\Gamma_1, \Gamma_2) \sum_\sigma \Gamma_1 \bullet_\sigma \Gamma_2$$

where $\varepsilon(\Gamma_1, \Gamma_2) \in \{\pm 1\}$. In the case that $\Gamma_1, \Gamma_2 \in \mathcal{HT}$, this sign is always $+1$. Since we will focus on diagrams in $\mathcal{HT}$, we omit the general definition of ε here. This shuffle product is graded-commutative and the differential d is a derivation with respect to this product. For details, see [16, Section 3.2.2], or [4, Section 3.1] for just the case of knots.

The following lemma is an important ingredient in the proof of our main result, Theorem 4.10. For a proof, see for example, the proof of Proposition 4.29 in [16]. Recall the discussion of the product of finite type homotopy string link invariants from the end of Section 2.2.

Lemma 2.10. *Via the isomorphisms $\mathcal{HW}_n^* \cong \mathcal{HV}_n/\mathcal{HV}_{n-1}$ from Theorem 2.5 (see the maps (5) and (6)), the shuffle product of diagrams corresponds to the product of finite type link invariants.* □

Remark 2.11. A proof of this fact appears in [KMV], but this shuffle product appears in earlier literature, such as [CCRL], [Tur], and even earlier, in a different guise, in [BN95]. This statement appears to be contained in [BN95, Exercise 3.10]. In that paper, invariants correspond to functionals on diagrams (weight systems), rather than the diagrams themselves, so the product of invariants corresponds to a product on such functionals, which is a *coproduct* on diagrams. For proving our result, we find it more convenient to think in terms of products of diagrams.

2.5. **Configuration space integrals.** We now review the generalization of the configuration space integrals of Bott and Taubes [3] to homotopy string links from [16]. However, we will do this for *embedded* string links, that is the space $\mathrm{Emb}(\coprod_1^m \mathbb{R}, \mathbb{R}^3)$ of embeddings of $\coprod_1^m \mathbb{R}$ in $\mathbb{R}^3$ with prescribed linear behavior outside of $\coprod_{i=1}^m [-1,1]$. This situation will illustrate all the main features of the construction and will avoid various technical issues that arise when dealing with homotopy string links (i.e. link maps instead of embeddings). In addition, the case of embeddings suffices for understanding the examples that appear in Section 3. We will then at the end of this section indicate what modifications are required for the case of homotopy string links.

Fix a trivalent diagram Γ with labeled vertices and oriented edges. Recall from the discussion following Definition 2.3 that a Lie orientation on Γ can be used to produce vertex labels and edge orientations (up to even permutations of the vertex labels and an even number of edge reversals). Suppose Γ has q_i vertices on the i-th segment and t free vertices. Consider the pullback square

(7)
$$\begin{array}{ccc} E[q_1, \ldots q_m; t] & \longrightarrow & C_{q_1+\cdots+q_m+t}[\mathbb{R}^3] \\ \downarrow & & \downarrow \\ \mathrm{Emb}(\coprod_1^m \mathbb{R}, \mathbb{R}^3) \times C_{q_1,\ldots,q_m}[\coprod_1^m \mathbb{R}] & \longrightarrow & C_{q_1+\cdots+q_m}[\mathbb{R}^3] \end{array}$$

Here

- The spaces $C_{q_1+\cdots+q_m}[\mathbb{R}^3]$ and $C_{q_1+\cdots+q_m+t}[\mathbb{R}^3]$ are the Axelrod–Singer compactifications of configuration spaces of $q_1 + \cdots + q_m$ and $q_1 + \cdots + q_m + t$ points in $\mathbb{R}^3$, respectively (see [16, Section 4]).
- The right vertical map is given by forgetting the last t points.
- The space $C_{q_1,\ldots,q_m}[\coprod_1^m \mathbb{R}]$ is a compactification of the configuration space of $q_1 + \cdots + q_m$ points, q_i of which are on the i-th copy of $\mathbb{R}$, which records all the relative rates of approach to infinity (see [16, Section 4]).
- The bottom horizontal map comes from the fact that an embedding of X into Y induces a map from configurations in X to configurations in Y.

Then we have the bundle

$$E[q_1, \ldots q_m; t] \longrightarrow \mathrm{Emb}(\coprod_1^m \mathbb{R}, \mathbb{R}^3)$$

given by the left vertical map in (7) followed by projection onto the first factor. Write $F = F[q_1, ..., q_m; t]$ for its fiber, which is a compactified configuration space of $q_1 + \cdots + q_m + t$ points in $\mathbb{R}^3$, q_i of which lie on the i-th strand of the given link and t of which can be anywhere in $\mathbb{R}^3$, including on the link. This fiber is a (finite-dimensional) manifold with corners.

There are maps

$$\varphi_{ij} : C_{q_1+\cdots+q_m+t}[\mathbb{R}^3] \longrightarrow S^2$$

given by the direction between the i-th and j-th configuration point. Via φ_{ij}, one can pull back the volume form sym_{S^2} on S^2 to $C_{q_1+\cdots+q_m+t}[\mathbb{R}^3]$ and then further to $E[q_1, ...q_m; t]$. Let θ_{ij} denote the resulting spherical form on $E[q_1, ...q_m; t]$. For our fixed diagram Γ, take the product β of all θ_{ij} such that vertices i and j are endpoints of an edge in Γ. Then let I_Γ be the integral of β over the fiber $F = F[q_1, ..., q_m; t]$ of the bundle above:

$$I_\Gamma = \int_F \beta = \int_{F[q_1,\ldots,q_m;t]} \prod_{\text{edges } ij \text{ of } \Gamma} \theta_{ij} \tag{8}$$

For details, the reader should consult [16, Section 4.4].

Thus I_Γ is a differential form on $\mathrm{Emb}(\coprod_1^m \mathbb{R}, \mathbb{R}^3)$. It is a 0-form, but it need not be closed, i.e. it need not be an invariant, because the fiber has boundary. Indeed, Stokes' theorem implies that $d\int_F \beta = \int_{\partial F} \beta$. However, taking appropriate linear combinations $I_{\sum \Gamma} := \sum I_\Gamma$ for various trivalent diagrams Γ leads to cancellation of the integrals along the boundaries of the fibers, and thus isotopy invariants. The linear combinations of diagrams Γ that produce invariants in this way are precisely the cocycles in the graph complex. In fact, the (isotopy analogue of the) map $\mathcal{I}$ appearing in the composite (5) is given by $\Gamma \mapsto I_\Gamma$; that composite (5) is the inverse map which establishes Theorem 2.5, the Fundamental Theorem of Finite Type Invariants.

In [16], the authors showed how to extend configuration space integrals to homotopy string links, that is, link maps which are not necessarily embeddings (for embeddings, one considers more general trivalent diagrams than described in Definition 2.3; they are essentially obtained by removing the condition that no two vertices on the same segment are joined by a path of edges). To adapt the construction to homotopy string links, one first takes into account the edges, as well as vertices, when making the compactified configuration spaces. More precisely, $C_{q_1+\cdots+q_m}[\mathbb{R}^3]$ and $C_{q_1+\cdots+q_m+t}[\mathbb{R}^3]$ are replaced by configuration spaces where one removes (and compactifies along) only those diagonals for which there exists a corresponding edge in Γ (see [16, Section 4.2.4]). In addition, the target of the bottom map (evaluation) in (7) is not simply $C_{q_1+\cdots+q_m}[\mathbb{R}^3]$ but the product of compactified configuration spaces determined by the *grafts* of Γ, namely the connected components of Γ obtained upon removing the segments (i.e. upon turning the trivalent diagram Γ into a unitrivalent diagram, in the language of Section 2.3.3). For details, see [16, Section 4.2.3]. This setup for link maps reduces to what has been described above in the case when the link map is an embedding.

The modification of configuration space integals to homotopy string links then provides the inverse in the link-homotopy version of the Fundamental Theorem of Finite Type Invariants, given in Theorem 2.5.

2.6. **Milnor's link homotopy invariants.** For each tuple $(i_1, ..., i_r, j)$ with $i_1, ..., i_r, j \in \{1, ..., m\}$, there is a Milnor invariant $\mu_{i_1,\ldots,i_r,j}$. Provided all the indices $(i_1, ..., i_r, j)$ are distinct, $\mu_{i_1,\ldots,i_r,j}$ is a link homotopy invariant of m-component string links [20]. The invariant $\mu_{i_1,\ldots,i_r,j}$ is defined as follows. The fundamental group of the link complement is generated by the meridians $m_1, m_2, ...$ of the components and their conjugates. The quotient by any term in the lower central series is generated by the m_i themselves [21]. So in this quotient, the j-th longitude can be written as a word w_j in the m_i. One then considers the Magnus expansion, which is a homomorphism from the free group on the m_i to the ring of power series in noncommuting variables $t_1, ..., t_m$. This map sends m_i to $1+t_i$ and m_i^{-1} to $1-t_i+t_i^2-\cdots$. Finally, one considers the image of w_j under this map and takes $\mu_{i_1,...,i_r,j}$ to be the coefficient of $t_{i_1}\cdots t_{i_r}$ in this power series. This number is well defined, provided one works modulo the n-th term in the lower central series with $n \geq r$. The dimension of the space of Milnor (link homotopy) invariants of n-component links is $(n-2)!$ [20].

The invariant $\mu_{i_1,...,i_r,j}$ is finite type of order r. There are several proofs in the literature [2, 18], so we will not provide one here. From now on, we will use the term "Milnor invariant" to refer to Milnor invariants with distinct indices, i.e. the link homotopy invariants. The simplest example is the case $r = 1$, where $\mu_{i;j}$ is the pairwise linking number of the i-th and j-th strands (which is a finite type 1 invariant). The next example is that of the *triple linking number* $\mu_{i_1,i_2;j}$ which has been the subject of much investigation, especially in recent years [22, 23, 8, 9, 19]. We will revisit both the linking number and the triple linking number in Section 3 from the configuration space integral point of view.

Each invariant $\mu_{i_1,...,i_r;j}$ is also an invariant of the $(r+1)$-component sublink determined by the strands labeled $i_1, ..., i_r, j$. Thus to study a given Milnor invariant, we may restrict to type n invariants of $(n+1)$-component string links, and from now on $m = n+1$.

3. Examples in low degrees

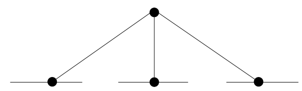
Before proving our theorem, we will illustrate it with the examples in the several lowest orders. The idea is as follows: Our main result, Theorem 4.10, leads to a correspondence between Milnor invariants and linear combinations of trivalent trees. Given a Milnor invariant, such a linear combination of trees is part of the integral formula for that invariant. The STU relation is not quite enough to determine the rest of the formula, but it is enough to determine the formula up to products of lower-order invariants. (The products of lower-order invariants correspond to cocycles in the graph complex which are linear combinations of *forests*.)

3.1. **The pairwise linking number.** The only type 1 invariant (of unframed string links) is the pairwise linking number. This invariant corresponds to a diagram with one chord with one endpoint on each of two segments. Thus, at this order, the correspondence between link homotopy invariants and trivalent trees is clear. The linking number can then be written as the integral associated to this one diagram, and this is essentially the Gauss linking integral (though for long links instead of closed links). That is, the linking number of strands i and j of a link L is

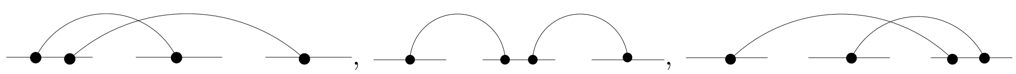
$$\mathrm{lk}(L_i, L_j) = (I_{\mathcal{H}})_\Gamma(L) = (I_{\mathcal{L}})_\Gamma(L) = \int_{C[1,1;\mathbb{R}\sqcup\mathbb{R}]} \left(\frac{L(x)-L(y)}{|L(x)-L(y)|}\right)^* \omega$$

where ω is the volume form on S^2 and $C[1,1;\mathbb{R}\sqcup\mathbb{R}]$ is the compactified configuration space of two points, one on each copy of $\mathbb{R}$; this compactified configuration space is just an octagonal disk (see [15, Section 1.2] for details).

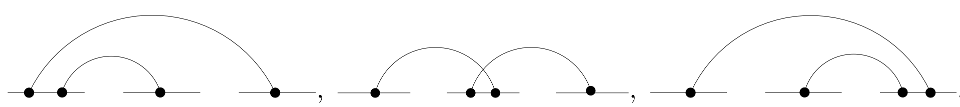
3.2. **The triple linking number.** For our discussion of invariants of type 2 or higher, it will be convenient to recall Lemmas 2.1 and 2.10, which respectively concern products of finite type invariants and products of graph cocycles. Recall also from Section 2.6 that the dimension of the space of Milnor (link homotopy) invariants of n-component links is $(n-2)!$ and that any such invariant is of type $n-1$. Thus at finite type 2, the space of Milnor invariants of 3-component links is one-dimensional, and we call a generator the triple linking number μ_{123}. Recall also that type n invariants correspond to diagrams with $2n$ vertices. It is easy to see that the space of trivalent trees on $2 \cdot 2 = 4$ vertices with leaves on distinct segments (modulo the IHX relation) also has one generator. It is the tripod T, mentioned earlier in Section 2.3.2 and pictured below:



Based on the correspondence of Habegger and Masbaum between Milnor invariants and such trivalent trees, one might naively expect the triple linking number to be given by the integral associated to T. However, the graph cocycle α_{123} for μ_{123} contains some chord diagrams as well. Thus the configuration space integral for μ_{123} has more terms than just the integral associated to T. Mellor established a recursive formula [18, Theorem 2] for calculating the weight system of any Milnor invariant. In [15], the first author used this formula to calculate the values of the weight system W_{123} for μ_{123}, or equivalently the graph cocycle α_{123}. A priori, there are, in addition to T, six link homotopy diagrams that touch all three segments and which one might thus expect to appear in α_{123}. They are the diagrams L, M, R,



and the diagrams L', M', R',



Applying Mellor's formula shows that $\alpha_{123} = L - M + R - T$ [15, Section 3.1]. (One can also use Mellor's formula to check that no other (chord) diagrams of order 2 appear in α_{123}.)

Thus in terms of configuration space integrals,

$$\mu_{123} = I_L - I_M + I_R - I_T \tag{9}$$

where the terms I_Γ above are the integrals over compactified configuration spaces associated to the diagrams $\Gamma = L, M, R, T$ as in (8): [3]

$$I_L = -\int_{F[2,1,1;0]} \theta_{13}\theta_{24} \qquad I_M = \int_{F[1,2,1;0]} \theta_{12}\theta_{34}$$

$$I_R = -\int_{F[1,1,2;0]} \theta_{13}\theta_{24} \qquad I_T = -\int_{F[1,1,1;1]} \theta_{14}\theta_{24}\theta_{34}$$

From the geometry of configuration space integrals, it makes sense that this is the formula for the triple linking number. Namely, the configuration space captured schematically by T – four points in $\mathbb{R}^3$, three of which are constrained to lie on the three strands of the string link – has three boundary components given by the free point colliding with the points on the link strands. There is no reason for the integral I_T over these boundary components to vanish, so the integral is not necessarily an invariant. However, each of the spaces corresponding to diagrams L, M, and R also has a boundary component given by the collision of two points on the same strand. The restrictions of the integrals I_L, I_M, and I_R to those boundaries thus precisely cancel the three boundary contributions from I_T in the sum above.

[3] Erratum to [15] regarding signs: The minus signs above come from the correspondence between Lie orientations and "integration orientations." In [15], these minus signs were erroneously absent. This was due to an erroneous identification of Lie orientations with integration orientations in the paragraph before Remark 3.1 of that paper. (However, all the signs in the two versions of the STU relation in that paper are correct, as are the calculated values of W_{123} on the Lie-oriented diagrams.)

A futher evidence that it is necessary to consider all four integrals is given by the fact that it is not hard to find a string link (even one with zero pairwise linking numbers) for which at least one of the integrals associated to L, M, R does not vanish. So the configuration space integral for μ_{123} is not merely I_T or $-I_T$ even in special cases. Nor does the STU condition give the coefficients of the other diagrams from the coefficient of T. However, one can ultimately conclude in this low-order example that the coefficient of T together with the STU condition *does* determine the coefficients of L, M, R, L', M', R' *up to linear combinations of* $\{L+L', M+M', R+R'\}$. By Lemma 2.10, these three elements correspond (up to sign) to the products of pairwise linking numbers. This is the first nontrivial example of our more general main result, and the "up to products of pairwise linking numbers" caveat is a good indicator of the type of statement we will establish in Section 4.

Contrast formula (9) with the formula of Habegger and Masbaum [11], which says that for a link with no pairwise linking, μ_{123} is given by just the Kontsevich integral for the tripod, i.e. the coefficient of T in the Kontsevich integral. This is essentially because in their setting, T is considered in the *quotient* of the diagram space by the STU relation. One could dualize to the corresponding "STU subspace" of diagrams in the graph complex (i.e., find the orthogonal complement to the STU relation) and ultimately reach the same conclusion as above regarding the possible diagrams in α_{123} in this example. However, the purpose of our work is to perform this combinatorial analysis more directly and systematically for all Milnor invariants and provide a clear correspondence between the diagrams appearing in the indeterminacy and products of lower-order Milnor invariants.

3.3. **The "quadruple linking numbers".** At finite type 3, Mellor's formula reveals that the graph cocycle α_{1234} for the invariant μ_{1234} has 24 terms, including 13 of the 72 chord diagrams, 9 of the 24 diagrams with one free vertex, and 2 of the 3 four-leaved trivalent trees. This points to the potential difficulty of quickly finding the integral formula for an arbitrary Milnor invariant. (This latter objective is the subject of work in progress of the authors and R. Komendarczyk.) Note however that there are only 3 isomorphism classes of trivalent trees with four leaves, distinctly labeled by 1, 2, 3, 4. The IHX relation says that the (signed) sum of these is zero, so the dimension of the space of these trees modulo IHX is 2. This is also the number of type 3 Milnor invariants of 4-component string links. Our main result will say that a set of coefficients of these trees which satisfy the IHX condition almost determines a sum of type 3 Milnor invariants; in fact, these coefficients determine it up to adding type-2 invariants, namely triple linking numbers and products of pairwise linking numbers.

4. Main Results

As mentioned in Section 2.6, to study type n Milnor invariants it suffices to only consider links with $n+1$ strands, so now let $\mathcal{HV}_n$ be the vector space of type n finite type, link homotopy invariants of string links on $n+1$ strands. This space contains type n Milnor invariants, as well as products of lower-order invariants, as guaranteed by Lemma 2.1.

4.1. The main definitions.

Definition 4.1. For any $k = 1, ..., n$, let $\mathcal{HV}_n^k$ be the subspace of $\mathcal{HV}_n/\mathcal{HV}_{n-1}$ spanned by the following type n invariants of $(n+1)$-component links: a generating element of $\mathcal{HV}_n^k$ is represented by a product of at least k Milnor invariants.

Since $\mathcal{HV}_n^k$ is a subspace of $\mathcal{HV}_n/\mathcal{HV}_{n-1}$, we may take the generating elements to be type n products of at least k Milnor invariants (since products which are of type less than n are set to 0 in this quotient).

If $r_1, ..., r_\ell$ are the orders of the ℓ invariants in such a product (with $\ell \geq k$), then by Lemma 2.1, we necessarily have $r_1 + \cdots + r_\ell = n$. Thus we may write $\mathcal{HV}_n^n \subset \cdots \subset \mathcal{HV}_n^1 \subset \mathcal{HV}_n/\mathcal{HV}_{n-1}$.

Similarly, we define the corresponding subspaces of the space of cocycles $\mathcal{HW}_n^*$.

Definition 4.2. Let $\mathcal{HW}_n^k$ denote the subspace of $\mathcal{HW}_n^*$ spanned by diagrams with at most k free vertices.

For ease of notation, we have omitted the $*$ in $\mathcal{HW}_n^k$, since we will now focus on $\mathcal{HW}_n^*$, the space of diagrams, and leave $\mathcal{HW}_n$, the space of weight systems, out of the picture.

We may write $\mathcal{HW}_n^0 \subset \mathcal{HW}_n^1 \cdots \subset \mathcal{HW}_n^{n-1} \subset \mathcal{HW}_n^*$. We claim that $\mathcal{HW}_n^{n-1} = \mathcal{HW}_n^*$. In fact, this can be seen using the H1T relation (that homotopy link diagrams have no cycles – see Remark 2.9), together with the following elementary lemma, where the trivalent vertices below are precisely the free vertices in our setup.

Lemma 4.3. *A trivalent tree on* $2n$ *vertices has exactly* $n-1$ *trivalent vertices. A trivalent forest on* $2n$ *vertices has at most* $n-1$ *trivalent vertices. Consequently, a trivalent forest on* $2n$ *vertices has at least* $n+1$ *leaves.*

Proof. First note that by valence considerations, a trivalent tree always has an even number of vertices. The statement about trivalent trees can then be proven easily by induction on n. A trivalent forest with $2n_1, ..., 2n_m$ vertices (where $n_1 + \cdots + n_m = n$) then has

$$(n_1 - 1) + \cdots + (n_m - 1) = n - m \leq n - 1$$

trivalent vertices. □

Finally, notice that the shuffle product of diagrams (or cocycles) restricts to maps

$$\mathcal{HW}_r^k \times \mathcal{HW}_s^\ell \longrightarrow \mathcal{HW}_{r+s}^{k+\ell}$$

while Lemma 2.1 shows that the product of invariants restricts to maps

$$\mathcal{HV}_r^k \times \mathcal{HV}_s^\ell \longrightarrow \mathcal{HV}_{r+s}^{k+\ell}.$$

4.2. **Describing the filtration quotients in terms of products.** We will now give a more detailed description of the cocycles $\mathcal{HW}_n^*$. We start by a review of the subspace of cocycles made up of *connected*, or *tree*, diagrams, meaning diagrams whose underlying unitrivalent diagrams are connected.

Lemma 4.4.

(1) *For* $n \geq 2$, *the vector space*

$$\mathcal{HW}_{n+1}^n/\mathcal{HW}_{n+1}^{n-1} = \mathcal{HW}_{n+1}/\mathcal{HW}_{n+1}^{n-1}$$

is spanned by connected diagrams.

(2) *This space is isomorphic to the space of linear combinations of (label-preserving isomorphism classes of) trivalent trees with* $n+2$ *leaves with distinct labels from the set* $\{1, ..., n+2\}$ *which satisfy (all) the IHX condition(s).*

(3) *The dimension of this space is* $n!$.

We say "(all) the IHX condition(s)" to emphasize that IHX condition is actually many conditions. This will be useful to remember when we apply linear algebra to these relations.

Proof. First note that diagrams in $\mathcal{HW}_{n+1}$ can be viewed as trivalent forests with labeled leaves (as loops of edges are not allowed), where labels correspond to the segments that the leaves are on. By Lemma 4.3, such a diagram with exactly n free vertices must be a tree. This proves statement (1).

For statement (2), we need to know (a) that elements of $\mathcal{HW}^n_{n+1}/\mathcal{HW}^{n-1}_{n+1}$ satisfy the IHX conditions and (b) that the IHX conditions are the *only* conditions defining this subspace. Both of these facts are proven in Bar-Natan's original paper [1] on finite type invariants (by dualizing between our "conditions" and his "relations"). Part (a) (i.e., that IHX implies STU) is similar to showing that a commutator in an associative algebra satisfies the Jacobi identity [1, Section 3.1]. Part (b) is considerably more involved and is part of [1, Theorem 8]. Statement (3) is the third part of Theorem 3 of [2]. □

The main purpose of this subsection is the following result. By Lemma 4.4, it says that $\mathcal{HW}^k_n/\mathcal{HW}^{k-1}_n$ is spanned by shuffle products of linear combinations of leaf-labeled trivalent trees such that each linear combination satisfies all of the IHX conditions.

Proposition 4.5. *The space $\mathcal{HW}^k_n/\mathcal{HW}^{k-1}_n$ is spanned by shuffle products of linear combinations of tree diagrams which satisfy the IHX conditions.*

Remarks 4.6.

(1) Note that this proposition is true only at the level of the filtration quotients $\mathcal{HW}^k_n/\mathcal{HW}^{k-1}_n$, and not at the level of $\mathcal{HW}^*_n$ itself. For example, we saw in Section 3 that the cocycle for the triple linking number is $\alpha_{123} := L - M + R - T$, which itself is not a linear combination of shuffle products of tree diagrams.

(2) Proposition 4.5 is in a way dual to Bar-Natan's description of $\mathcal{HW}_n$ as a polynomial algebra on leaf-labeled trivalent trees, which is the first part of Theorem 3 in [2]. However, the previous remark and the examples in Sections 3.2 and 3.3 show that one cannot merely take shuffle products of such trees to produce cocycles of diagrams and hence configuration space integral expressions for invariants.

Before we prove Proposition 4.5, we will need a few lemmas. We start by showing that $\mathcal{HW}^k_n/\mathcal{HW}^{k-1}_n$ is spanned by shuffle products of cochains (i.e., arbitrary linear combinations of diagrams).

Lemma 4.7. *The space $\mathcal{HW}^k_n/\mathcal{HW}^{k-1}_n$ is spanned by shuffle products of tree diagrams.*

Proof. An element $\alpha \in \mathcal{HW}^k_n/\mathcal{HW}^{k-1}_n$ can be represented by a linear combination $\sum_i a_i\Gamma_i$ of trivalent diagrams Γ_i with exactly k free vertices. Partition the Γ_i according to their underlying unitrivalent diagrams. Let $\mathcal{U}(\Gamma)$ denote the equivalence class of Γ in this partition. Next construct for each class $\mathcal{U}(\Gamma)$ an auxiliary "STU graph," with a vertex for each diagram $\Gamma' \in \mathcal{U}(\Gamma)$ and an edge between Γ' and Γ'' when there is an STU relation involving these two diagrams. (Necessarily, the two chord diagrams Γ', Γ'' are the diagrams T and U, since they have the same number of free vertices.) Notice that for each $\mathcal{U}(\Gamma)$, this STU graph is connected; in fact, any two trivalent diagrams in the same equivalence class are related by a sequence of moves, where each move swaps adjacent "legs" on the same segment, and in each such move, the two diagrams are T and U in some STU relation. As a result, the STU relation together with the fact that α has no diagrams with more than k free vertices imply that for each $\mathcal{U}(\Gamma)$, the coefficients of *all* the diagrams in $\mathcal{U}(\Gamma)$ are determined by any one of them. So the dimension of $\mathcal{HW}^k_n/\mathcal{HW}^{k-1}_n$ is at most the dimension of the space of shuffle products of connected diagrams. Furthermore, any such shuffle product represents an element of $\mathcal{HW}^k_n/\mathcal{HW}^{k-1}_n$. □

To prove that $\mathcal{HW}_n^k/\mathcal{HW}_n^{k-1}$ is spanned by shuffle products of cocycles, we need the following two basic linear algebra facts.

Lemma 4.8. *Let $V = V_1 \otimes \cdots \otimes V_\ell$ be a tensor product of finite-dimensional inner product spaces $V_1, ..., V_\ell$, equipped with the resulting inner product. For each i, let $U_i \subset V_i$ be a subspace. Then*

$$(U_1 \otimes V_2 \otimes \cdots \otimes V_\ell)^\perp \cap (V_1 \otimes U_2 \otimes V_3 \otimes \cdots \otimes V_\ell)^\perp \cap \cdots \cap (V_1 \otimes \cdots \otimes V_{\ell-1} \otimes U_\ell)^\perp = U_1^\perp \otimes \cdots \otimes U_\ell^\perp.$$

Proof. First prove the statement for $\ell = 2$ by counting dimensions and then prove the statement for any ℓ using the case $\ell = 2$ and induction. We leave the details to the reader. □

Lemma 4.9. *Let V be a finite-dimensional vector space with a basis and the resulting inner product. Let U be a subspace. Equip the m-fold symmetric power $S^m(V)$ with the inner product associated to the basis for $S^m(V)$ given by monomials in the basis for V. Let (U) denote the ideal in $S^m(V)$ generated by U, i.e. the image of $U \otimes V^{\otimes(m-1)}$ in $S^m(V)$. Then*

$$(U)^\perp \cong S^m(U^\perp).$$

Proof. By writing $V = U \oplus U^\perp$, it is easy to see that $S^m(V) = (U) \oplus S^m(U^\perp)$. □

We can now prove the main result of this section.

Proof of Proposition 4.5. We first describe $\mathcal{HW}_n^k/\mathcal{HW}_n^{k-1}$ in a slightly different way. The shuffle product is commutative, but we can order the factors in a product by ordering the set of subsets of leaves. Let $I \subset \{1, ..., n+1\}$ be a subset with $|I| \geq 2$. Let $\mathcal{T}_I$ denote the vector space with basis given by trivalent trees with leaves labeled by elements of I. Put an(y) ordering $<$ on the set of such I. By Lemma 4.4 (1), if we let $i = |I|$, we can identify $\mathcal{HW}_{i+1}^i/\mathcal{HW}_{i+1}^{i-1}$ with a subspace of $\mathcal{T}_I$. Then by viewing elements of the right side below as shuffle products of trivalent trees, Lemma 4.7 says that

$$\mathcal{HW}_n^k/\mathcal{HW}_n^{k-1} \subset V := \bigoplus_{\substack{I_1 < \cdots < I_\ell \\ n_1(|I_1|-1)+\cdots+n_\ell(|I_\ell|-1)=n}} S^{n_1}(\mathcal{T}_{I_1}) \otimes \cdots \otimes S^{n_\ell}(\mathcal{T}_{I_\ell}), \tag{10}$$

where the number ℓ of factors in the tensor product may vary over the direct sum.

Each $\mathcal{T}_I$ has a basis of trees (up to sign), which gives an inner product on each $\mathcal{T}_I$, given by $\langle T_i, T_j \rangle = \delta_{ij}$ for basis elements $T_i, T_j \in \mathcal{T}_I$. These basis elements also produce a basis for V (given by tensors of basis elements), and an inner product $\langle\, , \rangle : V \otimes V \to \mathbb{R}$.

Let $U_j \subset \mathcal{T}_{I_j}$ be the subspace generated by all possible IHX linear combinations, so that $U_j^\perp$ can be identified with $\mathcal{HW}_{i+1}^i/\mathcal{HW}_{i+1}^{i-1}$. As before, let (U_j) denote the ideal generated by U_j in a symmetric power $S^m(\mathcal{T}_{I_j})$. Then by Lemma 4.4, $\mathcal{HW}_n^k/\mathcal{HW}_n^{k-1}$ is precisely the subspace of the direct sum in (10) given by

$$\bigoplus_{\substack{I_1 < \cdots < I_\ell \\ n_1(|I_1|-1)+\cdots+n_\ell(|I_\ell|-1)=n}} ((U_1) \otimes \mathcal{T}_{I_2} \otimes \cdots \otimes \mathcal{T}_{I_\ell})^\perp \cap \cdots \cap (\mathcal{T}_{I_1} \otimes \cdots \otimes \mathcal{T}_{I_{\ell-1}} \otimes (U_\ell))^\perp.$$

Applying Lemma 4.8 and then Lemma 4.9 to each summand, we have

$$\mathcal{HW}_n^k/\mathcal{HW}_n^{k-1} \cong \bigoplus_{\substack{I_1 < \cdots < I_\ell \\ n_1(|I_1|-1)+\cdots+n_\ell(|I_\ell|-1)=n}} S^{n_1}(U_1^\perp) \otimes \cdots \otimes S^{n_\ell}(U_\ell^\perp). \tag{11}$$

In words, $\mathcal{HW}_n^k/\mathcal{HW}_n^{k-1}$ is spanned by shuffle products of linear combinations of trivalent trees, where each linear combination satisfies (all) the IHX condition(s). □

4.3. **Deducing the main theorem.** We are now ready to state and prove our main theorem.

Theorem 4.10. *For every* $k = 0, 1, ..., n-1$*, the isomorphism*

$$\mathcal{HV}_n/\mathcal{HV}_{n-1} \cong \mathcal{HW}_n^*$$

from Theorem 2.5 (given by the composite (6) of the canonical map (2) and linear dual in one direction, and configuration space integrals (5) in the other) restricts to an isomorphism of subspaces

$$\mathcal{HV}_n^{n-k} \cong \mathcal{HW}_n^k.$$

Proof. We proceed by induction on k.

The base case. For $k = 0$, we have that $\mathcal{HV}_n^n$ is spanned by products of n pairwise linking numbers (since those are the only type 1 invariants). By Lemma 2.10, the graph cocycles corresponding to these invariants are (linear combinations of) shuffle products of chords and hence contained in $\mathcal{HW}_n^0$. Thus the restriction of the canonical isomorphism $\mathcal{HV}_n/\mathcal{HV}_{n-1} \to \mathcal{HW}_n^*$ is an injection $\mathcal{HV}_n^n \to \mathcal{HW}_n^0$. By Proposition 4.5, it is also a surjection. Note that we have established the base case for all n.

The inductive step. Suppose we know that the canonical map restricts to an isomorphism $\mathcal{HV}_n^{n-j} \to \mathcal{HW}_n^j$ for all $j < k$ and for all n. We will complete the induction by showing that there is an isomorphism $\mathcal{HV}_n^{n-k}/\mathcal{HV}_n^{n-k+1} \to \mathcal{HW}_n^k/\mathcal{HW}_n^{k-1}$; indeed, since all the spaces involved are free modules, this will imply

$$\mathcal{HV}_n^{n-k} \cong \mathcal{HV}_n^{n-k}/\mathcal{HV}_n^{n-k+1} \oplus \mathcal{HV}_n^{n-k+1} \cong \mathcal{HW}_n^k/\mathcal{HW}_n^{k-1} \oplus \mathcal{HW}_n^{k-1} \cong \mathcal{HW}_n^k.$$

Part 1: Trivalent trees. We first need to consider the space $\mathcal{HV}_{k+1}^1/\mathcal{HV}_{k+1}^2$. By definition this space is spanned by the type $k+1$ Milnor invariants of $(k+2)$-component string links. As mentioned in Section 2.6, this space has dimension $k!$. By Lemma 4.4, the space $\mathcal{HW}_{k+1}^k/\mathcal{HW}_{k+1}^{k-1}$ has dimension $k!$ Thus $\dim(\mathcal{HV}_{k+1}^1/\mathcal{HV}_{k+1}^2) = \dim(\mathcal{HW}_{k+1}^k/\mathcal{HW}_{k+1}^{k-1})$.

Now restricting the canonical map $\mathcal{HV}_{k+1}/\mathcal{HV}_k \hookrightarrow \mathcal{HW}_{k+1}$ to $\mathcal{HV}_{k+1}^1$ gives an injection

$$\mathcal{HV}_{k+1}^1 \hookrightarrow \mathcal{HW}_{k+1}^k = \mathcal{HW}_{k+1} \tag{12}$$

By the induction hypothesis, $\mathcal{HV}_{k+1}^2$ maps isomorphically to $\mathcal{HW}_{k+1}^{k-1}$. Thus the kernel of $\mathcal{HV}_{k+1}^1 \to \mathcal{HW}_{k+1}^k/\mathcal{HW}_{k+1}^{k-1}$ is precisely $\mathcal{HV}_{k+1}^2$, and we have an injection

$$\mathcal{HV}_{k+1}^1/\mathcal{HV}_{k+1}^2 \hookrightarrow \mathcal{HW}_{k+1}^k/\mathcal{HW}_{k+1}^{k-1}. \tag{13}$$

Since these two spaces have the same dimension, the map is an isomorphism. Note that by the induction hypothesis, the same statement holds true if we replace k by any $j \leq k$. We will use this fact in Part 2 below.

Part 2: Trivalent forests. Consider $\mathcal{HV}_n^{n-k}$. We will first check that the canonical map takes this subspace into $\mathcal{HW}_n^k$. The space $\mathcal{HV}_n^{n-k}$ is spanned by type n (order n) products of at least $n-k$ Milnor invariants. Denote the orders of the factors in such a product by $r_1, ..., r_\ell$, where $\ell \geq n-k$. Then by Lemma 4.3, every diagram in the graph cocycle for the j-th factor has at least $r_j + 1$ segment vertices. The cocycle for the product of these ℓ invariants is a shuffle product of ℓ such cocycles and thus has at least $\sum_{j=1}^{\ell}(r_j+1)$ segment vertices. But $\sum_{j=1}^{\ell} r_j = n$, so the resulting cocycle has at least $n+\ell$ segment vertices and hence at most $n-\ell$ free vertices. Finally $\ell \geq n-k$ yields $n-\ell \leq k$, meaning that the resulting cocycle of a basis element of $\mathcal{HV}_n^{n-k}$ has at most k free vertices and is thus an element of $\mathcal{HW}_n^k$. Thus the canonical map $\mathcal{HV}_n/\mathcal{HV}_{n-1} \hookrightarrow \mathcal{HW}_n^*$ indeed takes $\mathcal{HV}_n^{n-k}$ into $\mathcal{HW}_n^k$.

Its restriction $\mathcal{HV}_n^{n-k} \to \mathcal{HW}_n^k$ is injective, and by the induction hypothesis, $\mathcal{HV}_n^{n-k+1}$ maps isomorphically to $\mathcal{HW}_n^{k-1}$. As a result, we have an injection

$$\mathcal{HV}_n^{n-k}/\mathcal{HV}_n^{n-k+1} \hookrightarrow \mathcal{HW}_n^k/\mathcal{HW}_n^{k-1}.$$

It remains to show surjectivity. By Proposition 4.5, $\mathcal{HW}_n^k/\mathcal{HW}_n^{k-1}$ is spanned by shuffle products of cocycles of connected diagrams. By Lemma 2.10 and the conclusion of *Part 1* of the inductive step, each such product of diagrams is hit by some product of Milnor invariants. Thus the map $\mathcal{HV}_n^{n-k} \to \mathcal{HW}_n^k/\mathcal{HW}_n^{k-1}$ is surjective, and hence so is its factor

$$\mathcal{HV}_n^{n-k}/\mathcal{HV}_n^{n-k+1} \longrightarrow \mathcal{HW}_n^k/\mathcal{HW}_n^{k-1}.$$

This completes the inductive step and the proof of the theorem. □

Corollary 4.11. *The space of type n Milnor invariants is isomorphic to the space of leaf-labeled trivalent trees modulo the IHX relations.*

Proof. By Theorem 4.10 (or alternatively, just Part 1 of its proof),

$$\mathcal{HV}_n^1/\mathcal{HV}_n^2 \cong \mathcal{HW}_n^{n-1}/\mathcal{HW}_n^{n-2}$$

where the left side is the space of type n Milnor invariants. Lemma 4.4 describes the right side as the space of linear combinations of leaf-labeled trivalent trees which satisfy IHX. Equivalently, by dualizing, this is the space of such trees modulo IHX. □

Remark 4.12. Corollary 4.11 is a result originally due to Habegger and Masbaum [11, Theorem 6.1, Proposition 10.6]. The advantage of our approach is that it establishes this correspondence through configuration space integrals and thus brings us closer to being able to write configuration space integral formulae for Milnor invariants. The fact that we work with filtration quotients above seems to correspond to the "first nonvanishing Milnor invariant" caveat in Habbeger and Masbaum's Theorem 6.1.

Corollary 4.13. *The n-th filtration quotient of finite type link homotopy invariants of string links is isomorphic to the homogeneous degree n part of the polynomial algebra on Milnor invariants with distinct indices.*

In other words, the set of type n products of Milnor invariants forms a basis for all type n invariants. This corollary implies that the the set of all finite-type homotopy string link invariants can be described as the polynomial algebra on all Milnor invariants. It is perhaps remarkable that the only facts about Milnor invariants that we have used here are that they are of finite type and that there are $(n-2)!$ of them at type n.

Proof of Corollary 4.13. By Theorem 2.5, we may consider cocycles $\mathcal{HW}_n^*$ instead of invariants in $\mathcal{HV}_n/\mathcal{HV}_{n-1}$. Consider the direct sum decomposition

$$\mathcal{HW}_n^* \cong \mathcal{HW}_n^{n-1}/\mathcal{HW}_n^{n-2} \oplus \cdots \oplus \mathcal{HW}_n^1/\mathcal{HW}_n^0 \oplus \mathcal{HW}_n^0. \tag{14}$$

Recall that Proposition 4.5 said that $\mathcal{HW}_n^k/\mathcal{HW}_n^{k-1}$ is a polynomial algebra on certain linear combinations of trees. Specifically, recall the isomorphism (11)

$$\mathcal{HW}_n^k/\mathcal{HW}_n^{k-1} \cong \bigoplus_{\substack{I_1<\cdots<I_\ell \\ n_1(|I_1|-1)+\cdots+n_\ell(|I_\ell|-1)=n}} S^{n_1}(U_{I_1}^\perp) \otimes \cdots \otimes S^{n_\ell}(U_{I_\ell}^\perp)$$

where each I_j is a subset of the segments $\{1, ..., n+1\}$ and $U_{I_j}^\perp$ is the subspace of trees with leaves on those segments satisfying all IHX conditions. If $i = |I_j|$, each $U_{I_j}^\perp$ was identified with $\mathcal{HW}_{i+1}^i/\mathcal{HW}_{i+1}^{i-1}$

by Lemma 4.4. By Theorem 4.10 (*Part 1*), $\mathcal{HW}^i_{i+1}/\mathcal{HW}^{i-1}_{i+1} \cong \mathcal{HV}^1_{i+1}/\mathcal{HV}^2_{i+1}$. The latter space is the space of type $(i+1)$ Milnor invariants, so the result follows. □

4.4. **Cohomology classes in spaces of link maps.** We will now use the fact that graph cocycles give rise to not only homotopy string link invariants in the classical dimension $d = 3$ but also cohomology classes of arbitrary degree in $\mathrm{Link}(\coprod_{i=1}^m \mathbb{R}, \mathbb{R}^d)$ for $d > 3$. Recall the integration maps[4] (3),

$$\mathcal{I} : \mathcal{HD}^k_n \longrightarrow \Omega^{n(d-3)+k}_{dR}\mathrm{Link}(\coprod_{i=1}^m \mathbb{R}, \mathbb{R}^d),$$

which are maps of differential algebras [16, Theorem 4.33]. Now consider the induced maps on cohomology in defect zero for arbitrary d:

$$\mathcal{I} : Z(\mathcal{HD}^0_n) \longrightarrow \mathrm{H}^{n(d-3)}\mathrm{Link}(\coprod_{i=1}^m \mathbb{R}, \mathbb{R}^d). \tag{15}$$

By the same argument used in Section 2 and Theorem 6.1 of [5], one can show that (15) is injective for any d. In fact, this argument is a generalization of the injectivity argument for $d = 3$ used in the proof of Theorem 2.5. One first constructs a cycle corresponding to each chord diagram Γ; the cycle is a product of n $(d-3)$-cycles, obtained by resolving double-points of a singular link in $\mathbb{R}^d$ corresponding to the chords in Γ. Then one shows that any integral $I_{\Gamma'}$ is nonzero on this cycle if and only if $\Gamma' = \Gamma$. Since every cocycle of trivalent diagrams has a chord diagram (see [5, Proposition 5.1] for the case of knots), this ultimately establishes the injectivity of (15).

For $d = 3$, the image of (15) is precisely the finite-type invariants [16, Theorem 5.8]. Thus we can deduce from Corollary 4.13 that the space of graph cocycles $\mathcal{HW}^*_n \subset \mathcal{HD}^0_n$ is also isomorphic to the polynomial algebra on Milnor invariants. Then applying the injectivity in cohomology and algebra structure to $d > 3$, we get a subspace of $\mathrm{H}^*(\mathrm{Link}(\coprod_{i=1}^m \mathbb{R}, \mathbb{R}^d))$ isomorphic to the polynomial algebra on Milnor invariants. In particular, we get a *nontrivial* cohomology class of degree $n(d-3)$ for every type n product of Milnor invariants. We will refer to such a cohomology class as a *generalized Milnor invariant.*

We conjecture that the map (3) from the whole graph complex induces a surjection in cohomology. We already know that in the case $d = 3$, the restriction (15) induces an isomorphism on H^0. In fact, the Vassiliev conjecture holds in this case [2], i.e., Vassiliev invariants separate homotopy string links. It would also be interesting to determine for arbitrary d how much of the cohomology of the space of link maps comes from the defect-zero part of the graph complex. Along these lines, we can loosely formulate the following:

Conjecture. All of the cohomology of the space of link maps $\mathrm{Link}(\coprod_{i=1}^m \mathbb{R}, \mathbb{R}^d)$, $d > 3$, comes from integrals corresponding to products of Milnor invariants.

We would also like to investigate geometric interpretations of our generalized Milnor invariants. In particular, it would be interesting to see if these classes are related to the invariants of link maps $\mathrm{Link}(S^{d_1} \sqcup S^{d_2} \sqcup \cdots \sqcup S^{d_r}, \mathbb{R}^d)$ defined by Koschorke [13]. These invariants are defined geometrically (they can be thought of as counting an "overcrossing locus" of a link) and can also be regarded as generalizations of Milnor invariants. An interesting connection could also be established between Munson's work [23] on relating manifold calculus of functors to Koschorke's generalizations of Milnor invariants. The connection between configuration space integrals for string links and manifold

[4]Note that the defect k in (3) is unrelated to the k in the filtrations of the space of cocycles in $\mathcal{HD}^0_n$ in the previous section.

calculus of functors was established by the first author in [14] who factored the integrals for links through the Taylor tower of these spaces. The functor calculus Taylor towers could thus serve as a common ground for configuration space integrals and Koschorke's invariants and provide the context for relating them to each other.

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