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Vassiliev measures of complexity of open and closed curves in 3-space

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In this article, we define Vassiliev measures of complexity for open curves in 3-space. These are related to the coefficients of the enhanced Jones polynomial of open curves in 3-space. These Vassiliev measures are continuous functions of the curve coordinates; as the ends of the curve tend to coincide, they converge to the corresponding Vassiliev invariants of the resulting knot. We focus on the second Vassiliev measure from the enhanced Jones polynomial for closed and open curves in 3-space. For closed curves, this second Vassiliev measure can be computed by a Gauss code diagram and it has an integral formulation, the double alternating self-linking integral. The double alternating self-linking integral is a topological invariant of closed curves and a continuous function of the curve coordinates for open curves in 3-space. For polygonal curves, the double alternating self-linking integral obtains a simpler expression in terms of geometric probabilities.

1. Introduction

Many physical systems are composed of entangled filamentous structures whose complexity affects their mechanical properties and their function [1–8]. Under some conditions, we can see these filamentous structures like mathematical curves in 3-space whose entanglement we can measure using tools from knot theory [9–25]. A knot (link) is one (or more) simple closed curve(s) in 3-space, and knots (links) are classified using the notion of topological equivalence. Many sophisticated topological invariants exist, such as knot and link polynomials [26–30]. However, there are two major throwbacks in measuring the entanglement complexity of filamentous structures in practice: these may be open curves in 3-space (i.e. they have a distinct starting point and endpoint) and entanglement in these systems is very complex, at least in terms of the number of crossings in diagrams, making the calculation of such polynomials intractable.

The only measure of entanglement of open curves in 3-space until recently was the Gauss linking integral [31]. This measures self or pairwise entanglement of open curves and has had a lot of success across disciplines [32–45]. Characterizing the entanglement of open curves in 3-space using stronger measures of entanglement that can detect knotting of open curves has attracted a lot of attention in the last 20 years (see [46–50] and references therein). However, all these approaches focused on approximating the open curve in 3-space by a knot (a simple closed curve in 3-space) or by a knotoid (a two-dimensional diagram of an open-ended knot). In 2020 [51], the Jones polynomial of open curves in 3-space was introduced, and it was shown that it is a polynomial with real coefficients that are continuous functions of the curve coordinates. Therein, it was shown that the Jones polynomial of open curves in 3-space generalizes the conventional Jones polynomial. In other words, the conventional Jones polynomial expression is a special case of the Jones polynomial introduced in [51].

The approach introduced in [51] provided a framework that we can use to study entanglement of both open and closed curves. This paper focuses on deriving Vassiliev invariant-type measures of entanglement of both open and closed curves. In addition, an integral formula of the second Vassiliev invariant measure is introduced that provides a way to compute such entanglement measures directly from the coordinates of an open curve in 3-space.

Vassiliev invariants are related to the coefficients of the Jones polynomial and can distinguish knots and links, as the polynomials do [52–56]. Combinatorial expressions for calculating some Vassiliev invariants from knot diagrams exist [53,54,56] and integral expressions for Vassiliev invariants also exist; however, their calculation remains elusive [57,58]. A major issue with computing Vassiliev invariants in practice is that physical filaments are usually composed by open curves in 3-space. The theory of knotoids provides a way to study the complexity of open-ended knot *diagrams* [59–61], for which Vassiliev invariants are rigorously defined [62]. However, these are not well defined for open curves in 3-space.

In this article, we define Vassiliev measures for open curves in 3-space using the coefficients of the Jones polynomial with enhanced states of the open curves in 3-space. We show that they are continuous functions of the curve coordinates. An integral formula for the second Vassiliev invariant from the enhanced Jones polynomial is introduced, which involves a Gauss map, the double alternating self-linking integral. For polygonal curves in 3-space, the double alternating self-linking integral is expressed as a finite sum of geometric probabilities. For open curves, the double alternating self-linking integral is a continuous function of the curve coordinates. The double alternating self-linking integral that we introduce provides a unique—to our knowledge—measure of the conformational complexity of open curves in 3-space that is stronger than the Gauss self-linking integral and does not require the computation of any knot polynomial. This can be extremely helpful in practice when studying entanglement in physical systems and we are aware of the potential impact this could have in the study of proteins and polymers. We point out that the method introduced here can be applied to other Vassiliev invariants as well. This generates well-defined integrals over closed or open curves in 3-space that capture higher degrees of entanglement.

More precisely, in §2, we derive the exact formulae of the Vassiliev invariants for knots and knotoids obtained from the enhanced Jones polynomial. In §3 we introduce the Vassiliev measures for open curves in 3-space and study their properties. In §4 we focus on the second Vassiliev invariant of the enhanced Jones polynomial and show that it can be computed using a Gauss code. In §5, a skein relation satisfied by the second Vassiliev invariant of the enhanced Jones polynomial for knotoids is derived and, in the case of knot-type knotoids, it is shown that this second Vassiliev invariant can be calculated by using a Gauss code diagram. In §6, we introduce

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the double alternating self-linking integral and we show that it is equal (up to some specified constants) to the second Vassiliev invariant of the enhanced Jones polynomial in the case of closed curves. In the case of open curves, it is a continuous function of the curve coordinates. Finally, in §7, we show that, for polygonal curves, the double alternating self-linking integral has a simpler expression as a finite sum of geometric probabilities and we give a finite form for the computation of those probabilities for polygonal curves with three or four edges in 3-space.

2. Vassiliev invariants of the enhanced Jones polynomial of knots and knotoids

In this section, we present the definitions of Vassiliev invariants of knots and knotoids defined through the coefficients of the Jones polynomial of knots and knotoids, respectively.

(a) Vassiliev invariants of the enhanced Jones polynomial of knots

The Jones polynomial is defined using the normalized bracket polynomial. An expression of the Jones polynomial, which is helpful for deriving Vassiliev invariants, relies on using enhanced states [63].

The bracket polynomial can be computed using the following relation:

$$\langle \bigcirc \rangle = q + q^{-1}. \tag{2.1}$$

The smoothings with coefficient 1 in the aforementioned equation are called A smoothings, and the smoothings with coefficient q are called B smoothings. Through A and B smoothings of the crossings in a diagram, we obtain a set of enhanced states. In enhanced states, circles have an associated sign in their diagram, and a circle with no sign is a sum of two such states. A circle with a positive sign corresponds to q and a circle with negative sign corresponds to q^{-1}.

For s an enhanced state, let $i(s)$ be the number of B smoothings and

$$\lambda(s) = \text{number of positive circles} - \text{number of negative circles}. \tag{2.2}$$

Then, each state corresponds to a term of the form $(-q)^{i(s)}q^{\lambda(s)} = (-1)^{i(s)}q^{j(s)}$, where $j(s) = i(s) + \lambda(s)$, and the bracket polynomial can be expressed as follows:

$$\langle K \rangle = \sum_{s \in S} (-1)^{i(s)} q^{j(s)}. \tag{2.3}$$

We define the enhanced Jones polynomial in q as follows:

$$J_K(q) = q^{n_+ - 2n_-}(-1)^{n_-}\langle K \rangle, \tag{2.4}$$

where n_+ is the number of positive crossings and n_- is the number of negative crossings. The enhanced Jones polynomial, J_K, is related to the Jones polynomial, V_K, through the relation

$$J_K(q) = (q + q^{-1})V_K(q), \tag{2.5}$$

with the substitution $q = t^{-1/2}$.

The enhanced Jones polynomial satisfies the following relation:

$$q^{-2}J_{K_+}(q) - q^2 J_{K_-}(q) = (q^{-1} - q)J_{K_0}. \tag{2.6}$$

We use the substitution $t = \mathrm{e}^x$, i.e. $q = \mathrm{e}^{-x/2}$, in $J_K(q)$ and then expand it in series of x.

$$\begin{aligned} J_K &= \sum_{s\in S} (-1)^{i(s)+n_-} q^{j(s)+n_+-2n_-} \\ &= \sum_{s\in S} (-1)^{i(s)+n_-} \mathrm{e}^{-(j(s)+n_+-2n_-)x/2} \\ &= \sum_{s\in S} (-1)^{i(s)+n_-} \sum_{k=0}^{\infty} \frac{1}{k!2^k} ((j(s)+n_+-2n_-)x)^k \\ &= \sum_{k=0}^{\infty} \frac{(-1)^k x^k}{2^k k!} \sum_{s\in S} (-1)^{i(s)+n_-} (j(s)+n_+-2n_-)^k. \end{aligned} \tag{2.7}$$

The coefficients of x^k are Vassiliev invariants of order k.

$$v_k = \frac{(-1)^k}{2^k k!} \sum_{s\in S} (-1)^{i(s)+n_-} (j(s)+n_+-2n_-)^k, \tag{2.8}$$

where S is the set of enhanced states of the knot diagram, $i(s)$ is the number of B smoothings, $j(s) = i(s) + \lambda(s)$, $\lambda(s)$ is the algebraic number of circles and n_- (resp. n_+) is the number of negative (resp. positive) crossings in the diagram.

To verify that v_k is a finite-type invariant of order k, we notice that, after substitution of $q = \mathrm{e}^{-x/2}$ in equation (2.6), we obtain

$$J_{K_+}(x) - J_{K_-}(x) = x(\text{other terms}). \tag{2.9}$$

For a singular knot K with k double points, $J_K(x)$ is divisible by x^k; thus, the coefficient of x^k does not vanish. However, if K has $k+1$ double points, the coefficient of $J_K(x)$ is divisible by x^{k+1}, which suggests that the coefficient of x^k vanishes. Thus, the coefficient of x^k, v_k, is a finite-type invariant of degree k.

(b) Vassiliev invariants of the enhanced Jones polynomial of knotoids

A knotoid is an open-ended knot diagram whose ends can be in different regions. Similarly, a linkoid is a diagram of a link with some open-ended components. Examples of knotoids and linkoids are shown in the electronic supplementary material, Supplementary Information and in [59,61]. We will use the enhanced states expression of the Jones polynomial. Note that, in enhanced states of knotoids, circles and arcs have an associated sign; if a circle or an arc has no sign, it is a sum of two states. A circle or an arc with a positive sign corresponds to q and a circle or an arc with a negative sign corresponds to q^{-1}.

The enhanced states expression of the Jones polynomial in q of a knotoid K is

$$J_K(q) = q^{n_+-2n_-} \sum_{s\in S} (-1)^{i(s)+n_-} q^{j(s)}. \tag{2.10}$$

We use the substitution $q = \mathrm{e}^{-x/2}$ and then expand $J_K(q)$ in series of x,

$$J_K(x) = \sum_{k=0}^{\infty} \frac{(-1)^k x^k}{2^k k!} \sum_{s\in S} (-1)^{i(s)+n_-} (j(s)+n_+-2n_-)^k. \tag{2.11}$$

The coefficient of x^k in $J_K(x)$ is a Vassiliev invariant of order k of the knotoid K,

$$v_k(K) = \frac{(-1)^k}{2^k k!} \sum_{s\in S} (-1)^{i(s)+n_-} (j(s)+n_+-2n_-)^k, \tag{2.12}$$

where S is the set of enhanced states of the knotoid K, $i(s)$ is the number of B smoothings, $j(s) = i(s) + \lambda(s)$, $\lambda(s)$ is the algebraic number of circles and n_- (resp. n_+) is the number of negative (resp. positive) crossings in the knotoid diagram.

3. Vassiliev measures of the enhanced Jones polynomial of open curves in 3-space

In this section, we define a set of new measures of entanglement of open curves in 3-space that we call Vassiliev measures because of the similarity of their definition to Vassiliev invariants. However, these are not invariants for open curves; to avoid any confusion, we will denote them w_k (instead of v_k). In the following, we will show that the same definition applies to both open and closed curves in 3-space. For this reason, we give the definition in general for any curve in 3-space.

Definition 3.1. Let l denote an open or closed curve in 3-space. We define the kth Vassiliev measure as follows:

$$w_k = \frac{(-1)^k}{4\pi 2^k k!}\int_{\xi\in S^2}\sum_{s_\xi\in S_\xi}(-1)^{i(s_\xi)+n_{-,\xi}}((j(s_\xi)+n_{+,\xi}-2n_{-,\xi})^k)\mathrm{d}A, \tag{3.1}$$

where S is the set of enhanced states of a projection of l, l_ξ, $i(s)$ is the number of B smoothings, $j(s)=i(s)+\lambda(s)$, $\lambda(s)$ is the algebraic number of circles and n_- (resp. n_+) is the number of negative (resp. positive) crossings in the diagram and where the integral is over all vectors in S^2 except a set of measure zero (corresponding to non-generic projections).

Proposition 3.2. *Let l denote an open or closed curve in 3-space. The kth Vassiliev measure, $w_k(l)$, is defined by the coefficients of the enhanced Jones polynomial of l.*

Proof. Let l denote a curve in 3-space. Let $(l)_\xi$ denote the projection of l on a plane with normal vector ξ. Let $K((l)_\xi)$ denote the knotoid corresponding to $(l)_\xi$.

The normalized bracket polynomial of l was defined in [51] as follows:

$$V_{K(l)} = \frac{1}{4\pi}\int_{\xi\in S^2}(-A^3)^{-wr(K(l)_\xi)}\langle K((l)_\xi)\rangle \mathrm{d}A, \tag{3.2}$$

where the integral is over all vectors in S^2 except a set of measure zero (corresponding to non-generic projections). The integrand is the Jones polynomial of the knotoid $K((l)_\xi)$.

Using the enhanced states expression of the Jones polynomial in this case, we get

$$J_K(q) = \frac{1}{4\pi}\int_{\xi\in S^2} q^{n_{+,\xi}-2n_{-,\xi}}\sum_{s_\xi\in S_\xi}(-1)^{i(s_\xi)+n_{-,\xi}}q^{j(s_\xi)}\mathrm{d}A. \tag{3.3}$$

We use the substitution $q=\mathrm{e}^{-x/2}$ and then expand this in series of x.

$$J_K(q) = \sum_{k=0}^{\infty}\frac{(-1)^k x^k}{2^k k!}\frac{1}{4\pi}\int_{\xi\in S^2}\sum_{s_\xi\in S_\xi}(-1)^{i(s_\xi)+n_{-,\xi}}((j(s_\xi)+n_{+,\xi}-2n_{-,\xi})^k)\mathrm{d}A. \tag{3.4}$$

Therefore, w_k is the coefficient of x^k in the enhanced Jones polynomial of l. ■

Corollary 3.3. *Let l denote an open curve in 3-space. The kth Vassiliev measure of l derived from the enhanced Jones polynomial of l is the average of the Vassiliev invariant in a projection over all possible projection directions, namely*

$$w_k(l) = \frac{1}{4\pi}\int_{\xi\in S^2} v_k(l_\xi) dA. \tag{3.5}$$

Proof. It follows directly from definition 3.1 and equation (2.12). ■

Proposition 3.4. *If l is a closed curve in 3-space, then the kth Vassiliev measure, $w_k(l)$, is equal to the kth Vassiliev invariant, $v_k(l)$, obtained from the enhanced Jones polynomial of l, i.e. $w_k(l)=v_k(l)$.*

Proof. If l is a closed curve in 3-space, then $v_k(l)$ is a topological invariant, independent of the projection direction. Thus,

$$w_k(l) = \frac{1}{4\pi}\int_{\xi\in S^2} v_k(l_\xi)\mathrm{d}A = v_k(l_\xi) = v_k(l). \tag{3.6}$$

■

Proposition 3.5. *Let l denote an open curve in 3-space, then w_k can be expressed as follows:*

$$w_k(l) = \sum_{K_i\in K(l)} p(K_i)v_k(K_i), \tag{3.7}$$

where K_i is a knotoid that appears in a projection of l and $p(K_i)$ is the geometric probability that the projection of l gives the knotoid K_i and $K(l)$ is the set of possible knotoids that can result as a projection of l.

Proof. Any fixed curve in 3-space can give projections that result in only a finite number of knotoids, we denote K_i, where $i = 1, \ldots, n$. Then, $p(K_i) = (1/4\pi)A_i$, where A_i is the sum of two antipodal spherical areas that define normal vectors to planes where the projection of l gives the knotoid K_i. Since $v_k(l_\xi)$ is constant in these areas,

$$\begin{aligned} w_k(l) &= \frac{1}{4\pi}\int_{\xi} v_k(l_\xi)\mathrm{d}A \\ &= \sum_{1\le i\le n}\frac{1}{4\pi}\int_{\xi\in A_i} v_k(l_\xi)\mathrm{d}A = \frac{1}{4\pi}\sum_{1\le i\le n} v_k(K_i)\int_{\xi\in A_i}\mathrm{d}A \\ &= \frac{1}{4\pi}\sum_{1\le i\le n} v_k(K_i)A_i = \sum_{1\le i\le n} p(K_i)v_k(K_i). \end{aligned} \tag{3.8}$$

■

Remark 3.6. We can also write w_k as follows:

$$w_k = \frac{(-1)^k}{2^k k!}\sum_{S,n_+,n_-} p_{K,S,n_-,n_+}\sum_{s\in S}(-1)^{i(s)+n_-}((j(s) + n_+ - 2n_-)^k), \tag{3.9}$$

where p_{K,S,n_+,n_-} denotes the geometric probability that a projection of K has n_+, n_- positive and negative crossings, respectively, and gives the set of enhanced states S and the sum is taken over all possible sets of states S that can be generated by projections of K with a given type of crossing n_+, n_-.

Proposition 3.7. *Let l denote an open curve in 3-space. Then, the kth Vassiliev measure of l, $w_k(l)$, is a continuous function of the curve coordinates.*

Proof. Let us consider a polygonal curve of n edges, l_n. Then, by proposition 3.5,

$$w_k(l_n) = \sum_{K_i\in K(l)} p(K_i)v_k(K_i), \tag{3.10}$$

where K_i is a knotoid that appears in a projection of l and $p(K_i)$ is the geometric probability that the projection of l gives the knotoid K_i and $K(l)$ is the set of possible knotoids that can result as a projection of l. In [51], it was shown that $p(K_i)$ is a continuous function of the curve coordinates. Thus, $w_k(l_n)$ is a continuous function of the coordinates of l_n. As $n \to \infty$, the result follows for any curve l. ■

4. The second Vassiliev invariant of the enhanced Jones polynomial of knots

In this section, we study the second Vassiliev invariant of knots derived by the enhanced Jones polynomial and show that it can be calculated using a Gauss code diagram from any knot diagram.

Theorem 4.1. *For a knot K, the first three Vassiliev invariants defined by the enhanced Jones polynomial satisfy the following equations:*

$$\left.\begin{aligned} v_0(K) &= v_0(\bigcirc) = 2, \\ v_1(K_+) &= v_1(K_-) \\ \text{and} \quad v_2(K_+) - v_2(K_-) &= -6lk(K_0), \end{aligned}\right\} \tag{4.1}$$

where K_0 is a link and lk denotes the linking number.

Proof. See electronic supplementary material, Supplementary Information. ■

Remark 4.2. It is interesting to point out that a similar relation exists for the Casson invariant, the second Vassiliev invariant obtained from the Conway polynomial [64].

Theorem 4.3. *For a two-component link, L, the first three Vassiliev invariants defined by the enhanced Jones polynomial satisfy the following equations:*

$$\left.\begin{aligned} v_0(L) &= v_0(\bigcirc\bigcirc) = 4, \\ v_1(L) &= -6lk(L), \\ v_2(L_+) - v_2(L_-) &= 12lk(L) - 6 \\ \text{and} \quad v_2(L) &= 2v_2(K_1) + 2v_2(K_2) + 12lk^2(L) - 6lk(L), \end{aligned}\right\} \tag{4.2}$$

where lk denotes the linking number and K_1, K_2 are the two knots obtained by smoothing the crossings in L to obtain two components.

Proof. See electronic supplementary material, Supplementary Information. ■

Remark 4.4. This result agrees with the statement in [65] that the second Vassiliev invariant of a two-component link is a linear combination of the second Vassiliev invariant of each component and the linking number of the link. Note that when $v_2(K_1) = v_2(K_2) = 0$, then $v_2(L) = 12lk^2(L) - 6lk(L)$.

Theorem 4.5. *Let $\hat{v}_2$ be defined as follows:*

$$\hat{v}_2(K) = \frac{1}{2} \sum_{j_1 > j_2 > j_3 > j_4 \in I_{\xi'}} \epsilon(j_1, j_3)\epsilon(j_2, j_4), \tag{4.3}$$

where $I_{\prime}$ denotes the set of pairs of alternating crossings in the diagram of the knot K.

$\hat{v}_2$ is a second Vassiliev invariant of knots, and $v_2 = \frac{1}{4} + 6\hat{v}_2$, where v_2 denotes the second Vassiliev invariant from the enhanced Jones polynomial.

Proof. The proof is similar to theorem 1.A in [54], and is given in the electronic supplementary material, Supplementary Information. ■

5. The second Vassiliev invariant of the enhanced Jones polynomial of knotoids

Here, we study the second Vassiliev invariant of the enhanced Jones polynomial of knotoids.

Definition 5.1. We will define a separated linkoid diagram of two components: a linkoid diagram where one of the two components is either all above or all below the other one.

Theorem 5.2. *Let K be a knotoid and let K_+, K_-, K_0 be derived by changing and smoothing a positive crossing of K. Let r be the algebraic sum of crossings needed to convert K to an ascending knotoid diagram and let l denote the algebraic sum of crossings needed to convert K_0 to a separated linkoid. Let $v_k(K_0^s)$ denote the kth Vassiliev invariant of the separated linkoid diagram obtained by K_0. The first three Vassiliev* *invariants defined by the coefficients of the enhanced Jones polynomial satisfy the equations*

$$\left.\begin{aligned} &v_0(K) = v_0(\quad) = 2,\\ &v_1(K_+) - v_1(K_-) = r v_0(K_0^s) - 4r\\ \text{and}\qquad &v_2(K_+) - v_2(K_-) = v_1(K_0^s) - (2l + 2r + 1) v_0(K_0^s) + 2l + 8r + 4. \end{aligned}\right\} \tag{5.1}$$

Proof. We follow the same steps as in the proof of theorem 4.1. Namely, by expanding the enhanced Jones polynomial of the knotoid K in the skein relation of the enhanced Jones polynomial and equating the coefficients of x^0 we get the following relation for knotoids:

$$\begin{aligned} 0 &= \sum_{s_+ \in S_+} (-1)^{i(s_+) + n_-^{(+)}} - \sum_{s_- \in S_-} (-1)^{i(s_-) + n_-^{(-)}}\\ &\Leftrightarrow \sum_{s_+ \in S_+} (-1)^{i(s_+) + n_-^{(+)}} = \sum_{s_- \in S_-} (-1)^{i(s_-) + n_-^{(-)}}\\ &\Leftrightarrow v_0(K_+) = v_0(K_-). \end{aligned} \tag{5.2}$$

Thus, v_0 is invariant upon a crossing change. So, if K is a knotoid, then we can change crossings so that we obtain an ascending diagram of a knotoid, which is the trivial knotoid [62]. Thus,

$$v_0(K) = v_0(\quad) = 2. \tag{5.3}$$

Similarly, if L is a linkoid of two components, we can change crossings in order to get a separated linkoid of two components,

$$v_0(L) = v_0(L^s). \tag{5.4}$$

By equating the coefficients of x in the expansion of the enhanced Jones polynomial of knotoids, we obtain the following relation:

$$v_1(K_+) - v_1(K_-) = v_0(K_0) - v_0(K_+) - v_0(K_-). \tag{5.5}$$

If K_+ is a knotoid and K_0 is a linkoid of two components, then equations (5.5) and (5.3) give

$$v_1(K_+) - v_1(K_-) = v_0(K_0^s) - 4, \tag{5.6}$$

from which we can get the relations

$$\left.\begin{aligned} &v_1(K_+) = v_1(K_-) + v_0(K_0^s) - 4\\ \text{and}\qquad &v_1(K_-) = v_1(K_+) - v_0(K_0^s) + 4. \end{aligned}\right\} \tag{5.7}$$

Thus, by repeatedly changing crossings to make K_+ into an ascending knotoid diagram (for which $v_1 = 0$), we get

$$v_1(K_+) = r v_0(K_0^s) - 4r, \tag{5.8}$$

where r is the algebraic sum of the signs of the crossings that need to be changed to make the knotoid K_+ into an ascending knotoid diagram.

If L_+ is a linkoid, then L_- is also a linkoid and L_0 is a knotoid. Then, equation (5.5) gives

$$v_1(L_+) - v_1(L_-) = v_0(L_0) - v_0(L_+) - v_0(L_-) = 2 - 2v_0(L^s), \tag{5.9}$$

from which we get the following relations:

$$\left.\begin{aligned} &v_1(L_+) = v_1(L_-) + 2 - 2v_0(L^s)\\ \text{and}\qquad &v_1(L_-) = v_1(L_+) - 2 + 2v_0(L^s). \end{aligned}\right\} \tag{5.10}$$

We can convert L_+ to a separated linkoid by repeatedly changing crossings. Suppose that the algebraic sum of crossings we need to change to get a separated linkoid diagram, L^s, is l. Then we get

$$v_1(L_+) = v_1(L^s) + 2l - 2lv_0(L^s). \tag{5.11}$$

By equating the coefficients of x^2 in the expansion of the enhanced Jones polynomial of knotoids, we get

$$v_2(K_+) - v_2(K_-) = v_1(K_0) - v_1(K_+) - v_1(K_-). \tag{5.12}$$

Thus, if K_+ is a knotoid,

$$\begin{aligned} v_2(K_+) - v_2(K_-) &= v_1(K_0^s) + 2l - 2lv_0(K_0^s) - [v_1(K_-) + v_0(K_0^s) - 4] - v_1(K_-) \\ &= v_1(K_0^s) + 2l - 2lv_0(K_0^s) - v_0(K_0^s) + 4 - 2v_1(K_-) \\ &= v_1(K_0^s) - (2l+1)v_0(K_0^s) + 2l + 4 - 2(rv_0(K_0^s) - 4r) \\ &= v_1(K_0^s) - (2l+2r+1)v_0(K_0^s) + 2l + 8r + 4. \end{aligned} \tag{5.13}$$

■

Definition 5.3. Let L define a linkoid of two components. We define the linking number of L, we denote $lk(L)$, to be half the algebraic sum of inter-crossings in a diagram of L, i.e. $lk(L) = \frac{1}{2}\sum_{c\in D} \mathrm{sign}(c)$, where D is the set of crossings between the two components in the diagram.

Remark 5.4. Note that the linking number of linkoids is an invariant of linkoids. The linking number of linkoids is not an integer in general, but, for a link-type linkoid, lk is an integer.

Proposition 5.5. *Let K denote a knot-type knotoid (a knotoid is said to be of knot-type if its ends are in the same region). The first three Vassiliev invariants defined by the coefficients of the enhanced Jones polynomial satisfy the equations*

$$\left.\begin{aligned} v_0(K) &= v_0(\sim) = 2, \\ v_1(K_+) &= v_1(K_-) \\ v_2(K_+) - v_2(K_-) &= -6lk, \end{aligned}\right\} \tag{5.14}$$

and

where lk is the linking number of the linkoid K_0.

Proof. If L^s is a separated link-type linkoid, it is the trivial linkoid; thus, $v_0(L^s) = 4$. The algebraic sum of crossings needed to change to get a separated linkoid diagram from any link-type linkoid diagram is $l = lk$, where lk denotes the linking number of a link-type linkoid. When K is a knot-type knotoid, then K_0 is a link-type linkoid. By using these facts, the results follow using the same method as in the proof of theorem 5.2. ■

In the following, we will refer to Gauss diagrams.

Definition 5.6. A Gauss diagram is a way to describe a knot diagram. A Gauss diagram is the immersing of a circle with the pre-images of each double point (associated with the knot diagram) connected with a chord. To incorporate the information on overpasses and underpasses, chords have an orientation from the over arc to the under arc. Gauss diagrams can have a base point and an orientation that matches a base point on a knot and the orientation of the knot. Given a knot K, we will denote $\langle$Gauss diagram 1 + Gauss diagram 2, $K\rangle$ the sum over all subdiagrams of K isomorphic to either Gauss diagram 1 or Gauss diagram 2.

A Gauss diagram can be used to describe knotoid diagrams as well. In this case, the Gauss diagram has a starting point and an endpoint matching those of the knotoid.

Theorem 5.7. *Let K denote a knot-type knotoid. Let $\hat{v}_2$ be defined as follows:*

$$\hat{v}_2(K) = \frac{1}{2}\sum_{j_1>j_2>j_3>j_4\in I_{\xi'}} \epsilon(j_1,j_3)\epsilon(j_2,j_4), \tag{5.15}$$

where $I_{\prime}$ denotes the set of pairs of alternating crossings in the diagram of the knotoid K.

$\hat{v}_2$ is a second Vassiliev invariant of knot-type knotoids, and $v_2 = \frac{1}{4} + 6\hat{v}_2$, where v_2 denotes the second Vassiliev invariant from the enhanced Jones polynomial.

Proof. The proof follows a similar approach to the proof of theorem 4.5.

Notice that, in terms of Gauss diagrams of knotoids,

$\hat{v}_2(K) = \langle$  $+$  $, K\rangle.$ (5.16)

To calculate v_2 of the knotoid K, we transform K to a descending knotoid, going from the starting point along the orientation of K and replacing an undercrossing by an overcrossing, if at the first passage through the point we go along the undercrossing. When we arrive at the endpoint of the diagram, it becomes descending. Each time we change a crossing s, the value of v_2 changes by $(-6)(-\epsilon(s))lk(\,)(\,)$, where $\epsilon(s)$ is the sign of the crossing. Since $v_2(\text{descending}) = \frac{1}{4}$, this gives

$$v_2(K) = \frac{1}{4} + 6\sum \epsilon(s) lk(L_s), \tag{5.17}$$

where L_s runs over linkoids that appeared as smoothings at points where the crossing changed.

To calculate $lk(L_s)$, we can sum up the signs of all the crossing points of L_s in which the component containing the endpoints goes below the other component. These points correspond to chords of G intersecting the chord $c(s)$ corresponding to s and directed to the side of $c(s)$ containing the endpoints. At the moment, all arrows of the original diagram G with heads between the starting point and the head of $c(s)$ have been inverted. Therefore, $lk(L_s)$ is equal to the sum of signs of arrows crossing $c(s)$ and having heads between the tail of $c(s)$ and the endpoints. In other words, $lk(L_s)$ is $\sum \epsilon(c_2)$, where the summation runs over all chords involved, together with $c(s)$, into subdiagrams of the type .

We can also calculate v_2 by transforming K to an ascending knotoid. By a similar argument we show that v_2 gets an expression similar to equation (5.17), where for a crossing change at a chord $c(s)$, $lk(L_s)$, is $\sum \epsilon(c_2)$, where the summation runs over all chords involved, together with $c(s)$, into subdiagrams of the type .

Thus, we obtain $v_2(K) = \frac{1}{4} + 6\hat{v}_2$. ■

6. The double alternating self-linking integral of curves in 3-space

In this section, we define the double alternating linking integral of open curves in 3-space and examine its relation to the second Vassiliev measure of open curves in 3-space.

Definition 6.1. Let l denote a curve in 3-space with parametrization γ. We define the double alternating self-linking integral as follows:

$$\begin{aligned} \mathrm{SLL}(l) = \frac{1}{8\pi} \int_0^1 \int_0^{j_1} \int_0^{j_2} \int_0^{j_3} & (\dot{\gamma}(j_1) \times \dot{\gamma}(j_3)) \\ & \cdot \frac{\gamma(j_1) - \gamma(j_3)}{|\gamma(j_1) - \gamma(j_3)|^3} (\dot{\gamma}(j_2) \times \dot{\gamma}(j_4)) \cdot \frac{\gamma(j_2) - \gamma(j_4)}{|\gamma(j_2) - \gamma(j_4)|^3} \\ & \chi(j_1, j_2, j_3, j_4) \mathrm{d}j_4 \mathrm{d}j_3 \mathrm{d}j_2 \mathrm{d}j_1, \end{aligned} \tag{6.1}$$

where $\Gamma(s,t) = (\gamma(s) - \gamma(t)/|\gamma(s) - \gamma(t)|)$, for $s,t \in [0,1]$, $0 \leq j_4 < j_3 < j_2 < j_1 \leq 1$, and where $\chi(j_1, j_2, j_3, j_4) = 1$, when $(j_1, j_2, j_3, j_4) \in E$ and $\chi(j_1, j_2, j_3, j_4) = 0$; otherwise, where $E \subset [0,1]^4$, such that $0 \leq j_1 < j_2 < j_3 < j_4 \leq 1$, $\Gamma(j_1, j_3) = -\Gamma(j_2, j_4)$.

Definition 6.2. Let $j_1 < j_2 < j_3 < j_4$ be points on a knot diagram. We will say that this 4-tuple corresponds to an alternating crossing when j_1, j_3 and j_2, j_4 are two crossing points in the diagram such that, if j_1 belongs to the over arc in the crossing, j_2 belongs to the under arc in the crossing or vice versa.

Theorem 6.3. *Let l denote a curve in 3-space with parametrization γ. The double alternating self-linking integral can be expressed as follows:*

$$SLL(l) = \frac{1}{8\pi}\int_{\boldsymbol{\xi}\in S^2}\sum_{j_1>j_2>j_3>j_4\in I^*_{\boldsymbol{\xi}}}\epsilon(j_1,j_3)\epsilon(j_2,j_4)dA, \tag{6.2}$$

where $\epsilon(s,t)=\pm1$ is the sign of the crossing between the projection of $\gamma(s)$ and $\gamma(t)$, and where $I^*_{\boldsymbol{\xi}}$ denotes the set of 4-tuples of alternating crossings in the projection to the plane with normal vector $\boldsymbol{\xi}$.

Proof. Let $\gamma(t)$ denote a parametrization of l and let $\Gamma(s,t)$ denote the Gauss map $\Gamma(s,t)=(\gamma(s)-\gamma(t)/|\gamma(s)-\gamma(t)|)$. Let $\gamma(j_1),\gamma(j_2),\gamma(j_3),\gamma(j_4)$ denote four points on l such that $\Gamma(j_1,j_3)=-\Gamma(j_2,j_4)$. Then, the projections of $\gamma(j_1),\gamma(j_3)$ and of $\gamma(j_2),\gamma(j_4)$ on the plane with normal vector $\boldsymbol{\xi}=\Gamma(j_1,j_3)$ coincide, creating two crossings, one where the arc containing $\gamma(j_1)$ is 'over' and one where the arc containing $\gamma(j_2)$ is 'under'. Thus, the crossings are 'alternating'.

Let l_n denote a polygonal approximation of l obtained from a partition of the interval $[0,1]$. Let $\gamma(t), t\in[0,1]$ be a parametrization of the polygonal curve l_n. Then, we can express the integral in the right-hand side of equation (6.2) as follows:

$$\frac{1}{8\pi}\int_{\boldsymbol{\xi}\in S^2}\sum_{j_1>j_2>j_3>j_4\in I^*_{\boldsymbol{\xi}}}\epsilon(j_1,j_3)\epsilon(j_2,j_4)\mathrm{d}A = \frac{1}{8\pi}\sum_{1\le i\le j\le k\le l\le n}\int_{\boldsymbol{\xi}\in S^2}\epsilon^*(j_1,j_3)\epsilon^*(j_2,j_4)\mathrm{d}A, \tag{6.3}$$

where i,j,k,l are indices of the edges of the polygonal curve l_n and where $\epsilon^*(s,t)$ can take values 0, or ±1, depending on whether the projection of $\gamma(s),\gamma(t)$ cross (and with what sign). We note that the integral in the latter expression may be non-zero, when either $i<j<k<l$ (thus, involving four edges) or when at most two of the edges are identified, i.e. $i=j<k<l$ or $i<j=k<l$ or $i<j<k=l$. If more indices are identified, thus only two edges or only one are involved, it is impossible to have two crossings in their projection. We focus on the case where $i<j<k<l$; thus, we have four different edges involved. (The case of three edges involved can be treated similarly and we will not discuss it in this proof.) Two edges cross on a spherical quadrangle (and its antipodal) [66]. Thus, two pairs of edges cross at the intersection of the two spherical quadrangles. Let us denote this intersection, which is a spherical polygon (and its antipodal), A. Then,

$$\begin{aligned}\frac{1}{8\pi}&\int_{\boldsymbol{\xi}\in S^2}\epsilon^*(j_1,j_3)\epsilon^*(j_2,j_4)\mathrm{d}A\\ &=\frac{1}{8\pi}\int_{\boldsymbol{\xi}\in S^2\setminus A}\epsilon^*(j_1,j_3)\epsilon^*(j_2,j_4)\mathrm{d}A+\frac{1}{8\pi}\int_{\boldsymbol{\xi}\in A}\epsilon^*(j_1,j_3)\epsilon^*(j_2,j_4)\mathrm{d}A\\ &=\frac{1}{8\pi}\int_{\boldsymbol{\xi}\in A}\epsilon(j_1,j_3)\epsilon(j_2,j_4)\mathrm{d}A,\end{aligned} \tag{6.4}$$

since $\int_{\boldsymbol{\xi}\in S^2\setminus A}\epsilon(j_1,j_3)\epsilon(j_2,j_4)\mathrm{d}A=0$. Let us denote $\gamma_1(j_1)$, $\gamma_2(j_2)$, $\gamma_3(j_3)$ and $\gamma_4(j_4)$, where $j_1,j_2,j_3,j_4\in([0,1])^4$, the parametrizations of the edges l,k,j,i, respectively. Let us define the map Γ^* from any 4-tuple in $[0,1]^4$ to $S^2\times S^2$, such that $\Gamma^*(j_1,j_2,j_3,j_4)=(\Gamma_1(j_1,j_3),\Gamma_2(j_2,j_4))$, where $\Gamma_1(j_1,j_3)=(\gamma_1(j_1)-\gamma_3(j_3))/|\gamma_1(j_1)-\gamma_3(j_3)|^3$ and $\Gamma_2(j_2,j_4)=(\gamma_1(j_2)-\gamma_3(j_4))/|\gamma_1(j_2)-\gamma_3(j_4)|^3$. Then, by changing variables in the integral, we obtain

$$\begin{aligned}\frac{1}{8\pi}\int_{\boldsymbol{\xi}\in A}\epsilon(j_1,j_3)\epsilon(j_2,j_4)\mathrm{d}A=\frac{1}{8\pi}\int_{0^*}^{1^*}\int_{0^*}^{1^*}\int_{0^*}^{1^*}\int_{0^*}^{1^*}&(\dot{\gamma}_1(j_1)\times\dot{\gamma}_3(j_3))\\ &\cdot\frac{\gamma_1(j_1)-\gamma_3(j_3)}{|\gamma_1(j_1)-\gamma_3(j_3)|^3}(\dot{\gamma}_2(j_2)\times\dot{\gamma}_4(j_4))\\ &\cdot\frac{\gamma_2(j_2)-\gamma_4(j_4)}{|\gamma_2(j_2)-\gamma_4(j_4)|^3}\mathrm{d}j_4\mathrm{d}j_3\mathrm{d}j_2\mathrm{d}j_1,\end{aligned} \tag{6.5}$$

where $|(\gamma(\dot{j}_1)\times\gamma(\dot{j}_3))\cdot((\gamma(j_1)-\gamma(j_3))/|\gamma(j_1)-\gamma(j_3)|^3)(\gamma(\dot{j}_2)\times\gamma(\dot{j}_4))\cdot(\gamma(j_2)-\gamma(j_4))/|\gamma(j_2)-\gamma(j_4)|^3|$ is the Jacobian of Γ^* and where the sign of $(\gamma(\dot{j}_1)\times\gamma(\dot{j}_3))\cdot(\gamma(j_1)-\gamma(j_3))/|\gamma(j_1)-\gamma(j_3)|^3$ is the sign of the crossing of the projections of the edges e_1,e_3 (when they cross in a projection direction) and the sign of $(\dot{\gamma}(j_2)\times\dot{\gamma}(j_4))\cdot(\gamma(j_2)-\gamma(j_4))/|\gamma(j_2)-\gamma(j_4)|^3$ is the sign of the crossing of the projections of the edges e_2, e_4 (when they cross in a projection direction). The symbol $*$ in the integral indicates integration over the subset of $[0,1]^4$, which defines 4-tuples of points on the knot that define vectors which give alternating crossings. This is the subset of $[0,1]^4$ whose image through Γ^* is A; we denote this subset $E=([0,1]^4)^*$. Since Γ is a continuous function and A is measurable, its pre-image, $E=([0,1]^4)^*$, is also measurable. Instead of integrating over E, we can integrate over $[0,1]^4$ as follows:

$$\begin{aligned}
&\frac{1}{8\pi}\int_{\xi\in A}\epsilon(j_1,j_3)\epsilon(j_2,j_4)\mathrm{d}A\\
&\quad=\frac{1}{8\pi}\int_0^1\int_0^1\int_0^1\int_0^1(\dot{\gamma}_1(j_1)\times\dot{\gamma}_3(j_3))\\
&\quad\cdot\frac{\gamma_1(j_1)-\gamma_3(j_3)}{|\gamma_1(j_1)-\gamma_3(j_3)|^3}(\dot{\gamma}_2(j_2)\times\dot{\gamma}_4(j_4))\cdot\frac{\gamma_2(j_2)-\gamma_4(j_4)}{|\gamma_2(j_2)-\gamma_4(j_4)|^3}\\
&\quad\chi(j_1,j_2,j_3,j_4)\mathrm{d}j_4\mathrm{d}j_3\mathrm{d}j_2\mathrm{d}j_1,
\end{aligned}\tag{6.6}$$

where $\chi(j_1,j_2,j_3,j_4)=1$, when $(j_1,j_2,j_3,j_4)\in E$ and $\chi(j_1,j_2,j_3,j_4)=0$, otherwise.

At the limit when $n\to\infty$, we obtain the formula

$$\begin{aligned}
&\frac{1}{8\pi}\int_{\xi\in S^2}\sum_{j_1>j_2>j_3>j_4\in I_\xi}\epsilon(j_1,j_3)\epsilon(j_2,j_4)\mathrm{d}A\\
&=\frac{1}{8\pi}\int_{j_1}\int_{j_2}\int_{j_3}\int_{j_4}(\dot{\gamma}(j_1)\times\dot{\gamma}(j_3))\cdot\frac{\gamma(j_1)-\gamma(j_3)}{|\gamma(j_1)-\gamma(j_3)|^3}(\dot{\gamma}(j_2)\times\dot{\gamma}(j_4))\cdot\frac{\gamma(j_2)-\gamma(j_4)}{|\gamma(j_2)-\gamma(j_4)|^3}\\
&\chi(j_1,j_2,j_3,j_4)\mathrm{d}j_4\mathrm{d}j_3\mathrm{d}j_2\mathrm{d}j_1\\
&=\mathrm{SLL}(l).
\end{aligned}\tag{6.7}$$

■

Proposition 6.4. *Let l denote a closed curve in 3-space. Then, the double alternating self-linking integral is a topological invariant and it is related to the second Vassiliev invariant of the enhanced Jones polynomial of l by*

$$v_2(l)=\frac{1}{4}+6\mathrm{SLL}(l).\tag{6.8}$$

Proof. By theorem 6.3 and by theorem 5.7,

$$v_2(l)=\frac{1}{4}+6\Big(\frac{1}{2}\sum_{j_1>j_2>j_3>j_4\in I^*_\xi}\epsilon(j_1,j_3)\epsilon(j_2,j_4)\Big),\tag{6.9}$$

where I^*_ξ denotes the set of pairs of alternating crossings in a diagram l_ξ.

Since $v_2(l)$ is an invariant, it is independent of the projection direction. We can also express $v_2(l)$ as follows:

$$\begin{aligned}
v_2(l)&=\frac{1}{4\pi}\int_{\xi\in S^2}\frac{1}{4}+6\Big(\frac{1}{2}\sum_{j_1>j_2>j_3>j_4\in I^*_\xi}\epsilon(j_1,j_3)\epsilon(j_2,j_4)\Big)\mathrm{d}A\\
&=\frac{1}{4}+6\frac{1}{8\pi}\int_{\xi\in S^2}\sum_{j_1>j_2>j_3>j_4\in I^*_\xi}\epsilon(j_1,j_3)\epsilon(j_2,j_4)\Big)\mathrm{d}A.
\end{aligned}\tag{6.10}$$

By theorem 6.3, $v_2(l)=\frac{1}{4}+6\mathrm{SLL}(l)$. ■

Remark 6.5. Note that this method of writing an integral in space for a Vassiliev invariant would work for any combinatorial expression for a Vassiliev invariant. The double alternating self-linking integral has similarities to the second Vassiliev invariant integral expression obtained from the perturbative expansion of Witten's integral [67]. This relation will be explored in a sequel to this study.

Proposition 6.6. *Let l denote an open curve in 3-space. SLL(l) is a continuous function of the coordinates of l.*

Proof. We will prove this first for a polygonal curve of n edges and the result will follow for any curve $l \in R^3$ as $n \to \infty$.

The double alternating self-linking integral of a polygonal curve can be expressed as follows:

$$\begin{aligned}\mathrm{SLL}(l_n) &= \frac{1}{8\pi}\int_{\boldsymbol{\xi}\in S^2}\sum_{j_1>j_2>j_3>j_4\in I^*_{\xi}} \epsilon(j_1,j_3)\epsilon(j_2,j_4)\mathrm{d}A \\ &= \frac{1}{8\pi}\sum_{1\le i\le j\le k\le l\le n}\int_{\boldsymbol{\xi}\in S^2}\epsilon(j_1,j_3)\epsilon(j_2,j_4)\mathrm{d}A \\ &= \frac{1}{2}\sum_{1\le i\le j\le k\le l\le n} p_{j_1,j_2,j_3,j_4}\epsilon(j_1,j_3)\epsilon(j_2,j_4), \end{aligned} \tag{6.11}$$

where p_{j_1,j_2,j_3,j_4} denotes the geometric probability that the edges e_{j_1}, e_{j_3} and e_{j_2}, e_{j_4} both cross in a projection direction and give an alternating crossing.

We can express p_{j_1,j_2,j_3,j_4} as the joint probability that e_{j_1}, e_{j_3} and e_{j_2}, e_{j_4} both cross. In [51], it was proved that the geometric probability that e_{j_1}, e_{j_3} cross, p_{j_1,j_3}, and the geometric probability that e_{j_2}, e_{j_4} cross, p_{j_2,j_4}, are continuous and are equal to the areas of the corresponding quadrangles on the sphere. Their intersection, p_{j_1,j_2,j_3,j_4}, is the area of the intersection of the two spherical quadrangles. Since both areas are continuous functions of the coordinates of the involved edges, so is their intersection. ■

Corollary 6.7. *Let l denote an open curve in 3-space. Then, as the endpoints of l tend to coincide,* SLL(l) *tends to* $\frac{1}{6}v_2(l) - \frac{1}{24}$.

Proof. It follows directly from propositions 6.4 and 6.6. ■

Definition 6.8. We define a tight open knot to be a fixed open curve in 3-space whose projections give only knot-type knotoids.

Proposition 6.9. *Suppose that l is a tight open knot. Then the double alternating self-linking integral is related to the second Vassiliev measure of l as* $w_2(l) = \frac{1}{4} + 6\mathrm{SLL}(l)$.

Proof. Let l denote a tight knot in 3-space. The second Vassiliev measure is defined as follows:

$$w_2(l) = \frac{1}{4\pi}\int_{\boldsymbol{\xi}\in S^2} v_2(l_{\boldsymbol{\xi}})\mathrm{d}A, \tag{6.12}$$

where $v_2(l_{\boldsymbol{\xi}})$ is the second Vassiliev invariant of the knotoid that results from the projection of l on the plane with normal vector $\boldsymbol{\xi}$.

Since l is a tight open knot, $l_{\boldsymbol{\xi}}$ is a knot-type knotoid for any $\boldsymbol{\xi}$ that defines a non-generic projection.

The result follows by theorems 5.7 and 6.3. ■

7. The double alternating self-linking integral of a polygonal curve

In the case of a polygonal curve, the double alternating self-linking integral has an expression as a finite sum of geometric probabilities.

Proposition 7.1. *The double alternating self-linking integral of a polygonal curve (open or closed) can be expressed as follows:*

$$\begin{aligned}\mathrm{SLL}(l) &= \frac{1}{2}\sum_{1\le j_4\le j_3\le j_2\le j_1\le n} p^*_{j_1,j_2,j_3,j_4}\epsilon(e_{j_1},e_{j_3})\epsilon(e_{j_2},e_{j_4}) \\ &\quad + \frac{1}{2}\sum_{1\le j_3\le j_2\le j_1\le n} p^*_{j_1,j_2,j_3}\epsilon(e_{j_1},e_{j_2})\epsilon(e_{j_1},e_{j_3}), \end{aligned} \tag{7.1}$$

Table 1. The spherical polygon $Q^*_{i,j,j+1}$ in the case where the signs satisfy $\epsilon_{i,j} = \epsilon_{i,j+1}$, depending on the conformation. The spherical polygon $Q^*_{i,j,j+1}$ contains the vectors that define planes where the projections of both e_i, e_j and e_i, e_{j+1} cross and they create an alternating crossing. $(\boldsymbol{w}_1, \boldsymbol{w}_2, \ldots, \boldsymbol{w}_n)$ denotes the spherical polygon bounded by the great circles with normal vectors $\boldsymbol{w}_i$, $i = 1, \ldots, n$, in the counterclockwise orientation (see [51]).

$\epsilon_{i,j} = \epsilon_{i,j+1}, w < 0, w_0 < 0$	$Q^*_{i,j,j+1}$
$c_{j+1,i+1} > 0, c_{j+2,i+1} > 0, c_{j+1,i} > 0, c_{j+2,i} > 0$	$(\boldsymbol{n}_4, \boldsymbol{n}_1, -\boldsymbol{u}_2, \boldsymbol{v}_3)$
$c_{j+1,i+1} < 0, c_{j+2,i+1} < 0, c_{j+1,i} > 0, c_{j+2,i} > 0$	$(\boldsymbol{n}_4, -\boldsymbol{u}_3, -\boldsymbol{u}_2, \boldsymbol{v}_3)$
$c_{j+1,i+1} > 0, c_{j+2,i+1} < 0, c_{j+1,i} > 0, c_{j+2,i} > 0$	$(\boldsymbol{n}_4, \boldsymbol{n}_1, -\boldsymbol{u}_3, -\boldsymbol{u}_2, \boldsymbol{v}_3)$
$c_{j+1,i+1} < 0, c_{j+2,i+1} > 0, c_{j+1,i} > 0, c_{j+2,i} > 0$	$(\boldsymbol{n}_4, -\boldsymbol{u}_3, \boldsymbol{n}_1, -\boldsymbol{u}_2, \boldsymbol{v}_3)$
otherwise	0

where $p^*_{j_1,j_2,j_3,j_4}$ denotes the probability that the projections of e_{j_1} and e_{j_2} as well as the projections of e_{j_3} and e_{j_4} both cross in a projection and form an alternating crossing, and $p(j_1,j_2,j_3)^*$ denotes the probability that one of the edges $e_{j_1}, e_{j_2}, e_{j_3}$ intersects the other two in a projection and forms an alternating crossing.

Proof. As explained in the proof of proposition 6.6, if j_1, j_2, j_3, j_4 all lie on the same edge, then there is no contribution to the integral. Similarly, if the four points lie only on two edges, they do not contribute to the integral any pairs of crossings. However, it is possible that they contribute when they lie in three or four edges. Similarly, if three edges or two pairs of edges cross in a projection, then they create two pairs of crossings. The result follows by separating these cases in equation (6.11). ■

This expression of SLL shows that for a polygonal curve its calculation relies on calculating the geometric probabilities $p^*_{j_1,j_2,j_3,j_4}$, $p^*_{j_1,j_2,j_3}$. We note that if all of j_1, j_2, j_3, j_4 are consecutive, then $p^*_{j_1,j_2,j_3,j_4} = 0$. Similarly, if all of j_1, j_2, j_3 are consecutive, then $p^*_{j_1,j_2,j_3} = 0$. The next proposition provides a closed formula for the computation of $p^*_{j_1,j_2,j_3}$ in the case where two of j_1, j_2, j_3 are consecutive.

Corollary 7.2. *Let e_i, e_j, e_{j+1} denote three edges in 3-space. Then, the joint probability of crossing between the projections of e_i, e_j and e_i, e_{j+1} so that they give an alternating crossing, namely, $p(i,j,j+1)$, is equal to $(1/2\pi)A(Q^*_{i,j,j+1})$, where $Q^*(i,j,j+1)$ is given in table 1, where $c_{4,1} = (\boldsymbol{p}_{4,1} \cdot \boldsymbol{n}_1)\epsilon_{1,3}$, $w = (u_2 \times (-n_2)) \cdot (u_2 \times n_4)$, $w_0 = (\boldsymbol{v}_3 \times (-\boldsymbol{n}_1)) \cdot (\boldsymbol{v}_3 \times \boldsymbol{n}_3)$ and the vectors $\boldsymbol{u}_2, \boldsymbol{n}_2, \boldsymbol{n}_4, \boldsymbol{v}_3, \boldsymbol{v}_2$ and $\boldsymbol{n}_1$ are normal to the planes containing the vertices $(i-1,i,j+1), (i-1,i,j), (i-1,j-1,i), (j-1,j+1,j), (j-1,j+1,i)$ and $(i-1,j-1,j)$, respectively.*

Proof. In order for them to form an alternating crossing, the signs of the two crossings must be the same. The geometric probability that three edges cross, two of which are consecutive, e_i, e_j, e_{j+1}, was found in theorem A.1 in [51]. To preserve the order of crossings, we need to ensure that, as we move along e_i in a projection, first we encounter the crossing with e_j and then with e_{j+1}. This imposes the extra constraint that the spherical area is on the side of the great circle defined by the vector $\boldsymbol{v}_3$ in the direction of $\boldsymbol{v}_3$. The results are presented in table 1. ■

(a) The double alternating self-linking integral of a polygonal curve with four edges

A polygonal curve with four edges is the shortest polygonal curve that can have a non-trivial double alternating self-linking integral. We will show that in this simple case the double alternating self-linking integral has an even simpler interpretation as the geometric probability that a projection of l gives the knotoid $k2.1$.

Proposition 7.3. *Let l_4 denote an open polygonal curve in 3-space. The double alternating self-linking integral of l_4 is equal to the signed geometric probability that it gives the knotoid $k2.1$ in a projection direction, i.e.* $\mathrm{SLL}(l_4) = \frac{1}{2}P(l_{\xi} = k2.1)$.

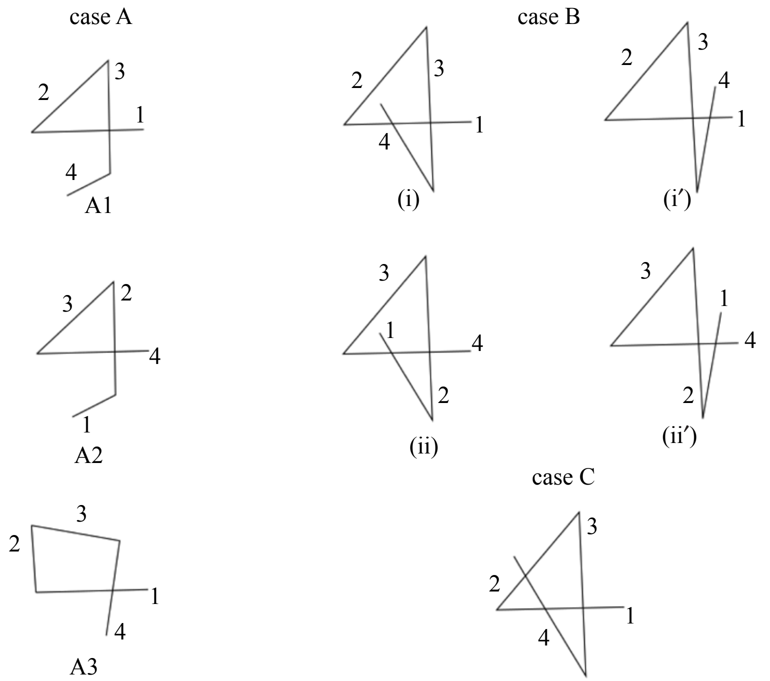

Figure 1. The possible projections with crossings of a polygonal curve with four edges.

Proof. From figure 1, we see that the only possibilities of a pair of alternating crossings in the projection of a curve with four edges are case B(i) or case B(ii), both of which correspond to the knotoid $k2.1$. In [51], it was proved that for a given curve l either B(i) or B(ii) is a possible outcome in the projections of l, but not both. The product of the two crossings is equal to 1 in both cases. ■

8. Conclusions

In this article, we defined Vassiliev measures for open curves in 3-space and showed that they generalize the conventional Vassiliev invariants. For open curves, these are continuous functions of the curve coordinates which tend to the Vassiliev invariants of the closed curves as the endpoints tend to coincide. A geometric interpretation of Vassiliev measures of closed and open curves was given, which allowed us to derive a well-defined integral expression of Vassiliev measures. More precisely, the double alternating self-linking integral was introduced, and it was shown that it coincides with the second Vassiliev invariant of closed curves. For open curves, this integral is a continuous function of the curve coordinates and, when the open curves have tight knots, the double alternating self-linking integral coincides with the Vassiliev measure of the open curves. For polygonal curves, the double alternating self-linking integral has a simpler expression as a sum of finitely many geometric probabilities. The double alternating self-linking integral allows us to rigorously define and capture entanglement and knotting in open curves in 3-space, avoiding the calculation of polynomials and avoiding artificial closures. The method introduced in this study provides a framework in which other Vassiliev invariants can also be generalized to open curves. These measures provide a novel and efficient method to measure entanglement and knotting in physical systems of filaments and can lead to many impactful applications.

Data accessibility. All the information required to reproduce the paper is contained within the paper and the electronic supplementary material.

Authors' contributions. Both authors made substantial contributions to the conception and design; drafting the article or revising it critically for important intellectual content; gave final approval of the version to be

published; and gave agreement to be accountable for all aspects of the work in ensuring that questions related to the accuracy or integrity of any part of the work are appropriately investigated and resolved.

Competing interests. We declare we have no competing interests.

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