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The second Vassiliev measure of uniform random walks and polygons in confined space

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Abstract

Biopolymers, like chromatin, are often confined in small volumes. Confinement has a great effect on polymer conformations, including polymer entanglement. Polymer chains and other filamentous structures can be represented by polygonal curves in three-space. In this manuscript, we examine the topological complexity of polygonal chains in three-space and in confinement as a function of their length. We model polygonal chains by equilateral random walks in three-space and by uniform random walks (URWs) in confinement. For the topological characterization, we use the second Vassiliev measure. This is an integer topological invariant for polygons and a continuous functions over the real numbers, as a function of the chain coordinates for open polygonal chains. For URWs in confined space, we prove that the average value of the Vassiliev measure in the space of configurations increases as $O(n^2)$ with the length of the walks or polygons. We verify this result numerically and our numerical results also show that the mean value of the second Vassiliev measure of equilateral random walks in three-space increases as $O(n)$. These results reveal the rate at which knotting of open curves and not simply entanglement are affected by confinement.

Keywords: polygons, Vassiliev invariants, random walks, knots, confinement

(Some figures may appear in colour only in the online journal)

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1. Introduction

Polymers and biopolymers are made of repetitive units that are bonded to form long filaments. Those macromolecules, entangle with each other and with themselves. Entanglement in systems of polymers has a very important effect to their mechanics and function [4, 18, 19, 34] and is affected by polymer architecture, polymer chemical composition, solvent quality, density and spatial confinement. Under the so-called theta conditions, long enough polymers, can be seen as random walks in Kuhn unit length [34]. A random walk representation of polymers allows to make theoretical predictions on the asymptotic behavior of polymer characteristics. For example, the radius of gyration, or the mean end-to-end distance of a polymer is well understood using random walks [34]. In this manuscript, we study theoretically the expected scaling of knotting complexity of a polymer chain in confinement, using the uniform random polygon (URP) and uniform random walk (URW) model, and we confirm our theoretical predictions with numerical results on URPs and URWs. We also compare these to numerical results on equilateral random walks of varying length in three-space.

Examples of confined polymers can be found in our cells, where biopolymers, like chromatin, which has approximately 6 billion base pairs, are confined in a space of radius 6–20 μm. [1]. Knotting in such systems would have significant impact on cell functions. To understand biological mechanisms of biomolecules in the cell and other confined spaces, it is important to compare the characteristics of these polymer conformations to those of random walks in the absence of any physical interactions. Previous results in studying knotting of random walks have focused on identifying knots in random polygons [2, 4–6, 8–11, 14, 16, 17, 20–23, 25, 26, 31, 35, 36, 38, 39]. It is well established that the probability of knotting and the complexity of knotting both increase with the length of the chains, as well as with confinement. In particular, it is shown that the probability of knotting increases exponentially with the length of a polygon. However, it is more difficult to answer how does the knotting complexity scale with the length of the polygons? A reason why this has been difficult is that the focus of previous work has been on identifying knot types in polygons, which provides a characterization of knotting that has been difficult to put in a simple quantitative measure of knotting complexity [39]. However, one could infer an answer to this question by examining how the maximum of the probability of a knot type scales with its length. An even more difficult question is how does knotting complexity of random walks (open polygons) increase with their length?

The problem with random walks is that they do not form topological knots. In order to study knotting of open curves in three-space, typically, a closure scheme is applied in order to approximate the open chain with a knot and then identify its knot-type [24]. Until recently, the only measure of entanglement that could be directly applied to open polygons with no closure scheme required, was the Gauss linking integral. When applied over one curve, the Gauss linking integral gives the Writhe and the average crossing number, ACN. The Writhe and the ACN are not topological invariants even for closed curves and do not detect knotting accurately. It is true that more complex knots and links have higher Writhe and the average crossing number, ACN, in general, but an unknot can have high Writhe and ACN as well. The Writhe and the ACN give real numbers which are continuous functions of the chain coordinates, for both closed and open polygons. Due to their simple definition however, the Writhe and ACN provide the best estimates in the literature of the question raised above. It has been shown that the Writhe and the ACN scale as $O(\sqrt{n})$ and $O(n\ln n)$, respectively, with the length, n, of equilateral random walks in three-space and as $O(n)$ and $O(n^2)$, respectively, for URWs in confinement [3, 12, 13, 15, 27, 30, 33, 37].

In [28, 29] new measures of entanglement of open curves in three-space were introduced. Namely, in [28] a framework by which knot polynomials -in particular the Jones polynomial—can be applied to measure knot complexity of open curves was introduced. In [29] it was shown that within the same framework, Vassiliev measures of complexity are well defined for open curves in three-space. These Vassiliev measures give continuous functions of knotting complexity for open curves and, as the endpoints of a chain tend to coincide, they tend to the corresponding Vassiliev invariant of the resulting knot. The second Vassiliev invariant of open and closed curves in three-space is a measure of knotting for both open and closed curves that has a simple geometric interpretation and can be calculated using an integral over one curve [29].

In this manuscript, we use the second Vassiliev measure to examine how knotting complexity increases with the length of random walks or polygons in confined space. One of the simplest models of random walks and polygons in confined space is the URW (resp. URP) model [3, 30]. In that model, each vertex of the walk or polygon is chosen with respect to the uniform distribution in a cube (or another convex space). We prove that the second Vassiliev measure scales as $O(n^2)$ with the length, n, of URPS and URWs. Moreover, we obtain estimates of the constants involved in this scaling, which we prove represent specific geometric probabilities in the space of URPs or URWs.

The manuscript is organized as follows: section 2 presents the second Vassiliev measure of open and closed curves in three-space, section 3 presents our analytical results on the scaling of the second Vassiliev measure of a URW or polygon as a function of its length. Section 4 presents our numerical data on the second Vassiliev measure of URWs and polygons of varying length in confined space and the second Vassiliev measure of equilateral random walks in three-space. In section 5 we discuss the conclusions of this study.

2. The second Vassiliev measure of open and closed curves in three-space

The second Vassiliev invariant, also known as the Casson invariant, is equal to the coefficient of x^2 in the Conway polynomial of a knot. It is also related to the coefficients of other knot polynomials [7]. In [32] an easy combinatorial formula for the second Vassiliev invariant of knots (closed curves) was derived. In [29], an integral formula for the second Vassiliev invariant, as a double alternating self-linking integral was derived which is applicable to both open and closed curves in three-space, namely:

Definition 2.1. Let l denote a curve in three-space with parametrization γ. We define the double alternating self-linking integral as:

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

where $\Gamma(s,t)=\frac{\gamma(s)-\gamma(t)}{|\gamma(s)-\gamma(t)|}$, for $s,t\in[0,1]$, $0\leqslant j_4<j_3<j_2<j_1\leqslant 1$ 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 $0\leqslant j_1<j_2<j_3<j_4\leqslant 1$, $\Gamma(j_1,j_3)=-\Gamma(j_2,j_4)$.

In [29], it was proved that the second Vassiliev invariant of the enhanced Jones polynomial of knots is related to the double alternating self-linking integral through the equation $v_2(l)=\frac{1}{4}+6\mathrm{SLL}(l)$. From [29], one can see that for the second Vassiliev invariant of the Conway polynomial, $v_2=\mathrm{SLL}(l)$. Due to this association of the double alternating self-linking integral with the second Vassiliev invariants, in the following, we will call the double alternating self-linking integral, simply second Vassiliev invariant.

The double alternating self-linking integral defined provides a well defined integral for the second Vassiliev invariant which has a simple geometric interpretation as an average of the algebraic sum of alternating pairs of crossings in a projection, over all possible projection directions. More precisely, we define an 'alternating' pair of crossings as follows:

Definition 2.2. Let $j_1 < j_2 < j_3 < j_4$ be points on a knot diagram. We will say that this four-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.

In [29] it was proved that for closed curves in three-space, the double alternating self-linking integral has a simple expression as an average of products of alternating signs of crossings:

Theorem 2.1. *Let l denote a curve in three-space with parametrization γ. The double alternating self-linking integral can be expressed as:*

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

where $\epsilon(s,t) = \pm 1$, is the sign of the crossing between the projection of $\gamma(s)$ and $\gamma(t)$, and where $I^*_{\vec{\xi}}$ denotes the set of four-tuples of alternating crossings in the projection to the plane with normal vector $\vec{\xi}$.

For closed curves, the double alternating self-linking integral is a topological invariant that can detect knots as the second Vassiliev invariant can. For open curves it was proved in [29] that it is a continuous function of the chain coordinates. As the endpoints of the chains tend to coincide, it tends to the Vassiliev invariant of the resulting knot.

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

Proposition 2.1. *The double alternating self-linking integral of a polygonal curve* (*open or closed*) *can be expressed as follows:*

$$\mathrm{SLL}(l) = \frac{1}{2}\sum_{1\leqslant j_4\leqslant j_3\leqslant j_2\leqslant j_1\leqslant n} p^*_{j_1,j_2,j_3,j_4}\epsilon(e_{j_1}, e_{j_3})\epsilon(e_{j_2}, e_{j_4}), \tag{3}$$

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.

3. The second Vassiliev measure of uniform random walks and polygons

In the URP model each coordinate of a vertex of the URW or polygon is drawn from a uniform distribution over $C = [0, 1]$. This generates a random walk or polygon confined in C^3.

We are interested in the average of the second Vassiliev measure (double alternating self-linking integral) over the space of configurations of URWs (or polygons, resp.) in confined space. We point out that the second Vassiliev invariant can take positive and negative values. However, mirror images contribute the same value instead of canceling. Therefore, the expected value of the second Vassiliev measure is not zero.

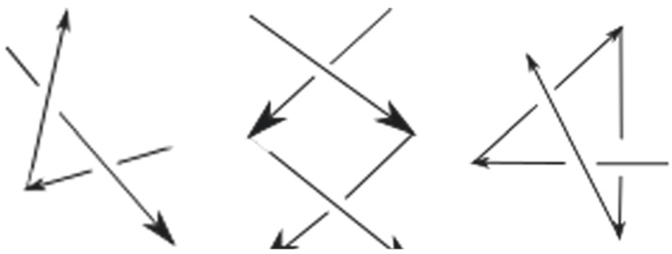

Figure 1. Examples of conformations contributing nonzero values to the product $\epsilon_1\epsilon_2$ in the case 4 (left), case 5 (middle) and case 6 (right), respectively, of lemma 3.1.

First, we study the expected value of the second Vassiliev measure of a URW (open polygonal chain) in confined space (theorem 3.1) and next we study the expected value of the second Vassiliev invariant of a URP (closed polygonal chain) in confined space (theorem 3.2).

Theorem 3.1. *The expected value of the second Vassiliev measure, $E[V_2(W_n)]$ of an oriented URW of n edges, W_n, contained in $\mathbf{C}^3$ is of the order $O(n^2)$. In particular, for URWs in confined space, $E[V_2(W_n)] = \alpha n^2 + \beta n + \gamma$, where $\alpha > 0, \beta < 0, \gamma > 0$.*

Remark 3.1. In the following it is shown that α, β and γ are the geometric probabilities of obtaining conformations like those shown in figure 1, in a diagram, independent of sign. More precisely, $\alpha = \frac{1}{2}u + \frac{1}{4}v$, $\beta = \frac{1}{2}(-5u - \frac{7}{2}v + w)$ and $\gamma = 3u + 3v - \frac{3}{2}w$, where u, v, w are defined as in lemma 3.1.

Let us consider two (independent) oriented random edges l_1 and l_2 of an oriented URW W_n and a fixed projection plane defined by a normal vector $\vec{\xi} \in S^2$. Since the end points of the edges are independent and are uniformly distributed in C^3, the probability that the projections of l_1 and l_2 intersect each other is a positive number which we will call $2p$. We define a random variable ϵ in the following way: $\epsilon = 0$ if the projection of l_1 and l_2 have no intersection, $\epsilon = -1$ if the projection of l_1 and l_2 has a negative intersection and $\epsilon = 1$ if the projection of l_1 and l_2 has a positive intersection. Note that, in the case the projections of l_1 and l_2 intersect, ϵ is the sign of their crossing. Since the end points of the edges are independent and are uniformly distributed in C^3, we then see that $P(\epsilon = 1) = P(\epsilon = 1) = p, E[\epsilon] = 0$ and $\mathrm{var}(\epsilon) = E[\epsilon^2] = 2p$. We will need the following lemma, modeled after the lemma 1 in [2], concerning the case when there are four edges involved (some of them may be identical or they may have a common end point): l_1, l_2, l_1' and l_2'. Let ϵ_1 be the random number ϵ defined above between l_1 and l_1' and let ϵ_2 be the random number defined between l_2 and l_2'. We are interested in the product $\epsilon_1\epsilon_2$, where the edges involved are ordered in the polygon as $l_1 < l_2 < l_1' < l_2'$, and such that, if $\epsilon_1, \epsilon_2 \neq 0$, then the pair of crossings is alternating. We will denote this statement as '$\epsilon_1\epsilon_2 \| \text{alternating}$'.

Lemma 3.1.

(*a*) *If the end points of l_1, l_2, l_1', and l_2' are distinct, then $E[\epsilon_1\epsilon_2 \| \text{alternating}] = 0$ (this is the case when there are eight independent random points involved).*

(*b*) *If $l_1 = l_2$, and the end points of l_1, l_1' and l_2' are distinct or if $l_1' = l_2'$ and the endpoints of l_1, l_2 and l_1' are distinct, or if $l_2 = l_1'$ and the endpoints of l_1, l_2, l_2' are distinct (this reduces the case to where there are only three random edges with six independent points involved), then $E[\epsilon_1\epsilon_2 \| \text{alternating}] = 0$.*

(*c*) *If l_1 and l_2, or l_1' and l_2', or l_2 and l_1', or l_2' and l_1 have a common end point, while the rest have distinct endpoints, then $E[\epsilon_1\epsilon_2 \| \text{alternating}] = 0$.*

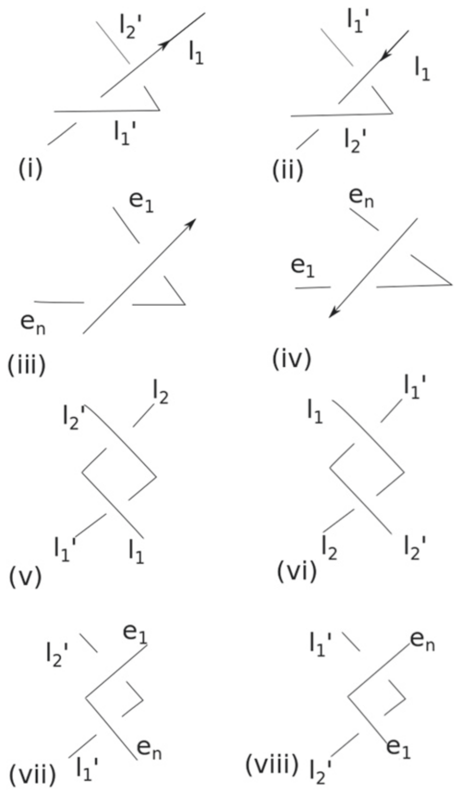

Figure 2. Cases (i) and (ii) are the only non-zero contributions to u in lemma 3.1. Cases (iii) and (iv) are the only non-zero contributions to u' in lemma 3.2. Cases (v) and (vi) are the only non-zero contributions to v in lemma 3.1. Cases (vii) and (viii) are the only non-zero contributions to v' in lemma 3.2.

(*d*) *In the case where* $l_1 = l_2$, *the endpoints of* l_1 *and* l_1' *and* l_1 *and* l_2' *are distinct, and* l_1' *and* l_2' *share a common point or if* $l_1' = l_2'$ *and the endpoints of* l_1' *and* l_1 *and* l_1' *and* l_2 *are distinct and* l_1 *and* l_2 *share a common point* (*so there are only five independent random points involved in this case*), *let* $E[\epsilon_1\epsilon_2||\text{alternating}] = u$. *Then* $u > 0$ *and* $u = P(\text{alternating})$ (*the probability that these edges form an alternating crossing*).

(*e*) *In the case where* l_1 *and* l_2 *share a common point, the endpoints of* l_1 *and* l_1' *and* l_1 *and* l_2' *are distinct, and* l_1' *and* l_2' *also share a common point* (*so there are four edges defined by six independent random points involved in this case*), *let* $E[\epsilon_1\epsilon_2||\text{alternating}] = v$. *Then* $v > 0$ *and* $v = P(\text{alternating})$ (*the probability that these edges form an alternating crossing*).

(*f*) *In the case where* l_1, l_2, l_1' *and* l_2' *are consecutive* (*so in this case, there are four edges defined by five independent random points*), *then* $E[\epsilon_1\epsilon_2||\text{alternating}] = w$, *where* $w < 0$ *and* $|w| = P(\text{alternating})$ (*the probability that these edges form an alternating crossing*).

Proof.

(a) In this case ϵ_1 and ϵ_2 are independent random variables, from which the result follows.

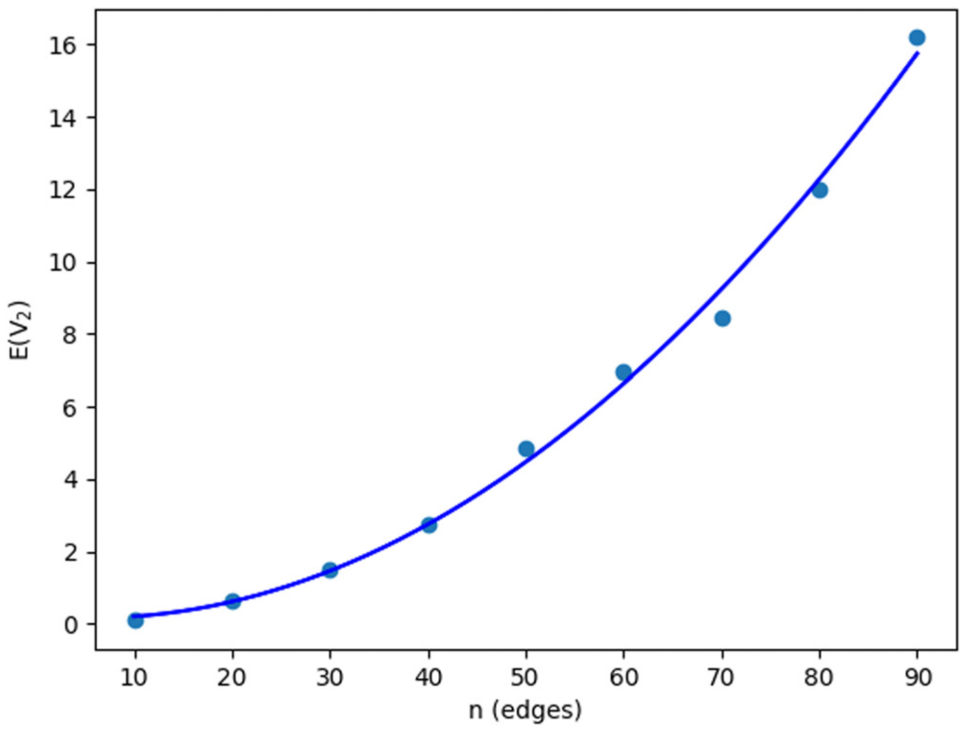

Figure 3. The expected values of the second Vassiliev measures obtained for URWs.

(b) First, note that in the configuration where the projections of l_1' and l_2' do not intersect the projection of l_1, we have $\epsilon_1\epsilon_2 = 0$. So we consider only configurations where the projections of l_1' and l_2' both intersect the projection of l_1. There are eight different ways to assign the orientations and labels to the edges. Four of them yield $\epsilon_1\epsilon_2 = -1$ and four of them yield $\epsilon_1\epsilon_2 = 1$. Since the joint density function of the vertices involved is simply $\frac{1}{V^6}$, where V is the volume of the confined space C^3, thus by a symmetry argument we have $E[\epsilon_1\epsilon_2] = 0$. The proof is similar when $l_1' = l_2'$ or $l_2 = l_1'$ and the rest of the endpoints are distinct.

(c) Since two edges have distinct endpoints from each other and from the other two, the crossing signs are independent in any projection direction and have equal probability of occurring.

(d) In the case where $l_1 = l_2$, the endpoints of l_1 and l_1' and l_1 and l_2' are distinct, and l_1' and l_2' share a common point, there are four possible cases of an alternating pair of crossings, all of which give $\epsilon_1\epsilon_2 = 1$. See figures 2(i) and (ii). The other two cases are obtained by taking the mirror image of these. Thus, $E[\epsilon_1\epsilon_2 || \text{alternating}] = u$, where u denotes the probability that we obtain a pair of alternating crossings from these three edges.

(e) In the case where l_1 and l_2 share a common point, the endpoints of l_1 and l_1' and l_1 and l_2' are distinct, and l_1' and l_2' also share a common point then there are only four cases, which both give $\epsilon_1\epsilon_2 = 1$. See figures 2(iii) and (iv). The other two cases are obtained by taking the mirror image of these. Thus, $E[\epsilon_1\epsilon_2 || \text{alternating}] = v$, where v denotes the probability that we obtain a pair of alternating crossings from these three edges.

(f) In the case where l_1, l_2, l_1' and l_2' are consecutive, then there are only four configurations possible, which contribute two pairs of alternating crossings each, with negative product of signs. Thus this configuration contributes a total $E[\epsilon_1\epsilon_2||\text{alternating}] = w$, where w is -1 times the geometric probability that the 4 edges create an alternating pair of crossings between l_1, l_1', l_2, l_2'.

□

Proof of theorem 3.1. Let $\vec{\xi} \in S^2$ and let $(V_2)_{\vec{\xi}}(W_n)$ denote the Vassiliev measure in the projection of W_n.

The second Vassiliev invariant in a projection is given as follows;

$$V_2((W_n)_{\vec{\xi}}) = \frac{1}{2}\sum_{\substack{i\leqslant j\leqslant k\leqslant l\\ \text{alternate}\\ \text{crossings}}} \epsilon_{ik}\epsilon_{jl}.$$

The expected value of the second Vassiliev invariant,

$$E[V_2((W_n)_{\vec{\xi}})] = \frac{1}{2}E\left[\sum_{\substack{i\leqslant j\leqslant k\leqslant l\\ \text{alternate}\\ \text{crossings}}} \epsilon_{ik}\epsilon_{jl}\right] = \frac{1}{2}\sum_{\substack{i\leqslant j\leqslant k\leqslant l\\ \text{alternate}\\ \text{crossings}}} E[\epsilon_{ik}\epsilon_{jl}].$$

We then split the sum according to lemma 3.1 and the only non-zero contributions are

$$\begin{aligned}
E[V_2((W_n)_{\vec{\xi}})] &= \frac{1}{2}\left[\sum_{1\leqslant i\leqslant n-3}\sum_{i+2\leqslant j\leqslant n-1} E[\epsilon_{ij}\epsilon_{i(j+1)}||\text{alt.}] + \sum_{1\leqslant i\leqslant n-3}\sum_{i+3\leqslant j\leqslant n} E[\epsilon_{ij}\epsilon_{(i+1)j}||\text{alt.}]\right. \\
&\quad \left. + \sum_{1\leqslant i\leqslant n-4}\sum_{i+3\leqslant j\leqslant n-1} E[\epsilon_{ij}\epsilon_{(i+1)(j+1)}||\text{alt.}] + \sum_{1\leqslant i\leqslant n-3} E[\epsilon_{i(i+2)}\epsilon_{(i+1)(i+3)}||\text{alt.}]\right] \\
&= \frac{1}{2}\left[\sum_{1\leqslant i\leqslant n-3}\sum_{i+2\leqslant j\leqslant n-1} u + \sum_{1\leqslant i\leqslant n-3}\sum_{i+3\leqslant j\leqslant n} u + \sum_{1\leqslant i\leqslant n-4}\sum_{i+3\leqslant j\leqslant n-1} v + \sum_{1\leqslant i\leqslant n-3} w\right] \\
&= \frac{1}{2}n^2\left(u + \frac{1}{2}v\right) + \frac{1}{2}n\left(-5u - \frac{7}{2}v + w\right) + 3u + 3v - \frac{3}{2}w. \qquad (4)
\end{aligned}$$

Then,

$$\begin{aligned}
E[V_2(W_n)] &= E\left[\frac{1}{4\pi}\int_{\vec{\xi}^2} V_2((W_n)_{\vec{\xi}})\mathrm{d}A\right] = \frac{1}{4\pi}\int_{\vec{\xi}^2} E[V_2((W_n)_{\vec{\xi}})]\mathrm{d}A \\
&= \frac{1}{2}n^2\left(u + \frac{1}{2}v\right) + \frac{1}{2}n\left(-5u - \frac{7}{2}v + w\right) + 3u + 3v - \frac{3}{2}w. \qquad (5)
\end{aligned}$$

Since $u, v > 0$ and $w < 0$, we obtain that

$$E[V_2(E_n)] = \alpha n^2 + \beta n + \gamma, \qquad (6)$$

where $\alpha, \gamma > 0$ and $\beta < 0$. □

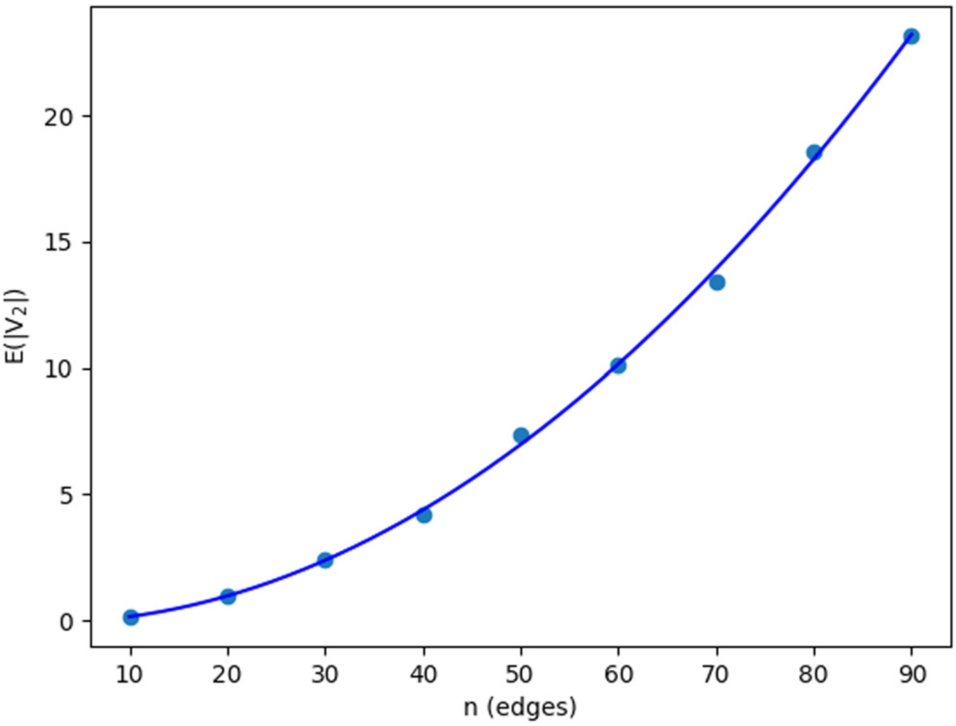

Figure 4. The expected values of the absolute second Vassiliev measures obtained for URWs.

Next, we study the expected value of V_2 for a URP. We will need lemma 3.1, but some additional cases need to be considered.

Lemma 3.2. *Let P_n denote a polygon of n edges, and let e_1, e_n denote the first and last edge of the polygon. Then $E[\epsilon_1\epsilon_2]$ for two pairs of crossings involving e_1, e_n satisfy:*

(*a*) *In the case where there are three edges edges involved, two of which are e_1, e_n and the third has no common point with those, $E[\epsilon_1\epsilon_2 || \text{alternating}] = u'$. Then $u' < 0$ and $|u'| = P(\text{alternating})$.*

(*b*) *In the case where there are four edges involved which belong to two pairs of consecutive edges, two of which are e_1, e_n and the two pairs have no points in common, then $E[\epsilon_1\epsilon_2 || \text{alternating}] = v'$. Then $v' < 0$ and $|v'| = P(\text{alternating})$.*

Proof. By inspection, (see figures 2(v)–(viii) and their mirror images) we notice that the only cases where (i) or (ii) give alternating crossings, have $\epsilon_1\epsilon_2 < 0$. □

Theorem 3.2. *The expected value of the second Vassiliev measure, $E[V_2]$ of an oriented URP of n edges, P_n contained in $\mathbf{C}^3$ is of the order $O(n^2)$. In particular, for URPs in confined space, $E[V_2(P_n)] = \alpha n^2 + \beta' n + \gamma'$, where $\alpha > 0$ and $\beta < 0$.*

Remark 3.2. We notice that the coefficient of n^2 in $E[\mathrm{V}_2(P_n)]$ is the same as that in $E[V_2(W_n)]$. β' and γ' are also related to the geometric probabilities of obtaining conformations as shown in figure 1 in a random projection direction. More precisely, $\alpha = \frac{1}{2}u + \frac{1}{4}v$,

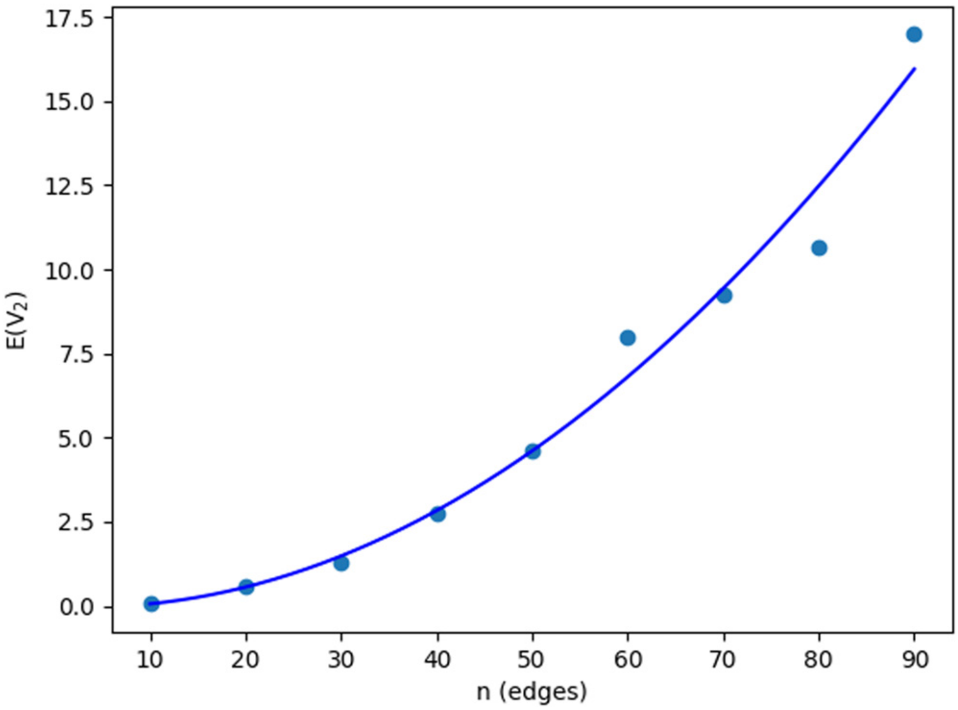

Figure 5. Expected Value of the second Vassiliev invariant, V_2, of URPs in confined space as a function of their length.

$\beta' = \frac{1}{2}(-5u - \frac{7}{2}v + 2w + u' + v')$, $\gamma' = -u - \frac{1}{2}v + \frac{3}{2}w - 2u' - \frac{5}{2}v'$, where u, v, w, u', v' are defined in lemmas 3.1 and 3.2.

Proof. Note that for a polygon, P_n, $V_2(P_n) = V_2((P_n)_{\vec{\xi}})$. To compute $E[V_2((P_n)_{\vec{\xi}})]$ we work as in theorem 3.1, by taking into account the contributions of the closure end. Namely,

$$
\begin{aligned}
E[V_2(P_n)] = \frac{1}{2}\Bigg[& \sum_{1\leqslant i\leqslant n-3}\ \sum_{i+2\leqslant j\leqslant n-1,\text{alt.}} E[\epsilon_{ij}\epsilon_{i(j+1)}] - E[\epsilon_{1,n-1}\epsilon_{1,n}] \\
& + \sum_{1\leqslant i\leqslant n-3}\ \sum_{i+3\leqslant j\leqslant n,\text{alt.}} E[\epsilon_{ij}\epsilon_{(i+1)j}] - E[\epsilon_{1,n}\epsilon_{2,n}] \\
& + \sum_{1\leqslant i\leqslant n-4}\ \sum_{i+3\leqslant j\leqslant n-1} E[\epsilon_{ij}\epsilon_{(i+1)(j+1)}] - E[\epsilon_{1,n-1}\epsilon_{2,n}] \\
& + \sum_{1\leqslant i\leqslant n-3} E[\epsilon_{i(i+2)}\epsilon_{(i+1)(i+3)}] \\
& + \sum_{i=3}^{n-2} E[\epsilon_{i,n}\epsilon_{i,1}] + \sum_{j=3}^{n-3} E[\epsilon_{n,j}\epsilon_{1,j+1}] \\
& + E[\epsilon_{n-2,n}\epsilon_{n-1,1}] + E[\epsilon_{n-1,1}\epsilon_{n,2}] + E[\epsilon_{n,2}\epsilon_{1,3}]\Bigg]
\end{aligned}
$$

$$
\begin{aligned}
&= \frac{1}{2}\left[\sum_{1\leqslant i\leqslant n-3}\ \sum_{i+2\leqslant j\leqslant n-1} u - u + \sum_{1\leqslant i\leqslant n-3}\ \sum_{i+3\leqslant j\leqslant n} u - u\right.\\
&\quad \left. + \sum_{1\leqslant i\leqslant n-4}\ \sum_{i+3\leqslant j\leqslant n-1} v - v + \sum_{1\leqslant i\leqslant n-3} w + \sum_{i=3}^{n-2} u' + \sum_{j=3}^{n-3} v' + 3w\right]\\
&= \frac{1}{2}n^2\left(u + \frac{1}{2}v\right) + \frac{1}{2}n\left(-5u - \frac{7}{2}v + w\right) + 3u + 3v\\
&\quad - \frac{3}{2}w - u - \frac{1}{2}v + \frac{3}{2}w + \frac{1}{2}(n-2-3+1)u' + \frac{1}{2}(n-3-3+1)v'\\
&= \frac{1}{2}n^2\left(u + \frac{1}{2}v\right) + \frac{1}{2}n\left(-5u - \frac{7}{2}v + 2w + u' + v'\right)\\
&\quad - u - \frac{1}{2}v + \frac{3}{2}w - 2u' - \frac{5}{2}v'. \qquad (7)
\end{aligned}
$$

Since, $u, v > 0$ and $u', v', w < 0$, we find that

$$E[V_2(P_n)] = \alpha n^2 + \beta' n + \gamma', \qquad (8)$$

where $\alpha > 0$ and $\beta' < 0$. □

4. Numerical results

In this section we present numerical results on the expected value of the second Vassiliev measure of URWs and polygons in confined space. We take averages of the second Vassiliev measure in the space of configurations of URWs and polygons of 10 to 100 edges with stepsize of 10. Each data point is an average over 500 random walks or polygons.

For URPs, the second Vassiliev measure is computed by using one projection of the polygon. The second Vassiliev measure of URWs was computed by averaging the algebraic sum of double alternating crossings in a projection over 500 projections. Projections were generated by selecting random vectors along the unit sphere. In practice, this was done by using the normal distribution to randomly select x, y, and z components and then dividing by the length of the vector, $\sqrt{x^2 + y^2 + z^2}$, to provide a unit vector that does not hold bias toward any directions on the unit sphere. (Indeed, then the probability density function of a vector $\vec{v} = (x, y, z)$ is $\frac{1}{(2\pi)^{3/2}}\,\mathrm{e}^{-\frac{1}{2}(x^2+y^2+z^2)} = \frac{1}{(2\pi)^{3/2}}\,\mathrm{e}^{-\frac{1}{2}\|v\|^2}$, independent of the direction.)

Section 4.2 presents our numerical results for URPs, section 4.1 presents our numerical results for URWs. For comparison, in section 4.3 we also present numerical results on the expected value of the second Vassiliev measure for equilateral random walks in three-space (un-confined random walks).

4.1. The second Vassiliev measure of uniform random walks in confined space

Figure 3 shows how the second Vassiliev measure of a URW scales in relation to its number of edges. The numerical show that $E(V_2(W_n))$ increases as $O(n^2)$, confirming theorem 3.1. In particular, we find that the data fit to a curve $\alpha n^2 + \beta n + \gamma$, where $\alpha = 0.0022$, $\beta = -0.0247$

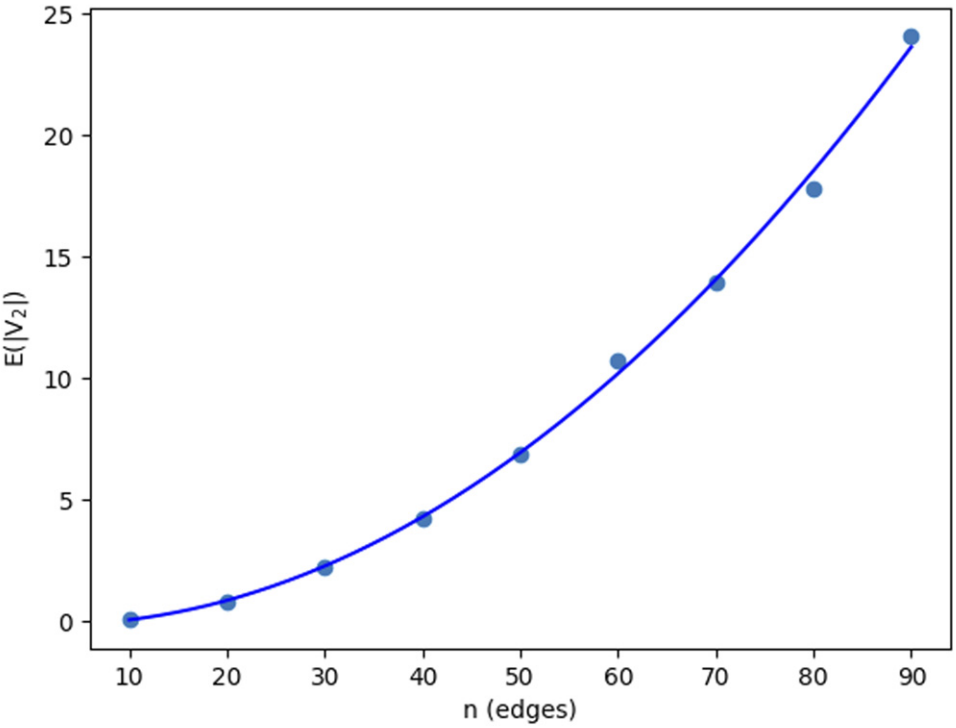

Figure 6. The expected value of the absolute second Vassiliev invariant, $|V_2|$, of URPs in confined space, as a function of their length.

and $\gamma = 0.2316$, with $R^2 = 0.9951$. These results also confirm that $\alpha > 0, \beta < 0, \gamma > 0$, as in theorem 3.1. It is also evident that the expected value of V_2 is always greater than zero, with V_2 taking positive values more often that negative values. Comparing these results to the Writhe and ACN of URWs in confined space, we find that $E[|V_2(W_n)|]$ scales faster that the Writhe, similar to the ACN. Our results suggest that at $N > 20$, $E[|V_2(W_n)|] > 1$, which suggests the presence of knots in most of these random walks. In the appendix, we see that knots (most likely open trefoils) appear already at $N = 10$.

Figure 4 shows how the expected value of $|V_2|$ for a URW scales in relation to its number of edges, also increasing as $O(n^2)$. In particular, we find that the data fit to a curve $\alpha n^2 + \beta n + \gamma$, where $\alpha = 0.0029$, $\beta = -0.0064$ and $\gamma = -0.0872$, with $R^2 = 0.9989$. As expected, the scaling is the same for $E[V_2]$ and $E[|V_2|]$ and $E[|V_2|] > E[V_2]$. Comparing the scaling of the expected value of $|V_2|$ to the expected value of the Writhe, $|Wr|$, of URWs, we find that $E[|V_2|] = O(n^2)$, while $E[|Wr|] = O(n)$. This suggests a big difference between the Writhe, which is affected a lot by the local geometry of a walk, and the second Vassiliev measure, which is a topological measure of knotting complexity.

4.2. The second Vassiliev measure of uniform random polygons in confined space

Figure 5 shows how the second Vassiliev measure of a URP scales in relation to its number of edges. The numerical results support the finding that $E(V_2(P_n))$ increases as $O(n^2)$. In partic-

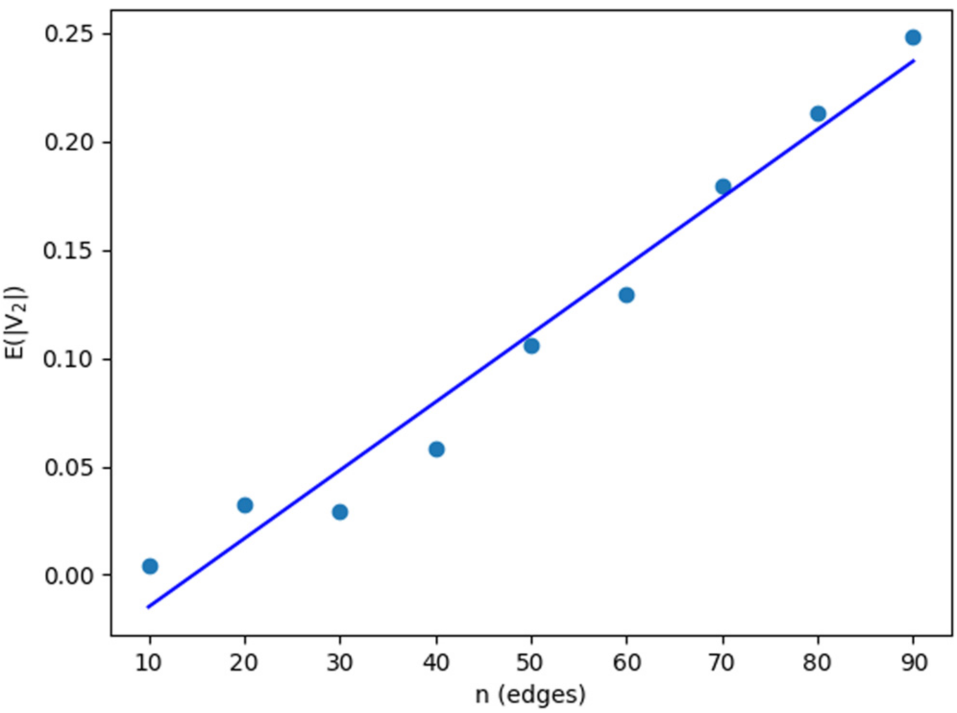

Figure 7. Expected values of the absolute second Vassiliev measure, $|V_2|$, of equilateral random walks, as a function of their length.

ular, we find that the data fit to a curve $\alpha n^2 + \beta n + \gamma$, where $\alpha = 0.0021$, $\beta = -0.0139$ and $\gamma = -0.016$, with $R^2 = 0.9772$. These results are in agreement with theorem 3.2. We also find that α is the same for URPs and URWs, as predicted.

Figure 6 shows how the expected value of $|V_2|$ for a URP scales in relation to its number of edges, also increasing as $O(n^2)$. In particular, we find that the data fit to a curve $\alpha n^2 + \beta n + \gamma$, where $\alpha = 0.0031$, $\beta = -0.0121$ and $\gamma = -0.1392$, with $R^2 = 0.998$. Note that the trefoil knot has $V_2 = 1$. We find that $E[|V_2(P_n)|] > 1$ at $N > 20$. This is in agreement with previous results on knotted polygons in confined spaces [14]. Comparing these results to the mean absolute Writhe of URPs, we find that V_2 increases faster than the Writhe. In fact, we find a scaling of the expected value of $|V_2|$ that is similar to that of the ACN.

4.3. The second Vassiliev measure of equilateral random walks

Figure 7 shows how the expected value of $|V_2|$ of an equilateral random walk scales in relation to its number of edges. We find that the second Vassiliev measure of equilateral random walks increases as $O(n)$. In particular, we find that the data fit to a curve $an + b$, where $a = 0.0031$ and $b = -0.0462$ with $R^2 = 0.9698$. As expected, confinement increases the asymptotic power scaling of V_2 and we find by a factor of two. A similar difference in the power by two was observed for the mean absolute Writhe [30]. We find that the expected value of the absolute second Vassiliev measure of equilateral random walks shows a scaling in between that of the Writhe, which is $O(\sqrt{n})$ [30], and that of the ACN, which is $O(n \ln n)$ [15].

5. Conclusions

We used a new measure of topological entanglement sensitive to knotting that is applicable to both closed and open curves to analyze the complexity of random walks and polygons in confinement. Using the URW, URP model, we proved that the second Vassiliev measure scales as $O(n^2)$ with the length n of a random walk or polygon. In fact, we found that the average Vassiliev measure follows a function of the form $\alpha n^2 + \beta n + \gamma$ and that the coefficients α, β, γ represent geometric probabilities of specific types of pairs of crossings in a projection. This scaling is comparable to that of the ACN of URWs in confined space and not that of the Writhe. We found that for $N > 20$, the mean Vassiliev measure is greater than 1. Indicatively, the trefoil knot has second Vassiliev invariant 1. This suggests that the open polygonal chains contain knots at $N > 20$. Our results on equilateral random walks in three-space showed a linear scaling of the second Vassiliev measure with the length of the chains, similar to that of ACN. The second Vassiliev measure of equilateral random walks is less than 1 for all the lengths analyzed here. This makes evident how confinement induces knotting in open chains.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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Appendix

In this section we present the distributions of the second Vassiliev measure and the second Vassiliev invariant for URWs and URPs, respectively of varying length.

Figure 8 shows the distribution of the second Vassiliev invariant for URPs of 10 to 90 edges. We see that for URPs of less than 30 edges the distributions of V_2 are narrow and centered at zero, indicating that the occurrence of knotting is rare. However, values of $V_2 = 1$ appear already at $N = 10$, indicating the presence of knots (likely trefoil knots). As the number of edges of a URP increases, the values of V_2 tend to broaden and deviate farther from the zero value, indicating an increase in knotting. A lean toward positive values also begins to become visible. Similar results are found for URWs in figure 9.

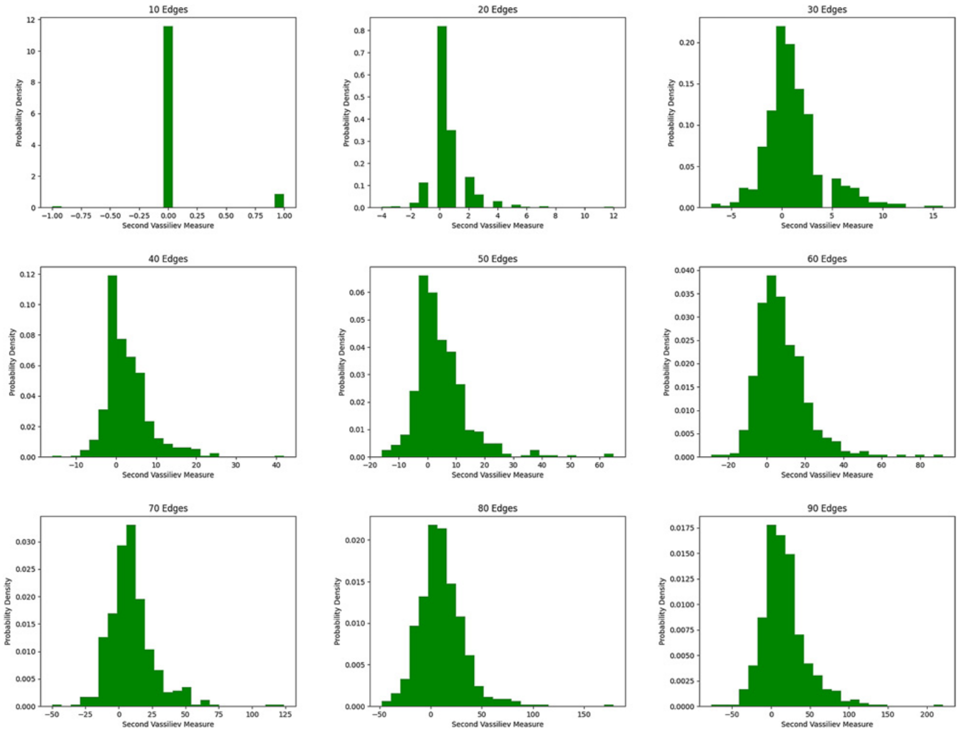

Figure 8. Distributions of the second Vassiliev measure for URPs of 10 to 90 edges.

Figure 10 shows the distribution of the absolute second Vassiliev measure for equilateral random walks in three-space of 10 to 90 edges. We see that equilateral random walks of few edges, $|V_2|$ is typically zero or very near zero, indicating that no or very little knotting is occurring. However, values of $v_2 \approx 0.8$ are populated, indicating the occurrence of open knots, even at $N = 10$. For longer chains, we see higher values of $|V_2|$ become more populated. The population of the zero value decreases, indicating a decreasing probability of obtaining an unknotted curve.

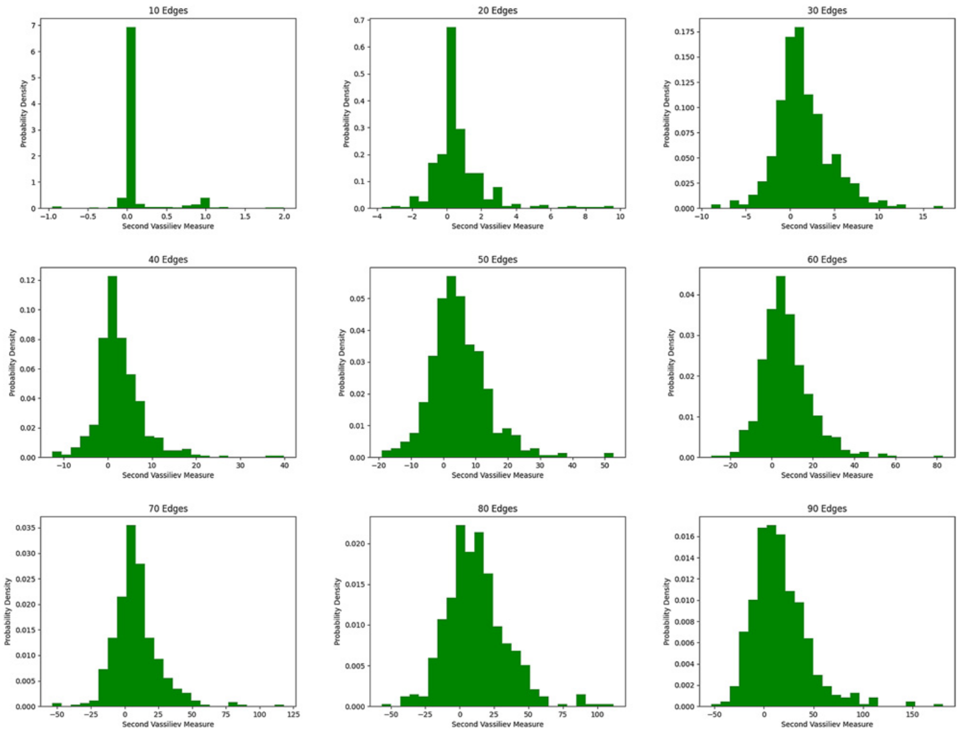

Figure 9. Distributions of the second Vassiliev measure for URWs of 10 to 90 edges.

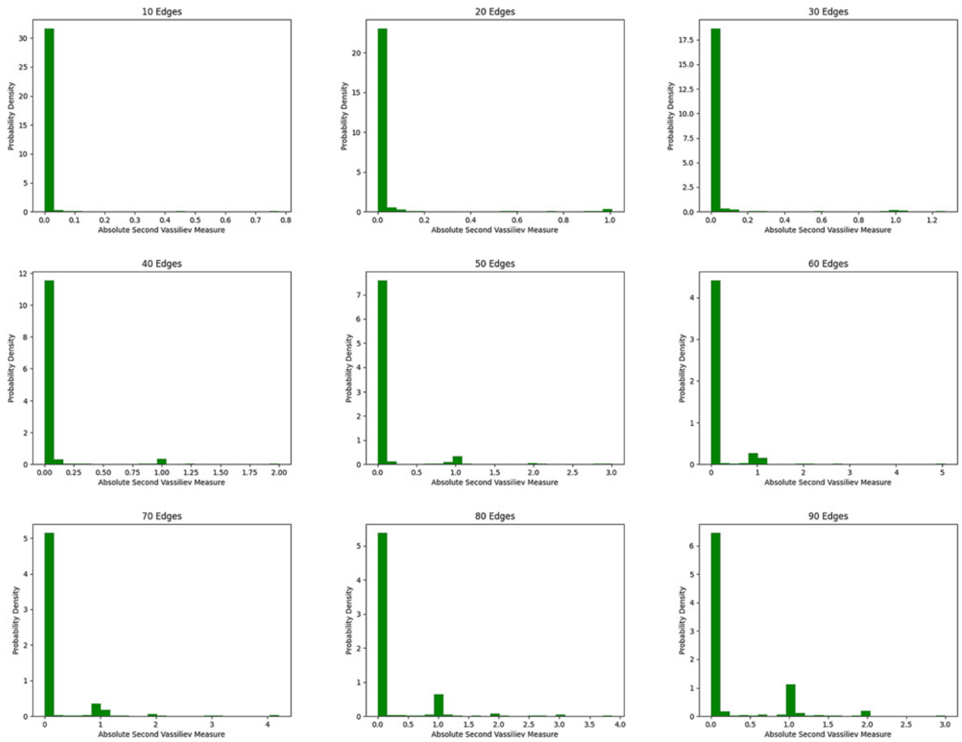

Figure 10. Distributions of the absolute second Vassiliev measure for equilateral random walks of 10 to 90 edges.

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