Reactive and Functional Polymers 131 (2018) 430–444

Contents lists available at ScienceDirect

Reactive and Functional Polymers

journal homepage: www.elsevier.com/locate/react

# Average crossing number and writhe of knotted random polygons in confinement

Yuanan Diao[a], Claus Ernst[b], Eric J. Rawdon[c,*], Uta Ziegler[d]

[a] Department of Mathematics and Statistics, University of North Carolina Charlotte, Charlotte, NC 28223, USA
[b] Department of Mathematics, Western Kentucky University, Bowling Green, KY 42101, USA
[c] Department of Mathematics, University of St. Thomas, Saint Paul, MN 55105, USA
[d] School of Engineering and Applied Sciences, Western Kentucky University, Bowling Green, KY 42101, USA

ARTICLE INFO

*Keywords:*
Confinement
Knot
Average crossing number
Writhe
Random polygons

ABSTRACT

In this paper we study the average crossing number and writhe of random freely-jointed polygons in spherical confinement. Specifically, we use numerical studies to investigate how these geometric quantities are affected by confinement and by knot complexity within random polygons. We report and compare our results with previously published results on knotted random polygons that are unconfined. While some of the results fall in line with what have been observed in studies of unconfined random polygons, some surprising results have emerged from our study, showing properties that are unique due to the effect of confinement. For example, under tight confinement, the average crossing number and the squared writhe grow proportional to the polygon length squared. However, the squared writhe of polygons with a fixed knot type (such as the trefoil) grows much slower than the squared writhe of all polygons. We also observe that while the writhe values at a given length and confinement radius are normally distributed, the distribution of the average crossing number values around their mean are not normal, but rather log-normal.

## 1. Introduction

Random equilateral polygons are often used as a coarse approximation for physical, rope-like objects that are circular and have a certain degree of randomness to their structure, such as circular polymers. In addition, polymers, e.g. DNA and RNA, may be subject to spatial confinement such as in a virus capsid or in an artificial nanopore. Here we use random equilateral free-jointed polygons in spherical confinement as a coarse model of biopolymers subject to spatial confinement. This article is the continuation of a study that explores the interplay between the topology (knotting) and geometry relative to the length and severity of confinement. In earlier papers [1–4] we have explored how confinement affects knotting by favoring certain classes of knot types and how confinement affects the total curvature (turning) and total torsion (twisting) of knotted polygons.

In this article we concentrate on how confinement affects the average crossing number (ACN) and writhe in the presence of knotting. In particular, we explore the interplay of these two quantities with confinement, length, and knot complexity. The ACN measures the complexity of a configuration by counting the average number of times the configuration passes over itself when viewed from all angles. Writhe is a measure of chirality of a configuration and plays an important role in knotted DNA (see e.g. [5–7]).

Three of the authors of this paper have developed a method for efficiently generating random polygons in confinement [8–10]. While these methods are not the first to generate confined random polygons [11], these methods are mathematical very clean (using explicit probability density functions in the generation process) and without any inherent bias in the generation method. The confinement generates higher complexity knots at shorter length values than is the case for unconfined knots, which allows us to analyze a wide range of knot types at relatively short lengths.

For these confined polygons we 1) fix the length and vary the confinement radius and 2) fix the confinement radius and vary the length, and observe the effects on the average crossing number and writhe. A few surprising results emerge from our study, showing some properties that are unique due to the effect of knotting in confinement. For example, under tight confinement, the squared writhe of polygons with a fixed knot type (such as the trefoil) grows much slower than the squared writhe of all polygons. We also observe that while the writhe values at a given length and confinement radius are normally distributed, the distributions of the ACN values around their means are not

* Corresponding author.
*E-mail addresses:* yuanandiao@uncc.edu (Y. Diao), claus.ernst@wku.edu (C. Ernst), ejrawdon@stthomas.edu (E.J. Rawdon), uta.ziegler@wku.edu (U. Ziegler).

https://doi.org/10.1016/j.reactfunctpolym.2018.07.028
Received 9 February 2018; Received in revised form 28 June 2018; Accepted 31 July 2018
Available online 11 August 2018

normal, but rather log-normal. Furthermore, a new proposed fit function for the ACN, as a function of the length of the random polygons and the confinement radius, provides an excellent fit over the whole range of the data.

This manuscript is organized as follows. In Section 2 we provide some background information on knot theoretic concepts from this article and explain how our data set was generated. Sections 3 and 4 deal with the interplay between topology (knotting complexity), confinement radius, and polygon length on the average crossing number and on the writhe, respectively. In both sections we show the numerical evidence from our data and then explain our observations. We conclude the article with Section 5 by summarizing the results and indicating open questions of future work.

## 2. Background

### 2.1. Knot theory background

For the convenience of our readers, we outline and discuss briefly some geometrical and topological concepts that are most relevant to this paper. For a more detailed exposition, please refer to a standard text on knot theory such as [12–15].

A *knot K* is a closed curve in $\mathbb{R}^3$ with no self-intersections. Here we assume that such a curve is a piece-wise smooth curve (this includes a space polygon without self-intersections). Two knots are topologically equivalent if one can be continuously deformed, together with the entire $\mathbb{R}^3$ space surrounding it and without being broken or causing self-intersection in the process, to the other. The class of all equivalent configurations is called a *knot type*. The knot type that contains the unit circle is called the *trivial knot* (type), and is denoted $0_1$.

For a fixed knot configuration $K$, a *regular projection* of $K$ is a projection of $K$ onto a plane such that no more than two segments of $K$ cross at the same point in the projection. An intersection in a regular projection is called a *crossing*. A regular projection of $K$ is typically drawn to show which strand passes over and which strand passes under at each crossing in the projection. A projection with this over/under information marked at the crossings is called a *knot diagram*. The minimum number of crossings among all possible knot diagrams of knots with the same knot type as $K$ is called the *crossing number* of $K$ and is denoted $cr(K)$.

A knot diagram is *alternating* if the strands alternate between under and over at crossings as one travels along the curve. A knot type is *alternating* if it has an alternating diagram and is non-alternating if it does not have any alternating diagram. If we switch the "over" and "under" at each crossing in a diagram of a knot type $K$ then we obtain a diagram of the *mirror image* of $K$, see Fig. 1(a).

A knot type is called a *composite knot* if it is realized by connecting two nontrivial knots as shown in Fig. 1(b). If a knot type is not composite, then it is a prime knot type. It is important to note that a composition of two alternating knot components always admits a minimum knot projection that is alternating, as well as a minimum knot projection that is non-alternating. Thus, in our study the composite knots are not included in either of the alternating or non-alternating knot groups.

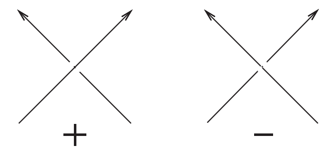


**Fig. 2.** A positive and a negative crossing.

A knot type is *amphichiral* or *achiral* if a configuration of the given knot type is equivalent to its mirror image (in which case all configurations of the given knot type are equivalent to their mirror images). We analyze knot types through 10 crossings. Oftentimes we focus on knot types through seven crossings, in which case there are three prime amphichiral knot types: $0_1$, $4_1$, and $6_3$. There are five prime 8-crossing and 13 prime 10-crossing amphichiral knot types. Knot types that are not amphichiral are called *chiral*. For the chiral knot types, we specify a positive and negative version of the knot type, e.g. the trefoil $3_1$ is divided into $+3_1$ and $-3_1$, based on the writhe of ropelength-minimized configurations from [16].

In this paper, we explore the average crossing number (ACN) and writhe of random polygons under confinement. The ACN of a knot configuration $K$ is defined as the average of the number of crossings over all regular projections of $K$. Given a knot diagram $D_K$ of $K$, the *projected writhe* of $D_K$ is the sum of the $\pm 1$ values assigned to the crossings of $D_K$ according to the convention in Fig. 2, and the *writhe* of $K$, denoted by $wr(K)$, is the average of the projected writhe taken over all regular projections of $K$. The writhe is similar to the ACN in that it measures the average of the crossing number of a projection over all projection directions – with the difference being that the writhe is a signed crossing number while the ACN is an unsigned crossing number.

We explore the effect of knot complexity on the ACN and writhe. Knot complexity can be measured in many different ways. There are quantities of classical knot theory (such as crossing number, genus, braid index, and bridge number) that can be found in any standard text on knot theory [12–15]. There are also physical or geometric measurements (such as ropelength or knot energies [17–27]) that become knot invariants by taking their minimum/infimum over all configurations of a particular knot type. We use the crossing number as our measure of knot complexity since the crossing number is the most widely used measure of knot complexity and none of the alternatives seem to have any intrinsic advantage over the crossing number.

### 2.2. Generating random polygons in confinement and knot identification

Our goal is to isolate the effects of confinement, and knotting within confinement, on the geometry of the configurations. Unfortunately, generating confined polygons is a difficult task. For unconfined freely-jointed polygons, many algorithms exist, such as the crankshaft algorithm [28, 29], the hedgehog algorithm [28, 30], and the generalized hedgehog algorithm [31]. However, using an existing unconfined algorithm in an accept-reject approach to generate polygons in confinement is not efficient for long polygons in tight confinement [32]. Lattice polygons and monte carlo approaches could provide a more realistic model of confined polymers with excluded volume. However, both of

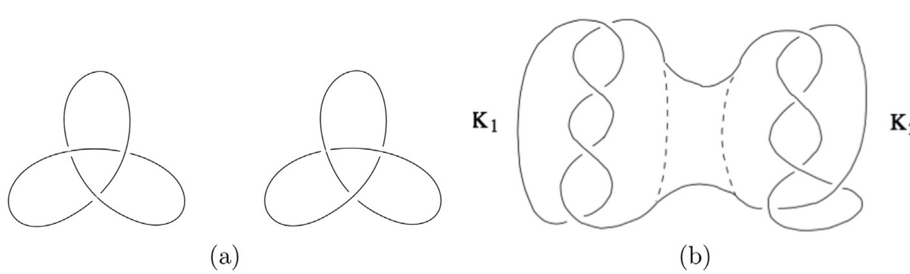


**Fig. 1.** (a) A knot and its mirror image; (b) a composite knot constructed from two nontrivial knots $K_1$ and $K_2$.