THE WRITHE OF KNOTS AND LINKS

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Abstract

We discuss the writhe of linked and knotted simple closed curves embedded in the simple cubic lattice, Z^3. We show that the writhe of a simple closed curve in Z^3 can be computed as the average of its linking numbers with certain pushoffs, and use this result to establish a lower bound on the rate of increase of the mean absolute writhe. We present Monte Carlo results on the distribution of writhe for particular knot types, and compare the mean values with values for ideal knots. Similar results are presented for links and we show that the mean writhe of $(2, 2k)$ torus links increases linearly with crossing number.

1 Introduction

A time-honoured model of the configurational properties of long linear polymer molecules in dilute solution in a good solvent is the self-avoiding walk. This is a walk (a sequence of edges and vertices) on a regular lattice, such as the simple cubic lattice, Z^3. No two vertices of the walk can occupy the same lattice point, and all self-avoiding walks with the same number (n) of edges have the same probability of occurence. The self-avoiding condition is designed to mimic the excluded volume effect in polymers, which says that no two monomers can occupy the same region of space. These lattice models have the advantage that they can be treated by combinatorial methods and, by using a computer, one can make use of efficient data structures because of the discrete nature of the space Z^3.

In the same way, ring polymers can be modelled by (self-avoiding) polygons. A polygon is an embedding of a simple closed curve in Z^3 and two polygons are considered distinct if they can not be superimposed by translation. If we write p_n for the number of polygons with n edges then $p_n = 0$ if n is odd, $p_4 = 3$, $p_6 = 22$, $p_8 = 207$, etc. In this paper we shall be concerned with the geometric properties of polygons and especially with their writhe, which is a measure of the geometrical entanglement complexity of space curves, and which we define in Section 2. Natural questions which one can ask are: "What is the distribution of the values of the writhe?", "How does the mean writhe, or mean square writhe, depend on n?", etc.

Calculating the writhe of a simple closed curve in R^3 is usually done by a stochastic numerical approximation, but we shall see in Section 2 that there is a considerable simplification when the curve is embedded in a lattice. Indeed, for polygons on the simple cubic lattice, four times the writhe is always an integer, and an exact calculation for the writhe can easily be performed. The approach described in Section 2 is an important ingredient in a proof, outlined in Section 3, that the expectation (over all polygons with n edges) of the absolute value of the writhe increases at least as fast as $\sqrt{n}$.

In Section 4 we describe a Monte Carlo method for estimating the distribution of the writhe when the polygons are conditioned to have a specified knot type, and in Section 5 we describe some results obtained in this way. It seems that the distribution of the writhe increases in width as n increases, but that the mean writhe is more or less independent of n. We shall see that these mean values are very close to the values estimated by Katritch *et al* [1] for the writhe of "ideal" knots. In addition we note that the mean writhe is a linear function of crossing number for knots in certain families (such as torus knots, twist knots with odd crossing number, twist knots with even crossing number, etc.), and seems to be additive under the process of connect sum when composite knots are formed from their prime components. This additivity under connect sum was also observed by Katritch *et al* [2]. In addition, our results suggest that linearity of writhe for certain homologous families of knots and links, and additivity of writhe, are not dependent on particular features of ideal representations of knot and link types.

Similar questions can be asked about the writhe of links, and we address these questions in Section 6. Perhaps the most striking result is the linear dependence of average writhe on crossing number in the sequence of $(2, 2k)$ torus links. This has been observed experimentally in circular DNA, and numerically in a particular model of DNA links[3]. Our results suggest that the feature is a more general one, and is not dependent on the particular features of DNA molecules.

2 Computing the writhe of lattice polygons

The writhe of a simple curve in 3-space is a geometric quantity intended to measure the signed non-planarity of a curve. The writhe of a space curve ω ($Wr(\omega)$) is defined in terms of orthogonal projections of ω onto 2-dimensional hyperplanes. We will restrict attention to simple closed curves ω. A projection direction is an oriented line in R^3; think of the projection plane as being below the curve ω. Given a knot diagram $\hat{\omega}$ determined by a regular orthogonal projection of the simple closed curve ω, orient the planar curve $\hat{\omega}$, and assign either +1 or -1 to each self-crossing of $\hat{\omega}$, according to the usual crossing sign convention for any diagram of a pair of oriented skew lines in 3-space (see figure 1). The sum of the signed crossings is the *signed crossing number* of that knot diagram; it is an integer-valued function of the space curve and the projection direction. For a fixed space curve, one averages this function over all projection directions (points on a reference 2-sphere) obtaining the writhe of the curve.

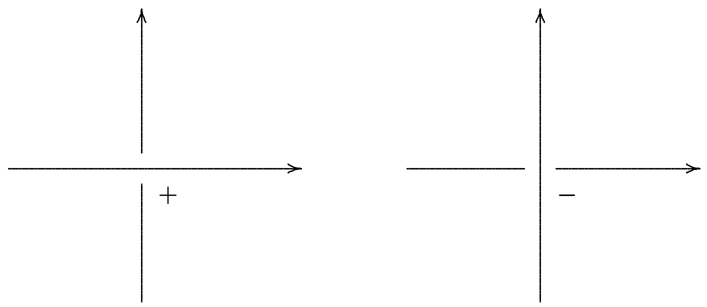

Figure 1: The sign-convention for projected arcs crossing each other in the plane.

In order to compute the writhe, this average value can be approximated in a stochastic fashion by randomly and uniformly choosing projection directions in which to sample the signed crossing number function. It is possible, however, to obtain exact calculations for curves constrained to live on spatially periodic lattices in R^3. In order to do this, one converts the signed crossing number of a planar diagram to a linking number; the topological invariance of linking number supplies the needed flexibility to achieve an exact calculation. The signed crossing number of a knot diagram can be viewed as a linking number of a pair of oriented space curves determined by the knot diagram as follows: travel along the projected curve $\hat{\omega}$ and push off by a small amount along a vector orthogonal to $\hat{\omega}$ in the direction of the unbounded region of the plane of the diagram. One obtains the planar pushoff $\hat{\omega}_p$, a companion planar curve which is parallel to $\hat{\omega}$. Orient $\hat{\omega}_p$ parallel to $\hat{\omega}$. Near each self-crossing of $\hat{\omega}$ (or $\hat{\omega}_p$) the overcrossing segment of the curve can be vertically pushed a small distance above the diagram plane, generating a pair of space curves (ω^*,ω_p^*) corresponding to the pair of planar curves ($\hat{\omega}$,$\hat{\omega}_p$). Thought of as 3-dimensional objects in this way, the linking number $Lk(\omega^*, \omega_p^*)$ is the signed crossing number of the knot diagram $\hat{\omega}$. The pair (ω^*, ω_p^*) cobound a small annulus in 3-space. Think of the small annulus as a curtain, and rotate the curtain downward until it hangs vertically downward from ω^* toward the diagram plane. The planar pushoff has now moved to the position of a spatial pushoff $\hat{\omega}_p^*$ of ω^* in the projection direction, and $Lk(\omega^*, \omega_p^*) = Lk(\omega^*, \hat{\omega}_p^*)$. The pair $(\omega^*, \hat{\omega}_p^*)$ is ambient isotopic by pushing vertically to the pair (ω, ω_p), where ω_p is a pushoff of ω vertically downward in the projection direction. Hence, the $Wr(\omega)$ is converted to the average value of linking numbers of ω with pushoffs in all projection directions.

If a simple closed space curve is constrained to lie on a regular space-filling lattice, the number of pushoffs needed for an exact computation of the writhe is finite. As will be argued below, this is because the “coordinate” planes of the lattice subtend finitely many compartments on a small 2-sphere about the origin, and the linking number of the curve and all pushoffs along directions in the interior of the same compartment have the same linking number. For simplicity, we argue[4] the case for the simple cubic lattice Z^3. Suppose that we wish to compute the writhe of the polygon ω in Z^3. Let S^2 be the 2-sphere in R^3 of radius $\frac{1}{2}$; S^2 is the space of directions for push-offs. The three coordinate planes in R^3 separate S^2 into eight connected regions (“octants”), characterized by constancy of sign in each coordinate. If $\mu \in S^2$, then $\omega_\mu = \omega + \mu$ is the push-off of ω in the direction μ.

Claim 1 *: If μ lies in the interior of any octant on S^2, then ω and ω_μ are disjoint space curves and $Lk(\omega, \omega_\mu)$ is defined.*

Proof: Suppose that $\mu = (\mu_1, \mu_2, \mu_3)$ lies in the interior of the first octant, where all three coordinates are positive; since μ lies on a 2-sphere of radius $\frac{1}{2}$, then $0 < \mu_i < \frac{1}{2}$ for i = 1,2,3. Now suppose that $(x, y, z) \in \omega$ and $(x + \mu_1, y + \mu_2, z + \mu_3) \in \omega \cap \omega_\mu$. Points in ω have the property that at least two of the coordinates are integers. By the pigeonhole principle, at least one of the following is true: both x and $x + \mu_1$ are integers; both y and $y + \mu_2$ are integers, or both z and $z + \mu_3$ are integers. This means that at least one of $\{\mu_1, \mu_2, \mu_3\}$ is an integer, which is impossible. A similar argument holds for the other seven octants.□

Claim 2 *: If μ and ν lie in the interior of the same octant, then $Lk(\omega,\omega_\mu) = Lk(\omega,\omega_\nu)$.*

Proof: Consider the shorter of the two great circle arcs connecting μ and ν on S^2; this arc lies in the interior of the same octant as do μ and ν. The points along this arc define a 1-parameter family of pushoff directions, starting with μ and ending with ν. Thus the pushoff ω_μ can be ambient isotoped to the pushoff ω_ν in the complement of ω, and the linking numbers are equal. Since all of the eight octants in S^2 have equal area, at this point we have shown that $Wr(\omega)$ is the average of eight linking numbers, one for each octant. We now use the symmetry of the simple cubic lattice to reduce the number of pushoffs needed to four.□

Claim 3 *: If μ is not on a coordinate plane, then $Lk(\omega,\omega_\mu) = Lk(\omega,\omega_{-\mu})$.*

Proof: Let t be a parameter such that $-1 \leq t \leq 0$. As in Claim 1, for each value of t, ω_μ and $\omega_{t\mu}$ are disjoint. To see this, suppose that $(x+\mu_1, y+\mu_2, z+\mu_3) = (x^* + t\mu_1, y^* + t\mu_2, z^* + t\mu_3)$ for some $(x,y,z),(x^*,y^*,z^*) \in \omega$. Suppose also that both x and x^* are integers. It follows that $(x - x^*) = (1-t)\mu_1$. But $(1-t)\mu_1$ cannot be an integer, because $1 \leq (1-t) \leq 2$, and $0 < |\mu_1| < \frac{1}{2}$. This means that we can ambient isotope ω to $\omega_{-\mu}$ in the complement of ω_μ, so $Lk(\omega_\mu,\omega) = Lk(\omega_\mu,\omega_{-\mu})$. Similarly, one can ambient isotope ω_μ to ω in the complement of $\omega_{-\mu}$, hence $Lk(\omega_{-\mu},\omega_\mu) = Lk(\omega_{-\mu},\omega)$. The claim now follows by symmetry of linking numbers in R^3.□

From the above three claims it is clear that $Wr(\omega)$ is the average of linking numbers of ω with pushoffs into four mutually non-antipodal octants. In particular, it follows that four times $Wr(\omega)$ is an integer for any polygon $\omega \in Z^3$. As we shall see, the fact that the writhe of a lattice polygon is the average of four linking numbers is useful in both calculational and theoretical (theorem proving) contexts.

3 Width of the writhe distribution

In this section we discuss how the width of the distribution of writhe of polygons in Z^3 depends on the number of edges in the polygon[5]. In particular, can we use the result in the previous section to examine the behaviour of the mean absolute writhe as a function of n? We expect the mean absolute writhe to increase with n, and we shall prove that this increase is at least as fast as $\sqrt{n}$.

We define two polygons in Z^3 to be identical if they can be superimposed by a translation. Let P_n be the set of polygons of length n in Z^3, and let the number of polygons in P_n be p_n. If ω is a polygon in P_n, then let $Wr(\omega)$ be the writhe of ω. The expected value of the writhe for a polygon with n edges in Z^3, $\langle Wr \rangle_n$, is defined by

$$\langle Wr \rangle_n = \frac{1}{p_n} \sum_{\omega \in P_n} Wr(\omega). \tag{1}$$

By symmetry, $\langle Wr \rangle_n = 0$. It will be more rewarding to study the expected absolute writhe, $\langle |Wr| \rangle_n$, or the expected square writhe, $\langle Wr^2 \rangle_n$, instead. We saw in the previous section that writhe of a given polygon can be computed by taking the average of linking numbers of the polygon with four pushoffs of itself into non-antipodal octants in Z^3. We use this result now to study the expectation of the absolute writhe. We shall divide the proof into two parts. In the first part, we show that small curly-cues can be truncated from a given polygon, and that the writhe is additive with respect to the truncation. In the second part we adapt a coin-tossing argument to study the expected absolute writhe.

Define a *curly-cue* to be the self-avoiding walk defined by the sequence of canonical unit vectors $\{i, i, -k, -j, -i, j, j, k, -i\}$.[a] The first and last vertices in a curly-cue can be joined by adding an extra edge in the j-direction giving a polygon $\mathcal{P}$ (see figure 2).

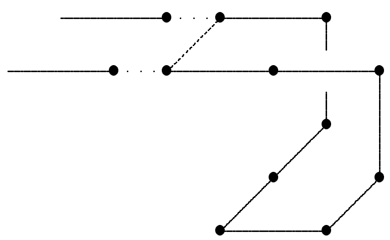

Figure 2: A curly-cue can be truncated from a polygon as shown here. The writhe of the polygon is additive with respect to this truncation.

In order to compute the writhe of $\mathcal{P}$, we construct its pushoffs and compute its linking numbers with its pushoffs. Let $\mathcal{P}_1$ be the pushoff of $\mathcal{P}$ obtained by

[a] Any rotation of this sequence in Z^3 is also a curly-cue.

adding $(i+j+k)/2$ to each point of $\mathcal{P}$. Direct computation show that the linking number is $Lk(\mathcal{P},\mathcal{P}_1)=1$. Push-offs by $(i-j+k)/2$ and $(-i-j+k)/2$ also give linking numbers equal to 1, but the push-off by $(-i+j+k)/2$ gives a linking number of -1. Hence, $Wr(\mathcal{P})=\frac{1}{2}$. Similarly, if $\mathcal{P}^*$ is the mirror image of $\mathcal{P}$, reflected through the xy-plane, then $Wr(\mathcal{P}^*)=-\frac{1}{2}$.

Let $\mathcal{C}$ be the cube formed by the union of the 3-cells dual to any translation in Z^3 of the set of vertices with coordinates in the set $\{0,1,2\}\times\{0,1,2\}\times\{0,1,2\}$. Let A be a polygon which intersects $\mathcal{C}$ in the curly-cue $\{i,i,-k,-j,-i,j,j,k,-i\}$ with first and last vertices P and Q. We can *truncate* this subwalk from A by removing it from A, and by joining P and Q with an edge in the j-direction in A. The subwalk can be turned into $\mathcal{P}$ by joining its ends with an edge in the j-direction. Suppose we obtain a polygon A' if we truncate the curly-cue from A. Then

$$Wr(A)=Wr(A')+Wr(\mathcal{P}). \tag{2}$$

To see this, consider push-offs A_1 of A and A'_1 of A' in the $(i+j+k)/2$ direction, as illustrated in figure 3. Define $Lk(A,A_1)$ to be linking number of A and A_1.

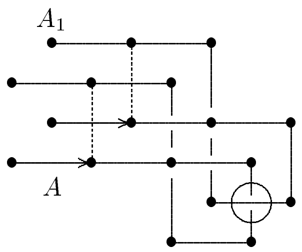

Figure 3: The projection in the xy-plane of a section of a polygon (and one of its push-offs) which contains a curly-cue. The curly-cue can be truncated at the dashed lines.

In figure 3 a projection of A and its push-off in the $(i+j+k)/2$ direction in the vicinity of the cube $\mathcal{C}$ is shown. If the crossing which is circled is reversed, then A and A_1 can be deformed by an isotopy in the cube $\mathcal{C}$ (for example, by performing Reidemeister moves on figure 3 after reversal of the crossing) to the pair A' and A'_1 (that is, with the curly-cue truncated at the dashed lines in figure 3). Thus, truncating the curly-cue is equivalent (in a topological sense) to reversing the single crossing encircled in figure 3. Let $\mathcal{P}$ and $\mathcal{P}_1$ be the polygons obtained by closing the curly-cues on truncation. Then

$$Lk(A,A_1)=Lk(A',A'_1)+1=Lk(A',A'_1)+Lk(\mathcal{P},\mathcal{P}_1). \tag{3}$$

The remaining three push-offs can be similarly analized, and the result is equation (2). This is an important result for us, since we know exactly the change in the writhe of a polygon if we truncate a curly-cue. We can now show that the expected value of the absolute writhe increases at least as fast as $O(\sqrt{n})$.

Let $\langle |Wr| \rangle_n$ be the mean of the absolute value of the writhe of polygons of length n.

Theorem 1 *The probability Prob($\langle |Wr| \rangle_n < f(n)$) approaches zero as $n \to \infty$ for any function $f(n) = o(\sqrt{n})$.*

Proof: Let $P = (C, B)$ be a ball-pair consisting of any translate of the cube C and the curly-cue $B = \{i, i, -k, -j, -i, j, j, k, -i\}$. We call P a pattern, and we define $P^* = (C, B^*)$ to be the mirror image of P (reflected through the xy-plane). Let $\epsilon > 0$ be given and let $\alpha_n(\epsilon)$ be the number of polygons of length n which have at least $\lfloor \epsilon n \rfloor$ occurances of the patterns P or P^*. (In other words, these polygons intersect at least $\lfloor \epsilon n \rfloor$ translated copies of the cube C in either B or B^*). A pattern theorem by Kesten[6] states than for sufficiently small ϵ and sufficiently large n, there exists a $\gamma > 0$ such that $(1 - e^{-\gamma n})p_n \geq \alpha_n(\epsilon)$, where p_n is the number of polygons of length n. Let a polygon counted by $\alpha_n(\epsilon)$ contain P or P^* exactly $D \geq \lfloor \epsilon n \rfloor$ times. Then P occurs exactly k times with probability

$$\binom{D}{k} \left(\frac{1}{2}\right)^k \left(\frac{1}{2}\right)^{D-k}.$$

This is a maximum when $k = \lfloor D/2 \rfloor$, and we obtain the upper bound $1/\sqrt{\lfloor \epsilon n \rfloor}$ on this probability. The writhe of a polygon ω counted by $\alpha_n(\epsilon)$ has contributions from the $D \geq \lfloor \epsilon n \rfloor$ copies of P or P^*, as shown by the truncation in figure 3 and by equation (2). Let ω' be the polygon obtained by truncating all the curly-cues from ω. Then by equation (2), $Wr(\omega) = Wr(\omega') + Wr(\text{curly-cues})$. If $|Wr(\omega)| \leq f(n)$, then this implies than $Wr(\text{curly-cues})$ can assume at most $\lceil 2f(n) + 1 \rceil$ different values. Thence, the probability that the absolute writhe of ω is less than $f(n)$ is bounded from above by the probability that $Wr(\text{curly-cues})$ assume one of at most $\lceil 2f(n) + 1 \rceil$ values. But

$$\text{Prob}(|Wr(\omega)| \leq f(n)) \leq \frac{\lceil 2f(n) + 1 \rceil}{\sqrt{\lfloor \epsilon n \rfloor}}, \tag{4}$$

Thus

$$\text{Prob}(\langle |Wr| \rangle_n \leq f(n)) \leq (1 - e^{-\gamma n}) \frac{\lceil 2f(n) + 1 \rceil}{\sqrt{\lfloor \epsilon n \rfloor}} + e^{-\gamma n} R, \tag{5}$$

where R is the contribution from polygons not counted by $\alpha_n(\epsilon)$. This approaches zero as $n \to \infty$ provided that $f(n) = o(\sqrt{n})$, as claimed above. □

In theorem 1 we have focussed entirely on the contribution of small curly-cues to the writhe of a polygon. In particular, this restriction enables us to prove that the expected absolute writhe of a random polygon grows at least as fast as the square root of its length. A model of self-avoiding walks with a fugacity coupled to writhe has recently been studied by an identification to the $N \to 0$ limit (N is the number of scalar components) of a complex scalar Chern-Simon theory[7]. In particular, they found that the conformation of the self-avoiding walk is decoupled from its writhe in the scaling limit. This can be interpreted as indicating that the total writhe (and therefore the total absolute writhe) of a self-avoiding walk is a consequence of contributions from local conformations in the walk, which are invisible from the long wavelength field theory (presumably, the local conformations are plectonemic wound conformations of size no larger than that of the persistence length of the walk). In our context, this suggests that the total writhe of a polygon is primarily determined by curly-cues. We therefore consider now the contribution to the absolute writhe of the polygon ω by the curly-cue pattern P and its mirror image P^*. Thus, if P occurs exactly k times, and there are a total of D occurances of P or P^*, the the contribution to the absolute writhe is $|2k - D|$. The expected value of this contribution for ω is given by

$$\begin{aligned} E_\omega(|2k-D|) &= \sum_k |2k-D| \binom{D}{k} 2^{-D} \\ &= 2^{-D+1} D \sum_{k<D/2} \binom{D}{k} - 2^{-D+2} \sum_{k<D/2} k \binom{D}{k}, \end{aligned} \tag{6}$$

after some algebra. This may be simplified to give

$$E_\omega(|2k-D|) = 2^{-D+1} D \binom{D-1}{(D-1)/2} \qquad \text{if } D \text{ is odd,} \tag{7}$$

and

$$E_\omega(|2k-D|) = 2^{-D} D \binom{D}{D/2} \qquad \text{if } D \text{ is even.} \tag{8}$$

But for any polygon counted by $\alpha_n(\epsilon)$, $\lfloor \epsilon n \rfloor \leq D \leq n$, and by noting that $\binom{D}{D/2} \sim 2^D D^{-1/2}$, we obtain the result that

$$E_\omega(|2k-D|) \sim n^{1/2}. \tag{9}$$

In other words, the contribution to the absolute writhe of the curly-cues grows as the square root of n. An important open question is to derive an upper bound on the n-dependence of the absolute writhe of the polygon, rather than focussing on the curly-cues. Numerical evidence[5] suggests that the mean absolute writhe might grow like $\sqrt{n}$. Using techniques similar to the above, we can compute the expectation values $E_\omega(|2k - D|^M)$.

4 Numerical methods

In this section we discuss a Monte Carlo algorithm for the sampling of knotted polygons in Z^3. In particular, we are interested in sampling polygons of a fixed (given) knot type. We shall show that the BFACF algorithm[8] is suitable for our purposes.

The BFACF algorithm has two elementary moves, illustrated in figure 4. The first of these moves changes the length of the polygon, while the second is a length preserving move. By applying these moves, the algorithm samples along a realisation of a Markov chain defined on the state space of polygons. It has one free parameter β, which can be set to control the expected length of polygons in the sample.

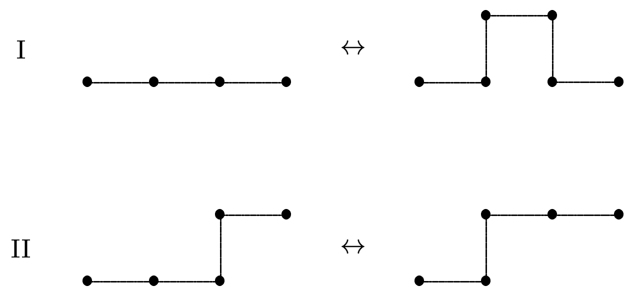

Figure 4: The elementary moves of the BFACF algorithm. Moves of type I can increase or decrease the length of the polygon by two edges. Moves of type II are length preserving.

The implementation of the algorithm is as follows: Let ω be the current state in the Markov chain. Select an edge uniformly in ω, and move the edge perpendicular to itself one lattice spacing in one of four possible lattice directions, while two new edges are inserted to keep the polygon connected. If this operation produces double edges then they are deleted. An enumeration of the possible outcomes shows that all possible results are one of the cases in figure 4. Let the new state be ν. If ν is not a polygon (i.e. if the vertices are not all of degree 2) then ν is rejected and ω is the next state of the Markov chain. If ν is a polygon then it is accepted or rejected as the next state by applying a Metropolis rule; if it is rejected, then ω will be taken as the next state in the chain. Let the number of edges in ω be $|\omega|$ and in ν be $|\nu|$. If $|\omega| \geq |\nu|$, then we accept ν as the next state in the chain; if $|\omega| = |\nu| - 2$, then we accept ν with probability β^2 as the next state. Since the edge is selected with probability $1/|\omega|$, and moved perpendicular to itself in one of four directions with probability $1/4$, the probability that ν is the next state in the Markov chains is given by

$$P(\omega \to \nu) = \big(\mathcal{I}(|\omega| \geq |\nu|) + \beta^2 \mathcal{I}(|\omega| < |\nu|)\big)/4|\omega|, \tag{1}$$

where $\mathcal{I}$ is an indicator function. On the other hand, by interchanging ω and ν in (1), we obtain the probability that ω is the next state in the Markov chain if ν is the current state. A comparison of these probabilities gives us the equation of detailed balance for this algorithm:

$$|\omega|\beta^{|\omega|} P(\omega \to \nu) = |\nu|\beta^{|\nu|} P(\nu \to \omega). \tag{2}$$

Notice that the algorithm is aperiodic (since there is a non-zero probability that a move will be rejected). The elementary moves in figure 4 are homeomorphisms on the polygon, and the knot type of the polygon along the Markov chain is therefore invariant. Therefore, the algorithm is reducible on the state space of all polygons, and we must find its *ergodicity classes*[b] if we are to understand its behaviour in any detail. The knot type of the polygon is set by the first polygon sampled by the chain. Let $\mathcal{P}(K)$ be the set of all polygons of knot type K. Then any ergodicity class, defined by an initial polygon of knot type K, is a subset of $\mathcal{P}(K)$. Remarkably, the ergodicity classes of the polygon are exactly the sets $\mathcal{P}(K)$, since it is known[9] that any two polygons of the same knot types can be connected by a finite sequence of the moves in figure 4. By summing the above over all possible states ν in a given ergodicity class, we see from the fundamental theorem of Markov chains that the invariant limiting distribution of the algorithm is given by

$$\Pi_\omega(K) = \frac{1}{Z_K(\beta)} |\omega|\beta^{|\omega|} \mathcal{I}(\omega \in \mathcal{P}(K)), \qquad \text{where } Z_K(\beta) = \sum_{\omega \in \mathcal{P}(K)} |\omega|\beta^{|\omega|}. \tag{3}$$

We conclude that this algorithm is suitable for sampling polygons with a given knot type. The invariant limit distribtion is given by (3), where polygons of the

[b]These are the subsets of the state space on which the algorithm is irreducible.

same length have the same weight. The expected length of polygons sampled by the algorithm is given by

$$\langle |\omega| \rangle_\beta = \sum_{\omega \in \mathcal{P}(K)} |\omega| \Pi_\omega(K). \tag{4}$$

This expected length is known to be infinite if β is larger than a critical value β_c. If $\beta < \beta_c$, then the expected length of polygons stays finite, and the algorithm can be used to sample finite polygons of a fixed knot type K from the distribution $\Pi_\omega(K)$ to compute their properties.

5 Writhe as a function of knot type

In 1980 Le Bret[10] computed the writhe of closed Gaussian piece-wise linear curves in R^3 as a model of closed circular DNA. If the knot type of the curve is fixed, he noticed that the mean writhe is zero for the unknot and for the achiral knot 4_1, but not for the chiral knots which he studied. These issues were revisited by Katritch *et al* [1] who published a similar study of "ideal knots" in $\mathcal{R}^3$ and of a simple model of circular DNA. These questions were also studied in the cubic lattice[11], and in this section we recount this study, and compare our findings with those of Le Bret and Katritch *et al.*

Any achiral knot K has a mirror image K^* of the same knot type. Since the writhe of K changes sign under reflection, but retains its magnitude, this observation proves that the mean writhe of any achiral knot is zero. Thus, if the mean writhe of a knot is not zero, then it is chiral.[c] If writhe can be computed by a Monte Carlo algorithm, then we have a good method for determining, up to numerical error, whether a given knot is chiral. It is fortunate that the writhe of a lattice knot can be computed exactly by taking the average of the linking number of the knot with its pushoffs into four non-mutually antipodal octants. This is a tremendous improvement, since the writhe is defined as the mean of the sum of the signed crossings over all regular projections of the knot.

We sampled along a Markov chain in the state space of lattice knots of a fixed knot type K by using the BFACF algorithm described in section 4. The writhe of the lattice knots along this chain was obtained by computing the linking numbers of the lattice knots with push-offs into four non-antipodal octants. The linking numbers were computed by performing heap sorting algorithms on the coordinates of the polygons. This allowed the calculation of

[c] Alas, the converse of this statement is not known to be true.

a linking number in $O(n \log n)$ CPU-time (as opposed to the $O(n^2)$ CPU-time which would be required for a naive search for intersections in projections of the knot and its push-offs.) Several runs were performed for each knot type, with several different values of the parameter β selected each time in an attempt to sample adequately polygons with length up to 250 edges. For each fixed value of n we tabulated the distribution of writhe, and computed a mean writhe over the distribution. The distribution is plotted in figure 5 for the knot 5_1. Notice that there are no data for $n < 34$; the best upper bound[12] on the number of edges necessary to tie the knot 5_1 is 34. The distribution widens as n increases, as we expect following the arguments in section 3, although this has not been made rigorous for the situation here. This increase in the width of the distribution was also observed by Le Bret[10]. The mean writhe of the knot seems to be independent of n, even though n increases from 34 up to 250. This observation seems to be true for every knot that we have examined. We can therefore estimate the mean writhe of the lattice knot by pooling all the data in figure 5 to arrive at a single estimate of the writhe.[d]

Our best estimate for the writhe of the trefoil is 3.441 ± 0.025, and estimating the writhe of 5_1 from the data in figure 5 gives 6.254 ± 0.011. The mean writhe for other knots are tabulated in the second column of table 1. All the knots in this table are chiral, since we know that achiral knots have mean writhe zero. We also compare our results with estimates obtained by Le Bret[10] and Katritch *et al* [1] (the estimates for the trefoil by Le Bret vary between 3.5 for the smallest polygons, and 3.15 for the largest polygons; we give the value obtained at the largest polygons in table 1). The data from the work of Katritch *et al* [1] are for an "ideal knot", and a model of circular DNA with 5400 base pairs and with 1800 base pairs respectively. The agreement in the data is remarkable. An interesting observation from table 1 is the appearance of linear relationships between the crossing number and the mean writhe in some knot families. (Katritch *et al* [1] also observed this in their model.) One such family is the family of $(2, 2k+1)$-torus knots with first members 3_1, 5_1, 7_1, 9_1, and so on. A linear fit to our data gives $\langle Wr \rangle \approx 1.409C - 0.789$ where C is the crossing number, and the accuracy of this fit is very good (the residual deviance is approximately 2×10^{-5}). Similar relationships can be obtained for other families of knots, such as the even crossing number twist knots (4_1, 6_1, 8_1, $\ldots$) and odd crossing number twist knots (3_1, 5_2, 7_2, $\ldots$). Linear fits to our data show that the rate of increase in mean writhe with crossing number is approximately 0.59 in both these families. These observations remain true

[d] We achieved this by plotting the mean writhe as a function of n, and carrying out a linear least squares analysis. The y-intercept was taken as the mean writhe, and we observed that the slope of the fitted line was very close to zero in every case.

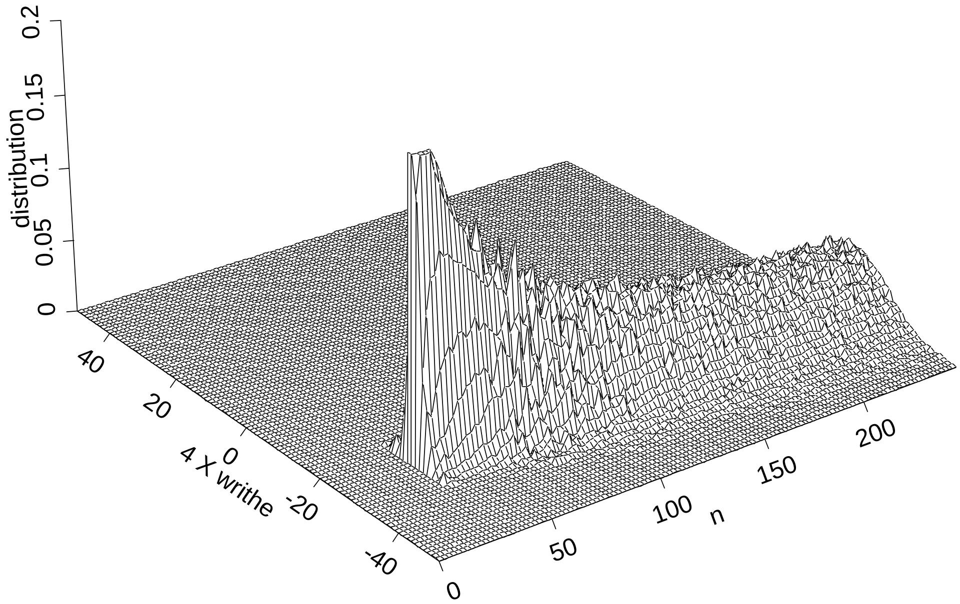

Figure 5: The distribution of writhe for a lattice knot of type 5_1. The distribution for each value of n has been normalised to 1. Notice that the minimal number of edges to tie the knot in $\mathcal{Z}^3$ is 34, so that there are no data for polygons shorter than 34 edges.

even in the case of more "complicated" knot families. We have considered the families of knots with Conway symbols $\langle 2k+1,1,2k\rangle$, $\langle 2k-1,1,2k\rangle$ and $\langle 1,2k-1,1,2k-1,2\rangle$, and we observe similar linear behaviour.

We can concatenate prime knots in the lattice to form composite knots by the following construction: The *top edge* of a polygon is the edge with lexicographically largest midpoint, and the *bottom edge* is that edge with lexicographically least midpoint. Two polygons are concatenated by translating one polygon (and rotating it if necessary) such that the midpoint of its bottom edge has first coordinate which is one more than the first coordinate of the midpoint of the top edge of the second polygon. We concatenate the two polygons by first deleting the bottom edge of the first and the top edge of the second polygon, before we add two edges incident with the endpoints of the deleted top and bottom edges to connect the two polygons into a single, larger polygon. If the first polygon had knot type K_1 and the second K_2, then the new polygon has knot type $K_1\#K_2$. The writhe of polygons is additive under concatenation.[11] This result suggests a much more general case: the possibility that writhe is additive under the connect sum of lattice knots: In other words, the mean writhe of a lattice knot of type $K_1\#K_2$ is the sum of the mean writhe of lattice knots

knot type	Janse van Rensburg *et al*		Le Bret	Katritch *et al*		
	average	minimal		ideal	5400bp	1800bp
3_1	3.44	3.44	3.5	3.41	3.43	3.41
5_1	6.25	6.25	6.3	6.26	6.30	6.21
5_2	4.55	4.49	4.7	4.54	4.56	4.59
6_1	1.16	0.93		1.23	1.20	1.18
6_2	2.83	2.69		2.70	2.83	2.76
7_1	9.07	9.28		9.15	9.10	8.95
7_2	5.74			5.82	5.79	5.77
8_1	2.35			2.33	2.47	2.43
8_{19}	8.73			8.64		
9_1	11.89			12.07	12.0	
9_2	6.95			6.84	6.94	
10_1	3.55			3.47	3.60	
10_{161}	9.30			9.45		
$3_1\#3_1$	6.91			6.81		

Table 1: Estimates of mean writhe for various chiral knots.

of types K_1 and K_2. Numerical work supports this notion strongly; for example, we measured $\langle Wr(3_1^-)\rangle = -3.441 \pm 0.025$, $\langle Wr(5_1^-)\rangle = -6.254 \pm 0.011$, while $\langle Wr(5_1^- \# 3_1^-)\rangle = -9.657 \pm 0.58$ and $\langle Wr(5_1^- \# 3_1^+)\rangle = -2.790 \pm 0.048$. Additivity under the connect sum operation was also observed by Katritch *et al.*[2]

6 Writhe as a function of link type

One can ask similar questions about the dependence of mean writhe on link type, though less work has been carried out in this area. Gee and Whittington[13] have recently used Monte Carlo methods to estimate the writhe of a polygon in a two component link of fixed type, as a function of the numbers of edges in the two polygons. We shall discuss these results and compare with work by Vologodskii and Cozzarelli[3] on torus links in a model of circular DNA.

Two component links can be symmetric or asymmetric. Colour the two circles red and blue. An unoriented link is *symmetric* if there is a ambient isotopy which interchanges the colours. That is, if there is a smooth deformation whereby the two circles in the link can be interchanged in space. $(2, 2k)$-torus links are symmetric. A link with one component knotted and the other unknotted (e.g. 7^2_8) is asymmetric. If the link is symmetric and the two polygons composing the link in Z^3 have the same number of edges, then each component of the link must have the same mean writhe, and this is the simplest case to consider. Suppose we consider $(2, 2k)$-torus links, where each polygon has n edges. Gee and Whittington[13] estimated the mean writhe for $k = 2, 3, 4, 5$ for $n \leq 140$. For each value of k the mean writhe seems to be more or less independent of n (except at very small values of n) and one can estimate the mean writhe on the assumption that it is really n-independent, and that the apparent small dependence is a mixture of statistical fluctuations and a slow convergence to a limiting value. It then seems that the mean writhe increases roughly linearly with increasing k. Vologodskii and Cozzarelli[3] observed similar behaviour in their model of circular DNA. Although the mean writhe values for the two models are different (for the same torus link), the mean writhe increases linearly with k in both cases, and the slope of the line is very similar.

This establishes that linking induces writhe and that the mean writhe increases (roughly linearly with k) within the family of $(2, 2k)$-torus links, when the two circles are the same length. If the circles have different lengths then the writhe can depend on the length of a circle and on the length (or relative length) of its partner. For instance, if a 20-gon and a 40-gon are linked to form a $(2, 4)$-torus link, the mean writhe of the 20-gon is 0.53 ± 0.03 while the mean writhe of the 40-gon is 3.35 ± 0.13 (so that the longer polygon has higher writhe, as found by Vologodskii and Cozzarelli[3]). More generally, consider a polygon with n edges linked to a polygon with m edges. Gee and Whittington[13] found that, for a fixed torus link type, the mean writhe of an n-gon decreases with increasing m at fixed n and increases with increasing n at fixed m. At fixed n the writhe of an n-gon seems to be approaching a limiting non-zero value as m increases, and this limiting value depends both on n and on the type of torus link, increasing both with n and with k.

7 Discussion

Lattice models have played an important role in the development of our understanding of the conformational properties of polymers and, since the recent interest in topological and geometrical entanglement in polymers, lattice models have proved important in these areas. The first proofs of the inevitability of knotting in sufficiently long ring polymers were constructed for lattice models[14,15] and we still know much more about the lattice version of this problem[16] than about its continuum analogues.[17,18,19]

The results which we described in Section 2 show that the computation of the writhe of a simple closed curve in Z^3 is much simpler than the corresponding calculation for curves in R^3. With some modifications this argument can be applied to other lattices such as the body-centred and face-centred cubic lattices. The result described in that section plays a key role in the proof of the theorem which we described in Section 3 which gives a lower bound on the rate of increase of $\langle |Wr| \rangle_n$.

The remainder of the paper is concerned with the mean writhe of circles of a fixed knot type or which are members of a link of two circles with specified link type. The mean writhe isn't strongly dependent on n and our estimates of the mean writhe as a function of knot type are very similar to the values found by Katritch *et al* [1] for ideal knots in R^3. In addition we observed that mean writhe is approximately additive under the connect sum operation (see also the results in Katritch *et al* [2]), and this might be an exact relation. We also observed that mean writhe increases linearly with crossing number in certain knot families, and that there is a similar behaviour in $(2, 2k)$-torus links.

For the moment the results described in Sections 5 and 6 are observations based on numerical data, and it would be interesting to establish these results rigorously.

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