The writhe of a self-avoiding polygon

1993 J. Phys. A: Math. Gen. 26 L981

(http://iopscience.iop.org/0305-4470/26/19/002)

J. Phys. A: Math. Gen. 26 (1993) L981–L986. Printed in the UK

LETTER TO THE EDITOR

The writhe of a self-avoiding polygon

E J Janse van Rensburg†, E Orlandini‡, D W Sumners§, M C Tesi‡ and S G Whittington‡

† Department of Mathematics, York University, Downsview, Ontario, Canada

‡ Department of Chemistry, University of Toronto, Toronto, Ontario, Canada M5S 1A1

§ Department of Mathematics, Florida State University, Tallahassee, Florida, USA

Received 2 July 1993

Abstract. We discuss the writhe of a self-avoiding polygon on a lattice, as a geometrical measure of its entanglement complexity. We prove a rigorous result about the dependence of the absolute value of the writhe on the number n of edges in the polygon, and use Monte Carlo methods to estimate the distribution of the writhe both for all polygons with n edges and for the subset of polygons that are trefoils.

Polymer molecules in solution are typically very flexible objects which can be highly self-entangled, as well as being entangled with other molecules. It is important to understand and to characterize the extent of this entanglement complexity since it influences crystallization behaviour (de Gennes 1984) as well as rheological properties (Edwards 1967).

Some work has appeared on measuring the topological entanglement complexity of a self-avoiding walk (Janse van Rensburg *et al* 1992), but most attention has focussed on polygons (as models of ring polymers), where knotting can occur. Knotting can be detected using invariants such as the Alexander polynomial (Vologodskii *et al* 1974). Monte Carlo methods have been used to estimate the knot probability, and knot distribution, in various models of ring polymers (Vologodskii *et al* 1974, Michels and Wiegel 1986, Janse van Rensburg and Whittington 1990, Koniaris and Muthukumar 1991). In addition, there are rigorous results on the asymptotic behaviour which establish that almost all sufficiently long lattice polygons are knotted (Sumners and Whittington 1988, Pippenger 1989), and that many measures of knot complexity diverge as the number of edges in the polygon goes to infinity (Soteros *et al* 1992). Similar asymptotic results are available for piece-wise linear polygons in $\mathbb{R}^3$ (Diao *et al* 1993).

These approaches focus on the topology of the system but it is also useful to have geometric measures of the polygonal entanglement. One interesting geometric property is the *writhe* of the polygon, which has proved to be useful in modelling the degree of supercoiling in DNA (Bauer *et al* 1980, White and Bauer 1986). Duplex DNA is modelled as a ribbon and there is an important conservation theorem (White 1969, Fuller 1971) relating the writhe of the centre line of a ribbon to the twist of the ribbon and the linking number of the two boundary curves. Although twist is only defined for a ribbon, writhe is well defined for a single curve.

Consider any simple closed curve in $\mathbb{R}^3$, and project it onto $\mathbb{R}^2$ in some direction $\hat{x}$. In general the projection will have crossings and, for almost all projection directions, these crossings will be transverse, so that we can associate a sign $+1$ or -1 with each crossing, as in figure 1. For this projection we form the sum of these signed crossing numbers, $S(\hat{x})$, and average over all projection directions $\hat{x}$. This average quantity is the writhe W of the curve (Fuller 1971). Writhe is a geometrical quantity (since it is not invariant under ambient isotopy) and is a real number which measures the extent to which the polygon is supercoiled.

If we compute the writhe of each self-avoiding polygon (in the simple cubic lattice, say) with n edges, and average over the set of polygons, clearly the expected value of the writhe $\langle W\rangle$ is zero by symmetry. Consequently, we shall be interested in the expectation of the absolute value of the writhe $\langle|W|\rangle$, or in the expectation of its square $\langle W^2\rangle$ or, more generally, in the distribution of W.

The primary difficulty with the computation of writhe is that it involves averaging the sum of signed crossing numbers over all projection directions. For self-avoiding polygons in Z^3, both the computation and theoretical considerations of writhe are greatly simplified by a theorem (Lacher and Sumners 1991) which reduces the writhe computation to the average of linking numbers of the given curve with four selected pushoffs. We make extensive use of this result.

Let $P = (0,0,0)$ and $Q = (0,1,0)$ on Z^3. Both P and Q are on the boundary of the solid cube C of size $2\times2\times2$ whose corners are

$$\{(0,-1,1),(0,1,-1),(0,-1,-1),(0,1,1),(2,-1,1),(2,1,-1),(2,-1,-1),(2,1,1)\}\,.$$

This cube is symmetric about the plane $z = 0$. Let i, j, k denote unit vectors in a right-handed coordinate system for Z^3. Consider the self-avoiding polygon B which is contained in C and described as follows: begin at P, and take the following sequence of steps in the directions $\{i, i, -k, -j, -i, j, j, k, -i, -j\}$. Let $W(B)$ denote the writhe of curve B.

Lemma 1.

$$W(B) = +\tfrac{1}{2}\,. \tag{1}$$

Proof. We use the theorem (Lacher and Sumners 1991) that the writhe of B is the average of the linking numbers of B with four curves pushed off into four mutually nonantipodal octants. We construct each pushoff of B by addition of one the following four vectors to each point of B: $\{v_1 = (i+j+k)/2, v_2 = (-i+j+k)/2, v_3 = (-i-j+k)/2, v_4 = (i-j+k)/2\}$. These vectors lie in the interiors of unit cubes in four non-mutually antipodal octants, all of which have a common edge. Let B_i denote the curve $B + v_i$, $1 \leqslant i \leqslant 4$. Orient B, and each pushoff B_i in parallel with B. The linking numbers of B with the B_i are $L(B, B_1) = L(B, B_3) = L(B, B_4) = +1$, but $L(B, B_2) = -1$. Hence $W(B) = +\frac{1}{2}$. □

If B^* denotes the mirror image of B (reflected in the plane $z = 0$), then B^* lies in C, and $W(B^*) = -\frac{1}{2}$.

Suppose now that A is a self-avoiding polygon which (given one of its two orientations) intersects cube C only in the self-avoiding walk B' which begins at P and ends at Q and traverses all the steps of B except the last one: that is, B' starts at P and consists of the steps $\{i, i, -k, -j, -i, j, j, k, -i\}$. We can truncate the polygon A by deleting the nine steps of B' and adding in the step i which connects P to Q on the boundary of C. This gives a new polygon A'.

Lemma 2.

$$W(A) = W(A') + W(B)\,. \tag{2}$$

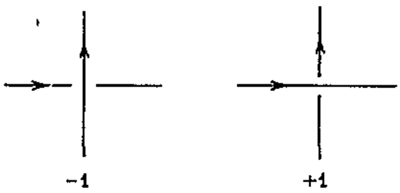

Figure 1. Positive and negative crossings are determined by a right-hand rule.

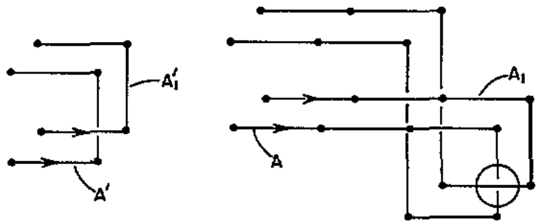

Figure 2. The additivity of linking numbers.

Proof. Consider the pushoffs A_1 of A and A'_1 of A'. Figure 2 shows the projection down the z axis of these pushoffs near cube C; the remainder of each polygon has been suppressed. In figure 2, the (+) crossing in the circle has curve A_1 over curve A. By a small move inside cube C, which does not alter the remainder of curves A and A_1, the (+) crossing in the circle in figure 2 can be changed to a (−) crossing (one in which A_1 goes under A), such that no other crossings between A and A_1 are changed. This gives a pair of curves which are isotopic (by an isotopy inside C) to the pair $\{A', A'_1\}$. In order to see this, first move A up through A_1 at the circle, then perform a Reidemeister I move inside C to convert A_1 to A'_1. This isotopy misses A. Then, perform a similar Reidemeister I move to convert A to A', missing A'_1. This proves that

$$L(A, A_1) = L(A', A'_1) + 1 = L(A', A'_1) + L(B, B_1)\ . \tag{3}$$

A similar computation for each of the other three pushoff directions proves that

$$L(A, A_i) = L(A', A'_i) + 1 = L(A', A'_i) + L(B, B_i) \qquad i = 3, 4 \tag{4}$$

but

$$L(A, A_2) = L(A', A'_2) - 1 = L(A', A'_2) + L(B, B_2)\ . \tag{5}$$

Averaging these equations over the four pushoffs gives us the desired writhe result. □

We are now ready to prove the main theorem of this letter.

Theorem 1. For every function $f(n) = o(\sqrt{n})$, the probability that the absolute value of the writhe is less than $f(n)$ goes to zero as n goes to infinity. □

Proof. The proof relies on a combination of Kesten's pattern theorem (Kesten 1963), and a coin tossing argument (Diao *et al* 1993). We call the ball pair consisting of any translate of the self-avoiding walk B' and the surrounding cube C a *pattern* $\mathcal{P} = \{C, B'\}$. Let the pattern $\mathcal{P}^*$ be the ball pair $\{C, B'^*\}$ where B'^* is the mirror image of B' (reflected in the plane $z = 0$). Kesten's theorem implies that there exists a positive number ϵ such that for all except exponentially few sufficiently long self-avoiding n-edge polygons, there are at least $\lfloor \epsilon n \rfloor$ pairwise disjoint translates of C each of which intersects the polygon in a translate of B' or B'^*. The distribution of the two patterns $\mathcal{P}$ and $\mathcal{P}^*$ is analogous to tossing a coin, because B' and B'^* occur independently with probability $\frac{1}{2}$ in each of the $\lfloor \epsilon n \rfloor$ translations of the cube C. Consequently the probability that B' occurs exactly k times among the $\lfloor \epsilon n \rfloor$

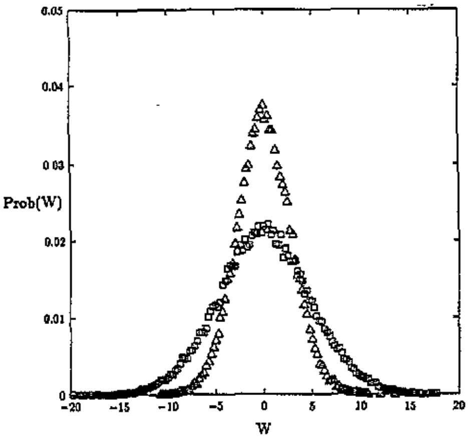

Figure 3. Distribution of the writhe for self-avoiding polygons of length $n = 400$ (Δ) and $n = 1100$ ($\square$).

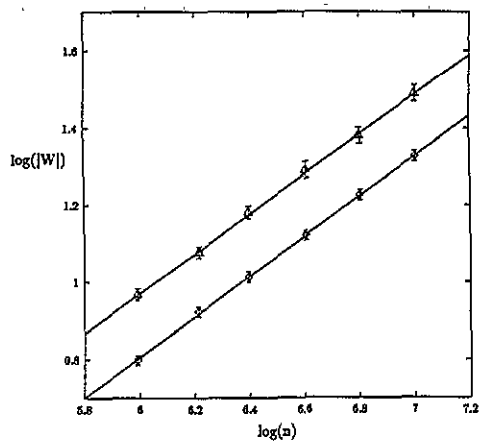

Figure 4. The dependence of $|W|$ on n for self-avoiding polygons in the good solvent ($\Diamond$) and poor solvent (Δ) regimes.

occurences of either B' or B'^* is less than $1/\sqrt{\lfloor\epsilon n\rfloor}$ for every $k \leqslant \lfloor\epsilon n\rfloor$ provided that n is sufficiently large. (This can be shown by applying Stirling's approximation to the binomial distribution.) The fraction of polygons with at least $\lfloor\epsilon n\rfloor$ occurrences of either $\mathcal{P}$ or $\mathcal{P}^*$ is at least $1 - e^{-\gamma n}$ for some positive γ. For each of these polygons, the writhe is the sum of two terms (lemma 2). The first term is from the polygon formed by truncating $\lfloor\epsilon n\rfloor$ times (which is some fixed number), and the second is from the $\lfloor\epsilon n\rfloor$ copies of B or B^* formed in these truncations. If the total writhe is numerically less than $f(n)$ then the contribution to the writhe from the $\lfloor\epsilon n\rfloor$ occurrences of the patterns must be one of at most $\lceil 2f(n) + 1\rceil$ different values. Hence

$$\mathrm{Prob}(|W| < f(n)) \leqslant \frac{(1 - e^{-\gamma n})(\lceil 2f(n) + 1\rceil}{\sqrt{\lfloor\epsilon n\rfloor}} \tag{6}$$

which goes to zero as $n \to \infty$ if $f(n) = o(\sqrt{n})$. $\square$

In order to obtain further information about the behaviour of the writhe, we have carried out some Monte Carlo calculations, generating polygons by a pivot algorithm (Madras *et al* 1990) and computing their writhe by the pushoff technique (Lacher and Sumners 1991). In figure 3 we show the distribution of the writhe for polygons with $n = 400$ and with $n = 1100$ edges. As expected the distribution is symmetric about the origin and is sharply peaked there, becoming less sharply peaked as n increases. The result of theorem 1 strongly suggests that

$$\langle |W| \rangle \sim n^{\alpha} \tag{7}$$

and this led us to plot $\log\langle |W| \rangle$ against $\log n$ in figure 4. The evidence for linear behaviour is excellent and we estimate that $\alpha = 0.522 \pm 0.004$.

Self-avoiding polygons can be regarded as a model of ring polymers in a good solvent. In order to investigate how the writhe depends on solvent quality we have introduced a contact potential between neighbouring pairs of vertices as follows. For a given polygon we count the number of pairs of vertices in the polygon which are unit distance apart but not incident

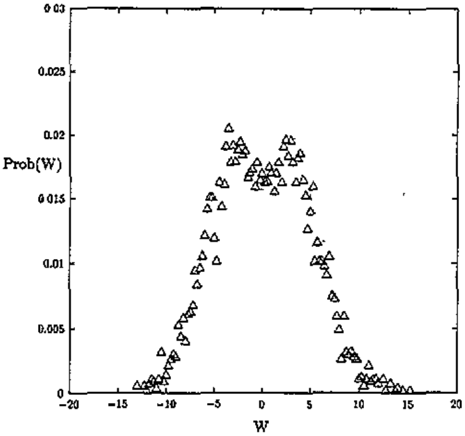

Figure 5. Distribution of writhe in trefoils with n = 400 in the poor solvent regime.

on a common edge. Let this number be m. We associate a (reduced) energy $(-m\beta)$ with the polygon so that the polygon has a weight proportional to $\exp(m\beta)$. Increasingly positive values of β correspond to decreasing solvent quality. We have calculated the distribution of the writhe for a range of values of n for $\beta = 0.26$, which is close to the collapse transition for the cubic lattice (Janse van Rensburg *et al* 1992). We plot $\log\langle|W|\rangle$ against $\log n$ for this value of β in figure 4. The behaviour is again linear with $\alpha = 0.515 \pm 0.006$ and is essentially parallel to the line for $\beta = 0$, the pure self-avoiding polygon (or good solvent) behaviour. This suggests that $\alpha \simeq 0.5$ for a wide range of solvent quality. However, at fixed n the value of $\langle|W|\rangle$ increases as the solvent quality decreases.

The results discussed above are for the set of all polygons with a fixed value of n. We have also considered the subset of polygons which are trefoils. (We sampled these as a subsample of the polygons generated in the above calculation, by checking the value of the Alexander polynomial, evaluated at $t = -1$.) In figure 5 we show the distribution of the writhe for polygons with $n = 400$, $\beta = 0.26$, which are trefoils. The distribution is bimodal. This presumably reflects the fact that trefoils are chiral knots. A corresponding calculation for the figure eight knot (which is achiral) shows a unimodal distribution.

In this letter we have reported the first calculations, as far as we are aware, of the distribution of writhe for self-avoiding polygons on a three dimensional lattice. We proved a theorem giving a lower bound on the rate of increase of the absolute value of the writhe with increasing n, and gave Monte Carlo evidence that this bound may be best possible. In addition we have investigated the distribution of writhe for polygons as a function the contact potential β, and have shown that the distribution is bimodal for trefoils.

We are pleased to acknowledge financial support from NSF and from NSERC.

References

Bauer W R, Crick F H C and White J H 1980 *Sci. American* **243** 118
de Gennes P G 1984 *Macromol.* **17** 703
Diao Y, Pippenger N and Sumners D W 1993 *J. Knot Theor. Ramif.* submitted
Edwards S F 1967 *Proc. Phys. Soc.* **91** 513
Fuller F B 1971 *Proc. Natl Acad. Sci.* **68** 815
Janse van Rensburg E J, Sumners D W, Wasserman E and Whittington S G 1992 *J. Phys. A: Math. Gen* **25** 6557
Janse van Rensburg E J and Whittington S G 1990 *J. Phys. A: Math. Gen* **23** 3573
Kesten H 1963 *J. Math. Phys.* **4** 960

Koniaris K and Muthukumar M 1991 *J. Chem. Phys.* **95** 2873
Lacher R C and Sumners D W 1991 Data structures and algorithms for the computation of topological invariants of entanglements: link, twist and writhe *Computer Simulations of Polymers* ed R J Roe (New York: Prentice-Hall) p 365
Madras N, Orlitsky A and Shepp L A 1990 *J. Stat. Phys.* **58** 159
Michels J P J and Wiegel F W 1984 *Proc. R. Soc.* A **403** 269
Pippenger N 1989 *Discrete Appl. Math.* **25** 273
Soteros C E, Sumners D W and Whittington S G 1992 *Math. Proc. Camb. Phil. Soc.* **111** 75
Sumners D W and Whittington S G 1988 *J. Phys. A: Math. Gen.* **21** 1689
Vologodskii A V, Lukashin A V, Frank-Kamenetskii M D and Anshelevich V V 1974 *Sov. Phys-.-JETP* **39** 1059
White J H 1969 *Am. J. Math.* **91** 693
White J H and Bauer W R 1986 *J. Mol. Biol.* **189** 329