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LETTER TO THE EDITOR

The writhe of a self-avoiding walk

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Abstract. The writhe of a self-avoiding walk in a three-dimensional space is the average over all projections onto a plane of the sum of the signed crossings. We compute this number using a Monte Carlo simulation. Our results suggest that the average of the absolute value of the writhe of self-avoiding walks increases as n^α , where n is the length of the walks and $\alpha \approx 0.5$. The mean crossing number of walks is also computed and found to have a power-law dependence on the length of the walks. In addition, we consider the effects of solvent quality on the writhe and mean crossing number of walks.

The concepts of writhing and twisting have become central to the understanding of polymer conformation and its effects on the physical and chemical properties of polymers. The degree of entanglement complexity of a polymer with itself (through knotting or writhing), or with neighbouring polymers (through linking), is believed to play a significant role in many physical and chemical processes involving a large number of very diverse polymers. These include the crystallization behaviour and rheological properties of a wide class of linear and closed (circular) polymers (Edwards 1967, de Gennes 1984), as well as the regulation of cellular processes by DNA molecules in the living cell (Wasserman *et al* 1985, Wasserman and Cozzarelli 1986). The geometry and topology of DNA molecules is particularly interesting and important, since both are actively manipulated by enzymes in order to enhance such processes as replication, transcription and recombination (see, for example, Bauer *et al* 1980 and White 1992).

A significant amount of literature is devoted to the entanglement complexity of closed self-avoiding walks (or *polygons*) as a model of ring polymers (Vologodskii *et al* 1974, Michels and Wiegél 1986, Janse van Rensburg and Whittington 1990, Koniaris and Muthukumar 1991, Janse van Rensburg *et al* 1993). These numerical simulations complemented the rigorous results involving the knottedness and writhing of polygons (Sumners and Whittington 1988, Pippenger 1989, Janse van Rensburg *et al* 1993). While all these studies applied to models of ring polymers, there are only a few studies devoted to the entanglement complexity of models of linear polymers (de Gennes 1984, Janse van Rensburg *et al* 1992, Arteca and Mezey 1992). This situation arises because there are few 'natural' topological definitions of the entanglement complexity of an arc. One 'natural' measure of the entanglement complexity of an arc is the number of crossings, averaged over

all projection directions (Janse van Rensburg *et al* 1992, Arteca and Mezey 1992). Other less 'natural' measures are derived from the knottedness of a curve obtained by closing the walk with parallel rays, or by joining the ends of the walk in a canonical way with a line segment (Janse van Rensburg *et al* 1992).

Writhing is an interesting *geometric* (as opposed to topological) measure of the entanglement complexity of a closed curve, and it has proved to be useful in modelling the degree of supercoiling in DNA (Bauer *et al* 1980, White and Bauer 1986). Duplex DNA can be modelled as a ribbon and there is a theorem relating the writhe of the centre line and the twist of the ribbon with the linking between its boundary curves (White 1969, Fuller 1971).

To define the writhe of a simple closed curve, or of an arc, in \mathcal{R}^3 first attach a direction to the curve and then consider the projection onto \mathcal{R}^2 in some direction specified by the unit vector \hat{x} . In general the projection will have crossings and, for almost all projection directions, these will be transverse so that we can assign a number $+1$ or -1 to each crossing (the signed crossing number) with the sign determined by a right-hand rule, as shown in figure 1. For each projection, form the sum of these signed crossing numbers, and then average over all projection directions \hat{x} . This quantity is the *writhe* of the simple closed curve or of the arc (Fuller 1971). If we consider two disjoint simple closed curves, A and B , the sum of the signed crossing numbers of the crossings of curve A under curve B , ignoring crossings of A with itself or B with itself, is the *linking number* of the two curves. This quantity is independent of the projection direction.

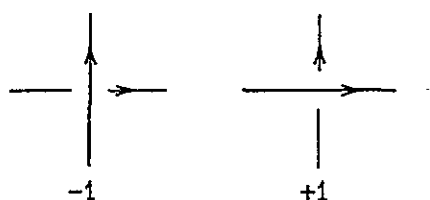


Figure 1. Positive and negative crossings are determined by a right-hand rule.

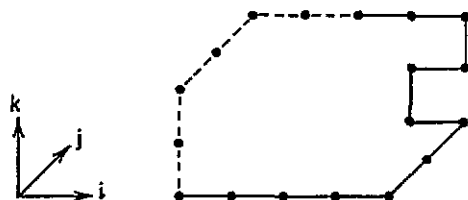


Figure 2. A polygon obtained from a self-avoiding walk by adding a lexicographic least path between the endpoints of the walk.

For polygons in \mathcal{Z}^3 the calculation of writhe is greatly simplified by a theorem of Lacher and Sumners (1991) which states that the writhe of a polygon equals the average of the linking numbers of the given polygon and its pushoffs (translates through a sufficiently small distance) into four non-antipodal octants. See also Janse van Rensburg *et al* (1993). We can define the writhe of a walk similarly by adding a 'lexicographic least' path between the endpoints of the walk, offset a small rational distance in a random direction (with rational direction cosines) to avoid self-intersections. See figure 2. One can then regard this closed walk as a polygon embedded in a cubic lattice which results from a subdivision of the original lattice. Thus, four pushoffs into non-antipodal octants can be used to compute the writhe of the polygon. Hence, we arrive at an alternative definition of the writhe of an open curve (or arc).

Arguing as we did for polygons (Janse van Rensburg *et al* 1993), we expect that the mean of the absolute value of the writhe (W_1) of a walk, defined now as the sum of the signed crossing numbers averaged over all projections of the walk, will have a power-law dependence on the length of the walk:

$$\langle |W_1| \rangle \sim n^{\alpha_1}. \quad (1)$$

We expect that $\alpha_1 \approx 0.5$, by considerations similar to those expressed in Janse van Rensburg *et al* (1993). If we consider the alternative definition of writhe (W_2) obtained by taking lexicographic least closing and using the theorem of Lacher and Sumners (1991), then we expect power-law dependence by the following heuristic argument. The number of edges needed to perform the lexicographic closing of the walk is of order n^ν , where ν is the metric exponent, and n the number of edges in the walk. The writhe of the resulting polygon is therefore expected to be proportional to $(n + An^\nu)^\alpha$, where α is the writhe exponent of a polygon, defined in Janse van Rensburg *et al* (1993). Consequently, $\langle |W_2| \rangle \sim n^\alpha (1 + An^{\nu-1})^\alpha \approx n^\alpha (1 + \alpha An^{-0.4})$, where A is a constant and where we take $\nu \approx 0.6$. For large n , we therefore expect that $\langle |W_2| \rangle$ will have the same power-law behaviour as the writhe of a polygon. Consequently, we postulate that

$$\langle |W_2| \rangle \sim n^\alpha \quad (2)$$

where $\alpha \approx 0.5$ is the exponent associated with the writhe of polygons.

The mean over all possible projections of the summed unsigned crossings (we refer to this as the *mean crossing number*) is a 'natural' measure of the entanglement complexity of a walk (Janse van Rensburg *et al* 1992, Arteca and Mezey 1992). Kesten's pattern theorem (Kesten 1963) implies that the mean crossing number is bounded from below by ϵn , where ϵ is a positive constant, and n is the number of edges in the walk. To see this, we consider a pattern which consists of a tight trefoil, and which has at least one crossing in any projection. There are exponentially few walks which do not contain this pattern at least ϵn times, for some $\epsilon > 0$, so the crossing number grows at least as ϵn . On the other hand, the maximum number of intersections in a projection of a walk occurs when every edge crosses every other edge. That is, the projection has at most $n(n-1)/2$ double points. Consequently, we expect that the mean crossing number will have a power-law dependence on n :

$$\langle C \rangle \sim n^{\alpha_C} \quad (3)$$

where $1 \leq \alpha_C \leq 2$.

To test equations (1)–(3), we carried out Monte Carlo simulations using the pivot algorithm for walks (Madras and Sokal 1987). The writhe was computed using the mean over all projections of the summed signed crossings to test (1), and using the lexicographic least closings followed by the pushoff technique to test (2). Simultaneously, we collected data to test (3). In figure 3 we show the writhe computed in the two ways for walks of lengths between 100 and 1500 edges. Least-squares fits to the data give $\alpha_1 = 0.519 \pm 0.004$, in (1), and $\alpha = 0.500 \pm 0.005$ in (2). Refitting using only the data for n between 400 and 1500, we obtain $\alpha_1 = 0.514 \pm 0.004$, and $\alpha = 0.495 \pm 0.005$. The error bars quoted correspond to two standard deviations and do not include any systematic error due to curvature, but the minor changes in the estimates when we include different numbers of data points suggest that the systematic errors are quite small. The estimates of α and α_1 are close to each other and to the expected (heuristic) lower bound of 0.5. The two sets of data in figure 3 are displaced by a roughly constant distance in the log-log plot, with data corresponding to the lexicographic least-closing calculation having the higher values. This is to be expected since adding the edges to the walk increases its length and therefore the linking number in the pushoff calculation. In addition, the arguments before (2) indicate a positive correction when the extra edges are added. In figure 3 we also plot the mean crossing number as a function of n in a log-log plot. This plot shows more curvature but a linear least-squares fit

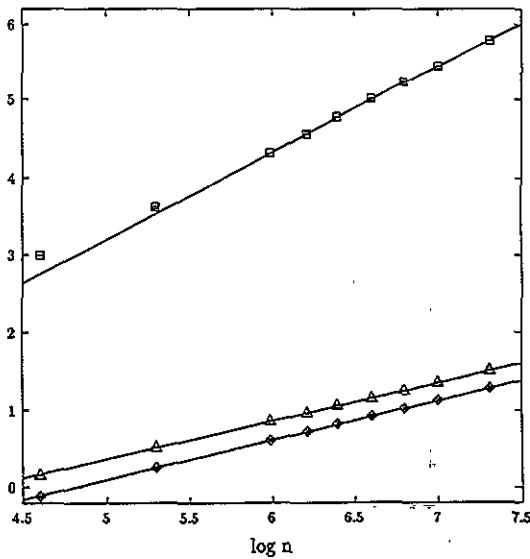


Figure 3. The lower two lines show the n -dependence of the logarithm of the mean of the absolute value of the writhe of a walk, computed in two ways. The upper line shows the n -dependence of the logarithm of the mean crossing number. In each case the lines are least-square fits of the data for n between 400 and 1500.

to the data for n between 400 and 1500 gives $\alpha_C = 1.122 \pm 0.005$. The upward curvature suggests that this value is likely to be an underestimate.

Self-avoiding walks can be regarded as a model of linear polymers in a good solvent. In order to investigate the effects of solvent quality on the writhe and crossing numbers of walks, we introduce a contact potential between vertices which are neighbours in a given conformation of the walk. The total (reduced) contact energy of a walk is determined by the number of neighbouring vertices (not adjacent in the walk), say m , and the contact potential β so that the walk has an associated weight proportional to $e^{m\beta}$. Increasing values of β are associated with decreasing solvent quality, and for $\beta \approx 0.26$ a 'collapse transition' is expected to occur (McCrackin *et al* 1973, Meirovitch 1991).

We carried out Monte Carlo simulations to test the effects of solvent quality on the writhe and mean crossing number of walks. We adjusted the contact potential to several values; e^β took values between 0.0 (simulating a strong short-ranged repulsion between monomers in the polymer), through the good solvent regime where $e^\beta = 1.0$ to the approximate location of the collapse transition where $e^\beta \approx 1.3$. We list the results in table 1, where the error bars given reflect only the statistical uncertainty and do not include any allowance for systematic errors. The exponent α_1 seems remarkably insensitive to the value of β , and over the whole range studied was found to be close to 0.52. In all these simulations the writhe of a walk was computed by the sum over the signed crossings, rather than the pushoff method. On the other hand, the crossing exponent α_C is insensitive to β in the repulsive and good solvent regimes, but it increases as we approach the collapse transition.

While the exponent α_1 is insensitive to β , the mean of the absolute writhe of a walk is dependent on β . We examine this dependence in figure 4, where we plot the mean absolute writhe of walks against the contact potential. We note a steady increase with increasing β . Since larger values of β assign larger weights to walks with many contacts, these conformations are more compact and therefore have larger writhe than conformations with low contact numbers. The crossing number has a similar dependence on β (figure 5). Conformations with larger contact numbers have larger crossing numbers.

In summary, the writhe of a walk can be defined in two alternative ways which give numerically consistent results. We take the fact that $\alpha \approx \alpha_1$ in (1) and (2) to mean that

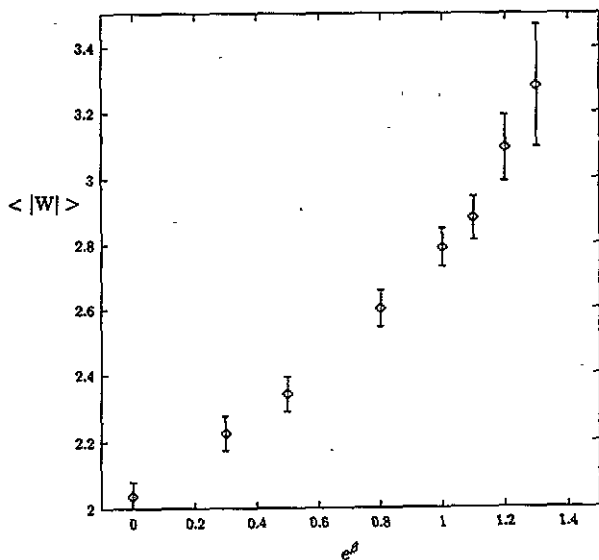


Figure 4. The dependence of the mean of the absolute value of the writhe on the contact potential β , for walks with $n = 900$.

Table 1. The writhe and crossing number exponents.

e^β	α_1	α_C
0.0	0.52 ± 0.01	1.115 ± 0.005
0.3	0.52 ± 0.02	1.110 ± 0.005
0.5	0.52 ± 0.01	1.118 ± 0.005
0.8	0.52 ± 0.01	1.112 ± 0.005
1.0	0.51 ± 0.01	1.122 ± 0.005
1.1	0.51 ± 0.01	1.131 ± 0.002
1.2	0.52 ± 0.01	1.160 ± 0.010
1.3	0.51 ± 0.02	1.180 ± 0.020

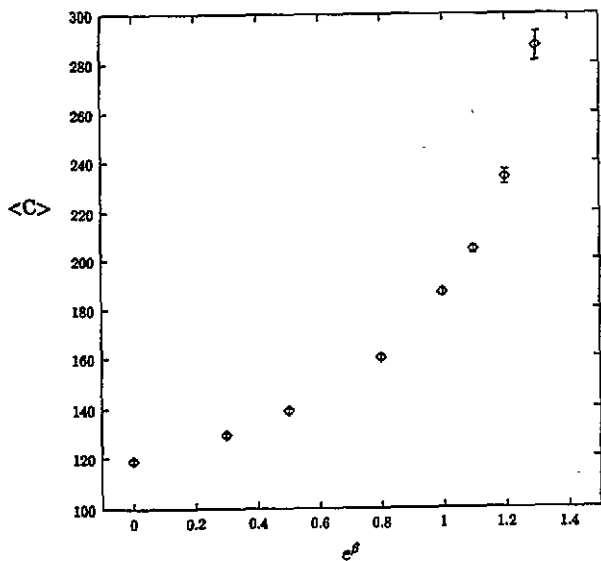


Figure 5. The dependence of the mean crossing number on the contact potential β , for walks with $n = 900$.

writhe can be considered an intrinsic property of a walk which can be measured in either of the ways suggested in this letter. This is because the number of edges which are needed to convert a walk into a polygon is proportional to $n^{0.6}$, which becomes small compared to n in the large n limit; and the geometric properties of a 'long' walk will look much like those of a polygon in this limit.

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