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LETTER TO THE EDITOR

The shapes of self-avoiding polygons with torsion

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Abstract. We consider self-avoiding polygons on the simple cubic lattice with a torsion fugacity. We use Monte Carlo methods to generate large samples as a function of the torsion fugacity and the number of edges in the polygon. Using these data we investigate the shapes of the polygons at large torsion fugacity and find evidence that the polygons have substantial helical character. In addition, we show that these polygons have induced writhe for any non-zero torsion fugacity, and that torsion and writhe are positively correlated.

There is considerable interest in geometrical measures of entanglement complexity of self-avoiding walks, and related structures such as polygons and ribbons, and these ideas have proved to be especially useful in describing models of double stranded polymers such as DNA (Bauer *et al* 1980). Two useful measures of geometrical entanglement complexity for a simple closed curve in three dimensions are writhe and torsion. Torsion characterizes the local helicity of the curve while writhe captures information about the non-local crossings of the curve with itself. The writhe of a polygon in Z^3 can be conveniently calculated by making use of a theorem due to Lacher and Sumners (1991) which shows that the writhe is the mean of the linking number of the polygon with its pushoffs into four mutually non-antipodal octants. This result is an essential ingredient in the proof that the expected value (over all n-gons) of the absolute value of the writhe of polygons in Z^3 increases at least as fast as $\sqrt{n}$ (Janse van Rensburg *et al* 1993). If the polygon has fixed knot type then the expected value of the writhe depends only weakly on n but is a function of the knot type of the polygon (Janse van Rensburg *et al* 1997), and is zero if the knot is achiral.

For a smooth curve in R^3 one can define the torsion in terms of a line integral (see, for example, Struik 1988) but, since we shall be concerned with piecewise linear curves, we define it in terms of dihedral angles (Alexandrov and Reshetniyak 1989). A polygon is made up of a sequence of line segments. Each consecutive triple of line segments defines a dihedral angle about the central segment of the triple. If the three line segments are coplanar this dihedral angle is either 0 or π. If they are non-coplanar it is $\pm\pi/2$. A *positive* dihedral angle is a dihedral angle of $\pi/2$ and a *negative* dihedral angle is a dihedral angle of $-\pi/2$. We associate a quantity τ_i with the ith line segment, and set $\tau_i = \pm 1$ according to whether

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the corresponding dihedral angle is positive or negative, and zero otherwise. We define the torsion of the polygon as

$$t = \sum_i \tau_i . \tag{1}$$

Let $p_n(t)$ be the number of *oriented* n-edge polygons with torsion t, and define the corresponding generating function

$$Z_n(\beta) = \sum_t p_n(t)\, \mathrm{e}^{\beta t} \tag{2}$$

where β is the torsion fugacity. We have shown that

$$\lim_{n\to\infty} \frac{\langle t\rangle}{n} = \frac{\mathrm{d}}{\mathrm{d}\beta} \lim_{n\to\infty} n^{-1} \log Z_n(\beta) \neq 0 \tag{3}$$

for any $\beta \neq 0$, and

$$\lim_{\beta\to\infty} \lim_{n\to\infty} \langle t\rangle / n = 1 \tag{4}$$

(Tesi *et al* 1997) so that at any non-zero torsion fugacity the mean torsion scales with n, and the proportionality constant goes to unity as β goes to plus infinity. At zero torsion fugacity $\langle t\rangle = 0$ but the expected value of the absolute value of the torsion increases at least as fast as $\sqrt{n}$ (Tesi 1997).

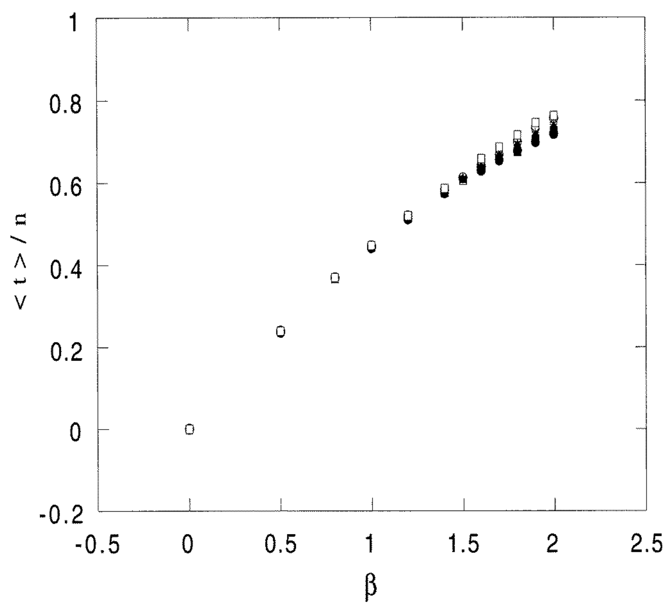

Figure 1. The mean torsion (per edge) as a function of the parameter β, for $n = 100$ (●), 200 (◊), 256 (×), 300 (+), 400 (△), 512 (○) and 600 (□).

The purpose of this letter is to use Monte Carlo methods to investigate the shapes of polygons with torsion as a function of the torsion fugacity and the number of edges in the polygon. We also compute the mean writhe as a function of the torsion fugacity and show that writhe is induced by torsion. The basic algorithm used is a pivot algorithm for polygons (Madras *et al* 1990) combined with a set of local moves which include the Verdier–Stockmayer moves (Verdier and Stockmayer 1961) as well as crankshaft moves.

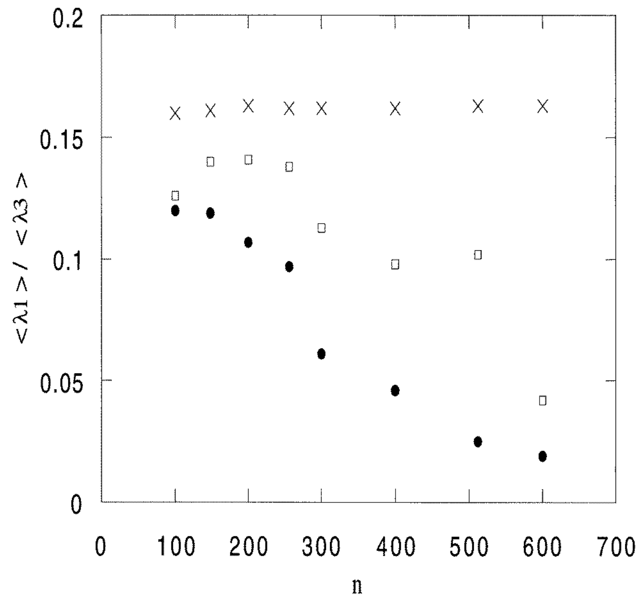

Figure 2. The n dependence of the ratio between the mean value of the lowest (λ_1) and the highest (λ_3) eigenvalue of the metric tensor. Different curves correspond to three different β values: 0.0 (×), 1.7 (□) and 2.0 (●).

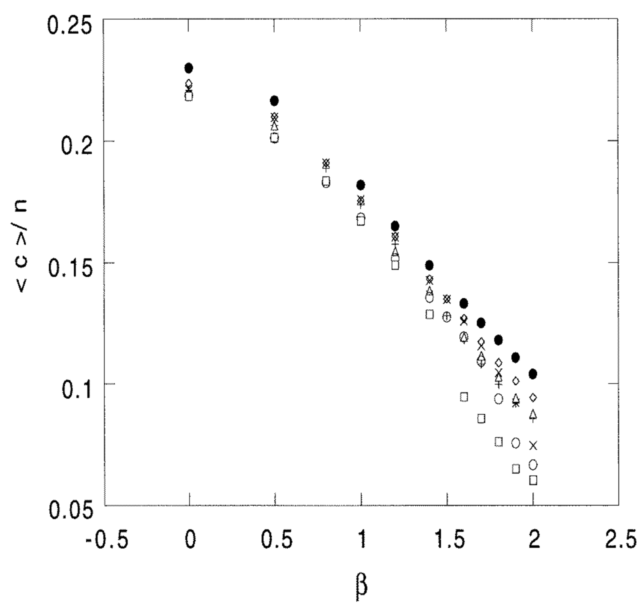

Figure 3. The β-dependence of the mean number of contacts (per edge) for different n values: 100 (●), 200 (◇), 256 (×), 300 (+), 400 (△), 512 (○) and 600 (□).

Although the pivot algorithm alone works well for $\beta = 0$ the local moves are essential for intermediate values of β since otherwise the autocorrelation time of the Markov chain becomes very large. At large β the inclusion of local moves is not enough to avoid the

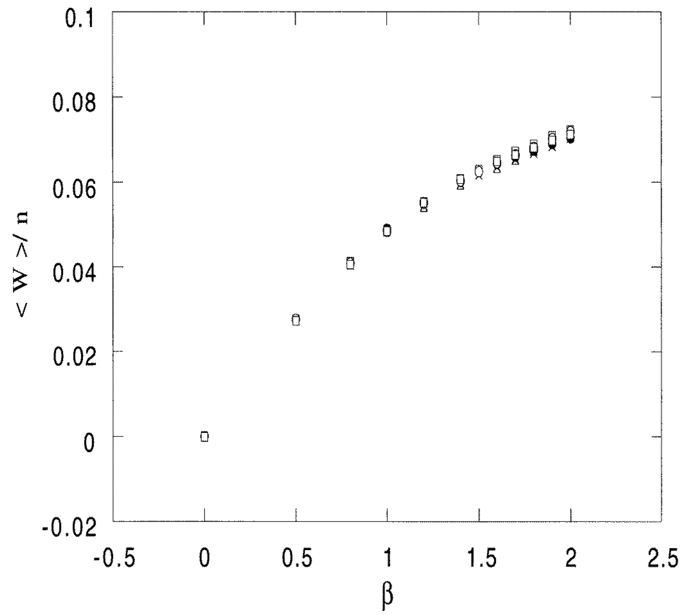

Figure 4. The mean induced writhe (per edge) as a function of the parameter β, for $n = 100$ (●), 200 (◊), 256 (×), 300 (+), 400 (△), 512 (○) and 600 (□).

quasi-ergodic problem and we combine the above algorithm with a multiple Markov chain algorithm originally invented by Geyer (1991). The idea is to run a set of Markov chains in parallel (at a fixed set of values of β) and swap configurations between the individual Markov chains. With appropriately chosen swapping probabilities the limit distribution of the composite Markov chain is the product distribution at the various values of β. For details see Tesi *et al* (1996) and Orlandini (1997).

We have estimated the torsion as a function of both the number, n, of edges in the polygon and the torsion fugacity β. In figure 1 we plot $\langle t\rangle/n$ as a function of β for various values of n. It is clear that the data approximately collapse to a single curve, consistent with the scaling law

$$\langle t\rangle \sim A(\beta)n \tag{5}$$

and the curve shown in figure 1 is a rough estimate of the function $A(\beta)$. Clearly $A(\beta) \leqslant 1$ and it seems to be approaching this value monotonically as β increases, consistent with (3) and (4).

The rigorous results on related topics of Tesi *et al* (1997) do not address directly the question of the shapes of polygons as a function of the torsion fugacity. To investigate this question we have calculated the mean square radius of gyration and also the metric tensor

$$Q_{\alpha\beta} = \frac{1}{2(n+1)^2}\sum_{k,m}(r_k^\alpha - r_m^\alpha)(r_k^\beta - r_m^\beta) \tag{6}$$

and its eigenvalues $\lambda_1 \leqslant \lambda_2 \leqslant \lambda_3$.

We have calculated the mean square radius of gyration $\langle S^2\rangle$ as a function of n and β and found that it is an increasing function of β at each value of n, increasing more sharply at larger n. We expect that

$$\langle S^2\rangle \sim D(\beta)n^{2\nu(\beta)} \tag{7}$$

and that the exponent $\nu(\beta)$ will have the self-avoiding walk value, $\nu = 0.588$ (Li *et al* 1995), at $\beta = 0$ and that $\nu(\infty) = 1$. We also expect a jump discontinuity in $\nu(\beta)$ and that it will otherwise be independent of β. The following argument suggests that the jump discontinuity occurs at $\beta = \infty$. Write x, y, z and $\bar{x}$, $\bar{y}$, $\bar{z}$ for unit vectors along, respectively, the positive and negative x-, y- and z-axes. For any $\beta \neq 0$ the ground state of a sequence of edges will be degenerate, consisting of sequences such as $(xyzxyzxyz\ldots)$, $(x\bar{y}\bar{z}x\bar{y}\bar{z}\ldots)$, etc. At any non-zero β there will be a tendency to form helical sections which will then be broken by random fluctuations (except at infinite β), and new helical sections will then follow the break. However, these helical sections might be different, leading to structures such as $(xyzxyzxyzxxxxxx\bar{y}\bar{z}x\bar{y}\bar{z}\ldots)$ where the axes of the two helical sections point in different directions. This lack of correlation between the directions of the helix axes suggests that we should have self-avoiding walk behaviour at large length scales, for every $\beta \neq \pm\infty$. At small length scales one will typically see helices. This leads us to expect that $\nu(\beta) = 0.588$ for every finite value of β but that longer polygons will be needed to see this asymptotic behaviour as β increases. We have been unable to confirm this behaviour numerically, presumably because longer polygons would be needed than those which we have been able to produce. As a result we regard the location of the jump discontinuity as an open question from the numerical point of view.

To confirm this general picture of helical sections whose length increases as β increases we have estimated the mean values of the eigenvalues of the metric tensor. At $\beta = 0 \langle\lambda_1\rangle/\langle\lambda_3\rangle$ is fairly constant as n increases while at $\beta = 2$ it decreases rapidly as n increases, indicating rod-like behaviour on the length scales which we can probe in this calculation. See figure 2. At large n it is clear that $\langle\lambda_1\rangle/\langle\lambda_3\rangle$ is a strongly decreasing function of β. On the other hand, $\langle\lambda_1\rangle/\langle\lambda_2\rangle$ is fairly constant (with a value around 0.3) for $0 \leqslant \beta \leqslant 2$ and for $100 \leqslant n \leqslant 400$.

We have also estimated the mean number of contacts (edges of the lattice incident on two vertices of the polygon which are not themselves edges of the polygon), $\langle c\rangle$, and we find that there is some tendency for the β-dependence of $\langle c\rangle/n$ to approach a limiting curve as n increases. See figure 3. Certainly $\langle c\rangle/n$ is a decreasing function of β. The decrease in the mean number of contacts (as β increases) is consistent with a less compact structure which could be elongating and becoming less spherically symmetric as β increases.

Taken together with the observation that the object is becoming more rod-like (on small and intermediate length scales) and the small and decreasing values of $\langle\lambda_1\rangle/\langle\lambda_3\rangle$ as β increases, these results indicate that the polygon aquires some helical character as the torsion fugacity increases.

One would expect that such helical regions would affect the writhe of the polygon and we have checked this by computing the mean writhe as a function of the torsion fugacity. Our results indicate that the mean writhe is non-zero at non-zero values of the torsion fugacity. That is, torsion induces writhe. In figure 4 we plot the mean writhe per edge of the polygon as a function of the torsion fugacity for various values of n. Again the data collapse to a single curve and suggest that the mean induced writhe scales with n. We write w for the induced writhe and

$$\langle w\rangle \sim B(\beta)n \tag{8}$$

for the apparent behaviour of the mean induced writhe. Clearly $\langle w\rangle \ll \langle t\rangle$ but $\langle w\rangle$ increases monotonically with increasing β. Although it is known (at least for the smooth case) that there are conformations of a simple closed curve which have writhe increasing like $n^{4/3}$ (Cantarella *et al* 1997) it appears that the writhe induced by torsion does not increase faster than linearly with n.

In this paper we have simulated a model of lattice polygons with a torsion fugacity. Positive torsion fugacity was found to induce positive writhe in this model. Our results are similar to those obtained in computer simulations of a rod model of DNA with a twist fugacity (Vologodski *et al* 1992): torsional energy is released as induced supercoiling (which manifests itself as writhe) (Vologodski *et al* 1992). Our results on the shape and size of the polygons indicate that for non-zero values of the fugacity the polygons have rod-like (helical) shapes on small and intermediate length scales. On the other hand, a density of random regions in the polygons will destroy all long-ranged correlations, and we expect the polygon to have self-avoiding walk exponents in the asymptotic limit, for any finite value of β. This model could also be of interest in the study of biopolymers such as polypeptides or proteins, since on small length scales the polygons appear to have helical regions.

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