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LETTER TO THE EDITOR

Induced writhe in linked polygons

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Abstract. We consider a pair of polygons on the simple cubic lattice forming a link of specified type. We investigate the mean writhe of the polygons as a function of the number of edges in each polygon, and of the link type. Although two unknotted polygons which are linked as a Hopf link have zero mean writhe, we show that other torus links induce writhe in the polygons. We also consider non-torus links, including a link in which one polygon is knotted.

There is considerable interest in the entanglement complexity of polymer molecules in dilute solution. One approach is to look at knotting in ring polymers or at corresponding local topological entanglements in linear polymers. Another approach is to focus on geometrical properties such as the writhe of the polymer. Writhe has been shown to be a useful measure of supercoiling in DNA (Bauer *et al* 1980, Vologodskii and Cozzarelli 1994). It can be defined (Fuller 1971) for any simple closed curve in $\mathbb{R}^3$ so it is a useful quantity for characterizing the conformations of single-stranded polymers, as well as double-stranded polymers such as DNA.

If ring polymers are modelled as polygons on the simple cubic lattice $\mathbb{Z}^3$ then there is a very convenient way of computing the writhe as the average of the linking number of a polygon with each of its pushoffs into four mutually non-antipodal octants (Lacher and Sumners 1991). This result is a key ingredient in a proof that the expectation of the absolute value of the writhe, $\langle|Wr(n)|\rangle$, over the set of polygons with n edges, increases at least as rapidly as $\sqrt{n}$ (Janse van Rensburg *et al* 1993).

Clearly the expectation of the writhe, over the set of n-gons, is zero by symmetry and this is also true if the polygons are conditioned to be unknotted. However, if the polygons are conditioned to be a particular knot type then the expectation of the writhe is zero if the knot is achiral, but (in general) non-zero if the knot is chiral (Janse van Rensburg *et al* 1993, 1996). If the sampling includes both the (+) and (−) knots in a chiral pair then the expectation of the writhe will be zero, but the distribution of writhe will be bimodal (Janse van Rensburg *et al* 1993). For chiral knots it has been found (Janse van Rensburg *et al* 1996) that the mean writhe is almost independent of n though the width of the distribution increases approximately as $\sqrt{n}$.

Circular DNA molecules often occur in nature as linked circles and the writhe of the DNA rings in these links has been studied experimentally (Wasserman *et al* 1988) and using Monte Carlo calculations (Vologodskii and Cozzarelli 1993). Vologodskii and Cozzarelli (1993) observed that linked pairs of circular DNA molecules had non-zero writhe, and that the writhe increased with increasing complexity of the link type. The purpose of this letter is to investigate the extent of the induced writhe when two polygons in $\mathbb{Z}^3$ are linked to form a particular link type. We are interested in how the writhe depends on the lengths (and relative lengths) of the two polygons and on the link type. We shall compare our results with those of Vologodskii and Cozzarelli (1993) since we are interested in the extent to which this phenomenon is a general one, rather than being a feature of a particular model of circular DNA.

The approach which we use is a grand-canonical Monte Carlo simulation using the BFACF algorithm (Berg and Foester 1981, Aragao de Cavalho and Caracciolo 1983, Aragao de Cavalho *et al* 1983). The BFACF algorithm samples on a realization of a Markov chain defined on the set of polygons with (in principle) all values of n, and the sampling is focused on a range of values of n determined by a parameter (the step fugacity). For a single polygon it is known that the ergodic classes of the Markov chain are the knot types (Janse van Rensburg and Whittington 1991) and the proof of that fact relies on showing that Reidemeister moves can be executed by BFACF moves. This implies that the ergodic classes of the BFACF algorithm applied to two polygons will be the knot and link classes of the polygons. This means that we can sample on a particular link type, and collect data at various values of the lengths of the polygons in a single Monte Carlo run.

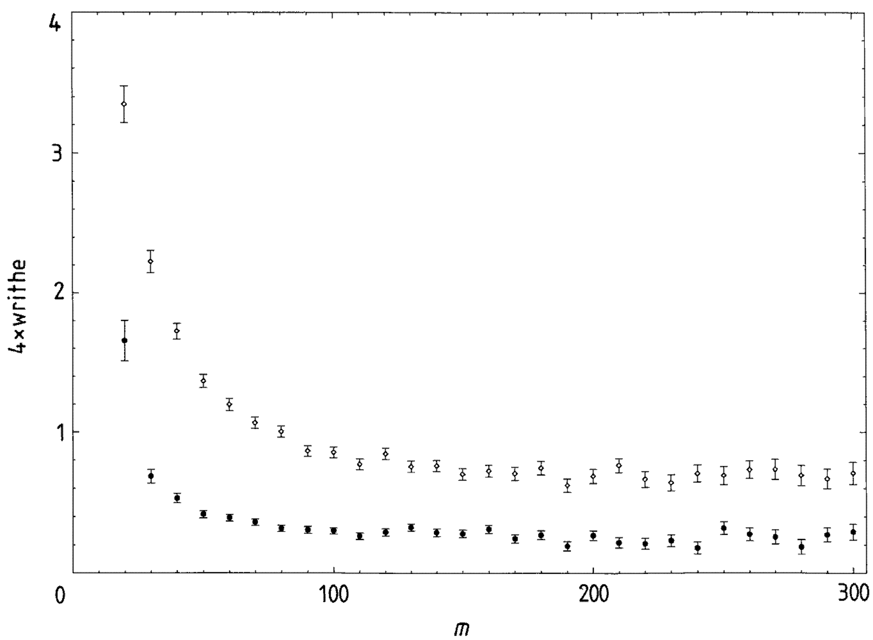

Figure 1. Four times the mean writhe of a 20-gon (○) and of a 40-gon (◇) as a function of the number (m) of edges in the second polygon in a (2,4)-torus link.

We begin by considering the family of $(2,2k)$-torus links whose first few members are (in Alexander–Briggs notation) 2_1^2 (the Hopf link), 4_1^2, 6_1^2 .... Drawings can be found in Rolfsen (1976) appendix C. If we consider any of the $(2,2k)$-torus links and colour the two circles red and blue then there is a series of Reidemeister moves and plane isotopies which interchanges the two colours. We call links with this property *symmetric* links. For each link type we consider pairs of polygons with m and n edges and compute the mean writhe of the n-gon, say, as a function of m and n. In the case of the Hopf link (the $(2,2)$-torus link, or 2_1^2) each polygon appears to have zero mean writhe, so that linking does not induce writhe for this type of link. For the $(2,4)$-torus link we show in figure 1 the mean writhe

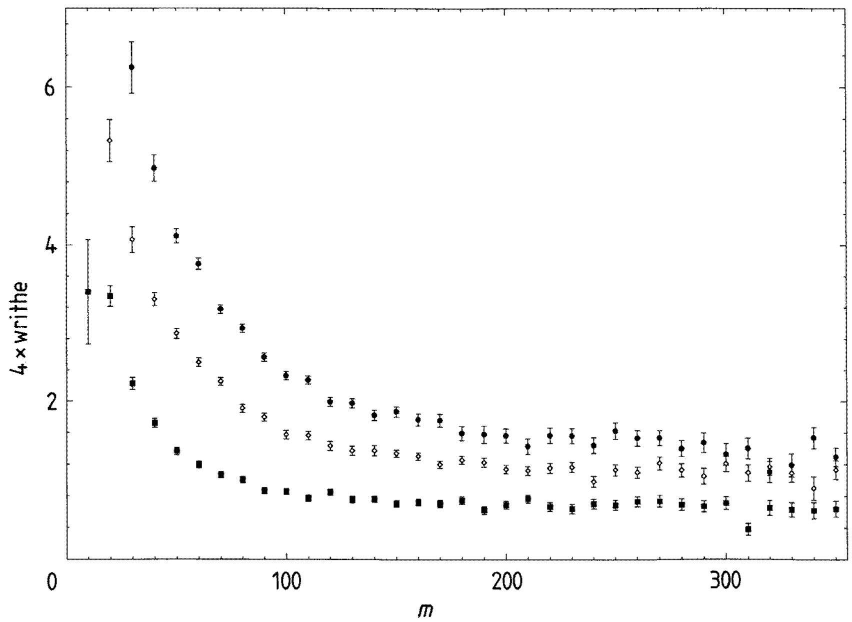

Figure 2. Four times the mean writhe of a 40-gon as a function of the number (m) of edges in the second polygon in a (2,4)-torus link (■), (2,6)-torus link (◊) and (2,8)-torus link (●).

of a 20-gon and of a 40-gon as a function of the number (m) of edges in the other polygon in the link. The writhe decreases at first as the length of the second polygon increases, and there is some evidence that the writhe is tending to a non-zero limit as m increases, though this needs further investigation. The writhe of the 40-gon is consistently higher than that of the 20-gon, and data for 60-gons and 80-gons (not shown) confirm that the writhe of the n-gon increases with increasing n at fixed values of m. In figure 2 we show the m-dependence of a 40-gon which is a member of a $(2, 4)$-, $(2, 6)$- and $(2, 8)$-torus link. Clearly the writhe of the 40-gon decreases as m increases, for each torus link, and increases as the complexity of the torus link increases. In figure 3 we show the mean writhe of an n-gon which is a member of a link of two n-gons, as a function of the torus link type. The mean writhe seems to be almost independent of n, after some initial transient behaviour, but increases as the complexity of the torus link increases. We have estimated the mean writhe for large n, assuming that (after the initial changes, say for $n \geqslant 40$), the results are simply fluctuations about a mean value independent of n. (There is some evidence (Janse van Rensburg *et al* 1996) for this type of behaviour for the writhe of polygons of fixed knot type.) These estimated values for the asymptotic writhe increase approximately linearly with k for (2,2k)-torus links. Similar behaviour was observed by Vologodskii and Cozzarelli (1993) for a model of linked circles of DNA. Although the values of the mean writhe are different in the two models the rate of increase is similar.

To summarize the situation for the (2,2k)-torus links, it seems that linking induces writhe in the polygons when $k \geqslant 2$. The writhe increases as the size (i.e. the number of edges) of the polygon increases and decreases as the size of the polygon to which it is linked increases. When the two polygons have the same size, the writhe is more or less independent of size provided that the polygons are not too small, and increases roughly linearly with k.

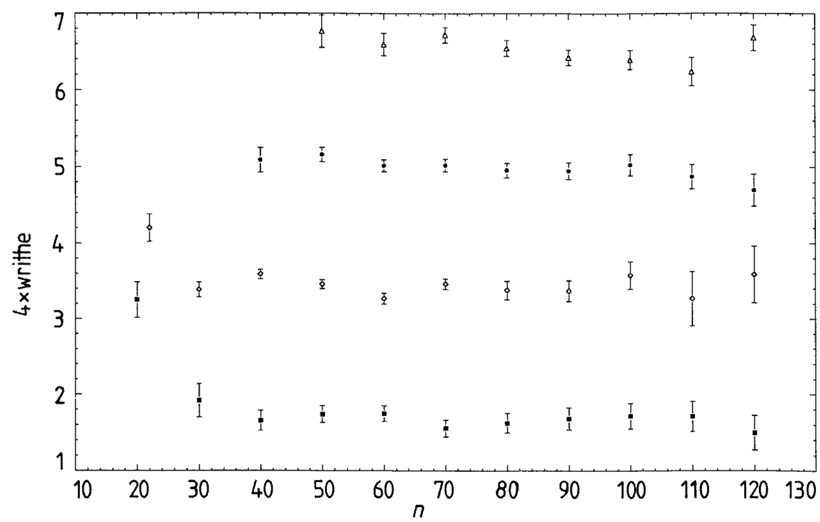

Figure 3. Four times the mean writhe of an m-gon in a link of two m-gons, for (2,4)-torus links (■), (2,6)-torus links (◇), (2,8)-torus links (●) and (2,10)-torus links (△).

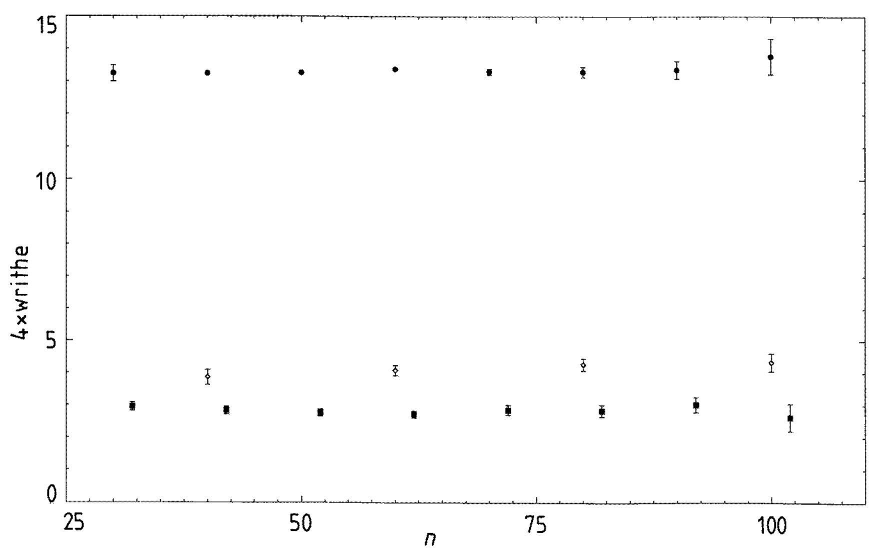

Figure 4. Four times the mean writhe of an n-gon in a link of two n-gons for the Whitehead link (■), the link 6^2_3 (◇) and the trefoil in the link 7^2_8 (●).

We have also examined several links other than torus links. The Whitehead link 5^2_1 is symmetric in the sense described above, and we have computed the writhe of one polygon (having n edges) in the link as a function of n and the size (m) of the second polygon in the link. The behaviour is similar to that found for the torus links, with the mean writhe increasing with n and decreasing with m, and apparently tending to a non-zero limit as m increases at fixed n. For comparison we have examined the link 6^2_3 (also a symmetric link). The behaviour is similar except that the induced writhe is larger. In figure 4 we show the n

dependence of the mean writhe when $m = n$ for the Whitehead link (5^2_1) and for 6^2_3. As a second comparison we have looked at the link 7^2_8 which is asymmetric. One of the circles is unknotted while the other is a trefoil. The unknotted polygon has mean writhe very close to zero while the knotted polygon has writhe comparable to the mean writhe of a trefoil which is not linked to another polygon. The mean writhe of the knotted polygon in this link (with $m = n$) is also shown in figure 4.

We have shown that the phenomenon of inducing writhe by linking is not confined to relatively realistic models of linked circular DNA but also occurs in simple lattice models. The importance of the effect increases as the complexity of the link increases and there are strong analogies with the phenomenon of writhe of knotted polygons (Janse van Rensburg *et al* 1993, 1996). Since the effect occurs in lattice polygons it might be possible to prove rigorous results about the effect and we are pursuing this approach.

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