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LETTER TO THE EDITOR

Knottedness in self-avoiding walks

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Abstract. In this letter we explore the knottedness of self-avoiding walks. We were not able to represent the data as a power law.

The study of self-avoiding walks (SAW) has been one of continuing interest for many years, especially since de Gennes (1972, 1979) has shown its relationship to critical phenomena. Much of the recent work on various models of SAW has involved fitting the results to some power-law form and then relating the exponents in the power law to the critical exponents obtained in phase transitions (de Gennes 1979).

Some recent work has been to characterise the topologically different classes of configurations of a single closed macromolecule (Michels and Wiegel 1982). It appears that Delbruck (1962) first proposed this problem and subsequently it has been taken up by a number of authors (see Michels and Wiegel (1982) for references).

Recently Sumners and Whittington (1988) proved two theorems concerning knot probability in self-avoiding walks and polygons.

Theorem 1. All except exponentially few sufficiently long self-avoiding polygons on the simple cubic lattice contain a knot.

A linear polymer is never knotted since the ends of the polymer can be rethreaded through the entanglements. Sumners and Whittington developed a suitable definition for knotting in SAW and hence their theorem 2.

Theorem 2. All except exponentially few sufficiently long self-avoiding walks on the simple cubic lattice contain a knotted arc.

Their results showed the validity of the Frisch–Wasserman–Delbruck conjecture (see Sumners 1986), namely: for a self-avoiding polygon of length n, the knot probability tends to unity as n tends to infinity.

There have been a number of numerical investigations, that of Vologodskii *et al* (1974) probably being the first. Their important result showed that for polygons of lengths less than about 150 the probability of finding a knot was of the order of 10^{-3} or less. Michels and Wiegel (1982) generated equilibrium configurations of a ring polymer in infinite space. Their results are compatible with power and scaling laws.

In this work we looked at the n dependence of the knot probability for self-avoiding walks and compared our results with those of Michels and Wiegel. In particular we tried to determine if the same power and scaling laws found for polygons are applicable to the knot probability in SAW.

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Self-avoiding walks of length n were generated on a 5-choice cubic lattice. The techniques for this kind of generation are well documented (Wall *et al* 1963, Windwer 1970). Once a successful SAW of length n was completed it was tested for knottedness. Whereas previous workers have used the Alexander polynomial (Alexander 1928) as a test for knottedness, in this work we used the knot invariant of crossings to determine if a knot exists in the SAW. This was accomplished in the following manner: the coordinates of the last step of the walk were compared with the coordinates of previous steps to determine if a crossing occurred. A crossing will occur if two of the coordinates of steps i and j are the same (the third coordinate could not be the same since this would mean closure, whereas these walks were tested already and were determined to be self-avoiding). A comparison of the values of the third coordinate of steps i and j determined whether the crossing was over (+) or under (−). In figure 1(a), the first crossing is + (over), the second is − (under), and the third is + (over). In figure 1(b), the signs are reversed, namely −, +, −, going from crossings 1 to 3. In figure 1(c), we have crossing +, +, −. This is an unknot. When two crossings, one immediately after the other, are of the same sign, +, + or −, − they cancel each other in the counting of crossings. In order to form a knot, one must have a minimum of three crossings (Rolfsen 1976).

When one is checking for the crossing invariant in this fashion it is necessary to distinguish between an actual knot and a twisted chain. Both will give the same results if the knot checking was terminated at this point. Referring to figure 2, figure 2(a) is a twisted chain whereas figure 2(b) is a trefoil knot. Both show +, −, + crossing as noted in the figure and determined by our crossing checking method. Each chain

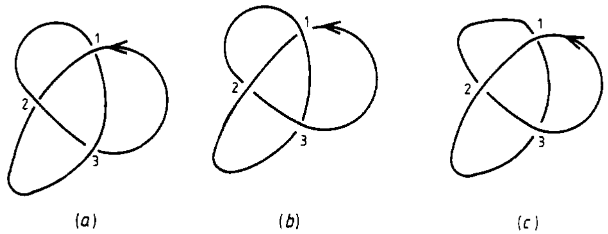

Figure 1. Two trefoil knots, (a) and (b), and an unknot (c). The knots (a) and (b) are mirror images of each other. In (a), if we start as 1 we get for crossings over (+) under (−) over (+). In (b) it is under (−) over (+) under (−). For (c), over (+) over (+) cancel each other out resulting in (c) being an unknot.

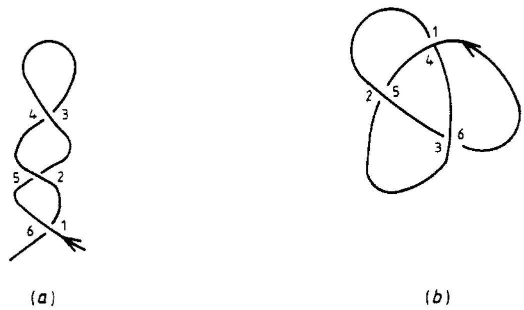

Figure 2. In (a) we have a twisted unknot whereas in (b) we have a trefoil knot. They both exhibit the crossings +−+.

which showed knot formation, by having three or more crossings, had to be distinguished from a twisted chain. This was done as follows. In figure 2, if one follows the initial arrows in both figures the crossings takes place in figure 2(a) as +, −, + and returns as −, +, − so that the first (1) and last (6) crossings in figure 2(a) are the same. Whereas when we examine the trefoil, in figure 2(b), we find that the first and fourth crossings are the same and the sixth and third crossings go together. In any knotted system, if there are n crossings one obtains $2n$ double points by travelling through the planar projection of the knot. Using this difference as our guide, twisted chains were found if the first and last crossings occurred with the same coordinates. In the checking for crossings, the coordinates of the last atom in the generated chain are tested against the coordinates of the other atoms in the chain. If a knot is found the checking of the atoms is reversed. That is, the last atom becomes the first atom and vice versa. The checking is repeated. When the first crossing in this fashion is found the coordinates of the two crossings are compared. If they are the same, the chain is termed a twisted chain and is not counted as a knotted chain.

The results of this work are shown in table 1. It is clear from the table that the number of knots increases strongly with the length of walks and then begins to taper off. For example, in going from size 100 to 200 the fraction of unknotted walks goes from 0.704 to 0.382; practically a 50% reduction. The same features are seen going from 200 to 300 and 300 to 400. However, the percentage change of size as well as knottedness is on a downward trend. In one run of length 1000 and sample size 100, 98 of the walks showed knottedness. This is in agreement with theorem 2 of Sumners and Whittington. Of course the term 'sufficiently long' gives us wide latitude.

Table 1. A summary of results. N is the length of the chain. S is the sample size for each value of N. B is the number of knots found per N and ζ is the fraction of unknotted SAW.

N	S	B	ζ
100	2000	592	0.704
150	2000	1009	0.496
200	1000	618	0.382
250	1000	740	0.260
300	1000	858	0.142
400	1000	916	0.084
500	500	472	0.056
1000	100	98	0.020

We also subjected our data to a number of plots of the fraction of unknotted walks as a function of the size of the walk to see whether this work would give the same straight line plots found by Michels and Wiegel (1982). We were unable to represent our data as a power law and could therefore find no appropriate scaling laws for this topological problem. Our work differs substantially from that of Michels and Wiegel in three respects. Whereas they studied the topology of polymer rings we looked at the topology of self-avoiding walks. Their sample size was superior to ours by an order of magnitude and finally they checked for knottedness by use of the Alexander polynomial whereas we used the invariant of crossings.

If we assume that our sample size is sufficiently large as to exhibit the trends looked for and that the knot checking by the different methods is equivalent it may be that we are looking at two different topological questions, although one can conceive of an arc connecting the two end-points of the self-avoiding walk without violating the excluded volume condition. In that case, the results of the two studies should differ by a scaling factor which we do not find. It would be very useful to have more information on the n dependence of knot probability in polygons and self-avoiding walks.

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