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Knots in self-avoiding walks

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Abstract. In this paper we discuss the existence of knots in random self-avoiding walks on a lattice. Using Kesten's pattern theorem, we show that almost all sufficiently long self-avoiding walks on the three-dimensional simple cubic lattice contain a knot.

1. Introduction

The problem of the occurrence of knots in a long linear polymer chain seems to have been first addressed by Frisch and Wasserman (1961) and by Delbruck (1962). Both groups formulated questions about the probability that a closed chain (i.e. a loop) with degree of polymerisation n would contain a knot. They conjectured that the probability that a loop would contain a knot would tend to unity as n tends to infinity. Edwards (1967) has emphasised the importance of topological constraints in the statistical mechanics of long polymer molecules and de Gennes (1984) has pointed out the possible importance of knots in long-time memory effects in melts of *linear* polymers. In addition, knots occur in circular DNA and provide information about enzyme mechanisms (see, for instance, Wasserman and Cozzarelli 1986). In spite of this, rather little theoretical work has appeared on knots in polymers.

In order to attack these questions theoretically we need a suitable model of an open or closed polymer chain. The model which we shall use in this work is a self-avoiding walk (or self-avoiding polygon) on the three-dimensional simple cubic lattice. It is well known that this model is a useful one for describing excluded-volume effects in polymers in dilute solution and it is an attractive model for looking at problems associated with knots since a self-avoiding polygon is topologically equivalent to a closed polymer chain.

This problem has been investigated numerically by several workers, of whom Vologodskii *et al* (1974) carried out the first Monte Carlo treatment of knotting in self-avoiding polygons. They generated a random sample of such polygons of fixed length and identified the knotted configurations by computing the Alexander polynomial. In fact they found that, for the polygon lengths which they studied (n less than about 150), the probability $\mathcal{P}_0(n)$, of finding a knot was very small (of the order of 10^{-3} or less). They also examined a random walk model (without the self-avoiding condition). When a self-intersection occurred they shifted the lattice by a small amount, along some randomly chosen direction, which has the effect of passing the chain under or over itself at each point which would otherwise be an intersection. They found that the knotting probability was much higher in this second model, and increased with increasing n. Several other Monte Carlo studies have been carried out more recently (des Cloizeaux and Mehta 1979, Michels and Wiegel 1984, 1986, Brinke and Hadziioannou 1987) with basically similar results. These studies all support a lattice version of the Frisch-Wasserman-Delbruck conjecture (see e.g. Sumners 1986) which can be stated as the following conjecture.

Conjecture. For a self-avoiding polygon of length n, the knot probability tends to unity as n tends to infinity.

In this paper we shall give a proof of the validity of this conjecture. The key to the proof is a result of Kesten (1963) which says that if a 'pattern' (i.e. a finite self-avoiding walk) can appear (more than twice) in a self-avoiding walk, then it will appear at least once in 'most' sufficiently long self-avoiding walks. By extending this result to polygons, and constructing a suitable knotted pattern, we prove the following theorem.

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

This implies the validity of the Frisch-Wasserman-Delbruck conjecture. Most polymers are linear, not ring polymers. In the standard definition of a knot, a linear polymer is never knotted since one can thread one of the free ends through any entanglement and eventually untangle the polymer. The question of the knotting probability for linear polymers would be answered immediately by Kesten's theorem if we had a suitable definition of 'knottedness'. We shall show that, for self-avoiding walks on the simple cubic lattice, it is possible to develop a suitable definition for knotting. This is because a self-avoiding walk on a lattice generates a unique three-dimensional excluded volume for itself. Sometimes this excluded volume is a 3-ball (homeomorphic to the set of all vectors of length less than or equal to one in 3-space). In this situation we can produce an arc (homeomorphic to the unit interval) embedded in the 3-ball, with its two boundary points trapped in the 2-sphere boundary of the 3-ball. Such an arc is said to be *properly embedded* in the 3-ball. Under these circumstances knotting is well defined and we can use Kesten's theorem to prove the following theorem.

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

2. Definitions

We take the standard knot theory definitions (Burde and Zieschang 1986). Let R^n denote Euclidean n-space. All homeomorphisms will be orientation preserving. The unit sphere in R^n is $S^{n-1} = \{x \in R^n \mid |x| = 1\}$. The unit ball in R^n is $B^n = \{x \in R^n \mid |x| \leq 1\}$. Let $f: S^1 \to R^3$ be an embedding (a placement of the circle in 3-space). Topologists usually restrict embeddings to be smooth or piecewise linear to avoid infinite (wild) pathology. We shall work in the piecewise-linear category, since we shall be considering self-avoiding walks on the simple cubic lattice in R^3. The embedding f determines a manifold pair, $(R^3, f(S^1))$. If we think of the standard embedding of R^2 (XY space) in R^3 (XYZ space), this defines a standard embedding of S^1 in R^3. This embedding determines the *unknot* (R^3, S^1). An embedding $f: S^1 \to R^3$ determines a *knot* if the pair $(R^3, f(S^1))$ is not homeomorphic to the standard pair (R^3, S^1). If f, g are a pair of embeddings of S^1 in R^3, they determine equivalent knots if there is a homeomorphism of pairs $H:(R^3, f(S^1)) \to (R^3, g(S^1))$. This definition agrees with the intuitive idea of a knot: two placements of the circle in 3-space are equivalent if it is possible to continuously deform one configuration (without cutting it or passing it through itself) until it can be superimposed upon the other. An embedding of a circle in 3-space is unknotted if it can be continuously deformed to a planar embedding.

There are analogous definitions of knotted arcs (B^1) in the 3-ball (B^3). Let $f: B^1 \to B^3$ denote a proper embedding; i.e. one in which $f^{-1}(\partial B^3) = \partial B^1$. That is, the boundary points of B^1 are sent into the boundary of B^3 under the embedding f, and no other points of B^1 are sent into the boundary by f. There is a standard embedding of B^1 in B^3, determined by the standard embedding of R^1 (X space) in R^3. This gives us the standard unknotted object in this context, (B^3, B^1). The embedding f determines a *knotted ball pair* if the pair $(B^3, f(B^1))$ is not homeomorphic to the standard ball pair. As before, two embeddings f, g determine *equivalent* ball pairs if there is a homeomorphism of pairs between them. The reason that one can get knotted arcs in this context is because the endpoints of the arc are trapped in the boundary 2-spheres of the 3-balls. In figure 1, configuration (a) is the standard (unknotted) ball pair, and (b) is a knotted ball pair. Note that for the unknotted ball pair the 1-ball can be continuously deformed so that it lies entirely in the surface of the 3-ball. This is not possible for the knotted ball pair. Configurations (c) and (d) of figure 1 illustrate the point that the 3-space surrounding an embedded arc is crucial in determining whether or not we have a knotted ball pair. This is a *relative* phenomenon, and an arc is knotted *relative* to certain 3-balls in which it is properly embedded, and unknotted *relative* to certain others. In configuration (c), for example, the apparently knotted arc determines an *unknotted* ball pair. The surrounding 3-space is 'knotted' in the same way as the arc, and together they determine the standard ball pair. In configuration (d) the apparently straight arc is in fact knotted, and determines the same knotted ball pair as that of configuration (b)!

Consider now the integer simple cubic lattice in R^3. A *step* is a directed edge joining two adjacent lattice points. A self-avoiding walk of n steps beginning at lattice point x_0 is an $(n+1)$-tuple of distinct lattice points $X = (x_0, x_1, \ldots, x_n)$, where x_i and

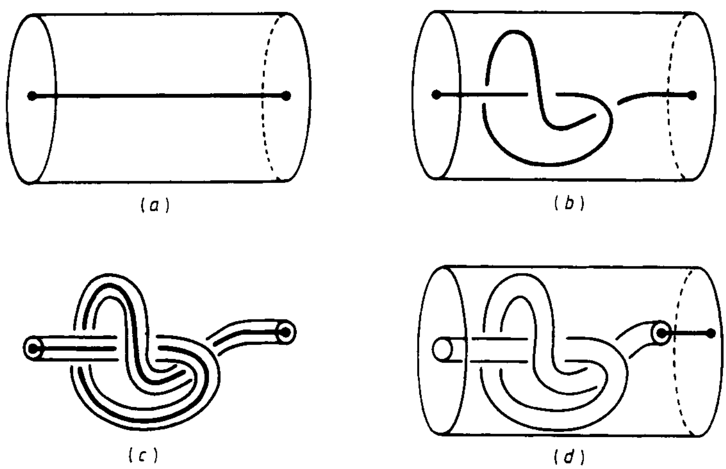

Figure 1. (a) The standard unknotted ball pair. (b) A knotted ball pair containing a trefoil. (c) is topologically equivalent to (a) and (d) is topologically equivalent to (b).

x_{i+1} are adjacent in the lattice. Each occupied lattice site in a self-avoiding walk sits in the middle (barycentre) of a dual 3-cube (the Wigner-Seitz cell), and one can think of this dual 3-cube as the 'excluded volume' generated by that occupied vertex. If one takes the union of all the Wigner-Seitz cells determined by the vertices of the self-avoiding walk X, one obtains the *lattice neighbourhood* of X, written $N(X)$. If X is a subwalk of a longer walk Y, let $(Y-X)$ denote the graph obtained by deleting the edges of X. The intersection of $(Y-X)$ with $N(X)$ consists of (at most) two half-intervals on the lattice, where the longer walk exits $N(X)$. Suppose that X is a self-avoiding walk of n steps, $(n \geq 3)$. X determines a unique derived walk X', where X' is the walk of $(n-2)$ steps obtained from X by deleting the first and last step. Suppose that $N(X')$ is homeomorphic to B^3. Let X'' denote the intersection of X with $N(X')$. We then have a unique ball pair $(N(X'), X'')$ determined by the self-avoiding walk X. It may happen that this ball pair is indeed knotted. If this is the case, we say that X is a knotted arc. If a self-avoiding walk Y contains a subwalk X, and X is a knotted arc, then we say that Y contains a knotted arc. If the self-avoiding walk X is a knotted arc, and X is a subwalk of a self-avoiding walk Y, then all the steps of $Y-X$ *must* avoid $N(X')$, and the 'knottedness' cannot be undone by 'threading back through the knot'. One thinks of such a knot as 'tight'. More precisely, if the self-avoiding walk X is closed into a circle in R^3 by adding an arc which misses $N(X')$, then this circle must be knotted, because it contains the knotted ball pair $(N(X'), X'')$. The proof of this fact involves computation of the fundamental group of the complements of the objects involved, and realising that an object (arc or circle) is knotted if the fundamental group of its complement is not the infinite cyclic group (Burde and Zieschang 1986). As an example of a (trefoil) knotted self-avoiding walk, let $\{i, j, k\}$ denote the unit vectors in the X, Y, Z directions, respectively, and let $\{-i, -j, -k\}$ denote the negatives of these unit vectors. If one is standing at an integral lattice point in R^3, one can take a step of length one in any of the six directions $\{i, -i, j, -j, k, -k\}$. Starting at the origin in R^3, take the following walk (T) of 18 steps:

$$T: \{i, i, j, k, k, -j, -j, -k, -i, -k, -k, j, j, k, k, -j, i, i\}.$$

In the above, T stands for trefoil, and the reader will verify (by drawing the relevant plug from the simple cubic lattice, or making a model out of matchsticks) that $N(T')$ is homeomorphic to B^3, so that T is a knotted arc. Moreover, any walk that has T as a subwalk has the trefoil in it. It is clear that the walk T can be closed up to yield the trefoil (three-crossing) knot. The above construction can in fact be performed for any arbitrary knot. Details will appear elsewhere.

3. Proof of results

Suppose that c_n is the number of n-step self-avoiding walks with the first vertex at the origin on the simple cubic lattice. Then Hammersley and Morton (1954) have shown that

$$0 < \lim_{n\to\infty} n^{-1} \log c_n = \inf_{n>0} n^{-1} \log c_n \equiv \kappa < \infty. \tag{3.1}$$

A *pattern* is any finite self-avoiding walk. We first state a lemma about the occurrence of patterns due to Kesten (1963).

Lemma 1. If there exists a self-avoiding walk on which a pattern (P) occurs three times then the number ($c_n(\bar{P})$) of n-step self-avoiding walks on which P does not occur is such that

$$\limsup_{n\to\infty} n^{-1} \log c_n(\bar{P}) = \lambda(\bar{P}) < \kappa. \tag{3.2}$$

Let u_n be the number of *directed* n-edge (self-avoiding) polygons *rooted* at the origin. Then (Hammersley 1961)

$$\lim_{n\to\infty} n^{-1} \log u_n = \lim_{n\to\infty} n^{-1} \log c_n = \kappa. \tag{3.3}$$

If p_n is the number of *directed* but *unrooted* polygons we have

$$u_n = np_n. \tag{3.4}$$

If we write $p_n(\bar{P})$ and $u_n(\bar{P})$ for the numbers of polygons and rooted polygons respectively which do not contain a pattern P then

$$u_n(\bar{P}) = np_n(\bar{P}) \tag{3.5}$$

since adding or removing a root does not affect the non-existence of a pattern.

If the last edge of a rooted polygon (i.e. the in-edge incident on the root) is deleted, the corresponding graph is a self-avoiding walk with $(n-1)$ edges. Moreover, deleting an edge cannot create a pattern so that

$$u_n(\bar{P}) \leqslant c_{n-1}(\bar{P}). \tag{3.6}$$

Equations (3.2) and (3.6) together establish the following lemma.

Lemma 2. If there exists a self-avoiding walk on which a pattern (P) occurs three times then the number of directed and rooted polygons on which P never occurs is such that

$$\limsup_{n\to\infty} n^{-1} \log u_n(\bar{P}) \leqslant \lambda(\bar{P}) < \kappa \tag{3.7}$$

with a corresponding result for $p_n(\bar{P})$.

Since T^3 (the concatenation of T with two suitably translated copies of T) is a self-avoiding walk, we can replace P by T in lemma 2. Hence, the number of polygons on which T never occurs is an exponentially small fraction of the number of polygons and we have theorem 1.

The probability that a polygon does not contain the pattern T is given by

$$u_n(\bar{T})/u_n \leqslant \exp[(\lambda-\kappa)n + o(n)] \tag{3.8}$$

where $\lambda = \lambda(\bar{T}) < \kappa$. The probability $\mathscr{P}_0(n)$ that an n-edge polygon is knotted is bounded below by the probability that it contains the knotted arc T, so that

$$1 \geqslant \mathscr{P}_0(n) \geqslant u_n(T)/u_n \geqslant 1 - \exp[(\lambda-\kappa)n + o(n)] \tag{3.9}$$

and $\mathscr{P}_0(n) \to 1$ as $n \to \infty$. Moreover the limit is approached exponentially rapidly. (Here $u_n(T)$ is the number of polygons which contain at least one copy of T.)

Similarly, taking $P = T$ in (3.2) immediately gives theorem 2. Again, the probability $\mathscr{P}(n)$ that a self-avoiding n-step walk contains a knotted arc is bounded below by the fraction of walks containing at least one copy of T, $c_n(T)/c_n$ and

$$1 \geqslant \mathscr{P}(n) \geqslant c_n(T)/c_n \geqslant 1 - \exp[n(\lambda-\kappa) + o(n)]. \tag{3.10}$$

Hence, the probability that a self-avoiding walk contains a knotted arc tends to unity, exponentially rapidly, as $n \to \infty$.

4. Discussion

The results presented in this paper establish the validity of the Frisch–Wasserman–Delbruck conjecture for self-avoiding polygons on the simple cubic lattice. In addition, we have shown that one can give a suitable definition of knotting in a self-avoiding walk and that the knot probability goes to unity as n goes to infinity.

This implies that the low value of the knotting probability found for self-avoiding polygons by Vologodskii *et al* (1974) is a small n effect. However, it would be very useful to have more information on the n-dependence of the knot probability. Our results on the rate of approach to the limit are weak and, except for the information available from Monte Carlo work, this is still an open question.

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