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Random linking of lattice polygons

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Abstract. We study the linking probability of polygons on the simple cubic lattice. In particular, we consider two polygons each having n edges, confined to a cube of side L, and ask for the linking probability as a function of n and L. We also consider other situations in which the polygons are restricted to be not too far apart, but not necessarily confined to a cube. We prove several rigorous results, and use Monte Carlo methods to address some questions which we are unable to answer rigorously. An interesting feature is that the linking probability is a function of L/n^{ν}, where ν is the exponent characterizing the radius of gyration of a polygon.

1. Introduction

Entanglements between polymer chains play an important role in the rheological properties of polymers (Prager and Frisch 1967, Edwards 1968, de Gennes 1979, Lacher *et al* 1986, Mikos and Peppas 1991, and many other references). One might hope to model entanglements between chains by considering *linking* between two ring polymers. Linking has the advantage of being well defined topologically, and links (or catenanes) are of interest chemically in their own right (Frisch and Wasserman 1961, Dietrich-Buchecker *et al* 1984, Logemann 1993, and references quoted therein). In addition, linked pairs of DNA rings occur in the mitochondria of malignant cells (Hudson and Vinograd 1967) and are intermediates in the replication of circular DNA (Sundin and Varshavsky 1981), so linking can have important biological consequences.

Ring polymers (such as closed circular DNA) can be modelled as n-step self-avoiding polygons on a lattice (such as Z^3) or in R^3, and the properties of linked pairs of polygons in these systems have been studied using Monte Carlo methods by a number of workers (Vologodskii *et al* 1975, Michels and Wiegel 1986, Klenin *et al* 1988). Little is known rigorously, but some work has been done on the linking probability for random embeddings of circles in R^3 (Pohl 1981, Duplantier 1981).

In this paper we shall be concerned with linking of pairs of polygons in Z^3. We consider two self- and mutually avoiding polygons, each with n edges, and ask for the probability that they are linked when they are subject to some constraint. (A constraint is necessary since n will be finite and Z^3 is an infinite space.) We shall consider several different constraints, such as requiring that the centres of mass of the two polygons are no more than a distance d apart, or that the two polygons are both contained in a cube of side L. In general, the linking probability will depend on n and d or on n and L, and we use both rigorous and numerical approaches to investigate these dependences. In section 2 we shall prove some results about the asymptotic behaviour for several cases, but we are unable to supply rigorous answers to many of the interesting questions. In section 3 we describe the Monte Carlo approach which we have used, and we present and discuss the numerical results in section 4.

2. Definitions and rigorous results

We define a *simple closed curve* in R^3 as the image of a smooth (C^∞) or piece-wise linear (PL) map of the circle S^1 into R^3. A *link* with k components is the image of a (smooth or PL) map of a disjoint union of k circles into R^3. In this paper we shall be concerned only with links with two components. Two links L_1 and L_2 are *equivalent* if there is a homeomorphism of R^3 onto itself which takes L_1 to L_2, and the equivalence class of a link is called its *link type*.

There are three distinct definitions of linking used in topology, and we first discuss the relation between these. Two disjoint simple closed curves C_1 and C_2 are *topologically unlinked* if there is a homeomorphism of R^3 onto itself, $H : R^3 \to R^3$, such that the images $H(C_1)$ and $H(C_2)$ are separated by a two-dimensional plane. The simple closed curve C_1 is *homotopically unlinked* from C_2 if there is a homotopy h_t from the embedding C_1 to the constant map (i.e. $h_0(C_1) = C_1$ and $h_1(C_1)$ is a point) such that $h_t(C_1)$ is disjoint from C_2 $\forall t \in [0, 1]$. It is possible for C_1 to be homotopically unlinked from C_2 but for C_2 to be homotopically linked to C_1, so homotopic linking is not a symmetric relation (Rolfsen 1976). Finally, C_1 is *homologically unlinked* from C_2 if C_1 bounds an orientable surface which is disjoint from C_2. Homological linking is a symmetric relation, and homological linking implies homotopic linking which implies topological linking. In this paper we shall be concerned mainly with homological and topological linking.

It is easy to detect whether or not two curves are homologically linked (Rolfsen 1976). One method, which is particularly useful for PL curves, is to orient each of the two curves C_1 and C_2, and to project them onto a plane so that no vertex in the projection of C_1 falls on the projection of C_2, or *vice versa.* At each point where C_1 crosses *under* C_2 we assign a value +1 or −1, according to the orientation of the crossing (see figure 1). The sum of these crossing numbers is called the *linking number* of the two curves, $l(C_1, C_2)$, and the curves are homologically linked if and only if $l(C_1, C_2) \neq 0$ (Rolfsen 1976). Detecting topological linking is a more difficult problem, and the method we use here offers only a partial solution, in that it fails to detect some links. We compute the two variable Alexander polynomial $\Delta(s, t)$ evaluated at $s = t = -1$ (see, for instance, Torres (1953) for a justification of the method and Vologodskii *et al* (1975) for details of the calculation). If $\Delta(-1, -1) \neq 0$ then the curves are topologically linked, but it is possible for a linked pair to have $\Delta(-1, -1) = 0$. However, this does not occur for any link with less than nine crossings.

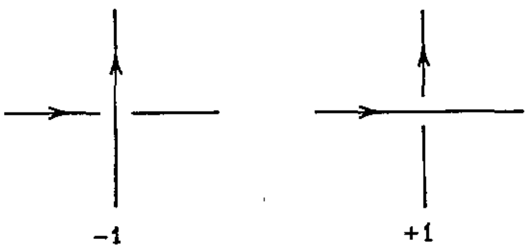

Figure 1. Positive and negative crossings determined by a right-hand rule.

We shall need a number of results for self-avoiding lattice polygons. We define an *n-step self-avoiding polygon* in Z^3 as an ordered set of n vertices such that vertices i and $i+1$ are a unit distance apart, $1 \leqslant i \leqslant n-1$, vertices n and 1 are also a unit distance apart, with the set of n edges joining vertex i to vertex $i+1$, $1 \leqslant i \leqslant n-1$, and vertex n to vertex 1. We shall be interested in the number, p_n, of these polygons, where two polygons are considered distinct if they cannot be superimposed by translation. For instance $p_4 = 3$, $p_6 = 22$ and $p_8 = 207$. Since $p_n = 0$ for all odd values of n we shall adopt the convention that n is even in most statements about self-avoiding polygons. The main rigorous result about the asymptotic behaviour of p_n is due to Hammersley (1961) who has shown that there exists a connective constant $\kappa > 0$ such that

$$p_n = \mathrm{e}^{\kappa n + \mathrm{o}(n)} \tag{2.1}$$

and similar techniques, together with the use of a pattern theorem (Kesten 1963), have been used (Sumners and Whittington 1988, Pippenger 1989) to prove that the number p_n^0 of *unknotted* polygons behaves as

$$p_n^0 = \mathrm{e}^{\kappa_0 n + \mathrm{o}(n)} \tag{2.2}$$

with $0 < \kappa_0 < \kappa$, so that the probability $P(n)$ that the polygon is a knot goes to unity exponentially rapidly as n goes to infinity, i.e.

$$P(n) = 1 - p_n^0/p_n = 1 - \mathrm{e}^{-\alpha_0 n + \mathrm{o}(n)} \tag{2.3}$$

for some positive constant $\alpha_0 = \kappa - \kappa_0$.

We first prove a theorem about pairs of polygons in a cubic box of side L.

Theorem 2.1. Let $p_n^{(2)}(L, \tau)$ be the number of ways of embedding two self- and mutually avoiding polygons, each with n edges, in a cube of side L such that the polygons are a link of type τ. Then

$$\lim_{n,L\to\infty} \frac{\log p_n^{(2)}(L,\tau)}{2n} = \kappa \tag{2.4}$$

provided that n and L both go to infinity such that $L \geqslant n + q$ and $L = \mathrm{e}^{\mathrm{o}(n)}$. Here q is independent of n and L, but may depend on τ.

Proof. Define the *bottom vertex* of a polygon as the vertex having smallest coordinates, taken in lexicographic order. To obtain an upper bound on $p_n^{(2)}(L, \tau)$, we consider embedding each polygon independently such that its bottom vertex is at each vertex of the cube of side L. This gives

$$p_n^{(2)}(L, \tau) \leqslant (L+1)^6 p_n^2 \tag{2.5}$$

so that

$$\limsup_{n,L\to\infty} \frac{\log p_n^{(2)}(L,\tau)}{2n} \leqslant \kappa + \lim_{n,L\to\infty} \frac{6\log(L+1)}{2n} \tag{2.6}$$

and the right-hand side is equal to κ if $L = \mathrm{e}^{\mathrm{o}(n)}$. To obtain a lower bound we note that, for any given link type τ, we can construct an embedding in Z^3 of a pair of polygons with this link type. This follows by an extension of the arguments of Soteros *et al* (1992). By subdivision and concatenation we can arrange this embedding so that an edge e_1 of one polygon lies in the plane $x = x_1$, containing vertices with smallest x-coordinate, and an edge e_2 of the other polygon lies in the plane $x = x_2$ containing vertices with largest x-coordinate. Moreover, both polygons can be arranged to have the same number of edges, say $m = m(\tau)$. With this pair of polygons fixed, we can translate each of $p_{n-m}/2$ polygons with $n-m$ edges so that the plane $x = x_2 + 1$ contains an edge of this polygon parallel to e_2, and no vertices of this polygon have x-coordinate less than $x_2 + 1$. These two polygons can now be concatenated by adding and deleting pairs of edges. The same construction can be carried out for the edge e_1, giving the bound

$$p_n^{(2)}(L,\tau) \geqslant p_{n-m}^2/4 . \tag{2.7}$$

For every value of n the resulting pair of polygons can always be contained in a cube of side $n+q$, for a suitable choice of q. This implies that

$$\liminf_{n,L\to\infty} \frac{\log p_n^{(2)}(L,\tau)}{2n} \geqslant \kappa \tag{2.8}$$

provided that $L \geqslant n+q$. The theorem follows from (2.6) and (2.8).

If we restrict our attention to non-trivially linked pairs of polygons (i.e. we exclude the unlinked pair), and count embeddings of pairs of polygons as distinct if they cannot be superimposed by translation, the above arguments work without the need for a confining cube, and we have the following theorem.

Theorem 2.2. If $p_n^{(2)}(\tau)$ is the number of embeddings in Z^3, per lattice site, of two polygons, each with n edges, forming a link of type τ, where τ is any link other than the unlink, then

$$\lim_{n\to\infty} \frac{\log p_n^{(2)}(\tau)}{2n} = \kappa . \tag{2.9}$$

Proof. It is convenient to fix the bottom vertex of one of the polygons at the origin. Then the lower bound

$$p_n^{(2)}(\tau) \geqslant p_{n-m}^2/4 \tag{2.10}$$

follows from a similar construction to that used in theorem (2.4). To construct an upper bound, we note that the two polygons cannot be linked if the bottom vertex of one is not within a cube of side n whose bottom vertex coincides with the bottom vertex of the other polygon. Hence we can construct each polygon in p_n ways, and translate one relative to the other in at most n^3 positions. Hence

$$p_n^{(2)}(\tau) \leqslant n^3 p_n^2 . \tag{2.11}$$

Taking logarithms, dividing by $2n$, and letting n go to infinity in (2.10) and (2.11) gives (2.9).

Each of the polygons making up a link (i.e. each component of the link) can be knotted, and we can ask for the probability that an embedding of a link (of type τ) has unknotted components. The answer is given by the following theorem.

Theorem 2.3. The probability $P^{(2)}(n,\tau)$ that both components (with n edges) of a link of type τ are knotted goes to unity as

$$P^{(2)}(n,\tau) = 1 - \mathrm{e}^{-\alpha_0 n + o(n)} \tag{2.12}$$

when $n \to \infty$.

Proof. Let $p_n^{(2)}(0,\tau)$ be the number of embeddings (per lattice site) of a pair of polygons, at least one of which is unknotted, each of which has n edges, and which are components of a non-trivial link of type τ. Then, by the argument used to obtain (2.11), but using unknotted embeddings of at least one of the polygons,

$$p_n^{(2)}(0,\tau) \leqslant n^3 \left(p_n^0\right)^2 + 2n^3 p_n^0 p_n. \tag{2.13}$$

Similarly,

$$p_n^{(2)}(0,\tau) \geqslant p_{n-m} p_{n-m}^0 / 4. \tag{2.14}$$

Then

$$\begin{aligned} P^{(2)}(n,\tau) &= 1 - p_n^{(2)}(0,\tau)/p_n^{(2)}(\tau) \\ &\leqslant 1 - \left[n^3 \left(p_n^0\right)^2 + 2n^3 p_n^0 p_n\right] / \left[p_{n-m}^2/4\right] \\ &= 1 - \mathrm{e}^{-(\kappa-\kappa_0)n + o(n)} \end{aligned} \tag{2.15}$$

and

$$\begin{aligned} P^{(2)}(n,\tau) &\geqslant 1 - \left[p_{n-m} p_{n-m}^0/4\right] / n^3 p_n^2 \\ &= 1 - \mathrm{e}^{-(\kappa-\kappa_0)n + o(n)} \end{aligned} \tag{2.16}$$

so that (2.12) follows with $\alpha_0 = \kappa - \kappa_0$.

3. Numerical methods

The theorems proved in section 2 do not address the regime in which the polygons are appreciably deformed by the applied geometrical constraint. To investigate the behaviour of the link probability in this situation we use Monte Carlo methods to generate a random sample of pairs of polygons. The algorithm used was invented by Madras *et al* (1990) and is a modification of a cut-and-paste algorithm, introduced by Lal (1969) for the simulation of self-avoiding walks in the canonical ensemble, and extensively studied by Madras and Sokal (1988), who called it the pivot algorithm. The idea is to sample along a realization of a Markov chain, defined on the set of polygons with fixed number of edges. The necessary elementary moves for the algorithm include several elements of the octahedral group, the symmetry group of the cubic lattice. In order to generate pairs of polygons we implemented a slight modification of the algorithm used by Janse van Rensburg and Whittington (1991) to sample the space of single polygons. Two pivots are chosen uniformly on each polygon and a symmetry operation (one for each polygon) is carried out on one of the two segments connecting the pivots. In addition to the usual self-avoidance condition for a single polygon, we require mutual avoidance between the two polygons; such requirements can be efficiently implemented by using hash-coding (Knuth 1973, Horowitz and Sahni 1976).

We are interested in studying situations in which the two polygons cannot be too far apart in space, since otherwise they will be unlinked. To focus the sampling on this regime we use an importance sampling method where polygons are sampled from the probability distribution function $f(d, d_0) = A \exp(-d^2/d_0^2)$ where d is the distance between the centres of mass of the two polygons, d_0 is an appropriately chosen parameter, and A is a normalization constant. Since we are sampling from a non-uniform distribution, in the data analysis we attach a weight w to each polygon pair in the sample, with $w = 1/f = A^{-1} \exp(d^2/d_0^2)$. In addition we pool the data from runs with different values of d_0 by using suitably weighted averages.

We studied polygon pairs of length n ranging from $n = 400$ up to $n = 1800$. For a fixed value of n we sampled with different values of d_0 in the interval $[n/4, 4n]$. For every state sampled in the Markov chain we computed the linking number, the Alexander polynomial evaluated at $s = t = -1$, $\Delta(-1, -1)$, the Alexander polynomial of each of the two components of the link, the distance d between the centres of mass of the two polygons, the mean-square radius of gyration of each polygon, and the spans in the three lattice directions, L_χ, where $\chi = x, y$ and z, of the pair of polygons. Averages were taken over 25 000 samples, sampled every 50 attempted pivots.

To investigate the dependence of the link probability on a geometrical constraint, such as a cube of side L, we used rejection techniques to choose, for a fixed L, the subset of pairs of polygons which could be contained in the L-cube. A pair of polygons fits a given L-cube if all the three spans are less than L. To count the number of ways in which a given pair can be contained in an L-cube we consider every two embeddings of pairs to be distinct even if they can be superimposed by translation in the x, y or z directions within the cube.

4. Numerical results

In this section we report results for two types of constraint. In section 4.1 we consider two polygons confined in a cube of side L, and examine the linking probability as a function of n and L. In section 4.2 we consider pairs of polygons which are constrained so that the distance between their centres of mass cannot exceed d, and investigate the linking probability as a function of n and d. We find strong qualitative similarities between the two cases.

4.1. Polygons confined to cubes

The results obtained in section 2, especially theorem 2.1, were for pairs of polygons whose configuration was not seriously affected by the presence of a constraint. For two polygons each with n edges, confined to a cube of side L, we would expect that this behaviour would continue until $L \sim n^\nu$, where ν is the exponent characterizing the n-dependence of the mean-square radius of gyration. For $L < n^\nu$, the polygons will be more compact, and this effect will increase as L decreases at fixed n. We shall focus on this regime.

In figure 2 we show the probability for polygon pairs to be homologically linked (i.e. of having a non-zero linking number) as a function of n and L. The qualitative features are clear. The linking probability increases with increasing n at fixed L, and with decreasing L at fixed n. Since there are two length scales in this problem (n^ν and L) one expects that it will be the *ratio* between these length scales which will govern the behaviour, and this is

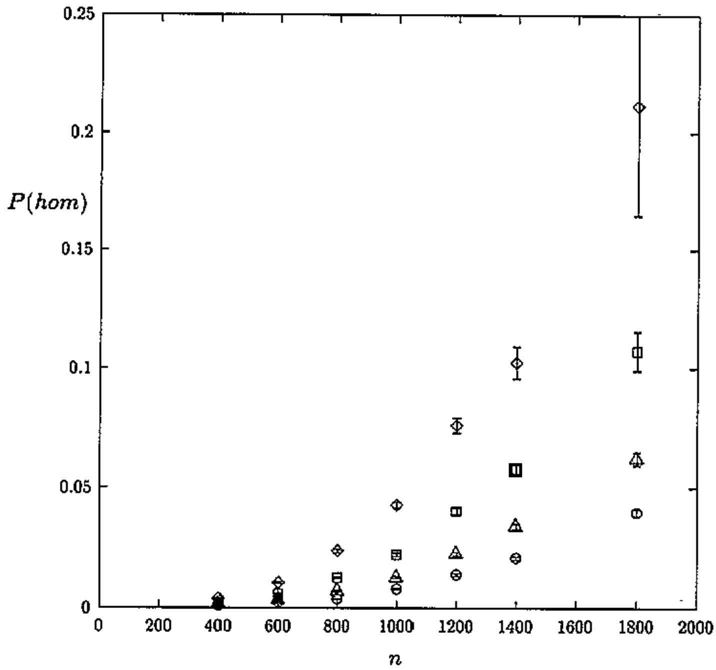

Figure 2. The homological linking probability for polygon pairs as a function of the number (n) of edges in each. Different curves correspond to different values of L: 72 (◇), 84 (□), 96 (△) and 108 (○).

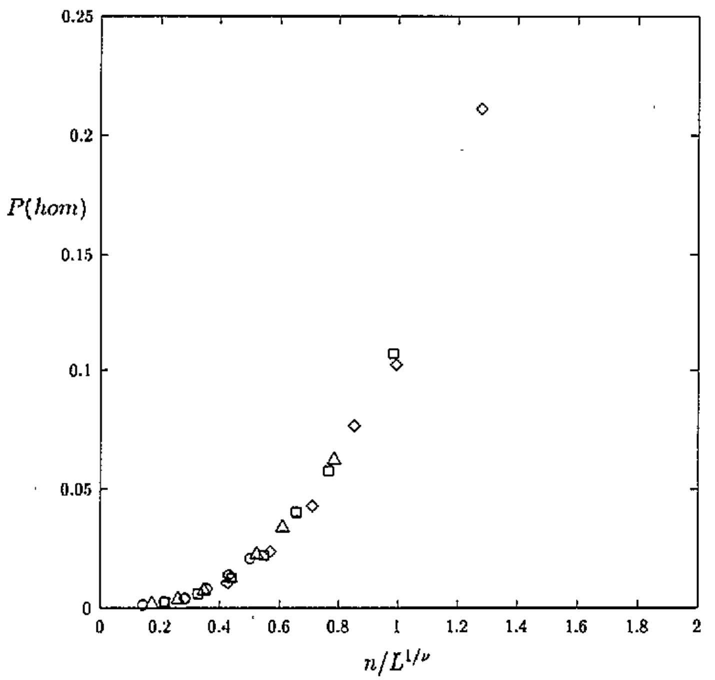

Figure 3. The homological linking probability plotted against the scaled variable $n/L^{1/\nu}$. The data are the same as those shown in figure 2, but the four curves collapse to a single curve.

indeed the case. In figure 3 we show the linking probability as a function of $n/L^{1/\nu}$, and it is clear that all the data for different values of n and L fall on a single curve. We note that the linking probability is still quite small for $n/L^{1/\nu} = 1$.

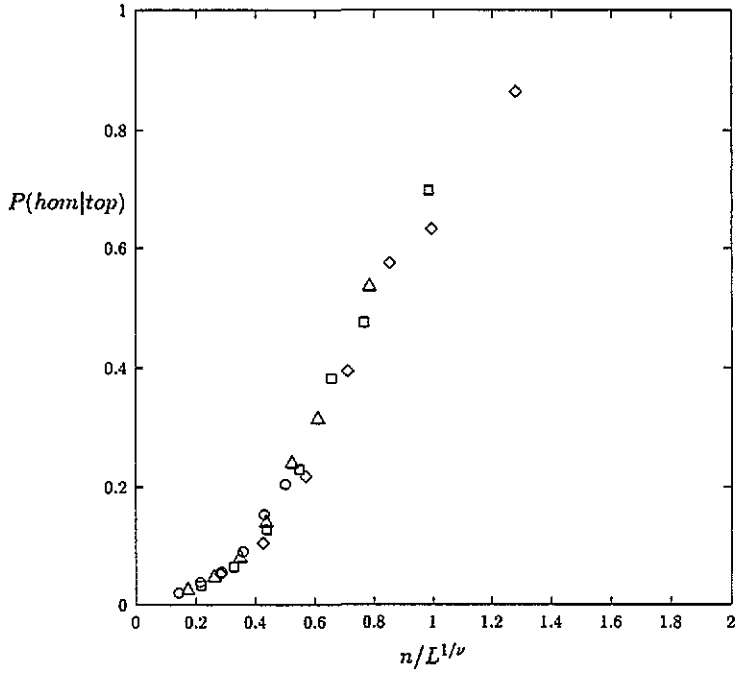

Figure 4. Probability of polygon pairs being homologically linked, given that the polygons are topologically linked, as a function of the scaled variable $n/L^{1/\nu}$.

Since homological linking is the weakest form of linking, it is interesting to investigate how effective it is as an indicator of topological linking. We consider the subset of pairs of polygons which have either $\Delta(-1,-1) \neq 0$ or $l \neq 0$ (or both), and we refer to these as topologically linked. (Although these invariants may miss some topologically linked pairs, we do not expect that this will be quantitatively serious at these values of n.) In figure 4 we plot the probability of being homologically linked, given that the polygons are topologically linked, as a function of $n/L^{1/\nu}$. As we see in figure 3, there are two different regimes corresponding to the dominance of one of the two length scales over the other. In particular for $n \ll L^{1/\nu}$, which corresponds to large boxes, almost all the topologically linked pairs are homologically unlinked. On the other hand, as $n/L^{1/\nu}$ increases, the fraction of topologically linked polygon pairs that are also homologically linked increases and goes to unity for $n \gg L^{1/\nu}$. This behaviour, which is not obvious *a priori*, suggests that homological linking is a good indicator of topological linking for configurations in which the two polygons are strongly interpenetrating, whereas it becomes a less efficient indicator for configurations in which the two components are, on average, further apart.

4.2. Centre-of-mass constraint

In this section we consider pairs of polygons (each with n edges) with distance between their centres of mass no greater than d. Once again we have two length scales (d and n^{ν}) and we expect that it will be the ratio of these length scales which will be important. In figure 5 we show the probability of being homologically linked as a function of $n/d^{1/\nu}$ and again the data for various values of n and d fall on a single curve. Also in this case we can see the presence of two different regimes. For $n \ll d^{1/\nu}$ the centres of mass of the two polygons are very far apart and, as expected, the linking probability is almost zero. As $n/d^{1/\nu}$ increases, the two polygons come closer together and are more likely to be linked. It is important to notice that for the limiting case $n \gg d^{1/\nu}$ the homological linking probability tends to a constant value strictly less than unity. This feature was also corroborated by performing a run in an extreme case with $n = 6400$ and with small d.

In figure 6 we show the probability of being homologically linked given that the polygons are topologically linked, as a function of $n/d^{1/\nu}$. Again, the values range from close to zero to close to unity, but homological linking seems to be a good indicator of topological linking for $n/d^{1/\nu}$ greater than about six.

5. Discussion

Although entanglements between polymer chains are clearly important in many areas of polymer physics, much less work has been done on this problem than on self-entanglement of a polymer chain, or knotting of a ring polymer. In this paper we have focused on linking of a pair of ring polymers, modelled as self-avoiding polygons on the simple cubic lattice.

All of the results reported in this paper are for links in which the two components have the same number of edges. We have shown rigorously that the number of embeddings of any non-trivial link has the same exponential behaviour, independent of the link type. Moreover, we have shown that each of the two components will almost surely be knotted, in the $n \to \infty$ limit.

In order to compare the behaviour of a non-trivial link with that of an unlinked pair of polygons, we have to impose some geometrical constraint, such as putting the polygons in a box, or demanding that their centres of mass be not too far apart. For polygons in a cube of side L we have proved that the exponential behaviour is the same for any link type as for the unlinked pair, under some mild conditions on L which ensure that the box is big enough for the constraint not to compress the polygons.

In order to investigate the behaviour when the geometrical constraint is more severe, we have developed a Monte Carlo algorithm which is a mixture of pivots and a rejection scheme. We have used this to examine the dependence of both the homological and topological linking probabilities on n and L, and on n and d, the maximum allowed distance between the centres of mass of the components. In each case we find that the behaviour is governed by the competition between two length scales (n^ν and L, or n^ν and d), and the linking probability is a function of either $n/L^{1/\nu}$ or $n/d^{1/\nu}$. Although the general behaviour is similar for polygons in a box, or with a centre-of-mass constraint, there are interesting quantitative differences. These may reflect the difference in the way in which the shape of a polygon responds to these two constraints. For polygons in a box, the constraint is isotropic and the decrease in the overall size of the polygons (as measured, for instance, by their radii of gyration) is also isotropic. When the polygons are pushed closer together by the centre of mass constraint, they shrink in a direction along the line joining their centres-of-mass, but expand in the directions normal to this line.

We have calculated the probability that one of the components is a knot and have found that this is very small at the values of n considered here. This is in contrast to the asymptotic result of theorem 2.3. In fact we know from other work (Vologodskii *et al* 1974, Janse van

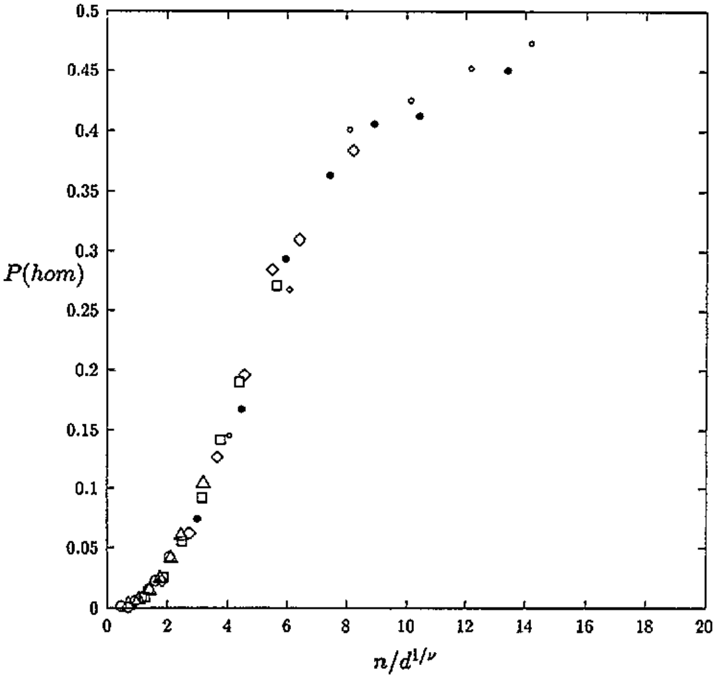

Figure 5. The homological linking probability for polygon pairs as a function of the scaled variable $n/d^{1/\nu}$. Different data points correspond to different values of d: 15 (○), 18 (●), 24 (◇), 30 (□), 42 (△) and 50 (○).

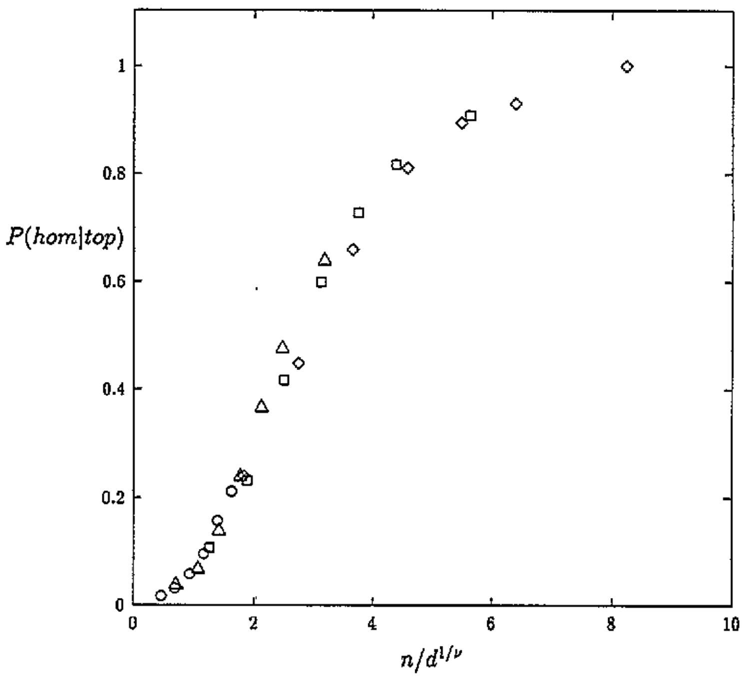

Figure 6. Probability of polygon pairs being homologically linked, given that the polygons are topologically linked, as a function of the scaled variable $n/d^{1/\nu}$.

Rensburg and Whittington 1990) that the knot probability for a single polygon is quite small at these values of n, but it is even smaller when the polygon is a component of a non-trivial link. Presumably this reflects the steric hindrance between the components.

In future work we intend to investigate the influence of other geometrical constraints on the linking probability.

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