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Asymptotics of knotted lattice polygons

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Abstract. We use Monte Carlo methods to investigate the asymptotic behaviour of the number and mean-square radius of gyration of polygons in the simple cubic lattice with fixed knot type. Let $p_n(\tau)$ be the number of n-edge polygons of a fixed knot type τ in the cubic lattice, and let $\langle R_n^2(\tau)\rangle$ be the mean square radius of gyration of all the polygons counted by $p_n(\tau)$. If we assume that $p_n(\tau) \sim n^{\alpha(\tau)-3}\mu(\tau)^n$, where $\mu(\tau)$ is the growth constant of polygons of knot type τ, and $\alpha(\tau)$ is the entropic exponent of polygons of knot type τ, then our numerical data are consistent with the relation $\alpha(\tau) = \alpha(\emptyset) + N_f$, where $\emptyset$ is the unknot and N_f is the number of prime factors of the knot τ. If we assume that $\langle R_n^2(\tau)\rangle \sim A_\nu(\tau)n^{2\nu(\tau)}$, then our data are consistent with both $A_\nu(\tau)$ and $\nu(\tau)$ being independent of τ. These results support the claims made in Janse van Rensburg and Whittington (1991a *J. Phys. A: Math. Gen.* **24** 3935) and Orlandini *et al* (1996 *J. Phys. A: Math. Gen.* **29** L299, 1998 *Topology and Geometry in Polymer Science (IMA Volumes in Mathematics and its Applications)* (Berlin: Springer)).

1. Introduction

The problem of knotting in long ring polymers was first discussed by Frisch and Wasserman (1961) and Delbruck (1962). They conjectured that the knot probability was unity in the limit of infinitely long ring polymers, and this has become known as the Frisch–Wasserman–Delbruck conjecture. The conjecture has been settled in the affirmative for a lattice model (Sumners and Whittington 1988, Pippenger 1989) and for some continuum models (Diao *et al* 1994). There has also been a considerable amount of numerical work on this problem, attempting to estimate the rate of increase of the knot probability with length (Vologodskii *et al* 1974, Michels and Wiegel 1984, 1986, Janse van Rensburg and Whittington 1990, Koniaris and Muthukumar 1991, Deguchi and Tsurusaki 1994). The problem has also been investigated experimentally for circular DNA molecules (Shaw and Wang 1993, Rybenkov *et al* 1993).

A related (and more delicate) problem which has only been addressed more recently is the relative frequency of occurrence of different knots. In the DNA literature there is considerable interest (Wasserman and Cozzarelli 1991, Wasserman *et al* 1985) in the properties of circular DNA molecules with fixed knot type since the knots produced by the action of certain enzymes on unknotted circular DNA can give useful information about the mechanism of enzyme action (Sumners 1995). This suggests a number of interesting questions about ring polymers with fixed knot type. For instance, how likely is a ring polymer to be of knot type τ_1 compared with being of knot type τ_2? Some preliminary numerical work has appeared on this question both for a lattice model (Orlandini *et al* 1996) and for a continuum model (Deguchi and Tsurusaki 1997). In a similar way one can ask for the mean dimensions (e.g. the mean square radius of gyration) of ring polymers as a function of their knot type (Janse van Rensburg and Whittington 1991a, Quake 1994). In this paper we use Monte Carlo methods to address both of these questions.

A *polygon* is an embedding of the circle graph in Z^3. We are interested in the number p_n of polygons of length n (i.e. composed of n lattice edges) where two polygons are considered distinct if they cannot be superimposed by translation. For instance, $p_4 = 3$ and $p_6 = 22$. Similarly we can define $p_n(\tau)$ to be the number of n-edge polygons with knot type τ. At present there are not many rigorous results for knotted polygons. It is known that all polygons with $n < 24$ are unknotted and that all non-trivial knotted polygons with 24 edges are trefoils (Diao 1992). Sumners and Whittington (1988) and Pippenger (1989) showed that

$$\lim_{n\to\infty} n^{-1} \log p_n(\emptyset) \equiv \kappa_0 < \lim_{n\to\infty} n^{-1} \log p_n \equiv \kappa \tag{1.1}$$

where $\emptyset$ is the unknot, so that unknots are (asymptotically) exponentially rare in the set of all polygons. A weaker result holds for polygons of knot type τ (Soteros *et al* 1992):

$$\liminf_{n\to\infty} n^{-1} \log p_n(\tau) = k_\tau \leqslant \limsup_{n\to\infty} n^{-1} \log p_n(\tau) = \kappa_\tau < \kappa. \tag{1.2}$$

It is not known that $k_\tau = \kappa_\tau$ for any knot type (other than the unknot), and generally, it is not known how the connective constants κ_τ are related to one another. If τ_1 is a factor knot of the (composite) knot τ, then concatenation of two polygons (one of knot type τ_1, and the other of knot type $\tau \setminus \tau_1$) will show that $\kappa_{\tau_1} \leqslant k_\tau \leqslant \kappa_\tau$ (Whittington 1992). Since the unknot is trivially a factor of any knot, concatenation of an unknot and a polygon of knot type τ proves that

$$k_\tau \geqslant \kappa_0. \tag{1.3}$$

An important open question is whether k_τ is dependent on the knot type.

The identification of polygons as a limit of a lattice $\mathrm{O}(N)$ model suggests that the asymptotic behaviour of p_n is given by

$$p_n = A n^{\alpha-3} \mu^n (1 + B n^{-\Delta} + C n^{-1} + \mathrm{o}(n^{-1})) \tag{1.4}$$

where $\mu = \mathrm{e}^\kappa$ and κ is lattice dependent. On the other hand, the exponents α and Δ are *critical exponents* and are believed to be universal for lattices of the same dimension.

The mean square radius of gyration $\langle R_n^2 \rangle$ of all polygons counted by p_n is expected to have the asymptotic form

$$\langle R_n^2 \rangle = A_\nu n^{2\nu} (1 + B_\nu n^{-\Delta} + C_\nu n^{-1} + \mathrm{o}(n^{-1})) \tag{1.5}$$

where the pedix ν on the coefficients A_ν, B_ν and C_ν of equation (1.5) distinguishes these from the coefficients in equation (1.4). The exponents ν and Δ have been estimated to have values

$$\begin{aligned} \nu &= 0.5882 \pm 0.0010 \\ \Delta &= 0.478 \pm 0.010 \end{aligned} \tag{1.6}$$

using field theoretic techniques (Guida and Zinn-Justin 1997, see also Le Guillou and Zinn-Justin 1980, 1989), whereas the best available numerical estimates for the self-avoiding walk are by Li *et al* (1995):

$$\begin{aligned} \nu &= 0.5877 \pm 0.0006 \\ \Delta &= 0.56 \pm 0.03. \end{aligned} \tag{1.7}$$

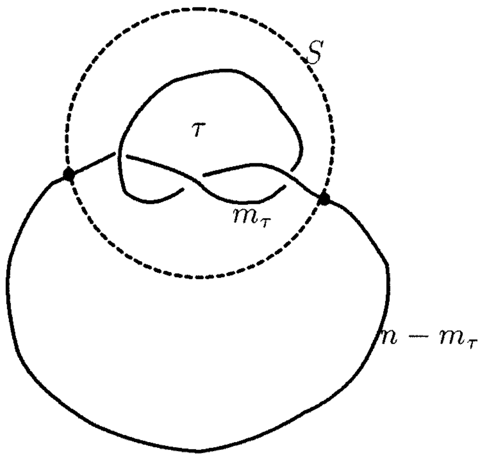

Figure 1. The sphere S separates the knotted polygon into two arcs, one of which will be knotted if it is closed by an arc on the sphere.

The scaling relations above are not rigorous, but have reasonably firm theoretical foundations, and there are numerous calculations which support equations (1.4) and (1.5). They are generally accepted as the correct approximations to p_n and $\langle R_n^2 \rangle$. Polygons of fixed knot type do not have similar connections to the O(N) model and we do not know the corresponding asymptotic expressions. Nevertheless, we note that $p_n(\tau)$ will grow exponentially with n, and that $Dn^{2/3} \leqslant \langle R_n^2(\tau) \rangle \leqslant n^2$, so that $\langle R_n^2(\tau) \rangle$ should increase as a power of n (with some corrections to scaling). Consequently it seems reasonable to assume that

$$p_n(\tau) = A(\tau) n^{\alpha(\tau)-3} \mu(\tau)^n \left(1 + \frac{B(\tau)}{n^{\Delta(\tau)}} + \cdots \right). \tag{1.8}$$

If this form is indeed correct then (1.2) implies that $\mu(\tau) < \mu$ for every τ. For the mean square radius of gyration, we similarly assume that

$$\langle R_n^2(\tau) \rangle = A_\nu(\tau) n^{2\nu(\tau)} [1 + B_\nu(\tau) n^{-\Delta(\tau)} + C_\nu(\tau) n^{-1} + \mathrm{o}(n^{-1})]. \tag{1.9}$$

In order to understand better the assumptions in equations (1.8) and (1.9), consider the following model of a polygon ω which is a prime knot. Let S be a geometric sphere which intersects ω in exactly two points. Then S divides ω into two segments, each of which can be closed by a curve on the sphere into an embedded circle. One of these segments, closed by a curve on the sphere, is a knot. Let the total length of this segment be m_τ, and assume that ω has n edges. We illustrate this situation in figure 1. Define M_τ to be the infimum of m_τ over all possible intersections with geometric spheres which cut ω in exactly two points. Define n_τ to be the expected value of M_τ taken uniformly over all polygons of knot type τ. We assume now that the mean square radius of gyration has the asymptotic formula $\langle R_n^2(\tau) \rangle \sim A_\nu(\tau) n^{2\nu_\tau}$. There are two possibilities: first we may have $n_\tau \sim n$ (assume that $n_\tau/n \to \gamma$ for some constant γ), or alternatively, $n_\tau = \mathrm{o}(n)$. If $n_\tau \sim n$, then the length of the segment of ω inside S grows, on average, proportionally to n, and the average radius of S grows at least as fast as $Dn^{1/3}$ where $D > 0$, and at most as fast as $\mathrm{O}(n^\nu)$. If $\langle R_n^2(\omega) \rangle^{1/2}$ grows faster than the average radius of S, then ω will start to assume the character of an unknotted polygon of length $(1-\gamma)n$, and we observe that $\nu(\emptyset) = \nu(\tau)$, while $A_\nu(\tau) = (1-\gamma) A_\nu(\emptyset) < A_\nu(\emptyset)$. If $\langle R_n^2(\omega) \rangle^{1/2}$ grows at the same rate as the average radius of S (this may be the case if $\gamma = 1$) then it is not possible to derive a relationship between the critical exponents or amplitudes. On the other hand, if we consider the case that $n_\tau = \mathrm{o}(n)$, then $\nu(\tau) = \nu(\emptyset)$ by the same arguments as in the case above. In addition, $\langle R_n^2(\tau)\rangle \approx A_\nu(\tau)(n-n_\tau)^{2\nu(\emptyset)} \approx A_\nu(\emptyset)n^{2\nu(\emptyset)}(1+\lambda n_\tau/n+\cdots)$. Thus, if $n_\tau = \mathrm{o}(n)$, then the knot has no effect on the amplitude ($A_\nu(\tau) = A_\nu$) and the effect of the knot only appears as corrections to the scaling. For example, if $n_\tau \sim \sqrt{n}$, then a correction term of the form $\lambda/\sqrt{n}$ will appear, and so on. There is conflicting evidence on the dependence of $A_\nu(\tau)$ on τ. It was first observed (Janse van Rensburg and Whittington 1991a) that $A_\nu(\emptyset) \approx A_\nu(\tau)$ for a variety of knots. On the other hand, simulations by Quake seemed to show the opposite: a strong dependence of $A_\nu(\tau)$ on τ (Quake 1994, 1995). These arguments also have implications for the entropic exponent: Indeed, if $n_\tau = \mathrm{o}(n)$, then in the large n limit, the 'average' knotted polygon looks like an unknotted polygon with a small sphere containing a knotted arc attached to it, and where its knot type is determined. We would expect that there exists a positive number γ such that we can place this sphere and its contents at γn places along the polygon, so that $p_n(\tau) \sim np_n(\emptyset)$. Substitution of equation (1.8) gives $\alpha(\tau) = \alpha(\emptyset) + 1$, if τ is a prime knot. This argument generalizes to cases where τ is a knot with N_f prime factors, and suggests that

$$\alpha(\tau) = \alpha(\emptyset) + N_f. \tag{1.10}$$

2. Monte Carlo approach

In this paper we aim to use high-quality Monte Carlo data to study the dependence of critical exponents and amplitudes of knotted polygons on knot types. In particular, we wish to test the relation in equation (1.10), and the dependence of $\nu(\tau)$ and $A_\nu(\tau)$ on τ. We shall sample along Markov chains in the state space of polygons in the cubic lattice using the BFACF algorithm (Berg and Foester 1981, Aragao de Carvalho and Caracciolo 1983, Aragao de Carvalho *et al* 1983). This is a grand canonical algorithm which samples along a Markov chain in the state space of polygons (not of fixed length) in a single run. The algorithm has a parameter (the step fugacity) which controls the mean length of polygons to be sampled. It is known that this algorithm is irreducible on classes of polygons with the same knot type τ (Janse van Rensburg and Whittington 1991b). This means that if the initial state is a polygon of a particular knot type, then only polygons of that knot type will appear in the sample and all such polygons have a non-zero probability of occurrence. This provides a very convenient way to sample polygons with a fixed knot type, even though the long autocorrelations of this algorithm makes it somewhat inefficient in many applications. To improve this situation we implement it with multiple Markov chain sampling (Geyer 1991, Geyer and Thompson 1994) by sampling along several Markov chains in parallel at different values of the step fugacity. States along the parallel Markov chains are swapped using a swapping probability which is chosen such that the overall invariant limit distribution of the composite chain is equal to the product of the marginal distributions of the individual Markov chains. As a result, the time series for the individual Markov chains can be analysed as though they had been obtained independently. The swapping procedure dramatically decreases the correlations within each Markov chain, and has little overhead since we are interested in sampling data at a number of different values of the step fugacity. (For a detailed discussion of the method and its implementation for a problem in statistical mechanics, see Tesi *et al* (1996) and Orlandini (1998).) The invariant limit distribution of the algorithm is

$$\pi_{\tau_0}(\omega) = \frac{1}{\Phi}|\omega|^q K^{|\omega|}\chi(\tau(\omega), \tau_0) \tag{2.1}$$

where q and K are parameters which can be chosen to optimize the sampling, $|\omega|$ is the number of edges in the polygon ω, $\tau(\omega)$ is the knot type of ω, χ is an indicator function which is 1 if ω has the same knot type (τ_0) as the first polygon in the realization of the Markov chain, and zero otherwise. Φ is a normalization factor. In this paper we use $q = 3$ in equation (2.1), which biases the sampling towards longer polygons. Each run corresponds to a multiple Markov chain implementation of the BFACF algorithm for fixed knot type, with 18 chains in parallel each sampled in increments of 2×10^5 BFACF iterations. Our data were obtained from 90 000 samples collected for each chain in the case of the unknot, resulting in a data-set of size 1.62×10^6, taken over a total of 3.24×10^{11} attempted BFACF moves. For the knots 3_1 and 4_1 we collected 150 000 sample points for each chain, and for the knots 6_2, $3_1\#3_1$ and $3_1\#4_1$, 100 000. The entire number of attempted BFACF moves for the whole project was 2.5×10^{12} iterations, consuming 15 months of CPU time on a SUN Ultrasparc workstation.

3. The entropic exponents

In this section we reconsider the entropic exponent $\alpha(\tau)$ for knotted polygons. Our main goal is to improve the results published previously (Orlandini *et al* 1996). The entropic exponent was also the subject of studies by Deguchi and Tsurasaki (1993, 1994, 1997). The mean length $\langle n(\tau)\rangle$ of polygons of knot type τ sampled at q and K can be shown to be given approximately by

$$\langle n(\tau)\rangle \approx \frac{[\alpha(\tau)+q-2]\mu(\tau)K}{1-K\mu(\tau)}\left(1-\frac{B(\tau)\Delta(\tau)[1-K\mu(\tau)]^{\Delta(\tau)}}{\alpha(\tau)+q-2}\right). \tag{3.1}$$

$\mu(\tau)$ can be estimated by considering the asymptotic behaviour of $\langle n(\tau)\rangle$ as $z = (1 - \mu(\tau)K) \to 0$ (or $K \to 1/\mu(\tau)$). In particular, to leading order, we can use (3.1) to approximate $1/\langle n(\tau)\rangle$:

$$\langle n(\tau)\rangle^{-1} \approx \frac{1-K\mu(\tau)}{[\alpha(\tau)+q-2]\mu(\tau)K} = \frac{1}{(\alpha+q-2)\mu(\tau)K} - \frac{1}{\alpha+q-2}. \tag{3.2}$$

and we see that an estimate of $\mu(\tau)$ can be obtained by extrapolating to that value of K for which $1/\langle n(\tau)\rangle$ is zero.

In figure 2 we plot $\langle n(\tau)\rangle^{-1}$ as a function of $1/K$ for runs carried out with $q = 3$ for the unknot, the trefoil and the composite knot $3_1\#4_1$. We note that as the complexity of the knot increases, the corrections to the linear scaling (3.2) become more and more important, but for K sufficiently close to the critical value ($K_c(\tau) = \mu(\tau)^{-1}$) linear behaviour is obtained (in figure 3 we enlarge the area close to the intersection in figure 2: the linear behaviour is clearly recovered). By extrapolating the data in figure 3, using a linear fit with equation (3.2), we obtain the following estimates:

$$\begin{aligned} \mu(\emptyset) &= 4.6852 \\ \mu(3_1) &= 4.6832 \\ \mu(4_1) &= 4.6833 \\ \mu(6_2) &= 4.6844 \\ \mu(3_1\#3_1) &= 4.6800 \\ \mu(3_1\#4_1) &= 4.6841. \end{aligned} \tag{3.3}$$

These values coincide to the second decimal place, and it seems reasonable to assume that they are indeed all equal. In fact, since we measured them from completely independent simulations, we can take their average to estimate the growth constant of polygons of a fixed knot type: we obtain $\mu(\emptyset) = \mu(\tau) = 4.6836 \pm 0.0038$ (95% confidence interval)

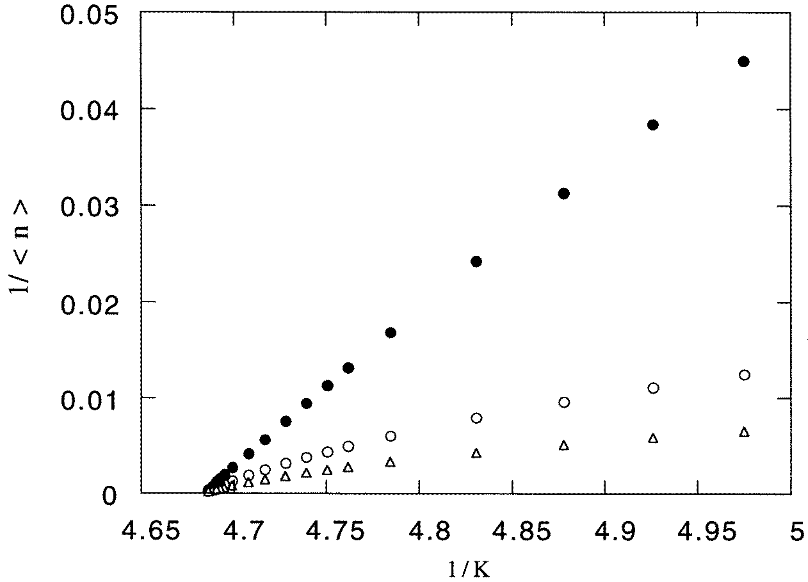

Figure 2. Plot of $\langle n(\tau)\rangle^{-1}$ as a function of $1/K$ for the unknot (●), the trefoil (○) and the composite knot $3_1\#4_1$ (△).

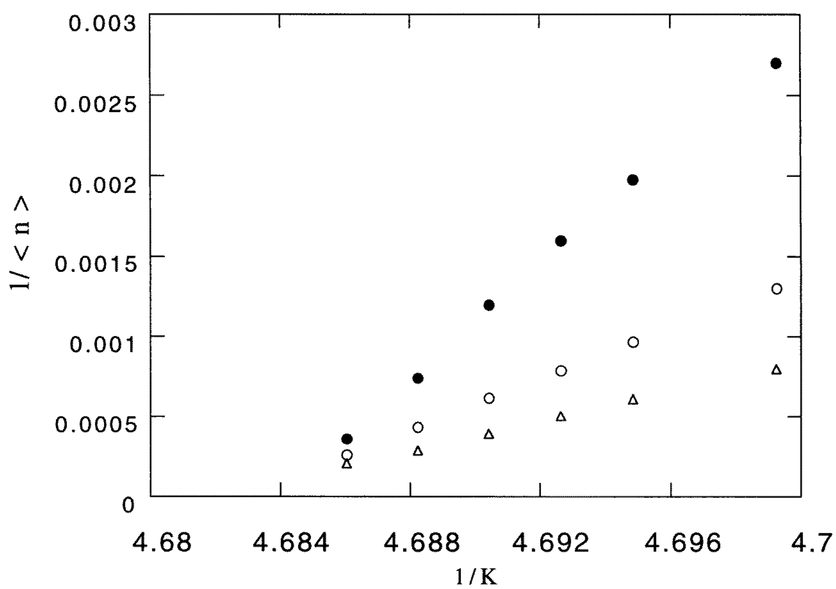

Figure 3. This graph focuses on the area where the data in figure 2 approach the critical value of K.

for any knot type τ. This estimate of $\mu(\tau)$ is remarkably close to the best available estimates of the growth constant for the self-avoiding walk. Guttmann (1989) estimated $\mu = 4.683\,93 \pm 0.000\,02$ using exact enumeration and series analysis. Our estimate is completely consistent with this. Observe that knotted polygons are extremely rare in polygons of lengths up to thousands of edges (see for example Janse van Rensburg and

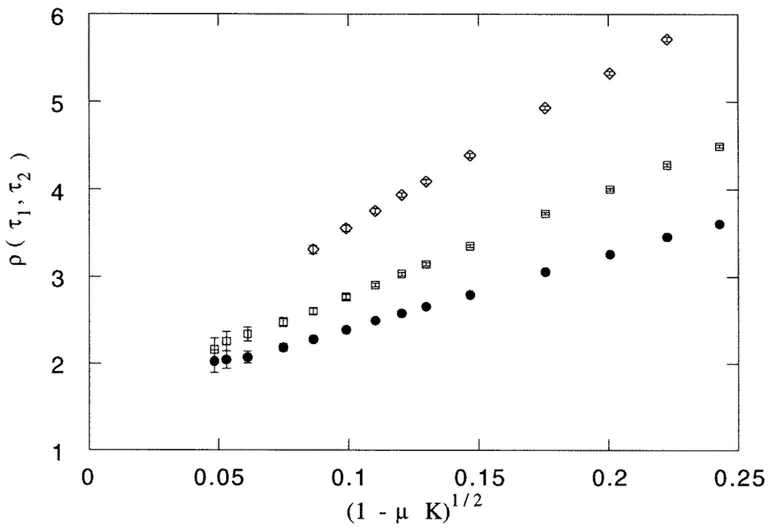

Figure 4. Plot of the ratio $\rho(\tau_1,\tau_2) = \langle n(\tau_1)\rangle/\langle n(\tau_2)\rangle$ versus $(1 - K\mu(\emptyset))^{1/2}$ for $\tau_1 = 3_1$ and $\tau_2 = \emptyset$ (●), $\tau_1 = 4_1$ and $\tau_2 = \emptyset$ (□), $\tau_1 = 6_2$ and $\tau_2 = \emptyset$ (◇). The extrapolation of the data indicates that the y intercept is somewhere between 1.6 and 1.8. This is consistent with $\alpha(\tau) = \alpha(\emptyset) + 1$ if τ is a prime knot.

Whittington 1990), so that knotted conformations have little or no effect on the estimated value of μ when this is computed over all polygon conformations with less than 10^3 or 10^4 edges. (In series enumerations of polygons on Z^3 by Guttmann (1989) there are precisely no knots encountered.) Consequently, we do not expect to see a numerical difference between the estimates of $\mu(\emptyset)$ and μ. If we then take into account the fact that $\mu(\tau)$ should be between these values, then the results above are perhaps not surprising. On the other hand, the estimates in equations (3.3) are obtained by extrapolating our data obtained *only* from polygons of fixed knot type.

We analyse the dependence of $\alpha(\tau)$ on τ by taking ratios of equation (3.1) for different knot types. If we assume that $\Delta = \min\{\Delta(\tau_1), \Delta(\tau_2)\}$, then we obtain for the first two terms in the expansion,

$$\frac{\langle n(\tau_1)\rangle}{\langle n(\tau_2)\rangle} \approx \frac{\alpha(\tau_1) + q - 2}{\alpha(\tau_2) + q - 2}[1 + c(1 - K\mu(\emptyset))^{\Delta}]. \tag{3.4}$$

Thus, a plot of $\langle n(\tau_1)\rangle/\langle n(\tau_2)\rangle$ against $(1 - K\mu(\emptyset))^{\Delta}$ should give a curve which will be linear for K close to $1/\mu(\emptyset)$ and have intercept $[\alpha(\tau_1)+q-2]/[\alpha(\tau_2)+q-2]$. For the set of all polygons, the confluent exponent Δ has a value close to $\frac{1}{2}$ (see equations (1.6) and (1.7)), and a plot of the ratio (3.4) against $\sqrt{1-\mu(\emptyset)K}$ supports linear dependence (figure 4). In this case, we set $\tau_2 = \emptyset$, while we took τ_1 equal to 3_1, 4_1 and 6_2, respectively. It appears that the three sets of points all approach a common value as $\sqrt{1-\mu(\emptyset)K}$ approaches zero. In order to estimate the limiting value, we could fit the ratio in equation (3.4) to a two-parameter expression of the form

$$\rho(\tau_1,\tau_2) = \frac{\langle n(\tau_1)\rangle}{\langle n(\tau_2)\rangle} = \frac{\alpha(\tau_1) + q - 2}{\alpha(\tau_2) + q - 2} + c_1(1 - K\mu(\emptyset))^{\Delta}. \tag{3.5}$$

However, the situation is not quite this simple: we are confronted with competing influences in our data. In the first case we note that confidence intervals are small for small values of K in figure 4; this is the region where we believe that corrections to equation (3.5) are important. On the other hand, for larger values of K, we have larger error bars, but it is in this region where equation (3.5) should be a good approximation. Thus, a naive fit to all the data points might produce values for $\rho(\tau_1, \tau_2)$ which are determined by points with small error bars in a range of K values where equation (3.5) is *not* a good approximation! In order to avoid this possibility, we took the four points at the largest values of K in each plot to extrapolate to the intercept. Our best estimates from the data in figure 4 give

$$\begin{aligned}\rho(3_1, \emptyset) &= 1.69 \pm 0.11\\ \rho(4_1, \emptyset) &= 1.67 \pm 0.11\\ \rho(6_2, \emptyset) &= 1.75 \pm 0.05\end{aligned} \tag{3.6}$$

where the error bars are 95% confidence intervals. These values are all consistent. By the argument accompanying figure 1 we note that if the smallest geometric ball containing the knot grows slower than linearly in n, then $\alpha(\tau) = \alpha(\emptyset) + N_f$, where N_f is the number of prime factors in τ. If we assume that $\alpha(\emptyset) = 0.237 \pm 0.004$ (obtained by using the hyperscaling relation $d\nu = 2 - \alpha$, and the best available numerical estimate of $\nu = 0.5877 \pm 0.0006$ (Li *et al* 1995)), then we find $\rho(3_1, \emptyset) \approx 1.81$. On the other hand, we also estimated the value of $\alpha(\emptyset)$ from our data from equation (3.2) to obtain $\alpha(\emptyset) = 0.27 \pm 0.02$, with the result that $\rho(3_1, \emptyset) \approx 1.79$. These results are consistent with our estimates in equation (3.6), and we take this as support for the notion that the length of knotted arc in the sphere in figure 1 grows slower than n.

We present more evidence by demonstrating that within numerical tolerances $\alpha(3_1) = \alpha(4_1)$, and $\alpha(3_1\#3_1) = \alpha(3_1\#4_1)$ in figure 5. Best fits to the data give

$$\begin{aligned}\rho(3_1, 4_1) &= 1.01 \pm 0.11\\ \rho(3_1\#3_1, 3_1\#4_1) &= 0.928 \pm 0.070.\end{aligned} \tag{3.7}$$

In figure 6 we plot ratios to estimate $\rho(\tau_1, \tau_2)$ with τ_1 a composite knot and τ_2 a prime knot. In all these cases we compute from equation (1.10) that $\rho(\tau_1, \tau_2) \approx 1.4$, and we expect that the data in figure 6 should reflect this value. We obtain

$$\begin{aligned}\rho(3_1\#3_1, 3_1) &= 1.25 \pm 0.16\\ \rho(3_1\#3_1, 4_1) &= 1.38 \pm 0.06\\ \rho(3_1\#4_1, 3_1) &= 1.27 \pm 0.02\\ \rho(3_1\#4_1, 4_1) &= 1.39 \pm 0.10.\end{aligned} \tag{3.8}$$

With the exception of the third value, these are all consistent with a value of 1.4. Finally, we summarize the results of this section as follows.

(i) Our results are consistent with the number of polygons with fixed knot type growing at the same exponential rate, independent of knot type.

(ii) All prime knots that we have examined appear to have the same entropic exponent, $\alpha(\tau)$.

(iii) Both composite knots with two factors ($3_1\#3_1$ and $3_1\#4_1$) that we examined appear to have the same entropic exponent.

(iv) It is clear that prime knots do not have the same exponent as the unknot, and knots with two factors do not have the same exponent as prime knots.

(v) The numerical estimates are consistent with equation (1.10).

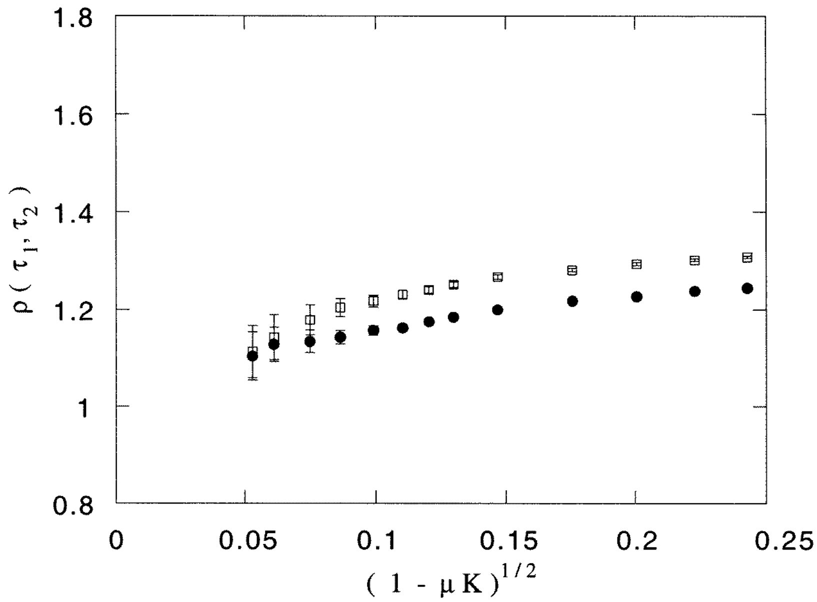

Figure 5. Plot of $\rho(\tau_1, \tau_2)$ against $(1 - K\mu(\emptyset))^{1/2}$ for $\tau_1 = 4_1$ and $\tau_2 = 3_1$ (●), $\tau_1 = 3_1\#3_1$ and $\tau_2 = 3_1\#4_1$ (□). These data points seem to approach 1 as K approaches its critical value. This suggests that polygons of knot types 3_1 and 4_1, and $3_1\#3_1$ and $3_1\#4_1$ respectively, have the same entropic exponent.

4. Mean size of knotted polygons

In this section we consider the mean sizes of knotted polygons and estimate the metric exponent of knots as well as the amplitudes of the mean square radii of gyration. This topic was first addressed in Janse van Rensburg and Whittington (1991a), where it was claimed that both the amplitude, and the metric exponent, are independent of the knot type of the polygon. Subsequent work by Quake (1994, 1995) agreed that the metric exponent is independent of the knot type, but indicated a dependence of the amplitude of the mean square radius of gyration on the knot type. We address these issues again, using the very large data sets generated by our simulations. The basic picture was presented in figure 1, where we argued that in the $n \to \infty$ limit the knot will be hidden in a small ball, and will be invisible in quantities such as the mean square radius of gyration. This point of view is supported by the results in the previous section. From another point of view, consider a small knot, and imagine the change in its conformation as its edges are multiplied. On entropic grounds, it seems to us to be more likely that the knot will expel a single loop which will acquire unknotted polygon statistics in the large n limit, rather than a number of loops which must interact with each other. (This argument can be made more precise if we consider a Hopf-link or a figure-of-eight graph embedded in the cubic lattice. Consider for example a figure-of-eight graph, which consists of two polygons which are attached to one another at a single vertex, and which are otherwise self-avoiding (Whittingon *et al* 1977, Guttmann and Whittington 1978). If there are n edges distributed among the two polygons with k edges in one polygon, and $(n - k)$ in the other, then the total number of conformations of the figure-of-eight is $S(n, k) = k(n - k)p_k p_{n-k} - \chi(n, k)$, where $\chi(n, k)$ is the number of conformations where the two polygons intersect one another. Observe

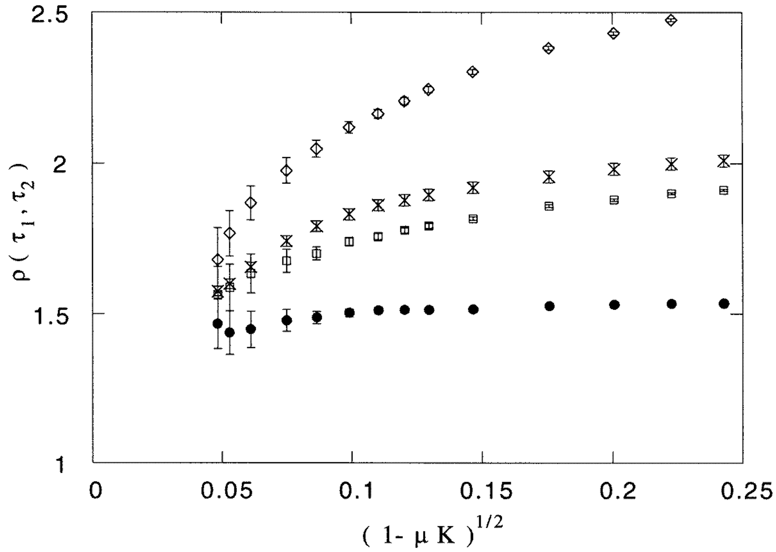

Figure 6. The ratio $\rho(\tau_1, \tau_2)$ against $(1-K\mu(\emptyset))^{1/2}$ for $\tau_1 = 3_1\#3_1$ and $\tau_2 = 3_1$ ($\Diamond$), $\tau_1 = 3_1\#4_1$ and $\tau_2 = 3_1$ ($\Box$), $\tau_1 = 3_1\#3_1$ and $\tau_2 = 4_1$ ($\times$), $\tau_1 = 3_1\#4_1$ and $\tau_2 = 4_1$ (●). These data points converge to somewhere between 1.3 and 1.4 which seems to indicate that the entropic exponent satisfies the relation $\alpha(\tau_1\#\tau_2) = \alpha(\tau_1) + 1 = \alpha(\tau_2) + 1$, where τ_1 and τ_2 are prime knot types.

that for fixed n, $\chi(n,k)$ increases as k approaches $n/2$, and that the product $p_k p_{n-k}$ is a minimum if $k = n/2$ (this is seen by noting that α in equation (1.4) is approximately $\frac{1}{4}$). Thus, $S(n,k)$ is a maximum if $k = 4$, or $k = n - 4$. In other words, figure-of-eights are dominated by those with one large and one small circle. This argument also applies to the Hopf-link.

4.1. The metric exponent

We postulated a basic scaling form for the mean square radius of gyration in equation (1.9). In order to estimate ν from our data, we compute the expected value of the mean square radius of gyration, $R^2_\tau(K,q)$, over polygons sampled from the distribution in equation (2.1). This gives the expression

$$R^2_\tau(K,q) = \frac{1}{G_\tau(K,q)} \sum \langle R^2_n \rangle n^q p_n(\tau) K^n. \tag{4.1}$$

If the assumed scaling form for $\langle R^2_n \rangle$ is substituted into equation (4.1), then after some simplification, we find the following approximation for $R^2_\tau(K,q)$:

$$R^2_\tau(K,q) \simeq h(\alpha,\nu) z^{-2\nu(\tau)} (1 + f(\alpha,\nu,\Delta) z^{\Delta} + g(\alpha,\nu) z + \cdots) \tag{4.2}$$

where $z = 1 - K\mu(\tau)$. The leading term in equation (3.1) can be used to eliminate z in the above; this produces the approximation:

$$R^2_\tau(K,q) \simeq h'(\alpha,\nu) \langle n \rangle^{2\nu(\tau)} (1 + f'(\alpha,\nu,\Delta) \langle n \rangle^{-\Delta} + g'(\alpha,\nu) \langle n \rangle^{-1} + \cdots) \tag{4.3}$$

where we now have a relation between $R^2_\tau(K,q)$ and $\langle n \rangle$. A log–log fit of our data to equation (4.3), where K takes a different value for each chain in our multiple Markov chain

Monte Carlo, can be used to estimate ν for each knot type. Our best estimates are

$$\begin{aligned}
\nu(\emptyset) &= 0.588 \pm 0.008 \\
\nu(3_1) &= 0.599 \pm 0.008 \\
\nu(4_1) &= 0.603 \pm 0.010 \\
\nu(6_2) &= 0.586 \pm 0.010 \\
\nu(3_1\#3_1) &= 0.604 \pm 0.020 \\
\nu(3_1\#4_1) &= 0.596 \pm 0.012.
\end{aligned} \tag{4.4}$$

Within the stated error bars, the above are all consistent with the best estimates of ν for polygons and self-avoiding walks (see equations (1.6) and (1.7)). These numbers also confirm the data in Janse van Rensburg and Whittington (1991a) and Quake (1995), and there seems to be no reason to suspect that, from a numerical point of view, there is a dependence of ν on the knot types. By averaging these results we can obtain an estimate of ν for polygons of fixed knot type, giving $\nu = 0.596 \pm 0.012$.

4.2. The amplitude of the mean square radius of gyration

In this section we consider the much more difficult issue of the behaviour of the amplitude of the mean square radius of gyration for polygons of different knot types. In this analysis, we assume that the metric exponent is independent of the knot type of the polygons, and we take its field theoretic value as the best possible estimate for its true value. We can expose the amplitude in equation (1.9) by division by $n^{2\nu}$ to find the equation

$$\langle R_n^2 \rangle / n^{2\nu} = A_\nu(\tau)[1 + B_\nu(\tau) n^{-\Delta} + C_\nu(\tau) n^{-1} + \mathrm{o}(n^{-1})]. \tag{4.5}$$

We plot our data in scatter plots in figure 7 to examine the behaviour of $\langle R_n^2 \rangle / n^{2\nu}$ as a function of $n^{-\Delta}$, where we assume that $\Delta = \frac{1}{2}$. The data should lie on curves which are, up to second order, parabolic in $n^{-\Delta}$. The deterioration in the data at large n values is due to poor statistics. Similar plots were presented in the studies by Janse van Rensburg and Whittington (1991a) and Quake (1995), but the data in figure 7 include measurements from polygons much longer than in those previous studies. Equation (4.5) indicates that we should be able to extrapolate $A_\nu(\tau)$ from our data by a three-parameter linear fit. Since these fits assume that all the data points are independent, we multiply the resulting confidence intervals by $\sqrt{2T}$, where T is the autocorrelation time of the underlying algorithm. Our best estimates are

$$\begin{aligned}
A_\nu(\emptyset) &= 0.103 \pm 0.028 \\
A_\nu(3_1) &= 0.1032 \pm 0.0016 \\
A_\nu(4_1) &= 0.0967 \pm 0.0022 \\
A_\nu(6_2) &= 0.0842 \pm 0.0012 \\
A_\nu(3_1\#3_1) &= 0.0889 \pm 0.0042 \\
A_\nu(3_1\#4_1) &= 0.089 \pm 0.012.
\end{aligned} \tag{4.6}$$

These estimates seem consistent, and if we keep in mind that there is an unknown systematic error present in the data (due to corrections to scaling that we did not control for, and to poor statistics for large values of n), then we conclude that these estimates are evidence that the amplitudes are independent of the knot type of the polygons. Indeed, the average of these results is 0.0942, and all the values in equation (4.6), with the exception of the knots 3_1 and 6_2, include the average within one standard deviation. Notice that there is also

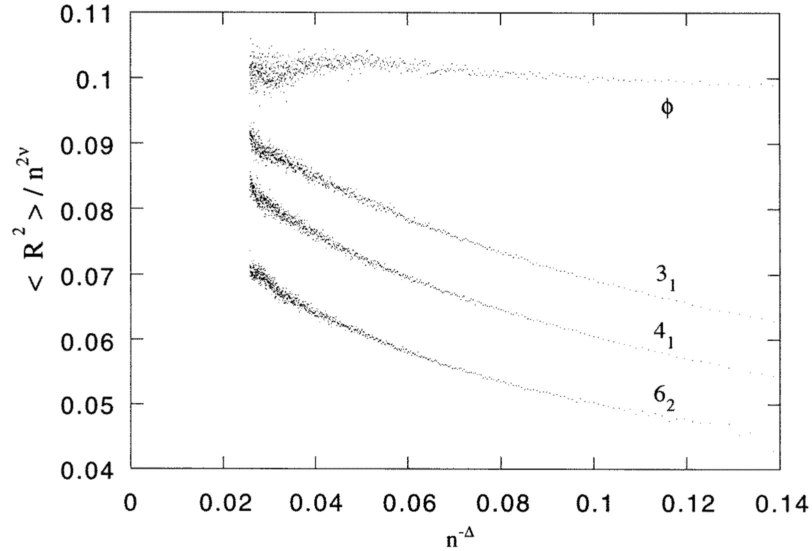

Figure 7. Scatter plot of $\langle R_n^2\rangle/n^{2\nu}$ against $n^{-\Delta}$. The data points from top to bottom correspond respectively to the unknot, 3_1, 4_1 and 6_2. Extrapolations of these data points indicate that they might approach the same value as $n \to \infty$. This suggests that the amplitude of the mean square radius of gyration of knotted polygons are independent of their knot type.

no systematic change in the estimated amplitudes with increasing crossing number in the knots, in contrast to the claim in the study by Quake (1995). There, it was claimed that the amplitude systematically decreases with increasing crossing number, and this observation was used as an argument supporting the notion that the amplitude is indeed dependent on the knot type. On the other hand, examination of the scatter plot in figure 7 shows that our data only slowly become asymptotic with increasing values of n, especially for the more complicated knots in our data. Quake's (1995) study included data sampled from the knots 10_1 and 20_1, which will be even less asymptotic than the data presented in figure 7. Note that the value of Δ is close to $\frac{1}{2}$, and that further simulations to sample data which will extrapolate further in figure 7 will require the generation of very long polygons. This remains a difficult challenge.

The ratio $\eta(\tau_1, \tau_2) = \langle R_n^2(\tau_1)\rangle/\langle R_n^2(\tau_2)\rangle$ can also be used to study amplitude ratios. In particular, if the amplitudes are independent of knot type, then $\eta(\tau_1, \tau_2) \to 1$ for any pair of knot types. In figure 8 we plot our estimates of $\eta(\tau_1, \tau_2)$ for the knots $\emptyset$, 3_1 and 4_1. All these points seem to approach 1 in the scaling limit, and we can fit them to the function $A + Bn^{-\Delta} + C/n$ to estimate the value of A, which should give us an estimate for $\eta(\tau_1, \tau_2)$. Our best estimates are

$$\begin{aligned} \eta(3_1, \emptyset) &= 1.044 \pm 0.044 \\ \eta(4_1, \emptyset) &= 1.005 \pm 0.028 \\ \eta(4_1, 3_1) &= 0.974 \pm 0.026. \end{aligned} \tag{4.7}$$

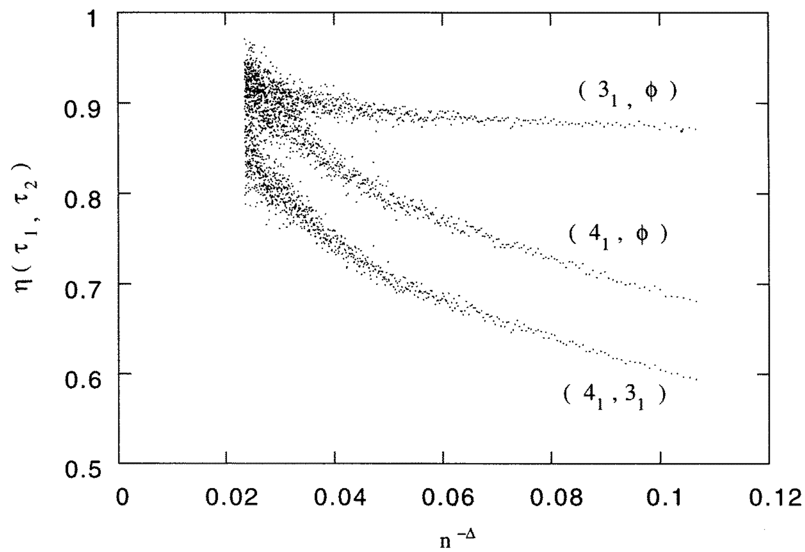

Figure 8. The ratio $\eta(\tau_1, \tau_2) = \langle R_n^2(\tau_1)\rangle / \langle R_n^2(\tau_2)\rangle$ versus $n^{-\Delta}$ for the following pairs of knots: $\tau_1 = 3_1, \tau_2 = \emptyset$; $\tau_1 = 4_1, \tau_2 = \emptyset$; $\tau_1 = 4_1, \tau_2 = 3_1$. All the data points seem to approach 1 as $n \to \infty$.

In addition to these, we also considered the ratios for the unknot, and the composite knots $3_1\#3_1$ and $3_1\#4_1$. In these cases we obtain

$$\begin{aligned} &\eta(3_1\#3_1, \emptyset) = 0.919 \pm 0.056 \\ &\eta(3_1\#4_1, \emptyset) = 0.917 \pm 0.092 \qquad (4.8) \\ &\eta(3_1\#4_1, 3_1\#3_1) = 0.91 \pm 0.11. \end{aligned}$$

These results are consistent with the idea that the amplitude ratios are independent of knot type.

5. Conclusions

We have used the BFACF Monte Carlo algorithm coupled with a multiple Markov chain approach to investigate two questions about polygons on the simple cubic lattice Z^3 with fixed knot type. In section 3 we investigated the number, $p_n(\tau)$, of polygons with knot type τ as a function of n, the number of edges in the polygon. We interpreted our results assuming the asymptotic form

$$p_n(\tau) \sim n^{\alpha(\tau)-3}\mu(\tau)^n \qquad (5.1)$$

where the symbol $\sim$ indicates the behaviour for large n with τ fixed. Our results indicate that $\mu(\tau)$ is independent of knot type and that $\alpha(\tau)$ is the same for all non-trivial prime knots. If τ is prime it seems likely that $\alpha(\tau) = \alpha(\emptyset) + 1$ where $\emptyset$ represents the unknot. If τ is composite with N_f prime factors then our results suggest that $\alpha(\tau) = \alpha(\emptyset) + N_f$.

We have also examined the behaviour of the mean-square radius of gyration of polygons for various knot types and our results are consistent with both the exponent and the amplitude being independent of knot type, suggesting that large polygons behave like unknots with one or more relatively small knotted ball pairs inserted somewhere along their length. This is in agreement with the conclusions of our earlier work, based on much less extensive Monte

Carlo calculations, but disagrees with the conclusions of Quake (1995). Quake interpreted his results as suggesting that the amplitude does depend on the complexity of the knot and he argued for a different scenario in which there is not a relatively localized knotted ball pair in the polygon. It may be that, for the more complex knots considered by Quake, correction to scaling terms are more important and one needs to collect data at much larger values of n in order to reach the asymptotic regime. This is our view, but there is considerable scope for more study.

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References

Aragao de Carvalho C and Caracciolo S 1983 *J. Physique* **44** 323
Aragao de Carvalho C, Caracciolo S and Fröhlich J 1983 *Nucl. Phys.* B **251** 209
Berg B and Foester D 1981 *Phys. Lett.* **106B** 323
Deguchi T and Tsurusaki K 1993 *J. Phys. Soc. Japan* **62** 1411
——1994 Statistical study of random knotting using Vasiliev invariants *Random Knotting and Linking* ed K C Millett and D W Sumners (Singapore: World Scientific) p 89
Deguchi T and Tsurusaki K 1997 *Phys. Rev.* E **55** 6245
Delbruck M 1962 *Mathematical Problems in the Biological Sciences* (Providence, RI: American Mathematical Society) p 55
Diao Y, Pippenger N and Sumners D W 1994 *J. Knot Theory Ramifications* **3** 419–29
Diao Y 1992 *J. Knot Theory and its Ramifications* **2** 413
Frisch H L and Wasserman E 1961 *J. Am. Chem. Soc.* **83** 3789
Geyer C J 1991 Markov chain Monte Carlo Maximum Likelihood *Computing Science and Statistics: Proc. 23rd Symp. on the Interface* ed E M Keramidas (Interface Foundation) p 156
Geyer C J and Thompson E A 1994 *Preprint* University of Minnesota
Guida R and Zinn-Justin J 1997 *Preprint* SPHT T97/040
Guttmann A J 1989 *J. Phys. A: Math. Gen.* **22** 2807
Guttmann A J and Whittington S G 1978 *J. Phys. A: Math. Gen.* **11** 721
Janse van Rensburg E J and Whittington S G 1990 *J. Phys. A: Math. Gen.* **23** 3573
——1991a *J. Phys. A: Math. Gen.* **24** 3935
——1991b *J. Phys. A: Math. Gen.* **24** 5553
Koniaris K G and Muthukumar M 1991 *Phys. Rev. Lett.* **66** 2211-4.
Le Guillou J C and Zinn-Justin J 1980 *Phys. Rev.* B **21** 3976
——1989 *J. Physique* **50** 1365
Li B, Madras N and Sokal A D 1995 *J. Stat. Phys.* **80** 661
Michels J P J and Wiegel F W 1984 *Phys. Lett.* **90A** 381
——1986 *Proc. R. Soc.* A **403** 269
Orlandini E 1998 *Numerical methods for Polymeric Systems (IMA Volumes in Mathematics and its Applications)* vol 102, ed S Whittington (Berlin: Springer)
Orlandini E, Janse van Rensburg E J, Tesi M C and Whittington S G 1998 *Topology and Geometry in Polymer Science (IMA Volumes in Mathematics and its Applications)* vol 103 (Berlin: Springer)
Orlandini E, Tesi M C, Janse van Rensburg E J and Whittington S G 1996 *J. Phys. A: Math. Gen.* **29** L299
Pippenger N 1989 *Discrete Appl. Math.* **25** 273
Quake S R 1994 *Phys. Rev. Lett.* **73** 3317
——1995 *Phys. Rev.* E **52** 1176
Rybenkov V V, Cozzarelli N R and Vologodskii A V 1993 *Proc. Natl Acad. Sci., USA* **90** 5307–11
Shaw S Y and Wang J C 1993 *Science* **260** 533
Soteros C E, Sumners D W and Whittington S G 1992 *Math. Proc. Camb. Phil. Soc.* **111** 75
Sumners D W 1995 *Not. Am. Math. Soc.* **42** 528

Sumners D W and Whittington S G 1988 *J. Phys. A: Math. Gen.* **21** 1689
Tesi M C, Janse van Rensburg E J, Orlandini E and Whittington S G 1996 *J. Stat. Phys.* **82** 155
Vologodskii A V, Lukashin A V, Frank-Kamenetskii M D, Anshelevich V V 1974 *Sov. Phys.–JETP* **39** 1059
Whittington S G 1992 *Proc. Symp. Appl. Math.* **45** 73
Wasserman S A, and Cozzarelli N R 1991 *J. Biol. Chem.* **266** 20 567
Wasserman S A, Dungan J M and Cozzarelli N R 1985 *Science* **229** 171
Whittington S G, Valleau J P and Torrie G M 1977 *J. Phys. A: Math. Gen.* **10** L111