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1996 J. Phys. A: Math. Gen. 29 L299

(http://iopscience.iop.org/0305-4470/29/12/003)

J. Phys. A: Math. Gen. **29** (1996) L299–L303. Printed in the UK

LETTER TO THE EDITOR

Entropic exponents of lattice polygons with specified knot type

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Received 4 April 1996

Abstract. Ring polymers in three dimensions can be knotted, and the dependence of their critical behaviour on knot type is an open question. We study this problem for polygons on the simple cubic lattice using a novel grand-canonical Monte Carlo method and present numerical evidence that the entropic exponent depends on the knot type of the polygon. We conjecture that the exponent increases by unity for each additional factor in the knot factorization of the polygon.

Linear polymer molecules can be highly self-entangled and these entanglements can be trapped as knots in circular polymers. There are a number of convenient models of circular polymers which can be studied to answer questions about knot probabilities and associated critical exponents but, in this letter, we shall be primarily concerned with polygons on the simple cubic lattice. Although polygons with no topological restriction are quite well understood, there are important open questions when the polygon is constrained to have a fixed knot type. In particular, little is known about the influence of the knot type on critical exponents.

We first review some rigorous results about knotted and unknotted polygons. Let p_n be the number of distinct (up to translation) n-edge polygons, and let $p_n(k)$ be the corresponding number when the polygon is conditioned to have a particular knot type k. We shall write $k = \emptyset$ for the unknot and otherwise use the Alexander–Briggs notation so that a trefoil is 3_1, a figure eight is 4_1, etc. It is known (Sumners and Whittington 1988, Pippenger 1989) that

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

so that unknots are exponentially rare in the set of all polygons. There is a similar result for any fixed knot type k (Soteros *et al* 1992)

$$\limsup_{n\to\infty} n^{-1} \log p_n(k) < \kappa \tag{2}$$

but there are important open questions about the relative numbers of polygons with different fixed knot types. It is easy to show that

$$\liminf_{n\to\infty} n^{-1} \log p_n(k) \geqslant \kappa_0 \tag{3}$$

for any knot type k, and that

$$\limsup_{n\to\infty} n^{-1}\log p_n(l) \leqslant \liminf_{n\to\infty} n^{-1}\log p_n(k) \tag{4}$$

for any compound knot k which has l as a factor (Whittington 1992). An important open question is whether the exponential growth rate depends on the knot type.

There are a few numerical results about the relative frequencies of lattice polygons with different knot types (see for instance Janse van Rensburg and Whittington 1990) and a detailed study of this question for Gaussian random polygons (Deguchi and Tsurusaki 1993, 1994). Using Monte Carlo methods, Deguchi and Tsurusaki showed that the relative frequency of occurence of each knot type (other than the unknot) increases as n increases, goes through a maximum, and then decreases. In fact (for lattice polygons) equation (2) implies that this decrease at large values of n must be exponential. The simpler knots have their maxima at smaller values of n and the location of the maximum generally moves to larger n as the knot increases in complexity (Deguchi and Tsurusaki 1993, 1994).

For the set of all (unrooted) polygons, it is believed that

$$p_n = An^{\alpha-3}\mu^n\left(1+\frac{B}{n^{\Delta}}+\cdots\right) \tag{5}$$

where $\mu = e^{\kappa}$. The plausible extension of this to polygons with knot type k is

$$p_n(k) = A(k)n^{\alpha(k)-3}\mu(k)^n\left(1+\frac{B(k)}{n^{\Delta(k)}}+\cdots\right). \tag{6}$$

If this form is indeed correct then (2) implies that $\mu(k) < \mu$ for every k.

The primary aim of this letter is to estimate the value of the entropic exponent, $\alpha(k)$, for some simple knots. Our approach is to use 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 polygons with a variety of lengths in a single run. The algorithm has a parameter (the step fugacity) which controls the range of values on which the sampling is focussed. The BFACF algorithm samples along a realization of a Markov chain defined on the set of all polygons but it is known (Janse van Rensburg and Whittington 1991b) that the ergodic classes of the Markov chain are the knot types. 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 occurence. This is a very convenient way to sample polygons with a fixed knot type but the algorithm has long correlation times. To improve this situation we have used multiple Markov chain sampling (Geyer 1991, Geyer and Thompson 1994). For this problem, it involves running several Markov chains in parallel at different values of the step fugacity, and swapping configurations between different chains with a probability chosen to make the limit distribution of the overall Markov chain 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 produces little overhead since, in any case, one is interested in obtaining data at a variety of 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.)

The BFACF algorithm realizes a Markov chain with limit distribution $\pi_{k_0}(\omega)$ given by

$$\pi_{k_0}(\omega) = \frac{1}{\Phi}|\omega|^q K^{|\omega|}\chi(k(\omega), k_0) \tag{7}$$

Table 1. Estimates of the mean number of edges as a function of knot type for various values of K when $q = 3$.

K	$\langle n(\emptyset)\rangle$	Error	$\langle n(3_1)\rangle$	Error	$\langle n(4_1)\rangle$	Error	$\langle n(3_1\#3_1)\rangle$	Error
0.203	26.11	0.09	89.84	0.12	111.34	0.13	222.50	0.29
0.205	32.00	0.11	104.08	0.15	127.68	0.16	253.76	0.37
0.207	41.45	0.15	126.07	0.21	153.50	0.23	300.42	0.53
0.209	59.55	0.23	165.97	0.35	199.47	0.40	380.96	0.96
0.210	76.23	0.33	200.77	0.56	240.56	0.59	451.7	1.5
0.2105	88.90	0.41	227.98	0.77	270.20	0.80	499.2	1.9
0.2110	107.21	0.54	264.0	1.2	310.7	1.1	568.9	2.9
0.2115	132.70	0.87	318.1	1.9	370.1	2	661.7	5.0
0.2120	179.3	1.45	408.3	4.1	466.9	4.5	812.9	7.6
0.2124	243.6	2.7	533.9	7.3	603.2	9.5	1019	12
0.2128	379	8	790	17	883	21	1394	35
0.2130	522	15	1067	37	1170	39	1857	140
0.2131	636	24	1293	60	1404	54	2286	285
0.2132	830	35	1658	115	1795	83	2853	483

where q and K are parameters which can be chosen to optimize the sampling, $|\omega|$ is the number of edges in the polygon ω, $k(\omega)$ is the knot type of ω, χ is an indicator function which is 1 if ω has the same knot type (k_0) as the first polygon in the realisation of the Markov chain and zero otherwise, and Φ is a normalization. Hence, the mean number of edges in polygons of knot type k sampled at q and K is given by

$$\langle n(k)\rangle \approx \frac{[\alpha(k)+q-2]\mu(k)K}{1-K\mu(k)}\left(1-\frac{B(k)\Delta(k)[1-K\mu(k)]^{\Delta(k)}}{\alpha(k)+q-2}\right) \tag{8}$$

where we have made use of (6). In table 1 we give estimates of $\langle n(k)\rangle$ as a function of K for runs carried out with $q = 3$. In each case we used 16 parallel Markov chains and sampled every 10^5 attempted BFACF moves. The results are based on 80 000 sample points (at each value of K) for the unknot, 85 000 sample points for the trefoil, 95 000 sample points for the figure eight knot and 110 000 sample points for the square knot.

In our analysis of the data we assume that $\mu(k_1) = \mu(k_2) = \mu(\emptyset)$. We know from equations (2) and (3) that $\mu(\emptyset) \leqslant \mu(k) < \mu = \mathrm{e}^{\kappa}$ for any knot k, and numerical evidence suggests that $\mu(\emptyset)$ is numerically very close to μ (Janse van Rensburg and Whittington 1990). Hence any error introduced by this assumption will be numerically very small. Taking the ratio of the averages in (8) for two different knot types k_1 and k_2, and assuming also that $\Delta = 1/2$ (LeGuillou and Zinn-Justin 1980, 1989, Li *et al* 1995) independent of knot type, gives

$$\frac{\langle n(k_1)\rangle}{\langle n(k_2)\rangle} \approx \frac{\alpha(k_1)+q-2}{\alpha(k_2)+q-2}\left[1+c(1-K\mu(\emptyset))^{\Delta}\right]. \tag{9}$$

Therefore plotting $\langle n(k_1)\rangle/\langle n(k_2)\rangle$ against $(1-K\mu(\emptyset))^{1/2}$ should give a curve which will become linear as K approaches $1/\mu(\emptyset)$ from below and have an intercept of $[\alpha(k_1)+q-2]/[\alpha(k_2)+q-2]$. In figure 1 we show results, with $q = 3$, for $k_1 = 4_1$ and $k_2 = 3_1$, $k_1 = 3_1$ and $k_2 = \emptyset$, $k_1 = 3_1\#3_1$ and $k_2 = \emptyset$.

The fact that the curve for 4_1 and 3_1 is clearly approaching a value very close to unity strongly suggests that $\alpha(4_1) = \alpha(3_1)$. For the other two cases the intercept is difficult to determine precisely but we estimate that

$$\frac{\alpha(3_1)+1}{\alpha(\emptyset)+1} = 1.8 \pm 0.2 \tag{10}$$

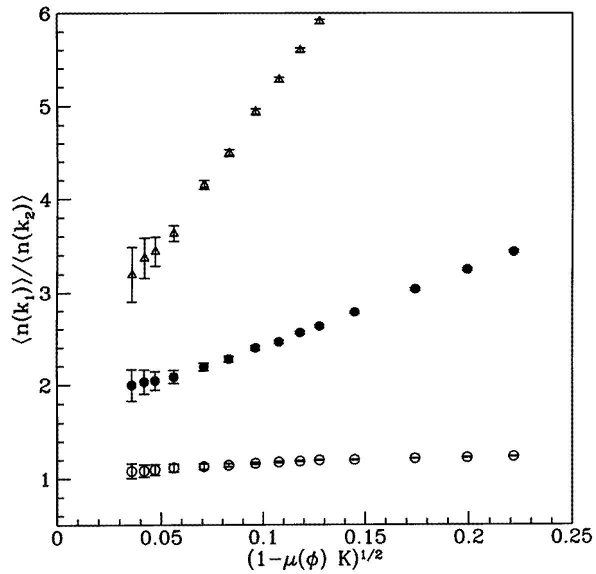

Figure 1. Plot of $\langle n(k_1)\rangle/\langle n(k_2)\rangle$ against $(1 - K\mu(\emptyset))^{1/2}$ for $k_1 = 4_1$ and $k_2 = 3_1$ ($\circ$), $k_1 = 3_1$ and $k_2 = \emptyset$ ($\bullet$), $k_1 = 3_1\#3_1$ and $k_2 = \emptyset$ ($\triangle$).

and that

$$\frac{\alpha(3_1\#3_1) + 1}{\alpha(\emptyset) + 1} = 2.6 \pm 0.2 \tag{11}$$

In forming these estimates we have given considerable weight to the estimates at large values of K, corresponding to large values of $\langle n\rangle$.

In order to estimate the value of $\alpha(3_1)$ from this intercept we need a value for $\alpha(\emptyset)$. We have used our data to make a direct estimate of this quantity with the result $\alpha(\emptyset) = 0.27 \pm 0.03$ (three standard deviations) . The value of the intercept given in (10), together with our direct estimate (0.27), is consistent with $\alpha(3_1) = \alpha(\emptyset) + 1$. Similarly, the intercept in (11) is consistent with $\alpha(3_1\#3_1) = \alpha(\emptyset) + 2$.

Our results show that the exponent α clearly depends on the knot type of the polygon, but the exponent ν characterising the radius of gyration is independent of knot type (Janse van Rensburg and Whittington 1991a). This implies that the hyperscaling relation $d\nu = 2 - \alpha$ does not apply in three dimensions when the polygons are conditioned to be a particular knot type, and suggests that there is no analogue of the connection between polygons and the $O(n)$ model when the polygons have fixed knot type. There are other examples known (e.g. c-animals) where the exponent controlling the growth of the number of objects depends on a topological restriction (Soteros and Whittington 1988) but the metric exponent is independent of such restrictions (Zhao *et al* 1992). In analogy with the c-animals case, for which it is believed (Lubensky and Isaacson 1979) that the entropic exponents for trees and animals are the same, one might expect that $\alpha(\emptyset)$ should be equal to α. The best estimate of α comes from a Monte Carlo estimate of ν together with hyper-scaling (Li *et al* 1995), giving $\alpha = 0.237 \pm 0.005$ (three standard deviations). On the basis of our estimate for $\alpha(\emptyset)$ we cannot say anything conclusive about this point.

Our results for the unknot, trefoil, figure eight and square knots suggest that, for any knot k, the exponent $\alpha(k)$ might be given by

$$\alpha(k) = \alpha(\emptyset) + N_{\mathrm{f}}(k) \tag{12}$$

where $N_{\mathrm{f}}(k)$ is the number of prime factors in the knot factorization of k.

We are pleased to acknowledge financial support from NSERC of Canada and from the European Community, in the form of a fellowship (to EO) under the EC Human Capital and Mobility Programme. We would like to thank Christine Soteros and De Witt Sumners for many pleasant and fruitful discussions.

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