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1975 J. Phys. A: Math. Gen. 8 56

(http://iopscience.iop.org/0305-4470/8/1/011)

J. Phys. A: Math. Gen., Vol. 8, No. 1, 1975. Printed in Great Britain. © 1975

Limiting ring closure probabilities in the self-avoiding walk problem

S G Whittington†, R E Trueman† and J B Wilker‡

† Department of Chemistry, University of Toronto, Toronto, Canada
‡ Department of Mathematics, University of Toronto, Toronto, Canada

Received 3 June 1974

Abstract. This paper is concerned with the limiting ring closure probability index (α). We obtain rigorous upper and lower bounds for the numbers of tadpoles weakly embeddable in a lattice. These bounds are used to prove the existence of a particular limit fcı tadpoles and to derive a lower bound on α. Using Monte Carlo methods we estimate that, for the face-centred cubic lattice, $\alpha = 2{\cdot}18 \pm 0{\cdot}07$.

1. Introduction

Although self-avoiding walks have been extensively studied as models of polymers with excluded volume, no satisfactory theory exists since there appears to be no convenient way of handling the long-range correlations inherent in the problem. A few rigorous results are known but most of our current knowledge in this area comes from Monte Carlo and exact enumeration studies. This paper is concerned with a particular aspect of this problem, ie with the probability of ring closure.

If we consider the addition of a step to a self-avoiding walk the resulting graph will be a self-avoiding walk or a polygon or a tadpole (this statement forms the basis of an important counting theorem (Sykes 1961)). The formation of a tadpole or a polygon corresponds to ring closure and we wish to investigate the relative probabilities of various types of ring closure.

It will be convenient to work with undirected graphs. A simple chain is a connected, undirected graph with two vertices of degree one and all other vertices of degree two. It is the undirected equivalent of a self-avoiding walk. A polygon is a connected, undirected graph with all vertices of degree two, while a tadpole has one vertex of degree one, one vertex of degree three and other vertices of degree two. Let the numbers of simple chains and polygons with n edges, weakly embeddable in a given lattice, be respectively $(n)_C$ and $(n)_0$. Let the number of tadpoles with h edges in the circuit and t edges in the simple chain from the vertex of degree one to the vertex of degree three be $(h, t)_\delta$. (The symbols used as subscripts are designed to suggest the topology of the graph concerned.)

Wall *et al* (1954) have distinguished between the initial and limiting ring closure probabilities which, in our notation, are

$$p_h^0 = h(h)_0/(q-1)(h-1)_C \tag{1}$$

and

$$p_h = \lim_{t\to\infty} [(h, t)_\delta/(q-1)(h+t-1)_C] \tag{2}$$

where q is the coordination number of the lattice.

Wall estimated that

$$p_h^0 \sim h^{-\alpha_0} \tag{3}$$

and

$$p_h \sim h^{-\alpha} \tag{4}$$

with $\alpha = \alpha_0 = 2$. The symbol $\sim$ is used in the sense that the ratio of the two sides of the expression tends to a finite positive limit as h tends to infinity. The initial ring closure probability has been extensively studied by exact enumeration methods with the conclusion that

$$\alpha_0 = \begin{cases} \frac{11}{6} & \text{in two dimensions} \\ \frac{23}{12} & \text{in three dimensions.} \end{cases} \tag{5}$$

The limiting ring closure index has recently been studied by Trueman and Whittington (1972) using Monte Carlo methods, and by Guttman and Sykes (1973) by exact enumeration. Both sets of authors agree that $\alpha > 2$ for all lattices studied. For the square lattice Trueman and Whittington estimated $\alpha \simeq 2{\cdot}13$ and the estimates of Guttman and Sykes were

$$\begin{aligned} &\alpha = 2{\cdot}10 \pm 0{\cdot}10 && \text{(triangular)} \\ &\alpha = 2{\cdot}15^{+0\cdot30}_{-0\cdot15} && \text{(square)} \\ &\alpha = 2{\cdot}15 \pm 0{\cdot}15 && \text{(face-centred cubic)} \\ &\alpha = 2{\cdot}10 \pm 0{\cdot}15 && \text{(simple cubic).} \end{aligned} \tag{6}$$

In spite of there being good numerical estimates of α there is no rigorous evidence that the limit in (2) exists. In this paper we prove a limiting theorem for tadpoles which, although not sufficiently strong to establish the existence of the limit, is a move in this direction. We also derive some rigorous bounds on the numbers of tadpoles which suggest some likely bounds on α. Finally we present a Monte Carlo estimate for α for the face-centred cubic lattice.

For the unrestricted random walk case the exponents can be calculated analytically (see eg Domb 1954), with the result $\alpha = \alpha_0 = 1$ in two dimensions and $1{\cdot}5$ in three dimensions.

2. Existence of a limit for tadpoles

Consider a tadpole with h edges in the head and t edges in the tail. If we delete an edge in the head, emanating from the vertex of degree three, we obtain a simple chain of $(h+t-1)$ edges. Each of the $(h, t)_\delta$ tadpoles will give rise to a different simple chain so that

$$(h, t)_\delta \leqslant (h+t-1)_C. \tag{7}$$

Hammersley and Morton (1954) showed that

$$\lim_{n\to\infty} n^{-1}\ln(n)_C = k \tag{8}$$

where k is a constant characteristic of the lattice, so that (7) and (8) imply that

$$\limsup_{(h+t)\to\infty} (h+t)^{-1}\ln(h,t)_\delta \leqslant k. \tag{9}$$

We now wish to find a lower bound on $(h, t)_\delta$. Consider the figure eights with h edges in one circuit and $(t+1)$ edges in the other. Let there be $(h, t+1)_8$ of these. Now consider deleting an edge, in the circuit of $(t+1)$ edges, emanating from the articulation point. The resulting graph is a tadpole so that

$$(h, t+1)_8 \leqslant (h, t)_\delta. \tag{10}$$

(On some lattices $t+1$ must be even. To establish a corresponding result for t even it is simply necessary to delete two edges giving $(h, t+2)_8 \leqslant (h, t)_\delta$.)

Whittington and Valleau (1970) have shown that

$$(m, n)_8 \geqslant (m)_0(n)_0 \tag{11}$$

on the square lattice and their argument is easily extended to other lattices. Then (10) and (11) give

$$(h+t)^{-1}\ln(h)_0+(h+t)^{-1}\ln(t+1)_0 \leqslant (h+t)^{-1}\ln(h,t)_\delta. \tag{12}$$

Hammersley (1961) has shown that

$$\lim_{n\to\infty} n^{-1}\ln(n)_0 = k \tag{13}$$

and (12) and (13) give

$$\liminf_{(h+t)\to\infty} (h+t)^{-1}\ln(h,t)_\delta \geqslant k \tag{14}$$

so that (9) and (14) give

$$\lim_{(h+t)\to\infty} (h+t)^{-1}\ln(h,t)_\delta = k. \tag{15}$$

3. Lower bound on the limiting ring closure index

To obtain a lower bound on α we require an upper bound on $(h, t)_\delta$. Consider the class of graphs formed by joining each simple chain of t edges, at each vertex of degree one, to each polygon of h edges, at each vertex. These graphs will include all tadpoles with h edges in the head and t edges in the tail so that

$$(h, t)_\delta \leqslant 2h(h)_0(t)_C. \tag{16}$$

Numerical evidence on $(n)_C$ and $(n)_0$ suggests that

$$(n)_C \sim n^\gamma\mu^n \tag{17}$$

and

$$(n)_0 \sim n^{-\beta}\mu^n \tag{18}$$

where $\gamma, \beta > 0$ and $\mu = \exp(k)$.

Consequently, from (17) and (18), we obtain

$$\lim_{t \to \infty} \left(\frac{2h(h)_0(t)_C}{(h+t-1)_C} \right) \sim h^{1-\beta} \tag{19}$$

and from (16) and (19) we obtain

$$\alpha \geqslant \beta - 1. \tag{20}$$

4. Monte Carlo data

We have estimated α for the face-centred cubic lattice by estimating the numbers of tadpoles and self-avoiding walks using the variance reduction scheme suggested by Hammersley and Morton (1954) and by Rosenbluth and Rosenbluth (1955). The method is very appealing but has seldom been used. We have found that it is especially useful for lattices of high coordination number. Consider the generation of the ith walk in a sample of N walks. As the jth step is to be added each of the possible $(q-1)$ vectors is examined to determine which of them do not lead to an immediate intersection. Let there be A_{ij} of these. The next step to be added is chosen from among these A_{ij} steps, each vector being accepted with probability A_{ij}^{-1}.

The weight of the ith walk is $\Pi_{j=1}^{n} A_{ij}$ and an unbiased estimate of the number of n step self-avoiding walks is

$$N^{-1} \sum_{i=1}^{N} \prod_{j=1}^{n} A_{ij}.$$

If A_{ij} is zero at any step, the walk is terminated and assigned a weight of zero. The extension to the estimation of tadpoles is completely straightforward and we do not pursue the details here.

We have estimated the numbers of tadpoles and self-avoiding walks with a total of up to thirty edges on the face-centred cubic lattice. Where the results could be checked against exact enumeration (Guttmann and Sykes 1973) the agreement is good. The total sample size of walks used was 250 000.

Since we are concerned with estimating $\lim_{t\to\infty} [(h, t)_\delta/(h+t)_C] = s(h)$ we have confined our attention to $h \leqslant 15$ so that the number of edges in the simple chain is at least as great as the number of edges in the circuit. Our estimates of these limits are in excellent agreement with those of Guttmann and Sykes (1973) for $h \leqslant 6$ but for $h = 7$, 8 and 9 our estimates are slightly lower than theirs. We have estimated α by plotting $\ln s(h)$ against $\ln h$ and the results are shown in figure 1.

The behaviour is quite linear for $h > 6$ and we estimate $\alpha = 2{\cdot}18 \pm 0{\cdot}07$.

5. Conclusions

The primary rigorous result of this paper is the establishment of the limit (15) and the proof that the value of the limit is the connective constant of the lattice. In fact our results also give an easy proof that

$$\lim_{h+t\to\infty} (h+t)^{-1} \ln(h, t)_8 = k.$$

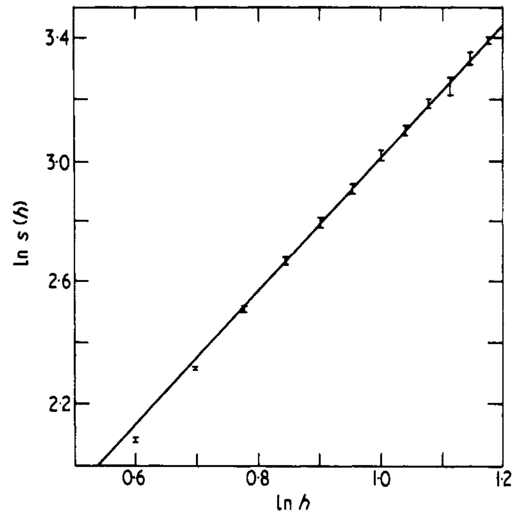

Figure 1. Dependence of ln $s(h)$ on ln h. The error bars represent subjective estimates of the reliability of the extrapolation to infinite tail length.

The lower bound on α has not been established rigorously since it depends on the assumption of the validity of (2) and (4) as well as (17) and (18). However, the numerical evidence for these results is very persuasive. If we insert the numerical estimates for β (Martin *et al* 1967) we obtain

$$\alpha \geqslant \begin{cases} 1{\cdot}75 & \text{(three dimensions)} \\ 1{\cdot}50 & \text{(two dimensions).} \end{cases}$$

These results are quite weak compared to numerical evidence but they do show that α cannot have the same value for self-avoiding walks as for random walks.

Finally, our Monte Carlo data for the face-centred cubic lattice yield an estimate of α in good agreement with the results of Guttmann and Sykes (1973). Unfortunately the Monte Carlo data are not sufficiently good to decide if α is different for the square and face-centred cubic lattices.

Acknowledgments

The authors gratefully acknowledge the financial support of the National Research Council of Canada.

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