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The end-point distribution of self-avoiding walks on a crystal lattice II. Loose-packed lattices

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Abstract. A study is made of the mean-square lengths of self-avoiding walks on a number of loose-packed lattices. It is found that the even–odd oscillations characteristic of this type of lattice may be largely removed by the use of an Euler transformation. From an analysis of the transformed series and of other moments from 1 to 10 of the distribution the mean-square length indices are estimated as $\gamma = 1{\cdot}500 \pm 0{\cdot}005$ in two dimensions and $\gamma = 1{\cdot}20 \pm 0{\cdot}02$ in three dimensions. These estimates are in good agreement with the exact simple fractions $\frac{3}{2}$ and $\frac{6}{5}$ favoured by several workers.

1. Introduction

Finite self-avoiding walks on lattices have been studied for some years now as a model of a single-chain polymer in dilute solution (Orr 1947, Domb 1969). This model provides a realistic representation of the excluded volume effect through the restriction that no lattice site may be visited more than once in the walk. The excluded volume, which is simply the fact that the segments of a polymer all occupy a finite volume, affects the average size of a polymer of n bonds. It is the purpose of this paper to investigate this effect by examining the average size of self-avoiding walks of n steps. The mean-square end-to-end length, ρ_n, is used as a measure of the average size.

For unrestricted walks ρ_n is readily shown to be proportional to the number of steps. There is good numerical evidence (Domb 1963) to suggest that for self-avoiding walks in two or three dimensions ρ_n behaves for large n as

$$\rho_n \sim \text{constant} \times n^{\gamma} \tag{1}$$

with γ greater than 1. The index γ, which measures the expansion of the polymer due to the excluded volume, appears to be a function only of the dimensionality of the lattice and not of its precise structure.

Most estimates for γ are close to 1·5 in two dimensions and to 1·2 in three and this has led several workers to conjecture that the true values are in fact the simple fractions $\frac{3}{2}$ and $\frac{6}{5}$ (Domb 1969). In a previous paper (Martin and Watts 1971), which will be referred to as I, we extended complete end-point distributions on several two- and three-dimensional lattices and presented an analysis of the mean-square lengths on the close-packed lattices. In the present paper the loose-packed lattices are studied. We show how the even–odd oscillations, which are usually present in mean-square length series on this type of lattice, may be greatly reduced by means of an Euler transformation. We also analyse other moments of the distribution which, if the distribution approaches a limiting shape (Fisher 1966), can also be used to find γ. By these means new estimates for γ are obtained which lend support to the hypothesis that

$$\gamma = \begin{cases} \frac{3}{2}, & d = 2 \\ \frac{6}{5}, & d = 3. \end{cases}$$

2. Analysis of mean-square lengths

We will assume that equation (1) correctly gives the asymptotic behaviour of ρ_n and further that the convergence to this form is given by

$$\frac{\rho_{n+1}}{\rho_n} = 1 + \frac{\gamma}{n}\left(1 + \frac{\alpha}{n}\right) + \mathrm{O}(n^{-2}). \tag{2}$$

Evidence for the above is given by Domb (1963) who plots $n(\rho_{n+1}/\rho_n - 1)$ against n^{-1} and, for each lattice, this approaches a limiting value with constant slope. If the assumptions of equations (1) and (2) are correct, the sequence of estimates

$$\gamma_{n,i}(\rho) = \frac{(\rho_{n+i} - \rho_n)(\rho_n - \rho_{n-i})}{(\rho_n^2 - \rho_{n+i}\rho_{n-i})}, \qquad i \text{ small} \tag{3}$$

will converge to γ with error $\mathrm{O}(n^{-1})$. Setting $i = 1$ in equation (3) gives the extrapolation formula used in I for the close-packed lattices. Setting $i = 2$ corresponds to extrapolating odd and even sequences separately and helps to reduce the oscillations on loose-packed lattices. Values of $\gamma_{n,2}$ are given in table 1 for the simple quadratic lattice and in table 2 for the simple cubic and body-centred cubic lattices.

The estimates indicate a value for γ which is very close to 1·2 for the three-dimensional lattices but is somewhat lower than 1·5 for the square lattice. In I from an analysis of the triangular lattice we estimated $\gamma = 1{\cdot}488 \pm 0{\cdot}002$ in two dimensions. Table 1 would suggest a value between this and 1·5 but we should also notice that the last few estimates on each of the two-dimensional lattices are rising slightly and so the possibility of $\gamma = 1{\cdot}5$ cannot be ruled out.

Table 1. Estimates for γ on the simple quadratic lattice

n	$\gamma_{n,2}(\rho)$	$\gamma_{n,1}(r)$	$v_n(r)$
10	1·4849	1·4518	1·5004
11	1·4793	1·4562	1·5012
12	1·4876	1·4600	1·5009
13	1·4815	1·4631	1·5006
14	1·4878	1·4658	1·5007
15	1·4846	1·4681	1·5008
16	1·4884	1·4702	1·5009
17	1·4863	1·4720	1·5009
18	1·4894	1·4736	1·5008
19	—	1·4750	—

Table 2. Estimates for γ on the simple cubic and body-centred cubic lattices

	simple cubic lattice			body-centred cubic lattice		
n	$\gamma_{n,2}(\rho)$	$\gamma_{n,1}(r)$	$u_n(r)$	$\gamma_{n,2}(\rho)$	$\gamma_{n,1}(r)$	$u_n(r)$
6	1·2137	1·2029	1·2338	1·2091	1·2052	1·1931
7	1·2031	1·2052	1·2087	1·2026	1·2043	1·1829
8	1·2038	1·2054	1·1911	1·2033	1·2029	1·1801
9	1·1995	1·2046	1·1793	1·1993	1·2016	1·1818
10	1·2009	1·2033	1·1730	1·2001	1·2006	1·1815
11	1·1979	1·2019	1·1736	—	1·1997	—
12	1·1989	1·2007	1·1781	—	—	—
13	1·1964	1·1998	1·1778	—	—	—
14	—	1·1990	—	—	—	—

The technique to be used in the following section identifies $-\gamma-1$ as the exponent of a singularity in the complex plane. This is the dominant singularity in the generating function for mean-square lengths and so defines the circle of convergence. An attempt is then made to distort the complex plane in such a manner that other singularities, which may be upsetting the smoothness of the estimates for γ, are mapped away from the circle of convergence. As this is shown to produce far smoother sequences we feel that it should form the basis of a reliable method for estimating γ.

3. Use of the Euler transformation

The generating function for mean-square lengths is defined by

$$G(x) = 1+\sum_{n=1}^{\infty} \rho_n x^n \tag{4}$$

and must have a dominant singularity at $x = 1$ to produce a series of all positive terms but may possess other, weaker, singularities also on the unit circle. In particular there are good reasons to expect a singularity at $x = -1$ (Sykes *et al* 1972) which would produce the observed even–odd oscillations in ρ_n. We will proceed as if a singularity at $x = -1$ does exist and show that an attempt to map this further from the origin almost entirely removes the oscillation.

A transformation is made from the x plane to a new plane z through the change of variable

$$z = \frac{2\xi x}{(\xi-1)x+(\xi+1)}. \tag{5}$$

This is chosen to map the points $x = 0$ and $x = 1$ into $z = 0$ and $z = 1$ and to map $x = -1$ into $z = -\xi$, ξ is real to preserve any symmetry about the real axis. For $\xi > 1$ the unit circle, $|x| = 1$, is mapped into a larger circle with centre $(1-\xi)/2$ and radius $(1+\xi)/2$, and this has the effect of moving any singularities originally on the circle of convergence, except of course the singularity at $x = 1$, away from the circle of convergence. The motion of points originally on the unit circle is shown in figure 1 for $\xi = 1$ (identity mapping), 2, 3 and 4.

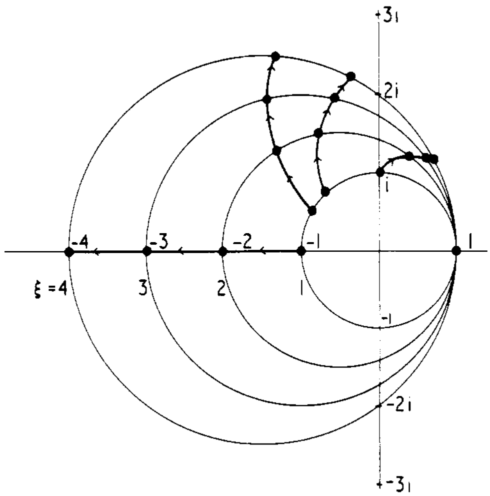

Figure 1. Motion of points originally on the unit circle as ξ takes the values 1 (identity mapping), 2, 3 and 4.

The above transformation will produce a new sequence r_n which has the same dominant asymptotic behaviour as ρ_n and is defined through the generating function

$$G(x(z)) = 1 + \sum_{n=1}^{\infty} r_n z^n.$$

The transformation was tried using a range of values for ξ and it was found that $\xi = 10$ gave the smoothest results.

4. Analysis of transformed series

4.1. *Simple quadratic lattice*

The new sequence, r_n, behaved sufficiently smoothly to enable the estimates $\gamma_{n,1}(r)$ to be formed (cf equation (3)). These are given in table 1 and are seen to be varying as n^{-1} and so the further sequence

$$v_n(r) = (n+1)\gamma_{n+1,1}(r) - n\gamma_{n,1}(r)$$

is also given in table 1. These are constant to within less than 0·1 % over the last nine entries and combining them with the estimate in I obtained from an analysis of the triangular lattice we obtain

$$\gamma = 1{\cdot}500 \pm 0{\cdot}005$$

in two dimensions.

4.2. *Three-dimensional lattices*

The sequences $\gamma_{n,1}(r)$ are given in table 2 for the simple cubic and body-centred cubic lattices. These are nearly constant and are close to 1·2. However, the last few terms in each of these two sequences are decreasing approximately as $n^{-1/2}$ and this suggests forming the further sequences

$$u_n(r) = \frac{(n+1)^{1/2}\gamma_{n+1,1}(r) - n^{1/2}\gamma_{n,1}(r)}{(n+1)^{1/2} - n^{1/2}}$$

which are also given in table 2. On this evidence we would estimate γ as $1{\cdot}18 \pm 0{\cdot}02$. This value is somewhat lower than the value of 1·2 which is often quoted and we feel that the linearity with $n^{-1/2}$ may in fact have been misleading. Further evidence for adopting an index of 1·2 is obtained by examining other moments of the distribution.

5. Other moments of the distribution

If the end-point distribution for self-avoiding walks approaches a limiting shape then it is easy to show that, for large n, the lth moment of the distribution is related to the second moment, or mean-square length, through

$$\langle r_n^l \rangle \sim \text{constant} \times \langle r_n^2 \rangle^{l/2}.$$

Hence if the assumption of equation (1) is correct the lth moment will behave for large n as

$$\langle r_n^l \rangle \sim \text{constant} \times n^{\gamma_l}$$

with

$$\gamma_l = \tfrac{1}{2} l \gamma.$$

Estimates for γ_l have been obtained for $l = 1, 2, \ldots, 10$ by forming the sequences $\gamma_{n,2}(\langle r_n^l \rangle)$ for each of the lattices (Watts 1972). Only the estimates are given (table 3) as the sequences would require a great deal of space. The γ_l are clearly linear with l and suggest

$$\gamma = \begin{cases} 1{\cdot}500 \pm 0{\cdot}01, & d = 2 \\ 1{\cdot}200 \pm 0{\cdot}015, & d = 3. \end{cases}$$

Table 3. Estimates for γ_l for l = 1 through 10

l	γ_l		
	SQ	SC	BCC
1	0·748 ± 0·01	0·595 ± 0·01	0·600 ± 0·01
2	1·495 ± 0·01	1·190 ± 0·01	1·200 ± 0·01
3	2·250 ± 0·02	1·790 ± 0·02	1·790 ± 0·02
4	3·000 ± 0·02	2·395 ± 0·02	2·400 ± 0·03
5	3·750 ± 0·02	3·000 ± 0·03	2·980 ± 0·05
6	4·500 ± 0·03	3·600 ± 0·03	3·600 ± 0·05
7	5·240 ± 0·03	4·200 ± 0·05	4·240 ± 0·05
8	6·010 ± 0·03	4·820 ± 0·05	4·850 ± 0·07
9	6·740 ± 0·04	5·400 ± 0·05	5·450 ± 0·07
10	7·520 ± 0·04	6·050 ± 0·05	6·000 ± 0·10

6. Conclusions

By use of the Euler transformation of equation (5) most of the even–odd oscillation has been removed from the mean-square length sequences on the loose-packed lattices. Combining estimates for γ obtained from the transformed sequences with those from an analysis of other moments, and the results in I from a study of the close-packed lattices, we obtain

$$\gamma = \begin{cases} 1{\cdot}500 \pm 0{\cdot}005, & d = 2 \\ 1{\cdot}20 \pm 0{\cdot}02, & d = 3. \end{cases}$$

These provide further support for the conjecture that γ is given exactly in two and three dimensions by the simple fractions $\frac{3}{2}$ and $\frac{6}{5}$ respectively.

It is possible that the initially low estimate of γ for the three-dimensional lattices is due to further irregular behaviour near the origin of the walk. Using higher moments directs attention towards the edge of the distribution. One would expect the immediate vicinity of the origin to have less effect on the behaviour in two dimensions than in three and this may explain why we were able to form considerably closer estimates for γ in two dimensions than in three.

An analogy with the Ising model suggests that the close-packed lattices will not possess a singularity at $x = -1$ in the corresponding generating function, and so would not be expected to benefit from the Euler transformation. This is indeed found to be the case. Application of the substitution (5) to the close-packed sequences produces no noticeable improvement.

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