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Exact enumeration of neighbour-avoiding walks on the tetrahedral and body-centred cubic lattices

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Abstract. The numbers and mean square lengths of short, neighbour-avoiding walks on the tetrahedral and body-centred cubic lattices have been determined exactly. Using standard extrapolation techniques, estimates have been made of the connective constants and mean square length exponents for these walks. Our estimate of the mean square length exponent is 1·22, but a value of 1·20 also appears plausible.

1. Introduction

Self-avoiding walks have been extensively studied as models of polymers with excluded volume and because of their importance in certain problems in the area of critical phenomena. Much of our current knowledge comes from exact enumeration and Monte Carlo studies, and one of the most important results which has emerged from this work is that certain exponents which characterize self-avoiding walks have values independent of which lattice is being studied and which depend only on the dimensionality.

Let the number of distinct self-avoiding n-step walks, weakly embeddable in a particular lattice, be C_n^0 and let the mean square end-to-end length of the walks be $\langle R_n^2\rangle_0$. Numerical evidence suggests that, for sufficiently large n,

$$C_n^0 \sim n^{\alpha_0}\mu_0^n \tag{1}$$

and

$$\langle R_n^2\rangle_0 \sim n^{\gamma_0} \tag{2}$$

where μ_0 is a constant characteristic of the lattice in question, and α_0, γ_0 are constants which appear to depend only on dimensionality. In three dimensions, evidence from exact enumeration strongly supports $\alpha_0 = \frac{1}{6}$ and $\gamma_0 = \frac{6}{5}$ (Domb 1963, Martin *et al* 1967, Wall and Hioe 1970); these results are consistent with Monte Carlo estimates (Gans 1965).

An important question remains: to what extent do the exponents depend on the range of the excluded volume potential? An obvious extension of self-avoiding walks is to self-avoiding walks with near neighbours excluded (or first-neighbour-avoiding walks) in which the walk cannot revisit a point already occupied, nor can it visit a point which is a first neighbour of a point already occupied. We will adopt symbols C_n and $\langle R_n^2\rangle$ for the number and mean square length of such walks. Hammersley's proof of the existence of the connective constant for self-avoiding walks goes over trivially to first-neighbour-avoiding walks so that

$$\lim_{n\to\infty} n^{-1}\ln C_n = \inf_{n>0} n^{-1}\ln C_n = k = \ln\mu \tag{3}$$

and since $C_n \leqslant C_n^0$ it follows that $\mu \leqslant \mu_0$.

The value of the mean square length exponent, γ, has been investigated by Monte Carlo and exact enumeration methods but there is disagreement amongst different workers. Mark and Windwer (1967) have carried out a Monte Carlo study on walks of up to about 200 steps on the tetrahedral lattice with the conclusion that $\gamma \simeq 1{\cdot}255$. Kumbar and Windwer (1971) enumerated neighbour-avoiding walks with up to 15 steps on the tetrahedral lattice and on the four-choice cubic lattice and estimated a value of γ between 1·25 and 1·26 for both lattices. Hioe (1967) investigated the square, triangular, simple cubic and face-centred cubic lattices using exact enumeration, with the conclusion that $\gamma = 1{\cdot}20$ in three dimensions and 1·50 in two dimensions.

The only rigorous result on this question appears to be a proof by Watson (1970) that the bond-site transformation is a bijection from the class of n-step self-avoiding walks on a lattice to the class of $(n-1)$-step neighbour-avoiding walks on the covering lattice. From this it also follows that the mean square length exponent for self-avoiding walks on a lattice L is equal to the mean square length exponent for neighbour-avoiding walks on the covering lattice L′, ie $\gamma_0(\mathrm{L}) = \gamma(\mathrm{L}')$. Watson points out that, since there is good numerical evidence that γ_0 depends only on the dimensionality of the lattice, it is likely that γ is equal to γ_0 for all lattices of a given dimension.

Although this argument is persuasive, it should be treated with some caution since the final step relies on the conjecture that γ_0 depends only on dimensionality. In two dimensions it is well established that γ_0 is equal to 1·50 for the square, hexagonal and triangular lattices, but it is worth noting that, although the covering lattice of the hexagonal lattice (ie the Kagome lattice) has received some numerical attention, the covering lattices of the square and triangular lattices are not planar, and the exponents on such lattices have not been investigated (of course, Watson's work indicates that $\gamma = 1{\cdot}50$ for these lattices but, unfortunately, it is *not* certain that $\gamma_0 = 1{\cdot}50$).

In the same way, although Watson's work throws doubt on the results of Kumbar and Windwer, it does not disprove them. These disagreements have led us to extend the enumerations on the tetrahedral lattice by a further four terms and to enumerate the walks up to 12 steps on the body-centred cubic (BCC) lattice.

2. Exact enumerations

The method which we have adopted for enumeration of short walks is somewhat different from the methods which have been used previously (Martin 1962, Hioe 1970, Chay 1971, 1972) and is closely related to the dimerization approach used by Suzuki (1968) and by Alexandrowicz (1969), in Monte Carlo studies of self-avoiding walks.

In order to enumerate all first-neighbour-avoiding walks of $(m+n)$ steps we first enumerate all first-neighbour-avoiding walks of m steps and of n steps using standard methods (Martin 1962). Let these sets of walks be S_m and S_n and let each walk start from the same origin. For each walk $W_m \in S_m$ and $W_n \in S_n$ we superimpose W_m and W_n and reverse each step in W_n. The resulting directed graph is an $(n+m)$-step walk and the set of such graphs will include all $(m+n)$-step first-neighbour-avoiding walks.

To determine *which* of these walks are first-neighbour-avoiding we begin by constructing $\mathscr{L}_m$, the set of N_m lattice sites that are excluded by (ie that are visited by, or are near neighbours of sites visited by) at least one member of S_m. Each W_m can then be represented by a sequence of N_m bits in which each bit is associated with one site in $\mathscr{L}_m$ and only those bits corresponding to sites excluded by that particular walk are nonzero. For each W_n a similar sequence of N_m bits is used to represent those lattice sites in $\mathscr{L}_m$ visited by that particular walk. The superposition of any W_m and W_n will then result in a first-neighbour-avoiding walk if the intersection of the corresponding bit patterns is zero (ie if no 'ones' are common to the two bit patterns). For the lattices and walk sizes considered here, the bit representation is not unwieldy; for the tetrahedral lattice $N_8 < 350$. The enumeration of 19-step walks on the tetrahedral lattice required less than nine minutes on an IBM 370/165; before multiplication by the customary symmetry factors, this represents a counting rate of over three million successes per minute.

The numbers of walks and their mean square end-to-end lengths are given in tables 1 and 2.

3. Analysis of results

We have analysed the exact enumeration data using standard ratio methods. Assuming that

$$C_n \sim n^\alpha \mu^n \tag{4}$$

then

$$C_{n+1}/C_n \sim (1+\alpha/n)\mu \tag{5}$$

Table 1. Numbers (C_n) and mean square lengths ($\langle R_n^2\rangle$) of neighbour-avoiding walks on the tetrahedral lattice.

n	C_n	$\langle R_n^2\rangle$
1	4	3
2	12	8
3	36	13·6666
4	108	19·5555
5	300	27·3200
6	852	35·04225
7	2364	43·85279
8	6636	52·51356
9	18492	61·77742
10	51660	71·05970
11	143508	80·90083
12	399492	90·71281
13	1107324	101·03925
14	3074940	111·30195
15	8510868	122·03163
16	23591796	132·68004
17	65229852	143·75115
18	180566076	154·74085
19	498813708	166·12132

Table 2. Numbers (C_n) and mean square lengths ($\langle R_n^2 \rangle$) of neighbour-avoiding walks on the BCC lattice.

n	C_n	$\langle R_n^2 \rangle$
1	8	3
2	56	6·85714
3	296	13·37838
4	1640	20·25365
5	8984	27·98308
6	49256	36·01753
7	266600	44·83525
8	1448072	53·76872
9	7820984	63·22801
10	42316952	72·74976
11	227940584	82·75354
12	1229803016	92·75876

so that we can form a sequence of estimates $\mu_n = C_{n+1}/C_n$ of μ. Because of the odd–even alternation on these lattices, it is more convenient to notice that

$$C_{n+2}/C_n \sim (1+2\alpha/n)\mu^2 \tag{6}$$

and to form the sequence of estimates

$$\mu_n^+ = (C_{n+2}/C_n)^{1/2}. \tag{7}$$

The behaviour of μ_n and μ_n^+ as a function of n is shown in figure 1 for the tetrahedral lattice and in figure 2 for the BCC lattice.

For the tetrahedral lattice we estimate

$$\mu_{\text{tet}} = 2{\cdot}742 \pm 0{\cdot}002 \tag{8}$$

in good agreement with the results of Kumbar and Windwer (1971), who suggested $\mu = 2{\cdot}74$. For the BCC lattice the behaviour of μ_n and μ_n^+ is shown in figure 2. We estimate

$$\mu_{\text{BCC}} = 5{\cdot}33 \pm 0{\cdot}01. \tag{9}$$

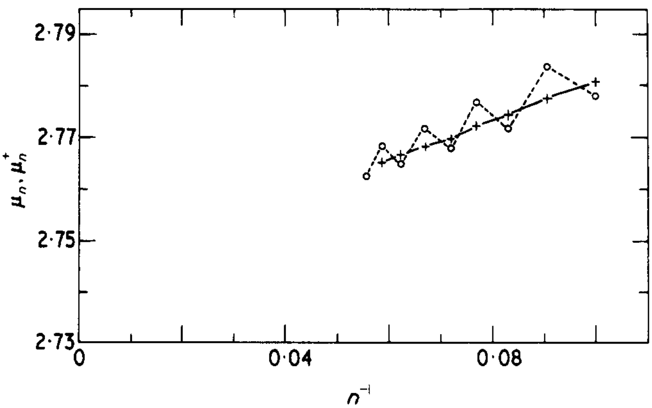

Figure 1. Extrapolations against n^{-1} of $\mu_n = C_{n+1}/C_n$ and $\mu_n^+ = (C_{n+2}/C_n)^{1/2}$ for the tetrahedral lattice.

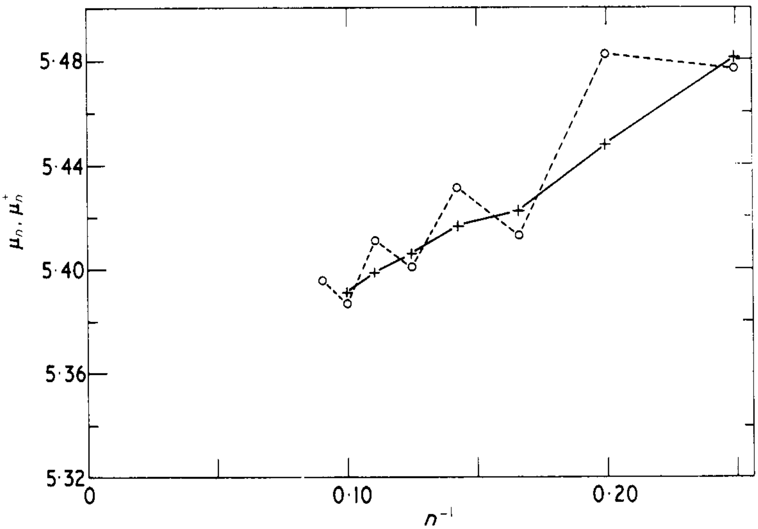

Figure 2. Extrapolations against n^{-1} of $\mu_n = C_{n+1}/C_n$ and $\mu_n^+ = (C_{n+2}/C_n)^{1/2}$ for the BCC lattice.

In attempting to estimate the value of the mean square length exponent, γ, we have removed much of the odd–even alternation by forming the series of linear extrapolants

$$\gamma_n^+ = \tfrac{1}{2}n[(\langle R_{n+2}^2\rangle/\langle R_n^2\rangle)-1]. \tag{10}$$

The n dependence of γ_n^+ is shown in figure 3 for both the tetrahedral and BCC lattices. For the tetrahedral lattice, including the four extra terms over those derived by Kumbar and Windwer (1971) indicates a considerable amount of curvature in the data and it is clear that their estimate of $\gamma = 1{\cdot}25$ is much too high. The curvature makes the data difficult to extrapolate with confidence but an estimate based on the last four points for the tetrahedral lattice would suggest a value of γ between 1·22 and 1·23. However,

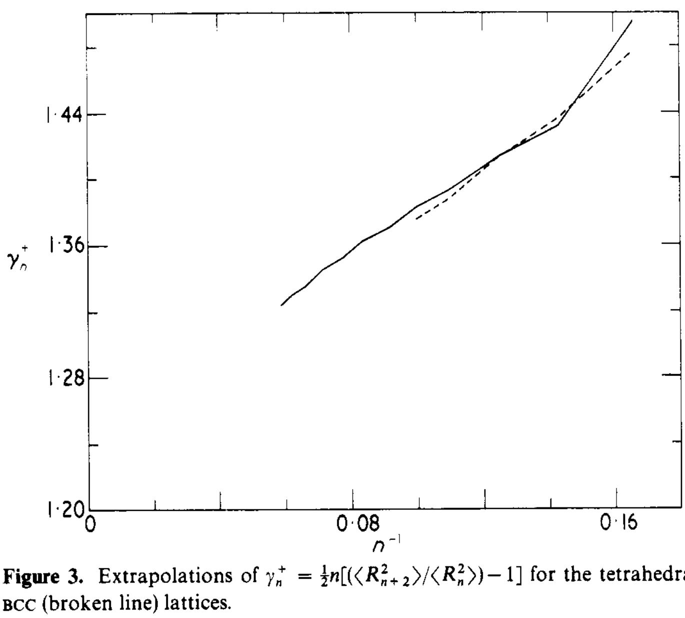

Figure 3. Extrapolations of $\gamma_n^+ = \frac{1}{2}n[(\langle R_{n+2}^2\rangle/\langle R_n^2\rangle)-1]$ for the tetrahedral (full line) and BCC (broken line) lattices.

since some curvature is still present at these values of n it is likely that this value would be too high, and our final, somewhat subjective, estimate is

$$\gamma = 1{\cdot}22^{+0{\cdot}01}_{-0{\cdot}02}$$

for both lattices.

4. Discussion

When the data discussed here are compared with data for self-avoiding walks, the most noticeable feature is that convergence, for data on neighbour-avoiding walks, is very slow, as suggested by Mazur and Joseph (1963).

Since both lattices are loose-packed one would expect (Sykes *et al* 1972) that the generating function of mean square lengths would have a singularity where the circle of convergence cuts the negative real axis, in addition to the singularity on the positive real axis. On the suggestion of a referee we attempted to make use of this to improve the convergence. Following Watts (1974) we used a conformal transformation which maps the unit circle centred at the origin into a circle centred at $(1-\xi)/2$ with radius $(1+\xi)/2$, $\xi > 1$. This leaves the dominant singularity unchanged but moves the second singularity away from the circle of convergence. The effect of this transformation is to remove the odd–even alternation but, unfortunately, it does little to improve the convergence of the γ_n^+ series.

Our estimates of γ are considerably lower than those of Windwer and co-workers for the tetrahedral lattice. Our best estimate of γ is above the estimate for self-avoiding walks (1·20) but this value lies within our estimated error bounds. Our disagreement with Kumbar and Windwer (1971) simply stems from our use of four more terms in the mean square length sequence. Including these extra terms shows that some downward curvature appears in the sequence of γ_n^+ values. It is more difficult to reconcile our estimates with the Monte Carlo results of Mark and Windwer (1967). They consider walks with up to 208 steps which our data would indicate to be sufficiently long to yield good estimates of γ. Unfortunately they do not give any indication of the standard deviations or sample sizes for their Monte Carlo work. Their data (figure 2 of their paper) in the range $n = 50$–120 would indicate a value of γ less than 1·25 and it may be that their data for longer walks suffer from relatively large sampling errors.

Acknowledgments

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