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The asymptotic behaviour of selfavoiding walks and returns on a lattice

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Abstract. New data for the number of selfavoiding walks and selfavoiding returns to the origin on two and three dimensional lattices are presented and studied numerically by the ratio method. Estimates for the critical attrition and critical indices are given. For a loose-packed lattice the selfavoiding walk generating function appears to have a singularity on the negative real axis. This singularity is at the same distance from the origin as the physical singularity, and is found to be cusp-like with an exponent of $\frac{1}{2}$ in two dimensions and $\frac{3}{4}$ in three dimensions. This behaviour enables a close analogy to be drawn between the behaviour of the Ising model high temperature susceptibility and the walk generating function.

1. Introduction

Recently the derivation of extended series for the high temperature susceptibility of the Ising model in two and three dimensions has enabled a detailed theory of asymptotic behaviour to be developed (Sykes *et al* 1972a, 1972b to be referred to as I and II). It is the purpose of the present paper to develop an analogous theory for selfavoiding walks; to do this we have extended the data on the square, simple cubic and body-centred cubic lattices.

A detailed introduction to the problem, and a lead into the literature, is given by Martin *et al* (1967). Interest centres on the generating functions for selfavoiding chains and rings defined by

$$C(x) = \sum_{n=0}^{\infty} c_n x^n \qquad c_0 = 1 \text{ (chain-generating function)} \tag{1.1}$$

$$U(x) = \sum_{n=0}^{\infty} u_n x^n \qquad u_0 = 1 \text{ (ring-generating function)} \tag{1.2}$$

where c_n is the number of n step selfavoiding walks and u_n the number of n step self-avoiding returns to the origin. These generating functions are analogous in many respects to the susceptibility and energy of the corresponding Ising model.

For close-packed lattices data for $C(x)$ on the triangular lattice through $n = 17$ and on the face-centred cubic through $n = 12$ are given by Martin *et al* (1967); slightly extended data on the rings through $n = 18$ and $n = 14$ respectively are given by

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Sykes *et al* (1972c). In the light of recent developments we have re-examined the evidence and report on this briefly in § 2.

For loose-packed lattices data for $C(x)$ through $n = 18$ on the square lattice are given by Hiley and Sykes (1961) and through $n = 16$ for the simple cubic lattice by Sykes (1963); again slightly extended data on the rings are given by Sykes *et al* (1972c). We have extended the data for $C(x)$ on the square lattice a further six terms to $n = 24$, on the simple cubic lattice a further three terms to $n = 19$ and on the body-centred lattice a further six terms to $n = 15$. We use the new data to make a more detailed analysis in § 3. We summarize the walks on loose-packed lattices in the Appendix.

Throughout our treatment we shall assume a familiarity with I and II and only describe briefly the results of applying the same approach to the excluded volume problem.

2. Close-packed lattices

The elementary treatment supposes that near $x = 1/\mu$

$$C(x) \sim A(1-\mu x)^{-g-1}. \tag{2.1}$$

A detailed numerical analysis of this assumption is given by Martin *et al* (1967) and reference should be made to this paper for a general discussion of the evidence. The data are found to be reasonably consistent with the hypothesis

$$g = \tfrac{1}{3} \text{ in two dimensions}$$

$$g = \tfrac{1}{6} \text{ in three dimensions.}$$

The corresponding attrition parameters, which are lattice dependent, are there estimated as

$$\begin{aligned} \mu &= 4{\cdot}1515 \qquad \text{(triangular lattice)} \\ \mu &= 10{\cdot}035 \qquad \text{(face-centred cubic lattice).} \end{aligned} \tag{2.2}$$

To apply the more detailed theory of I and II we investigate the assumption that, more generally

$$C(x) \sim (1-\mu x)^{-g-1}\Phi(x)+\Psi(x) \tag{2.3}$$

where Φ and Ψ are regular in the disc $|x| \leqslant 1/\mu$. Then the quantity

$$\beta_n = \frac{n\mu_n}{n+g} \qquad \mu_n = \frac{c_n}{c_{n-1}} \tag{2.4}$$

should, for large n, approach linearity against $1/n^2$. Following II we form a sequence of estimates by solving for μ and ξ

$$\beta_n = \mu\left(1+\frac{\xi}{n^2}\right) \tag{2.5}$$

using successive pairs of ratios. We illustrate the results for the triangular lattice in figure 1. The estimates for $n > 12$ are all very close together (within a few parts in a million); in fact they are slightly closer together than the corresponding estimates for the susceptibility. In contrast a smooth behaviour is less well defined and apparently only develops for slightly higher values of n (about 14 in place of 11 for the susceptibility);

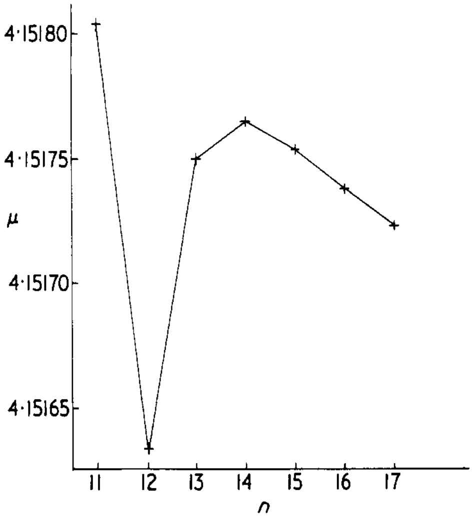

Figure 1. Triangular lattice. Estimates for the attrition (μ) obtained by solving $\beta_n = \mu(1+\xi/n^2)$ using successive pairs of ratios.

it seems that convergence is slower. The data are difficult to extrapolate more precisely; the last estimate is within 6 parts in 100 000 of the 1967 estimate. We conclude that the assumption (2.3) fits the data well, and that

$$\mu = 4{\cdot}1517 \pm 0{\cdot}0001 \tag{2.6}$$

which represents no significant change.

Since convergence is slower than for susceptibilities we would not expect the much shorter data for the face-centred cubic lattice to have reached the smooth region. We give the last six solutions to (2.5) in table 1. It will be seen that nevertheless the range

Table 1. Successive solution of (2.5) for face-centred cubic lattice

n	μ
7	10·03306
8	10·03453
9	10·03447
10	10·03454
11	10·03468
12	10·03481

of variation is already quite small; the last entry is within 2 parts in 100 000 of the 1967 estimate. We conclude that β is linear against $1/n^2$ within narrow limits and estimate

$$\mu = 10{\cdot}0355 \pm 0{\cdot}0010. \tag{2.7}$$

Our general inference for close-packed lattices is that, while convergence is somewhat slower, the qualitative behaviour of $C(x)$ closely resembles that of $\chi(v)$ found in

I and II. If the assumption (2.3) is correct, the estimates (2.6) and (2.7) are likely to be precise to within a few parts in 100 000.

3. Loose-packed lattices

For loose-packed lattices the situation is complicated by the presence of a characteristic even–odd oscillation in the ratios μ_n. We investigate the assumption that

$$C(x) \sim A(1-\mu x)^{-g-1} + A^*(1+\mu x)^{-h-1} \tag{3.1}$$

where the second term is included to account for the oscillatory behaviour. The introduction of a singularity at $x = -1/\mu$ (corresponding to a notional antiferromagnetic walk) is difficult to justify rigorously; one such must be present in the ring generating function since this is an even function of x. For the susceptibility it appears likely (Sykes 1961, Sykes and Fisher 1958) that the oscillation is caused by a singularity with exponent equal to the exponent characterizing the behaviour of the internal energy at this point. The internal energy is derived by differentiation of the free energy, and this latter is dependent on polygons (and other no-field graphs). For the polygons, differentiation results in contributions proportional to u_n (Sykes 1961). By analogy we suppose that the second index in (3.1) may well be that of *the ring generating function*. Alternatively we observe that the successive coefficients for $C(x)$ are usually calculated recursively from the number of dumb-bells, figure-eights and rings (Sykes 1961), and that any singularity in the ring generating function $U(x)$ *could* impress itself on $C(x)$. The argument is not rigorous since we have not proved that the singularity is not cancelled by the generating functions of dumb-bells and figure-eights. Without adjudicating on these somewhat tenuous arguments we investigate (3.1) numerically.

We illustrate three approximations for the square lattice in figure 2.

$$\beta_n = \mu\left(1+\frac{\eta}{n^2}\right) \tag{3.2}$$

which, following II and by analogy, we still denote by $\beta(1\text{F})$ and regard as the first

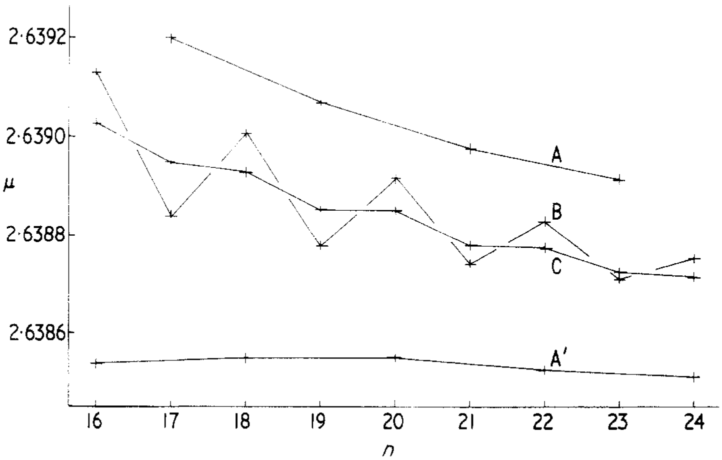

Figure 2. Square lattice. Estimates for the attrition (μ) obtained from: A, A′ the approximation $\beta(1\text{F})$; B the approximation $\beta(1\text{A})$ with $\theta = 1{\cdot}833$ and C with $\theta = 1{\cdot}860$.

order 'ferromagnetic' approximation; it takes no account of the oscillation except in so far as the successive solutions are obtained from alternate pairs of ratios. The other two approximations are of 'antiferromagnetic' type, $\beta(1\text{A})$, and correspond to

$$\beta_n = \mu\left(1+(-1)^n\frac{\zeta}{n^\theta}\right). \tag{3.3}$$

These ignore the quadratic approach term of the first singularity but take account of the oscillation. From (3.1) and the arguments of II it follows that the oscillation should decline as $1/n^{g-h}$ where g and h are defined by (3.1), so that the index θ in (3.3) is now that of *initial ring closure* (Hiley and Sykes 1961). We illustrate the results obtained by adopting the estimate of Martin *et al* (1967) of $\theta = 1{\cdot}833$ and also $\theta = 1{\cdot}860$ which latter value is more effective in smoothing the oscillation and is within $1\frac{1}{2}\%$ of the former. There are two points to be made: first we have investigated numerically numerous algebraic functions of type (3.1) and found that the true index is not always the one which gives the smoothest set of solutions but is always very close to it (Roberts 1971). Second, the observed smoothness is only in the last four estimates; the previous four can be made smooth by adopting $\theta = 1{\cdot}87$ but this does less well for the last four. Thus as the number of terms increases the index found in this way approaches the ring closure index within narrow limits.

We conclude the data are quite consistent with all our hypotheses. We present in table 2 the last six solutions of the combined approximation $\beta(1\text{F}, 1\text{A})$ corresponding to

$$\beta_n = \mu\left(1+\frac{\eta}{n^2}+(-1)^n\frac{\zeta}{n^{1\cdot 833}}\right). \tag{3.4}$$

Table 2. Successive solutions of (3.4) for square lattice

n	η	ζ	μ
19	−0·075189	−0·313711	2·638727
20	−0·092443	−0·313122	2·638860
21	−0·069912	−0·312436	2·638703
22	−0·083188	−0·312035	2·638787
23	−0·064622	−0·311530	2·638681
24	−0·074143	−0·311272	2·638730

The chief difference from the corresponding results for the susceptibility is that ζ now dominates and η is relatively small and ill defined. We estimate

$$\mu = 2{\cdot}6385\pm 0{\cdot}0001 \tag{3.5}$$

which is within reasonable agreement with Hiley and Sykes (1961) who give $\mu = 2{\cdot}6390\pm0{\cdot}0005$ from 18 terms, and in precise agreement with Guttmann *et al* (1968) who give $\mu = 2{\cdot}6385\pm0{\cdot}0001$ from 18 terms.

For the simple cubic lattice we illustrate in figure 3 the approximation $\beta(1\text{F})$ and also $\beta(1\text{A})$ for $\theta = 1{\cdot}9167$ which corresponds to the ring closure index of Sykes *et al* (1967) and further $\theta = 1{\cdot}94$ which is more effective in smoothing the oscillation. As in two dimensions the second index is only some $1\frac{1}{2}\%$ above the first and the same

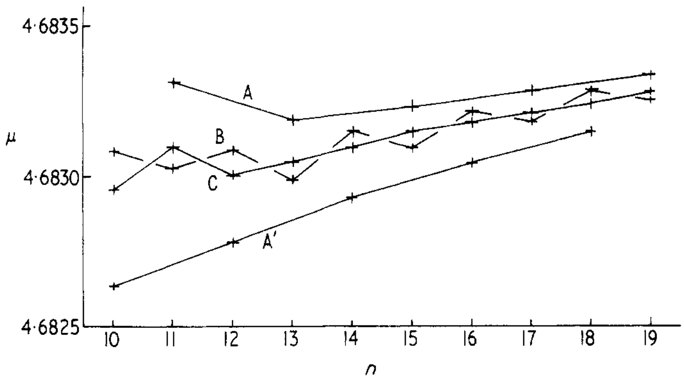

Figure 3. Simple cubic lattice. Estimates for the attrition (μ) obtained from: A, A' the approximation $\beta(1\text{F})$; B the approximation $\beta(1\text{A})$ with θ = 1·9167 and C with θ = 1·94.

observations apply. We regard the general trend as satisfactory and estimate

$$\mu = 4{\cdot}6835 \pm 0{\cdot}0005 \tag{3.6}$$

which is only 0·02% higher than the earlier estimates (Sykes 1963, Guttmann *et al* 1968) based on 16 terms.

The behaviour of the body-centred cubic lattice, for which we have derived 15 terms, is qualitatively the same. We give the last few solutions of the combined first order approximation using the initial ring closure index for both three dimensional lattices in table 3. For the body-centred cubic lattice we estimate

$$\mu = 6{\cdot}5295 \pm 0{\cdot}0005. \tag{3.7}$$

Table 3. Successive solutions of $\beta(1\text{F}, 1\text{A})$ with θ = 1·9167 for the simple cubic lattice and body-centred cubic lattice

	n	η	ζ	μ
Simple cubic	14	−0·02315	−0·13870	4·68313
	15	−0·02100	−0·13858	4·68308
	16	−0·02680	−0·13825	4·68320
	17	−0·02472	−0·13815	4·68316
	18	−0·03072	−0·13786	4·68327
	19	−0·02864	−0·13776	4·68324
Body-centred cubic	12	−0·00183	−0·12477	6·52892
	13	−0·00558	−0·12504	6·52915
	14	−0·00670	−0·12496	6·52915
	15	−0·00820	−0·12505	6·52921

This result is also in good agreement with earlier estimates based on only 9 terms in the series. These were μ = 6·54 ± 0·01 by Fisher and Sykes (1959) and $\mu \simeq$ 6·527 by Guttmann *et al* (1968). As in two dimensions, the parameter ζ dominates while η is relatively small and ill defined.

While (3.1) appears sufficient to describe the data for the lattices we have examined, additional terms are required to account for the more complex behaviour of walks on the honeycomb and diamond lattices; a similar complexity is found for the susceptibility (see paper I).

4. Conclusions

We have investigated the assumption that for a close-packed lattice the chain-generating function $C(x)$ may be written, near $x = 1/\mu$

$$C(x) \sim (1-\mu x)^{-g-1}\Phi(x)+\Psi(x) \tag{4.1}$$

where Φ and Ψ are regular in the disc $|x| \leqslant 1/\mu$. By a numerical study we have found the data consistent with this assumption; extended data are in close agreement with the values $g = \frac{1}{3}$ in two dimensions (triangular lattice) and $g = \frac{1}{6}$ in three dimensions (face-centred cubic lattice).

For a loose-packed lattice we have investigated the more general assumption

$$C(x) \sim (1-\mu x)^{-g-1}\Phi(x)+(1+\mu x)^{-h-1}\Phi^*(x)+\Psi(x) \tag{4.2}$$

where Φ, Φ^* and Ψ are regular in the disc $|x| \leqslant 1/\mu$. We have suggested some theoretical reasons for identifying h with the critical index for rings. Again by numerical study we have found the data consistent with this assumption; extended data are in close agreement with the values $g = \frac{1}{3}$ and $h = -1\frac{1}{2}$ in two dimensions (square lattice) and $g = \frac{1}{6}$ and $h = -1\frac{3}{4}$ in three dimensions (simple cubic and body-centred cubic lattices). In other words we have found that the characteristic even–odd oscillation in the ratios for a loose-packed lattice declines to leading asymptotic order as $n^{-\theta}$, with θ equal to the initial ring closure index, namely, $\theta = 1\frac{5}{6}$ in two dimensions and $\theta = 1\frac{11}{12}$ in three dimensions. This is in complete analogy with the result for the Ising model, where the oscillations are found to decrease with index $\theta = 2\frac{3}{4}$ in two dimensions and $\theta = 2\frac{1}{8}$ in three dimensions (Sykes *et al* 1972b).

The detailed theory of the asymptotic behaviour of coefficients in high temperature series expansions for the Ising model finds a close parallel in that of selfavoiding walks.

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Appendix. Selfavoiding walks

n	c_n honeycomb lattice	c_n square lattice	c_n simple cubic lattice	c_n body-centred cubic lattice
0	1	1	1	1
1	3	4	6	8
2	6	12	30	56
3	12	36	150	392

n	c_n honeycomb lattice	c_n square lattice	c_n simple cubic lattice	c_n body-centred cubic lattice
4	24	100	726	2648
5	48	284	3534	17960
6	90	780	16926	120056
7	174	2172	81390	804824
8	336	5916	387966	5351720
9	648	16268	1853886	35652680
10	1218	44100	8809878	236291096
11	2328	120292	41934150	1568049560
12	4416	324932	198842742	10368669992
13	8388	881500	943974510	68626647608
14	15780	2374444	4468911678	453032542040
15	29892	6416596	21175146054	2992783648424
16	56268	17245332	100121875974	
17	106200	46466676	473730252102	
18	199350	124658732	2237723684094	
19	375504	335116620	10576033219614	
20	704304	897697164		
21	1323996	2408806028		
22	2479692	6444560484		
23	4654464	17266613812		
24	8710212	46146397316		
25	16328220			
26	30526374			
27	57161568			
28	106794084			
29	199788408			
30	372996450			
31	697217994			
32	1300954248			
33	2430053136			
34	4531816950			

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