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The end-to-end length distribution of self-avoiding walks

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Abstract. The distribution of end-to-end lengths of an n step self-avoiding walk has been calculated for walks of up to 10 steps on the face-centred cubic lattice and up to 12 steps on the triangular lattice. The data on both lattices have been extended to higher step lengths for walks with short end-to-end lengths. The regions of short end-to-end lengths and long end-to-end lengths have been analysed separately. The results show that the region of long end-to-end lengths behaves predictably in contrast to the region of short end-to-end lengths. A new analytical form for the distribution close to the origin is suggested. The results throw considerable light on the scaling laws first introduced to explain critical phenomena. It is suggested that the strong-scaling hypothesis is untenable in both two and three dimensions. A new characteristic length is introduced and its magnitude is calculated.

1. Introduction

A self-avoiding walk on a regular crystal lattice is a well-known model of a polymer molecule. The self-avoiding condition, that no lattice site may be simultaneously occupied by two segments of the polymer chain, allows the model to take account of 'excluded volume' effects (see Domb 1969 for a recent review). The theoretical elucidation of the properties of polymer solutions including excluded volume effects has proved a particularly intractable problem. This study follows one of the perhaps more successful of the various approaches.

The method has been to make an exact enumeration of all possible self-avoiding walks with given end points and up to a certain number of steps. The introduction of a lattice model greatly simplifies the numerical calculations. Furthermore, it accounts crudely for some of the internal chemical structure of a real molecule. This paper will be concerned with studies on two lattices, the face-centred cubic FCC in three dimensions and the triangular in two dimensions. We calculate the distribution exactly for short walks and extrapolate the data to obtain the asymptotic behaviour of long walks. We have calculated the distribution for walks of up to 10 steps on the FCC and up to 12 steps on the triangular.

The model has been studied previously using the same method by Domb *et al* (1965). We corroborate and extend their results which were obtained for the simple-quadratic and simple-cubic lattices. There have been many Monte-Carlo studies of self-avoiding walks of which that by Mazur and McCrackin (1968) is most relevant to the subject of this paper. Our results compare favourably with the Monte-Carlo studies. Recently there have been several attempts to determine the distribution analytically using self-consistent field methods. This approach is associated with Edwards (1965), Reiss (1967) and Yamakawa (1968). The numerical work gives an independent test of the success of such theories.

It has been realized for a number of years that there is a close relation between the excluded volume problem and the Ising model of ferromagnetism. This relation has been explored in detail by Domb (1970). The end-to-end length distribution is analogous to the spin–spin correlation function of the Ising model. By exploiting this analogy McKenzie and Moore (1971) have suggested an analytical form for the end-to-end length distribution which is valid for walks with a large number of steps and large end-to-end lengths. If $p_n(r)$ is the probability that a walk of n steps reaches the point r from the origin, McKenzie and Moore suggest that for large n

$$p_n(r) \sim \frac{A}{R_n^d}\left(\frac{r}{R_n}\right)^g \exp\left\{-\left(\frac{r}{R_n}\right)^\delta\right\} \tag{1}$$

for $r \gg R_n$. In this equation A is a constant, R_n is a 'scaling' length and δ and g are indices which determine the shape of the distribution. If it is assumed that the scaling length behaves as

$$R_n \sim R_0 n^\nu, \qquad n \to \infty, \tag{2}$$

where R_0 is a constant then one can deduce that δ and ν are related by

$$\delta = \frac{1}{1-\nu}. \tag{3}$$

This relation was earlier suggested by Fisher (1966). McKenzie and Moore also predicted a scaling relation involving g. One of the major aims of this paper is to examine the data in the light of equation (1). We shall show that the numerical data are consistent with equation (1) if $\nu = \frac{3}{5}$ for the FCC lattice and $\nu = 0{\cdot}745$ for the triangular lattice. (Note that $\nu = \frac{1}{2}$ corresponds to a gaussian distribution.) The scaling relations involving δ and g are also found to be correct within the errors implicit in this type of study. This work is contained in §§ 3 and 4. The spherical symmetry of the distributions has been assumed (Domb *et al* 1965).

The derivation of the form of the distribution in (1) is correct only for $r \gg R_n$. The contrary limit of fixed r and $n \to \infty$ will be considered in § 5. The major suggestion concerning the behaviour of the distribution close to the origin is the so-called 'strong scaling' hypothesis, which we shall state as

$$p_n(\boldsymbol{r}) \sim \frac{1}{R_n^d} F\left(\frac{r}{R_n}\right) \tag{4}$$

for all $\boldsymbol{r}$ and $n \to \infty$. Since the numerical data show a dip in the distribution close to the origin it is reasonable to assume that F behaves as

$$F(y) \sim y^h \tag{5}$$

as $y \to 0$ or in the context of (4) for fixed r and $n \to \infty$. McKenzie and Moore predicted a scaling relation involving h. The numerical data have been used to calculate h and it will be shown that the scaling relation is not obeyed on the FCC but is obeyed on the triangular lattice. However, further analysis shows that the agreement for the triangular lattice is fortuitous and that for both lattices a better fit to the numerical data is obtained with a logarithmic dependence on r when r is small. This result is impossible to reconcile with the scaling form (4) and we suggest that for neither lattice is the strong-scaling hypothesis useful.

Although our main results are of direct interest in the study of magnetic systems and more generally in the theory of second-order phase transitions, they are also of interest in the field of polymers. Most experimental and theoretical studies of polymer solutions are applicable close to the Flory 'theta' point, which is defined by those conditions of temperature, solvent and polymer solute such that the excluded volume effect is balanced by net attractive forces between the segments of the polymer chain so that the average shape of the molecule is gaussian. The theta point is always close to the gel point of the solution so that the thermodynamic properties of the solution are varying rapidly as the transition is approached. Experimentally it is more convenient to work with athermal solutions, that is, solutions for which the heat of dilution is zero. The self-avoiding walk model corresponds to an athermal solution. Our results are therefore of interest to experimenters studying polymers dissolved in 'good' solvents.

2. Preliminaries

In this section we shall describe how the data were calculated and describe some preliminary calculations.

The data for the distribution up to 10 lines on the FCC were calculated on the KDF9 computer at the National Physical Laboratory using a program developed by Dr J L Martin of King's College, London. The calculation took approximately 20 hours even taking considerable account of symmetry. The data on the points closest to the origin at 11 lines on the FCC were calculated by Watts and Martin and are published by Sykes *et al* (1972a). The data for the distribution up to 12 lines on the triangular lattice were calculated on the IBM 360/65 computer at University College, London using the same program. The time taken was $27\frac{1}{2}$ minutes. The data on the points closest to the origin up to 15 lines on the triangular were calculated on the same computer and took about 4 hours. The data on the points closest to the origin are tabulated in the Appendix.

An important quantity derived from the distribution data is the total number of self-avoiding walks C_n. This number gives an important check on the data and is also the normalization constant for the distribution. Following Domb (1969) we assume that C_n behaves as

$$C_n \sim C_0 n^{\gamma-1} \mu^n \tag{6}$$

for large n where C_0 is a constant and μ is the 'effective coordination number' or 'connective constant'. The existence of μ has been proved by Hammersley (1957). We confirm the results of Sykes *et al* (1972b), who have more extensive data, that for the FCC lattice $\mu = 10{\cdot}035$ and $\gamma = \frac{7}{6}$ and for the triangular lattice $\mu = 4{\cdot}1517$ and $\gamma = \frac{4}{3}$. In the Ising model γ describes the critical behaviour of the high-temperature susceptibility in zero field.

A second quantity of interest is U_n, the number of self-avoiding walks of n steps which return to one step from the origin. It is assumed that

$$U_n \sim U_0 n^{\alpha-2} \mu^n \tag{7}$$

where U_0 is a constant. The identification of μ in (6) and (7) has been proved by Hammersley (1961). It has been shown that $\alpha = \frac{1}{4}$ for the FCC lattice and $\alpha = \frac{1}{2}$ for the triangular lattice (Sykes *et al* 1972b). In magnetic systems α describes the behaviour of the specific heat as the critical temperature is approached from above in zero field.

Finally, we may calculate the mean square end-to-end length $\mu_n(2)$. It is assumed that

$$\mu_n(2) \sim \rho^2 n^{2\nu'} \qquad \text{as } n \to \infty. \tag{8}$$

The index $2\nu'$ can be estimated by extrapolation using Neville tables. Table 1 shows that for the FCC lattice $2\nu' = 1{\cdot}200 \pm 0{\cdot}005$ and for the triangular lattice $2\nu' = 1{\cdot}49 \pm 0{\cdot}01$. The uncertainties in $2\nu'$ are estimated from table 1. We deduce that $\nu' = 0{\cdot}600 \pm 0{\cdot}003$ for the FCC and $\nu' = 0{\cdot}745 \pm 0{\cdot}005$ for the triangular. The corresponding values of ρ are $\rho = 0{\cdot}9594$ for the FCC and $\rho = 0{\cdot}865$ for the triangular. On each lattice the bond length is taken as unit length.

Table 1. Neville tables of estimates to $2\nu'$ for the FCC and triangular lattices, derived from the second moment $\mu_n(2)$ where $\mu_n(2) \sim \rho^2 n^{2\nu'}$

FCC	n	Estimates		
	2	1·1818		
	3	1·2044	1·2270	
	4	1·2118	1·2265	1·2263
	5	1·2140	1·2205	1·2144
	6	1·2135	1·2117	1·1984
	7	1·2122	1·2057	1·1937
	8	1·2110	1·2040	1·1999
	9	1·2100	1·2026	1·1983
	10	1·2090	1·2013	1·1966
Triangular	n	**Estimates**		
	2	1·4000		
	3	1·5145	1·6290	
	4	1·5167	1·5210	1·4670
	5	1·5063	1·4754	1·4298
	6	1·5002	1·4754	1·4754
	7	1·5000	1·4991	1·5465
	8	1·4973	1·4815	1·4376
	9	1·4960	1·4866	1·5018
	10	1·4951	1·4879	1·4924
	11	1·4942	1·4859	1·4781
	12	1·4936	1·4874	1·4943

3. Higher moments

We propose to investigate the shape of the end-to-end length distribution by studying the behaviour of the moments of the distribution. If $\mu_n(t)$ is the tth moment of an n step walk and $C_n(\boldsymbol{r})$ is the number of self-avoiding walks which start at the origin and end at the lattice site $\boldsymbol{r}$ then we define formally

$$\mu_n(t) = \sum_{\boldsymbol{r}} C_n(\boldsymbol{r}) r^t \Big/ \sum_{\boldsymbol{r}} C_n(\boldsymbol{r}) = \sum_{\boldsymbol{r}} C_n(\boldsymbol{r}) r^t / C_n. \tag{9}$$

By analogy with (8), let us assume that

$$\mu_n(t) \sim R_t n^{\lambda_t}, \qquad n \to \infty, \tag{10}$$

where R_t is a constant and λ_t is to be determined by extrapolation. With t in the range $-10 \leqslant t \leqslant 10$ and using Neville tables, we obtain the results for λ_t shown in figures 1 and 2. The figures show a striking difference in behaviour between positive and negative moments. For the positive moments we obtain a good fit to the data with $\lambda_t = \nu t$ with $\nu = \frac{3}{5}$ for the FCC and $\nu = \frac{3}{4}$ for the triangular. Within the limits of error these values of ν agree with those obtained from the second moment alone. There is a certain amount of curvature in figure 2 which is probably related to the slowness of convergence

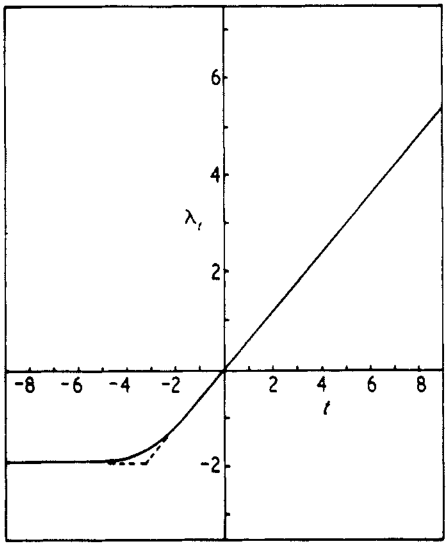

Figure 1. FCC lattice: plot of λ_t against t. λ_t is defined from the tth moment $\mu_n(t)$ by $\mu_n(t) \propto n^{\lambda_t}$. The broken lines represent $\lambda_t = 0{\cdot}6t$ and $\lambda_t = -1{\cdot}92$.

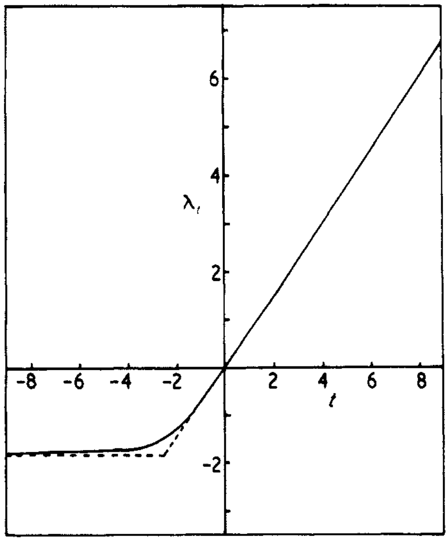

Figure 2. Triangular lattice: plot of λ_t against t. λ_t is defined from the tth moment $\mu_n(t)$ by $\mu_n(t) \propto n^{\lambda_t}$. The broken lines represent $\lambda_t = 0{\cdot}75t$ and $\lambda_t = -1{\cdot}83$.

of the data for the triangular lattice. The linear dependence of λ_t on t for $t > 0$ suggests the introduction of a quantity R_n such that

$$\mu_n(t) \propto R_n^t \tag{11}$$

and

$$R_n \sim R_0 n^{\nu}, \qquad \text{for large } n. \tag{12}$$

Since the positive moments weight disproportionately the 'tail' of the distribution, we therefore suggest that the decay of the distribution for large r can be represented by a single scaling length R_n. Along with (12) this is one of the main assumptions in the derivation of equation (1) by McKenzie and Moore.

In contrast, for $t < 0$, λ_t rapidly tends to a limiting value. The origin of this behaviour can be seen directly. As t becomes more negative the configurations with small end-to-end lengths make the dominant contribution to the moments. In the limit $t \to -\infty$ only the walks whose end points are unit distance apart make a contribution. That is,

$$\mu_n(t) \to C_n(1)/C_n \qquad \text{as } t \to -\infty.$$

But $C_n(1)$ is just U_n, so that for large n,

$$\begin{aligned}\mu_n(t) &\to U_n/C_n \\ &\sim \frac{U_0}{C_0} n^{\alpha-1-\gamma}.\end{aligned} \tag{13}$$

But $\alpha - 1 - \gamma = -\frac{23}{12}$ for the FCC lattice and $-\frac{11}{6}$ for the triangular lattice. The lines $\lambda_t = \alpha - 1 - \gamma$ have been inserted in figures 1 and 2. It can be seen that the limiting value is obtained at about $t = -6$ for the FCC lattice but that convergence is much slower for the triangular lattice.

On the basis of figures 1 and 2 we postulate that the distribution shows different behaviour for short end-to-end lengths and long end-to-end lengths and that there is a sharp transition between the two types of behaviour as shown by the intersection of the broken lines $\lambda_t = \alpha - 1 - \gamma$ and $\lambda_t = \nu t$ in figures 1 and 2. The deviation of the real data from this ideal behaviour in the region close to the intersection would be expected because of the limited amount of data and difficulties in extrapolation. With the values of α, γ and ν given above, the lines intersect at $t = -3\frac{7}{36}$ for the FCC lattice and $t = -2\frac{4}{9}$ for the triangular lattice.

4. Large end-to-end lengths

Assuming the existence of two types of behaviour, we now investigate each in turn. We shall postpone study of the region of small end-to-end lengths until the next section and concentrate first on the behaviour of the distribution for large end-to-end lengths. For $r \gg R_n$ it is plausible to expect the distribution to be described by equations (1) and (2) together with the 'scaling relations' deduced by McKenzie and Moore namely

$$\delta = \frac{1}{1-\nu} \tag{14}$$

and

$$g = \frac{1 - \frac{1}{2}d + d\nu - \gamma}{1-\nu}. \tag{15}$$

Our purpose in this section is to verify that these relations are satisfied by calculating g and δ, and that equation (1) adequately describes the distribution with the calculated values of g and δ. To accomplish this we define 'reduced' moments $\sigma_n(t)$ by

$$\sigma_n(t) = \mu_n(t)/(\mu_n(2))^{t/2}. \tag{16}$$

Because the decay of the distribution is governed by a single scaling length R_n as demonstrated in the previous section, the reduced moments should become independent of n for large n, that is,

$$\sigma_n(t) \to \sigma_t, \qquad n \to \infty. \tag{17}$$

The σ_t depend therefore only on the shape of the distribution and hence can be used to determine the shape parameters g and δ. Neville tables of $\sigma_n(4)$ and $\sigma_n(6)$ are shown in table 2, and the estimated values of σ_t are shown in table 3. As can be seen from table 2, the $\sigma_n(t)$ converge slowly so that our confidence in the values of σ_t obtained by this method is not high.

To obtain a better guide to the errors introduced by the extrapolation we have proceeded indirectly. From (1) it is readily deduced that

$$\sigma_t = \frac{\Gamma((d+g+t)/\delta)}{\Gamma((d+g)/\delta)}\left(\frac{\Gamma((d+g)/\delta)}{\Gamma((d+g+2)/\delta)}\right)^{t/2}. \tag{18}$$

By choosing suitable values of g one can find a value of δ such that $\sigma_t = \sigma_n(t)$ for each

Table 2. Neville tables of estimates to the reduced moments σ_4 and σ_6 for the FCC and triangular lattices. σ_t is defined by equation (17)

FCC	n	Estimates to σ_4			Estimates to σ_6		
	1	1·0000			1·0000		
	2	1·2222	1·4444		1·6806	2·3611	
	3	1·2932	1·4352	1·4307	1·9642	2·5314	2·6166
	4	1·3290	1·4362	1·4372	2·1182	2·5804	2·6294
	5	1·3513	1·4404	1·4468	2·2175	2·6144	2·6654
	6	1·3671	1·4462	1·4577	2·2889	2·6463	2·7101
	7	1·3792	1·4518	1·4659	2·3441	2·6753	2·7476
	8	1·3888	1·4564	1·4702	2·3885	2·6993	2·7715
	9	1·3968	1·4602	1·4736	2·4253	2·7196	2·7906
	10	1·4034	1·4635	1·4764	2·4565	2·7369	2·8063
Triangular	n	Estimates to σ_4			Estimates to σ_6		
	1	1·0000			1·0000		
	2	1·3000	1·6000		2·0500	3·1000	
	3	1·3083	1·3249	1·4873	2·0547	2·0640	1·5460
	4	1·3305	1·3972	1·4696	2·1291	2·3522	2·6405
	5	1·3473	1·4146	1·4408	2·1924	2·4459	2·5864
	6	1·3592	1·4187	1·4267	2·2378	2·4647	2·5022
	7	1·3686	1·4249	1·4406	2·2737	2·4890	2·5499
	8	1·3765	1·4317	1·4520	2·3043	2·5183	2·6063
	9	1·3831	1·4362	1·4521	2·3304	2·5391	2·6117
	10	1·3888	1·4399	1·4547	2·3530	2·5565	2·6260
	11	1·3938	1·4433	1·4585	2·3729	2·5724	2·6441
	12	1·3981	1·4460	1·4595	2·3907	2·5857	2·6519

Table 3. Estimates of σ_4, σ_6, σ_8 and σ_{10} obtained by extrapolation using Neville tables, compared with the estimates obtained by substituting equations (20) and (21) for δ and g into (19). The error limits in the latter estimates correspond to those quoted in (20) and (21)

FCC	t	σ_t (extrapolated)	σ_t (by substitution)
	4	1·48	1·481 ± 0·007
	6	2·87	2·85 ± 0·04
	8	6·75	6·75 ± 0·15
	10	18·5	18·5 ± 0·7
Triangular	4	1·46	1·455 ± 0·008
	6	2·65	2·64 ± 0·04
	8	5·65	5·61 ± 0·14
	10	13·9	13·4 ± 0·5

moment and each value of n. That is, for each moment and each value of n a set of values of g and δ can be found such that (18) is satisfied exactly. We have then extrapolated the values of δ for a given value of g so as to produce an asymptotic relation between g and δ for each moment. We have therefore eight asymptotic relations between g and δ for $3 \leqslant t \leqslant 10$ which satisfy both the numerical data and equation (18). The spread between the relations for different moments is small and gives confidence in the extrapolation procedure. The hatched areas in figures 3 and 4 summarize the results of the numerical calculations. The error bars were estimated from the spread of the results between different moments and different methods of extrapolation. (Ratio plots were also used.)

A second theoretical relation between g and δ is obtained by eliminating ν between equations (14) and (15) and substituting the appropriate values of d and γ. We obtain

$$\delta = \frac{g+d}{1+\frac{1}{2}d-\gamma} = \begin{cases} \frac{3}{4}g+\frac{9}{4} & \text{for the FCC lattice} \\ \frac{3}{2}g+3 & \text{for the triangular lattice.} \end{cases} \qquad (19)$$

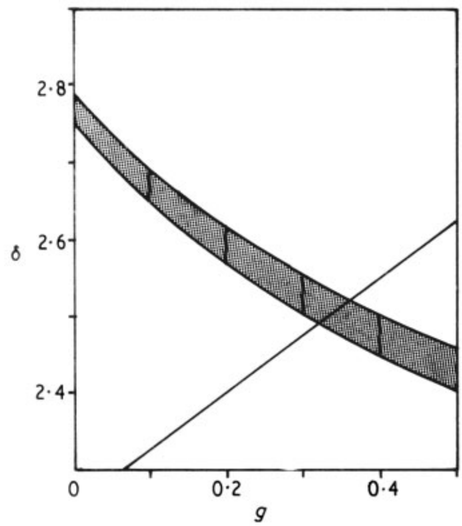

Figure 3. FCC lattice: the relation between δ and g. The hatched area is the relation derived from the numerical data by extrapolation. The straight line represents $\delta = \frac{4}{3}g+\frac{9}{4}$.

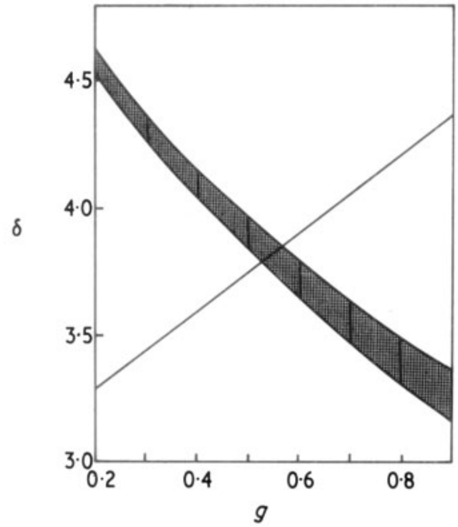

Figure 4. Triangular lattice: the relation between δ and g. The hatched area is the relation derived from the numerical data by extrapolation. The straight line represents $\delta = \frac{3}{2}g + 3$.

This relation is shown by the straight line in figures 3 and 4. The intersection of this line with the hatched area gives the values of δ and g which are consistent with the numerical data and equation (19). We estimate

$$\delta = \begin{cases} 2{\cdot}51 \pm 0{\cdot}02 & \text{for the FCC lattice} \\ 3{\cdot}82 \pm 0{\cdot}04 & \text{for the triangular lattice} \end{cases} \qquad (20)$$

and

$$g = \begin{cases} 0{\cdot}35 \pm 0{\cdot}03 & \text{for the FCC lattice} \\ 0{\cdot}55 \pm 0{\cdot}03 & \text{for the triangular lattice.} \end{cases} \qquad (21)$$

The error limits in (20) and (21) are taken from figures 3 and 4. We may now check equation (14) by calculating ν using (20) and comparing with the values of ν' obtained from the second moment. Substituting (20) into (14) we obtain

$$\nu = \begin{cases} 0{\cdot}602 \pm 0{\cdot}003 & \text{for the FCC lattice} \\ 0{\cdot}739 \pm 0{\cdot}003 & \text{for the triangular lattice.} \end{cases} \qquad (22)$$

These values of ν agree closely with those of ν' obtained previously.

Finally, the reduced moments σ_t can be calculated by substituting (20) and (21) into (18). For the 4th, 6th, 8th and 10th moments we obtain the values shown in table 3. The close agreement with the extrapolated values gives added weight to the internal consistency of our approach.

To summarize our conclusions so far, there is convincing evidence that for $r \gg R_n$, the end-to-end length distribution can be described by

$$p_n(r) = \frac{A}{R_n^d}\left(\frac{r}{R_n}\right)^g \exp\left\{-\left(\frac{r}{R_n}\right)^\delta\right\}$$

which is a function of a single scaling length R_n. Furthermore, if $R_n \sim R_0 n^{\nu}$ for large n then the relations

$$g = \frac{1-\frac{1}{2}d+d\nu-\gamma}{1-\nu}$$

and

$$\delta = \frac{1}{1-\nu}$$

are consistent with the numerical data when $\nu = \frac{3}{5}$ and $\gamma = \frac{7}{6}$ for the FCC lattice and $\nu = 0{\cdot}745$ and $\gamma = \frac{4}{3}$ for the triangular lattice. We also obtain $R_0 = 0{\cdot}879$ for the FCC lattice and 1·048 for the triangular lattice.

5. Small end-to-end lengths

The major hypothesis to be tested in this section is the so-called 'strong scaling' hypothesis, which states that $p_n(\boldsymbol{r})$ can be described by a single scaling length R_n such that

$$p_n(\boldsymbol{r}) = \frac{1}{R_n^d} F\left(\frac{r}{R_n}\right) \tag{23}$$

for *arbitrary* values of r/R_n. We have shown that when $r \gg R_n$ the evidence in favour of a scaling form for $p_n(\boldsymbol{r})$ is strong. We now examine the region of the distribution given by $r \ll R_n$. In particular, we shall consider the asymptotic behaviour of the distribution for fixed values of the end-to-end length.

In these circumstances, it is reasonable to assume that the distribution behaves in a manner similar to U_n (equation 7). That is we assume that

$$C_n(r) \sim f(r) n^{\alpha-2} \mu^n \tag{24}$$

for fixed r and $n \to \infty$. This hypothesis is supported by Hammersley (1961) who showed that for walks whose end points are O(n) apart, μ in (24) exists and is identical with μ occurring in (6). With $\mu = 10{\cdot}035$ for the FCC and $\mu = 4{\cdot}1517$ for the triangular lattice, we can check (24) by extrapolating the data for various values of r to find $\alpha - 2$. A sample of the results are shown in table 4. Allowing for the paucity of data, it is reasonable to conclude that $\alpha = \frac{1}{4}$ for the FCC and $\alpha = \frac{1}{2}$ for the triangular lattice for all values of r. The function $f(r)$ has been estimated by extrapolating the values of $C_n(r)/n^{\alpha-2}\mu^n$. The results are shown in table 5 where it can be seen that $f(r)$ is a slowly increasing function of r.

From the definition of $p_n(\boldsymbol{r})$ it immediately follows from (24) that

$$p_n(\boldsymbol{r}) = \frac{C_n(\boldsymbol{r})}{C_n} \sim \frac{n^{\alpha-1-\gamma} f(r)}{C_0} \tag{25}$$

with r fixed and $n \to \infty$. Since there is no explicit mention of a scaling length in (25), one does not anticipate satisfying the scaling hypothesis. However it was argued by McKenzie and Moore that if $F(y)$ had the form

$$F(y) \propto y^h \tag{26}$$

Table 4. Neville tables of estimates to the index $\alpha-2$ for walks which return to the points (0,0,2) and (1,1,2) for the FCC lattice and the points (0,2) and (1,1) for the triangular lattice on the assumption that the number of walks behaves as $n^{\alpha-2}(10{\cdot}035)^n$ for the FCC and $n^{\alpha-2}(4{\cdot}1517)^n$ for the triangular lattice

FCC	n	Estimates for (0,0,2)			Estimates for (1,1,2)		
	6	−1·239	−1·524	−1·784	−1·134	−1·745	−1·811
	7	−1·308	−1·651	−1·904	−1·227	−1·694	−1·591
	8	−1·349	−1·600	−1·474	−1·287	−1·647	−1·530
	9	−1·386	−1·639	−1·753	−1·332	−1·649	−1·654
	10	−1·416	−1·656	−1·717	−1·369	−1·665	−1·720
	11	−1·441	−1·674	−1·746	−1·400	−1·678	−1·731
Triangular	n	**Estimates for (0,2)**			**Estimates for (1,1)**		
	10	−1·561	−1·247	−1·765	−1·525	−1·203	−2·068
	11	−1·534	−1·243	−1·222	−1·508	−1·325	−1·935
	12	−1·517	−1·304	−1·641	−1·491	−1·285	−1·063
	13	−1·502	−1·320	−1·412	−1·482	−1·361	−1·820
	14	−1·492	−1·347	−1·524	−1·474	−1·368	−1·410
	15	−1·484	−1·367	−1·506	−1·469	−1·392	−1·561

Table 5. Estimates of $f(r) = \lim_{n\to\infty} C_n(r)/(10{\cdot}035)^n n^{-1{\cdot}75}$ for the FCC lattice and $f(r) = \lim_{n\to\infty} C_n(r)/(4{\cdot}1517)^n n^{-1{\cdot}5}$ for the triangular lattice

FCC			Triangular		
Point	r	$f(r)$	Point	r	$f(r)$
0,1,1	1·000	0·186	0,1	1·000	0·36
0,0,2	1·414	0·225	1,1	1·732	0·50
1,1,2	1·732	0·242	0,2	2·000	0·53
0,2,2	2·000	0·255	1,2	2·646	0·60
0,1,3	2·236	0·267	0,3	3·000	0·62
2,2,2	2·449	0·274	2,2	3·461	0·66
1,2,3	2·646	0·283	1,3	3·606	0·67
0,3,3	3·000	0·300	0,4	4·000	0·70

for $y \to 0$, then (23) and (25) could be made consistent with

$$h = \frac{\gamma+1-d\nu-\alpha}{\nu}. \tag{27}$$

With $\gamma = \frac{7}{6}$, $\alpha = \frac{1}{4}$ and $\nu = \frac{3}{5}$ (27) predicts that $h = \frac{7}{36}$ ($= 0{\cdot}194$) for the FCC lattice, and with $\gamma = \frac{4}{3}$, $\alpha = \frac{1}{2}$ and $\nu = 0{\cdot}745$ we predict $h = 0{\cdot}46$ for the triangular lattice. The index h can be obtained from the extrapolated values of $f(r)$ (table 5) whose dependence on r must be identical with that of $F(y)$. A least squares fit of the data to the equation

$$\ln f(r) = h \ln r + \ln b \tag{28}$$

where b is a constant gives $h = 0{\cdot}42$ for the FCC and $h = 0{\cdot}46$ for the triangular lattice. The value of h for the triangular is identical with the predicted value, a result which is almost too good to be true. However, the prediction is clearly contradicted for the FCC lattice.

To determine the source of the discrepancy for the FCC lattice we must examine the assumptions we have made in more detail. There appear to be three main assumptions: the scaling form (25) for $p_n(r)$; equation (24) describing the behaviour of $C_n(r)$; and the form (26) for $F(y)$. The evidence in favour of (24) is strong and has been described above. We shall therefore concentrate first on the assumption (26). Of course there are many possible functions one might choose to represent $F(y)$, but let us first consider the addition of a constant term B to (27) so that

$$F(y) \propto B + y^h. \tag{29}$$

The presence of a constant would have a marked effect on the log–log plot which was used to determine h. We have fitted the data using least squares to the function

$$f(r) = a + br^h \tag{30}$$

for different values of h. If (26) were correct, one would expect the sum of the squares of the deviations from (30) to have a minimum when a is zero and h has the value found previously. The results are shown in table 6. The sum of the squares of the deviations is monotonically decreasing with h down to $h = 0{\cdot}04$ for the FCC and $h = 0{\cdot}01$ for the triangular lattice. At the same time a becomes increasingly negative. These results suggest that the best fit to the data is

$$f(r) = a + b \ln r \tag{31}$$

for *both* lattices with, of course, different values for a and b. The fact that the sum of the squares of the deviations for the FCC lattice increases slightly below $h = 0{\cdot}04$ is not considered significant. Using (31) we find

$$a = \begin{cases} 0{\cdot}187 & \text{for the FCC lattice} \\ 0{\cdot}363 & \text{for the triangular lattice} \end{cases} \tag{32}$$

Table 6. Least squares fit of $f(r)$ to the form $f(r) = a + br^h$ where a and b are constants for various values of h. The column labelled SSQ is the sum of the squares of the deviation of the numerical data from the best fit for each value of h

	FCC lattice			Triangular lattice		
h	a	b	SSQ $\times 10^6$	a	b	SSQ $\times 10^5$
1·0	0·143	0·054	30·46	0·296	0·106	46·65
0·9	0·132	0·064	25·39	0·268	0·129	38·99
0·8	0·118	0·077	20·81	0·235	0·159	31·89
0·7	0·100	0·094	16·75	0·192	0·198	25·40
0·6	0·076	0·117	13·22	0·134	0·251	19.58
0·5	0·043	0·149	10·24	0·054	0·328	14·48
0·4	−0·007	0·198	7·826	−0·067	0·444	10·15
0·3	−0·091	0·280	5·992	−0·267	0·641	6·640
0·2	−0·257	0·446	4·746	−0·669	1·038	3·991
0·1	−0·756	0·944	4·095	−1·872	2·238	2·236
0·09	−0·867	1·055	4·062	−2·140	2·505	2·110
0·07	−1·184	1·372	4·016	−2·904	3·269	1·887
0·05	−1·755	1·942	3·993	−4·279	4·643	1·702
0·03	−3·086	3·273	3·995	−7·488	7·852	1·553
0·01	−9·742	9·929	4·020	−23·53	23·90	1·441

and

$$b = \begin{cases} 0{\cdot}10 & \text{for the FCC lattice} \\ 0{\cdot}24 & \text{for the triangular lattice.} \end{cases} \tag{33}$$

It may be objected that the data of table 5 are not sufficiently precise to support these conclusions. However, the extrapolation technique used to calculate the data of table 5 was repeated several times for each lattice as new data became available without changing appreciably the results from those tabulated. The changes had no significant effect on the results of the least squares procedure subsequently employed.

Considerable ingenuity may be expended in postulating other possible forms than (26) and (31) for $f(r)$. However, on the grounds that the best hypothesis is the simplest one that fits the data, we conclude that for short end-to-end lengths the distribution behaves as

$$n^{\alpha-1-\gamma}(a+b\ln r)/C_0 \tag{34}$$

with the values of a and b given in (32) and (33). The agreement of h with the predicted value for the triangular lattice must now be viewed as a mere accident. Indeed, experimenting with equation (31) it is easy to see that a log–log plot of $f(r)$ against r would give an apparent slope which depends only on a and is relatively insensitive to changes in a. Both the FCC and the triangular lattices would therefore give a slope of about the same value which would be in the range 0·4 to 0·5 when a is in the range 0·1 to 0·5.

We conclude therefore, that the assumption (26) for $F(y)$ is incorrect. This result casts strong doubt on the strong-scaling hypothesis. Furthermore, the logarithmic dependence of $f(r)$ on r is impossible to reconcile with the hypothesis. An additional difficulty arises from the fact that equation (31) implies $h = 0$, which, on substitution in (27), gives the scaling relation

$$d\nu = \gamma+1-\alpha. \tag{35}$$

It is easy to verify that the extrapolated values of γ, α and ν do not support this relation in either two or three dimensions. Moreover, if the behaviour of the end-to-end distribution approximates more and more closely to that of a random walk as the dimensionality is increased (Edwards 1965, Rubin 1952), then substitution of the random walk values, $\gamma = 1$, $\alpha = 0$ and $\nu = \frac{1}{2}$, in (35) clearly leads to an absurdity as $d \to \infty$. On the basis of these arguments we conclude that the strong-scaling hypothesis is not adequate to describe the behaviour of the end-to-end length distribution on the triangular and FCC lattices.

6. Comments

Our value of 0·745 for ν for the triangular lattice is slightly lower than the value of $\frac{3}{4}$ found by Domb (1963). The lower value is supported by Hioe (1967). Corresponding to the lower value of ν we find $\delta = 3{\cdot}84$ instead of $\delta = 4$, the value found by Domb *et al* (1965) for the simple quadratic lattice. In three dimensions $\delta = 2{\cdot}5$ was found by Domb *et al* (1965) for the simple cubic lattice. The Monte-Carlo calculations of Mazur and McCrackin find $\delta \simeq 2{\cdot}9$ for the FCC and simple-cubic lattices, but the shape parameter g was not included in their calculations. Putting $g = 0$ in figure 3 gives a value of δ in approximate agreement with their results.

The main result of this work is that the distribution shows different behaviour for short end-to-end lengths and long end-to-end lengths. For long end-to-end lengths the theory of McKenzie and Moore gives a good description of the behaviour. However, for short end-to-end lengths the inadequacy of the strong-scaling hypothesis has been demonstrated in both two and three dimensions.

It has been recognized for some time that for the Ising model and the self-avoiding walk problem in three dimensions, the scaling relation $d\nu = 2-\alpha$ proposed by Kadanoff *et al* (1967) is not confirmed by numerical calculations. This scaling relation, like equations (27) and (35) relates the long-range behaviour characterized by ν to the short-range behaviour characterized by α. Our main result suggests that such a relation does not exist. Rather there are *two* characteristic lengths in the problem: the first is R_n which characterizes the decay of the distribution; the second, is a length of the order of the lattice bond length and which characterizes the short-range behaviour. This length can be determined by rewriting (34) in the form

$$n^{\alpha-1-\gamma}(b \ln r/Kr_0)/C_0$$

where Kr_0 is the characteristic length and r_0 is the lattice bond length. From (32) and (33) we obtain $K = 0{\cdot}155$ for the FCC lattice and $K = 0{\cdot}224$ for the triangular lattice.

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Appendix

We tabulate below the counting data for the first eight points nearest to the origin for the FCC lattice up to 11 steps and the triangular lattice up to 15 steps. The data for the 11 step walks for the FCC have been published by Sykes *et al* (1972a) but is included here for completeness. The data for the full distribution are not tabulated since they would require considerable space. The FCC data are available in McKenzie (1967).

FCC lattice

Number of steps	1	2	3	4	5	6	7	8	9	10	11
Point											
0,1,1	1	4	22	140	970	7196	56092	452064	3735700	31484244	269613896
0,0,2	—	4	24	152	1080	8152	63976	518232	4299728	36360872	312284536
0,2,2	—	1	12	114	940	7568	61728	512996	4334884	37164700	322624804
1,1,2	—	2	18	136	1030	7992	63796	522474	4369840	37179840	320861342
0,1,3	—	—	9	96	835	7020	58857	497360	4251804	36765592	321262541
0,3,3	—	—	1	24	360	4000	39330	367912	3370604	30630980	277824572
1,2,3	—	—	3	52	575	5470	49303	436446	3850752	34063392	303790797
2,2,2	—	—	6	72	690	6192	53946	466800	4053816	35450940	312411672

Triangular lattice

Number of steps	1	2	3	4	5	6	7	8	9	10
Point										
0,1	1	2	4	10	30	98	328	1140	4040	14 542
0,2	—	1	6	18	50	156	508	1724	6018	21 440
1,1	—	2	6	16	46	140	464	1580	5538	19 804
0,3	—	—	1	12	54	188	636	2168	7556	26 826
1,2	—	—	3	16	57	184	601	2036	7072	25 088
0,4	—	—	—	1	20	130	576	2218	8170	29 830
1,3	—	—	—	4	35	166	633	2276	8107	29 086
2,2	—	—	—	6	40	174	644	2268	8020	28 666

Number of steps	11	12	13	14	15
Point					
0,1	53 060	195 624	727 790	2728 450	10 296 720
0,2	77 632	284 706	1055 162	3944 956	14 858 934
1,1	71 884	264 204	980 778	3671 652	13 843 808
0,3	96 724	353 390	1305 126	4864 450	18 272 804
1,2	90 503	330 836	1222 783	4561 058	17 145 990
0,4	109 192	402 258	1492 746	5578 742	20 986 424
1,3	105 460	386 320	1428 664	5327 738	20 014 741
2,2	103 696	379 450	1402 276	5227 366	19 633 732

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