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Self-avoiding lattice walks with high coordination and small excluded volume†

A J Barrett and A Pound

Department of Mathematics, Royal Military College of Canada, Kingston, Ontario K7L 2W3, Canada

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Abstract. A self-avoiding walk on a lattice may be characterised by the 'excluded volume ratio'

$$V = \frac{\text{closest approach of two centres}}{\text{step length}}.$$

Walks to other than nearest-neighbour sites on a simple cubic lattice have high coordination numbers and low values of the excluded volume ratio. Some general results are presented for a class of these walks. Exact enumerations and Monte Carlo simulations have been made of the total number C_N and the mean square length $\langle R_N^2 \rangle$ for two examples of this class. These measurements are used to test the 'universality hypothesis' which contends that

$$C_N \sim N^{1/6} \mu^N$$
$$\langle R_N^2 \rangle \sim N^{6/5}$$

as $N \to \infty$, irrespective of the value of V. The data are in reasonable agreement with these statements, and the universality hypothesis is found to provide a good basis for the description of a self-avoiding walk.

1. Introduction

As with many other fundamental problems, that of a self-avoiding walk on a lattice defies exact solution. Consequently, analytic results are rare; numerical studies have been, and are, plentiful. The challenge lies in interpreting intelligently the vast collection of numbers which has been produced.

The self-avoiding walk is of interest to polymer theorists, who see it as a model of a real polymer chain, and also to students of critical phenomena. The feature common to both problems is a long-range interaction. The excluded volume effect operates between any two monomers of a polymer, no matter how much they are separated along the chain; the interesting features of critical phenomena are also dominated by long-range interaction. One hopes that the analogy may be further extended and that for polymer chains, as for critical phenomena, the essential features are independent of the details of short-range structure.

The consequences of this supposition have been examined elsewhere (e.g. Domb 1969, Lax *et al* 1978), but it will be useful to summarise briefly some of the features.

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Consider the following two equations which figure prominently in numerical studies of self-avoiding walks:

$$\langle R_N^2 \rangle = CN^{\gamma} \tag{1a}$$

$$C_N = DN^{g}\mu^{N}. \tag{1b}$$

$\langle R_N^2 \rangle$ is the mean square end-to-end length of an N-step self-avoiding walk, and C_N is the total number of such walks. μ is the exponential of the connective constant defined by Hammersley (1957), and the values of C, D, γ and g are to be established. If the quantities $\langle R_N^2 \rangle$ and C_N in fact depend on short-range structure, then one can expect γ and g to vary from chain to chain. If, on the other hand, only long-range effects are important, then γ and g are effectively *critical exponents*. In other words γ will be the same for all chains, as will g. We shall refer to this proposition as the 'universality hypothesis'. The values most often quoted for three-dimensional chains are

$$\begin{aligned} \gamma &= 6/5 \\ g &= 1/6. \end{aligned} \tag{2}$$

It is most important to note that the expressions (1), incorporating the values (2), are expected to be valid only in the vicinity of the 'critical point', which for a self-avoiding chain means that N must be 'sufficiently large'.

The universality hypothesis is an obvious target of numerical investigation. Numerous enumerations of short chains and simulations of longer ones have been performed with the intent of measuring γ and g. The evidence, which is well summarised in McKenzie (1976) and Smith and Fleming (1975) is far from conclusive. One reason for this is that one is never sure whether or not N is 'sufficiently large'. If, for instance, $\langle R_N^2 \rangle$ has a Darboux type expansion (see appendix 2)

$$\langle R_N^2 \rangle = N^{6/5}\left(A + \frac{B}{N} + \dots\right) \tag{3}$$

then the asymptotic region will be achieved only for exceedingly large values of N, and estimates obtained by fitting data to the simple form (1a) are unreliable. It should be clear from the above that simple measurements of g and γ are not likely to prove or disprove the universality hypothesis. A more valid test is surely to see whether or not the principle of universality can provide an adequate description for self-avoiding walks with widely varying short-range structures. That is the approach of this paper.

There are, then, essentially two features of interest. The first is the introduction of a class of walks, which provides the opportunity for study of self-avoiding walks over a wide range of excluded volume. The second is an analysis of the numerical data which is more sophisticated than a simple log–log plot. Most investigators have indeed relied upon this device to establish the value of γ in (1a), and failing to find universal values have suggested that universality is a false concept. We believe that a less naive approach will show this suggestion to be premature.

Numerical data can furnish estimates of parameters only within the framework of a given theory, and care must be taken in the selection of that theory. The particular expression (3), which is consistent with the principle of universality, is made plausible by the theorem of Darboux cited in appendix 2.

The presentation is as follows: in § 2, we define non-nearest-neighbour walks and give some useful results. Section 3 is concerned with the numerical results. Data for two examples of non-nearest-neighbour walks are compared with the predictions of the universality hypothesis. Some conclusions are stated in § 4.

2. Non-nearest-neighbour walks

One means of fundamentally altering the short-range structure of a self-avoiding walk is changing the excluded volume represented by the walk. Define (Smith and Fleming 1975) the *excluded volume ratio* of the familiar 'pearl necklace chain' (see figure 1) by

$$V = d/a$$

where d is the bead diameter and a is the step length. The analogous quantity for a lattice walk may be defined as (Barrett 1976)

$$V = \frac{d}{a} = \frac{\text{closest approach of two centres}}{\text{step length}}. \tag{4}$$

(The two centres must not be adjacent along the chain.)

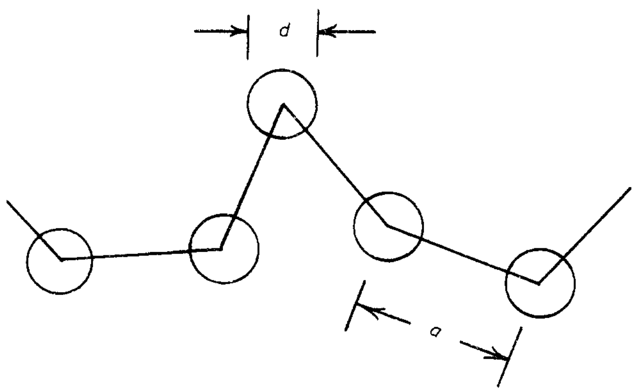

Figure 1. Pearl necklace model. $V = d/a$.

Most of the studies which have been done have dealt with the cubic lattices (SC, BCC and FCC) and the diamond lattice, for which $V = 1$ (e.g. Domb 1963, Wall *et al* 1954). Recently, however, some work has been done on neighbour-avoiding walks for which $V > 1$ (Torrie and Whittington 1975) and on off-lattice walks for which $V < 1$ (Smith and Fleming 1975, Bruns 1977). To our knowledge no measurements have been made on lattices for which $V < 1$ (except, of course, in this work).

A self-avoiding walk with an excluded volume ratio less than 1 is obtained by permitting steps only to non-nearest-neighbour sites on a simple cubic lattice, and by forbidding self-intersections. To illustrate the concepts involved, nearest-neighbour, non-nearest-neighbour, and neighbour-avoiding walks on the simple quadratic lattice are shown in figure 2.

Consider a simple cubic lattice with unit lattice spacing. Any lattice point may be specified by the vector $\boldsymbol{l} = (l_1, l_2, l_3)$. Generally, a walk on this lattice may be specified by permitted step vectors (p, q, r). We shall therefore designate as a pqr walk, a walk such that each permitted step vector has one component of length p, one component of length q, and the third component of length r. A random pqr walker has 48 choices for

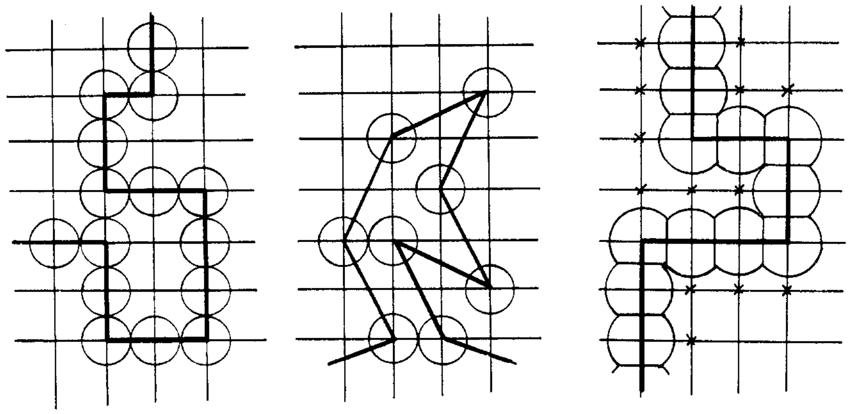

Figure 2. (a) Nearest-neighbour walk. $V=1$. (b) Non-nearest-neighbour walk. $V=1/\sqrt{5}<1$. (c) Neighbour-avoiding walk. $V=\sqrt{2}>1$.

the next step if $p \neq q \neq r \neq 0$, corresponding to the 3! permutations of p, q, r and the 2^3 possible sign combinations.

We now restrict ourselves to $11P$ walks. If $p=0$, this is a nearest-neighbour walk on the FCC lattice and if $P=1$, it is a nearest-neighbour walk on the BCC lattice. Otherwise a $11P$ walk is a 24 choice walk.

The proofs of the following three theorems may be found in appendix 1.

Theorem 1. The lattice point $(1, 0, 0)$ is not accessible to any $11P$ walk.

Theorem 2. A necessary and sufficient condition for the lattice point $(1, 1, 0)$ to be accessible to a $11P$ walk is that p be even.

Theorem 3. A necessary and sufficient condition for the lattice point $(1, 1, 1)$ to be accessible to a $11P$ walk is that p be odd.

We note that any lattice vector is a linear combination of the vectors $(1, 0, 0)$, $(1, 1, 0)$ and $(1, 1, 1)$, and state the following corollary:

Corollary. All $11P$ walks with p even (odd) have the same set of accessible points.

With the aid of these results it is not hard to compute the excluded volume ratio of a $11P$ walk:

$$\begin{aligned} V &= \frac{\sqrt{2}}{a} = \left(\frac{2}{2+p^2}\right)^{1/2} \qquad p \text{ even} \\ V &= \frac{\sqrt{3}}{a} = \left(\frac{3}{2+p^2}\right)^{1/2} \qquad p \text{ odd.} \end{aligned} \tag{5}$$

Now, define $P_N(\boldsymbol{l})$ to be the probability that the random walker occupies the lattice site $\boldsymbol{l}$ on the Nth step. The lattice walk generating polynomial may be defined by

$$\phi(x_1, x_2, x_3) = \sum_{\boldsymbol{l}} p_1(\boldsymbol{l}) x_1^{l_1} x_2^{l_2} x_3^{l_3}$$

so that

$$\phi(\boldsymbol{x})=\tfrac{1}{24}[(x_1+x_1^{-1})(x_2+x_2^{-1})(x_3^p+x_3^{-p})+(x_1+x_1^{-1})(x_2^p+x_2^{-p})(x_3+x_3^{-1}) \\ +(x_1^p+x_1^{-p})(x_2+x_2^{-1})(x_3+x_3^{-1})]. \tag{6}$$

$P_N(\boldsymbol{l})$ can be obtained by extracting the coefficients of $x_1^{l_1}x_2^{l_2}x_3^{l_3}$ from ϕ^N.

Following Montroll and Weiss (1965) we write the Green function of the walk as

$$P(\boldsymbol{l},x)=\frac{1}{(2\pi)^3}\iiint_{-\pi}^{\pi}\frac{e^{i\boldsymbol{k}_1\boldsymbol{l}}\,d^3k}{1-x\lambda(\boldsymbol{k})}. \tag{7}$$

$\lambda(\boldsymbol{k})$ is the function obtained from (6) by writing

$$x_j=e^{ikj} \qquad j=1,2,3.$$

Thus

$$\lambda(\boldsymbol{k})=\tfrac{1}{3}(\cos k_1\cos k_2\cos pk_3+\cos k_1\cos pk_2\cos k_3+\cos pk_1\cos k_2\cos k_3).$$

To obtain an asymptotic expression for $P(\boldsymbol{l},x)$, note that for $x\leqslant 1$ and l large, the dominant contribution to the integral arises from those points where $\lambda(\boldsymbol{k})=1$. Therefore, expand $1-x\lambda(\boldsymbol{k})$ in powers of k, ignoring terms of $O(k^3)$. Then perform the integral to obtain

$$P(\boldsymbol{l},x)\sim\frac{3g}{2\pi a^2 l}\exp\frac{-\sqrt{6}l(1-x)^{1/2}}{a} \tag{8}$$

where $l=(l_1^2+l_2^2+l_3^2)^{1/2}$ and g is a factor which accounts for the number of effective points, in the cube of side 2π, where $\lambda(\boldsymbol{k})=1$ (see Joyce 1972, Barrett and Domb 1979).

If P is even there is the point $(0,0,0)$ and the eight points $(\pm\pi,\pm\pi,\pm\pi)$. These latter points are at the corners of the cube, and each is shared by eight similar cubes. The weight for each corner point is therefore $\frac{1}{8}$. Similarly, if P is odd, there is the point $(0,0,0)$ and the twelve points $(0,\pm\pi,\pm\pi)$. The latter are on the edges of the cube and are to be weighted by $\frac{1}{4}$. Finally then

$$\begin{aligned} g&=2 \qquad p \text{ even} \\ g&=4 \qquad p \text{ odd.}\end{aligned} \tag{9}$$

The asymptotic form (8) is identical to that of the Green functions for the cubic lattices. The asymptotic results proved by Barrett and Domb (1979) will therefore be valid for $11P$ walks.

It is possible to make a connection between the usual two-parameter variable

$$z=\left(\frac{3}{2\pi}\right)^{3/2}\frac{N^{1/2}\beta}{a^3} \tag{10}$$

and the excluded volume ratio V. β is the binary cluster integral. Domb and Joyce (1972) have introduced a model which leads to a slightly different definition of z (see also Domb and Barrett 1976). Each self-intersection of a random walk is assigned a statistical weight $1-w$. $w=0$ thus corresponds to a random walk and $w=1$ to a fully self-avoiding one. For this model

$$z=h_0N^{1/2}w \tag{11}$$

where h_0, the *lattice parameter*, is defined by

$$h_0 = \left(\frac{3}{2\pi}\right)^{3/2} \frac{g}{a^3}. \tag{12}$$

We shall use this definition of z. Note that for a self-avoiding lattice walk

$$z = h_0 N^{1/2}.$$

One can make use of this formalism to devise a scaling relationship between excluded volume ratios. Let h_0 and h_0^* be the lattice parameters of two walks exhibiting the same values of z. Then

$$h_0^* N^{1/2} w = h_0 N^{1/2} \qquad w < 1$$

which implies

$$w = h_0 / h_0^*.$$

If both walks have the same value of g and d, and $V^* = 1$, then

$$w = \frac{h_0}{h_0^*} = V^3. \tag{13}$$

Once z has been calculated, the expansion factor

$$\alpha_N^2 = \frac{\langle R_N^2 \rangle}{Na^2}$$

may be computed using an approximate universal formula such as the one proposed by Lax *et al* (1978):

$$\alpha^2 = [1 + 20z 156z^2 + 592z^3 + 325z^4 + 1670z^6]^{1/15}. \tag{14}$$

3. Numerical studies

Exact enumerations and Monte Carlo simulations were performed on two examples of $11P$ walks; the 112 walk which is 'close packed' and the 113 walk which is 'loose packed'. The results follow.

3.1. *Exact enumerations*

The results of the exact enumerations are shown in table 1. The first five terms of the 113 series were computed using the methods described in Barrett (1977). G M Torrie of the University of Toronto kindly agreed to check these results, and in doing so supplied the next two terms of the series, and all seven terms of the 112 series!

Estimates of the exponent γ may be obtained (see Domb 1963) by defining

$$\gamma_N = \frac{N}{2}\left(\frac{\langle R_N^2 \rangle}{\langle R_{N-2}^2 \rangle} - 1\right)$$

and extrapolating the sequences $\gamma_3, \gamma_5, \gamma_7, \ldots,$ and $\gamma_4, \gamma_6, \ldots.$ These ratios are plotted for the 113 walk in figure 3, and unfortunately all that can be said is that $\frac{6}{5}$ is not an inconceivable limit.

Table 1. Exact enumerations

112			113		
N	$C_N/24$	$\langle R_N^2\rangle$	N	$C_N/24$	$\langle R_N^2\rangle$
2	23	12·522	2	23	22·957
3	527	19·139	3	529	34·955
4	12 025	25·869	4	12 091	47·250
5	273 695	32·689	5	276 421	59·548
6	6216 581	39·597	6	6296 699	72·101
7	140 975 467	46·585	7	143 487 903	84·652

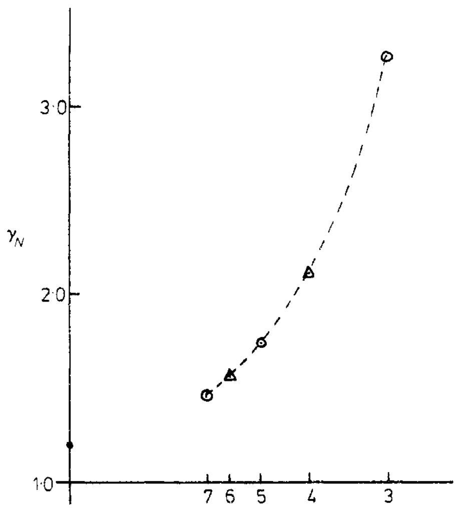

Figure 3. Ratios of exact enumerations, 113 walk. ●, universal value 1·2; ○, odd ratios; △, even ratios.

Similarly, very little can be done to estimate μ and g. S G Whittington (private communication) has noted a modification to Hammersley's inequality in the form

$$\lg \mu \leqslant \frac{1}{N} \lg\left(\frac{q-1}{q} C_N\right) \tag{15}$$

where q is the coordination of the lattice. We thus obtain the following upper bounds on μ:

$$\mu \leqslant 22{\cdot}898 \qquad (113)$$

$$\mu \leqslant 22{\cdot}840 \qquad (112).$$

All attempts to obtain an estimate of g from these series were fruitless.

3.2. *Monte Carlo simulations*

For each of the 112 and 113 walks, a sample in excess of 500 000 walks from 1 to 100 steps was generated, in blocks of 10 000 walks each. The method used is that of

Rosenbluth and Rosenbluth (1955), which yields an unbiased estimate of the total number of walks, and a biased estimate of the mean square length (McCrackin 1972, McCrackin *et al* 1973). Computed estimates of this bias are less than 1% of one standard deviation, and we have therefore ignored it. The data are displayed in table 2; the uncertainties shown are two standard deviations of the block averages. It can be seen that the first seven terms are comfortably within one standard deviation of the exact values.

Table 2. Monte Carlo data.

	112			113	
N	$C_N/24\times 23^{N-1}$	$\langle R_N^2\rangle$	N	$C_N/24\times 23^{N-1}$	$\langle R_N^2\rangle$
2	1·000	12·515±0·131	2	1·000	22·895±0·232
3	0·996	19·125±0·239	3	1·000	34·921±0·382
4	0·988	25·879±0·344	4	0·994	47·174±0·559
5	0·978	32·709±0·490	5	0·988	59·451±0·820
6	0·966	39·613±0·561	6	0·978	71·938±1·08
7	0·952	46·655±0·635	7	0·969	84·501±1·22
50	0·360	389·173±6·69	50	0·462	691·134±10·6
60	0·280	476·173±8·78	60	0·379	843·294±12·4
70	0·216	564·736±10·1	70	0·310	998·812±15·9
80	0·167	655·023±12·1	80	0·254	1157·741±19·6
90	0·129	746·575±13·7	90	0·207	1317·465±22·4
100	0·099	840·680±17·5	100	0·168	1480·655±28·5

A plot of $\lg\langle R_N^2\rangle$ versus $\lg N$ for all the data (of the 112 walk) is shown as figure 4. The mere fact that there is curvature present in this plot indicates that the simple formula (1) is inadequate, and that correction terms are needed. However, a weighted

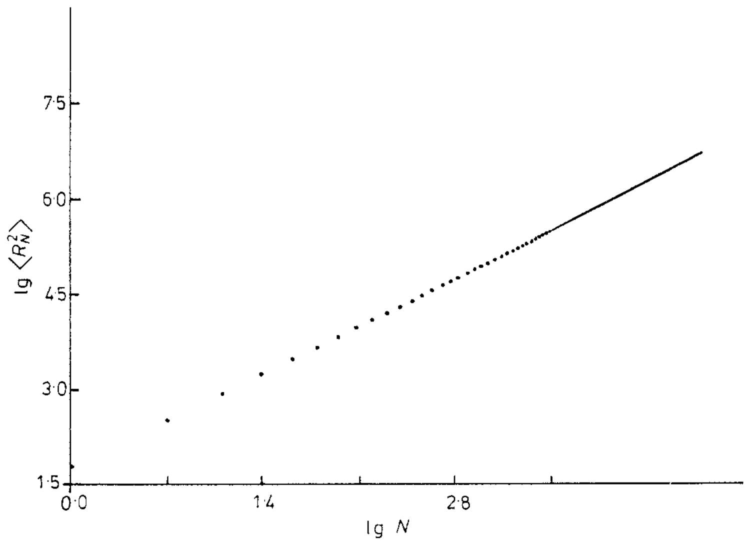

Figure 4. Monte Carlo data, 112 walk. Note curvature.

least squares fit of the 'linear' portion of the curves ($N > 50$) yields

$$\gamma = 1\cdot1008, C = 9\cdot303 \qquad (113)$$

$$\gamma = 1\cdot1098, C = 5\cdot062 \qquad (112).$$

The values of γ are certainly less than the predicted 'universal' values 1·2.

A weighted least squares fit of the same data ($N \geqslant 50$) to the Darboux form (3) yields

$$A = 5\cdot489, B = 42\cdot25 \qquad (113)$$

$$A = 3\cdot134, B = 21\cdot80 \qquad (112).$$

Figure 5 shows a comparison of the Monte Carlo data to the fitted forms (1) and (3). The difference between the two is not significant, but the second is perhaps to be preferred on theoretical grounds.

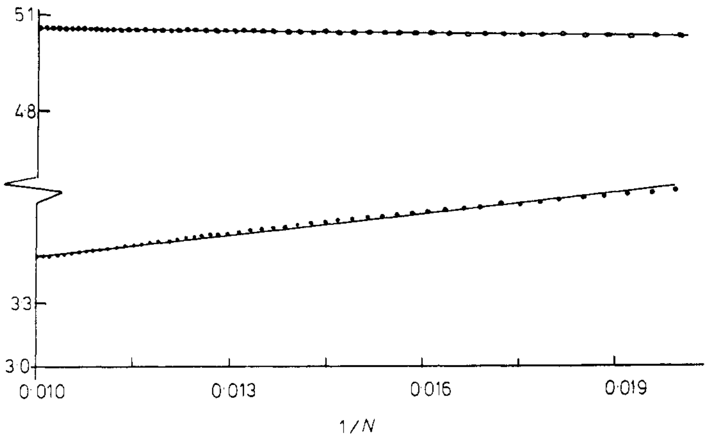

Figure 5. Comparative fit of Monte Carlo data with fitted expressions, 112 walk. ● $\langle R_N^2\rangle/N^{1\cdot11}$, ● $\langle R_N^2\rangle/N^{1\cdot2}$. Upper full line, $C = 5\cdot062$; lower full line $A + B/N = 3\cdot134 + 21\cdot8/N$.

It has been proposed (Barrett 1975, 1976) that

$$A = (2\sqrt{\pi}h_0)^{2/5}a^2 \qquad (16)$$

for the cubic lattices. Assuming the same relation for the $11P$ walks, we expect

$$A = 4\cdot837 \qquad (113)$$
$$A = 2\cdot877 \qquad (112)$$

which differs by approximately 10% from the Monte Carlo values. The agreement may not be convincing, but it is tempting.

Finally, the data for $N \geqslant 50$ has been compared with the predictions of the universal formula (14). The difference is at most a satisfying 2% (agreement this good is probably fortuitous).

The total number of walks C_N has been fitted to the relation

$$\lg C_N = \lg D + N \lg \mu + g \lg N$$

by non-linear regression (see, for example, Nielson 1964). The results are:

$$\begin{aligned} \lg D &= -0{\cdot}108 \pm 0{\cdot}001,\ g = 0{\cdot}120 \pm 0{\cdot}001,\ \lg \mu = 3{\cdot}114 \pm 0{\cdot}001 \qquad (113) \\ \lg D &= -0{\cdot}086 \pm 0{\cdot}001,\ g = 0{\cdot}125 \pm 0{\cdot}001,\ \lg \mu = 3{\cdot}108 \pm 0{\cdot}001 \qquad (112). \end{aligned} \tag{17}$$

The corresponding estimates of μ are

$$\begin{aligned} \mu &= 22{\cdot}503 \qquad (113) \\ \mu &= 22{\cdot}373 \qquad (112). \end{aligned}$$

Since $\lim_{N\to\infty} (1/N) \lg C_N = \lg \mu$, it is possible to estimate μ by extrapolating the sequence $\{(1/N) \lg C_N\}$. The values obtained in this way are:

$$\begin{aligned} \lg \mu &= 3{\cdot}115 \pm 0{\cdot}001 \qquad (113) \\ \mu &= 22{\cdot}539 \\ \lg \mu &= 3{\cdot}109 \pm 0{\cdot}001 \qquad (112) \\ \mu &= 22{\cdot}410. \end{aligned} \tag{18}$$

If μ is known then one may estimate g by fitting $\lg(C_N/\mu^N)$ versus $\lg N$. However, no reasonable value of g is obtained in this fashion if the estimates (18) are used. g is clearly a very sensitive function of μ.

Alternatively one can assume $g = \frac{1}{6}$ and then fit $\lg(C_N/N^g)$ versus N to obtain $\lg \mu$. The results are:

$$\begin{aligned} \lg \mu &= 3{\cdot}1130 \pm 0{\cdot}0004 \qquad (113) \\ \mu &= 22{\cdot}490 \\ \lg \mu &= 3{\cdot}107 \pm 0{\cdot}001 \qquad (112) \\ \mu &= 22{\cdot}361 \end{aligned} \tag{19}$$

in close agreement with (17). Clearly, $g = \frac{1}{6}$ cannot be excluded.

4. Conclusions

We have assumed particular expressions for the numbers of self-avoiding walks and their mean square lengths based on the principle of universality, and a theorem of Darboux. We have examined the 112 and 113 self-avoiding walks to determine whether or not these walks fit into the 'universal' scheme. We find, in fact, that they fit reasonably well. Indeed we find that the formulae (3), (14) and (16) provide a good description of the 112 and 113 walks as well as of the cubic lattice self-avoiding walks. We regard this as additional evidence of an 'experimental' nature supporting the universality hypothesis.

Acknowledgments

S G Whittington and G M Torrie have made a handsome contribution to this work, as have R Benesch, R Swift and E Allen. D DeKee provided the non-linear regression program. Thanks are also due to CVW.

Appendix 1. Proof of theorems

Proof of theorem 1. The lattice walk generating function is defined by (6). The probability that the random walker arrives at the point (l_1, l_2, l_3) on the Nth step is the coefficient of $x_1^{l_1}x_2^{l_2}x_3^{l_3}$ in $[\phi(x_1, x_2, x_3)]^N$. ϕ^N is a linear combination of terms of the form

$$x_1^{j_1+j_2(-1)+j_3p+j_4(-p)}x_2^{k_1+k_2(-1)+k_3p+k_4(-p)}x_3^{m_1+m_2(-1)+m_3p+m_4(-p)}$$

with the following conditions on the j_i, k_i, m_i:

(1) $j_i \geq 0, k_i \geq 0, m_i \geq 0; i = 1, 2, 3, 4.$

(2) $\sum_{j=1}^{4} j_i = \sum_{i=1}^{4} k_i = \sum_{i=1}^{4} m_i = N.$

(3) $j_1 + j_2 + k_1 + k_2 + m_1 + m_2 = 2(j_3 + j_4 + k_3 + k_4 + m_3 + m_4).$

(4) $j_1 - j_2 + (j_3 - j_4)p = l_1$

$k_1 - k_2 + (k_3 - k_4)p = l_2$

$m_1 - m_2 + (m_3 - m_4)p = l_3.$

The third condition arises from the fact that two of the x_i have an exponent ± 1, while only one has an exponent $\pm p$, in each term of ϕ.

Define

$$A = j_1 - j_2 + k_1 - k_2 + m_1 - m_2$$
$$B = j_3 - j_4 + k_3 - k_4 + m_3 - m_4.$$

Since $j_1 - j_2$ has the same parity (even or odd) as $j_1 + j_2$, it follows from condition (3) that A is even. It follows from condition (2) that B has the same parity as $3N$, and hence as N.

Setting $l_1 = 1$, $l_2 = l_3 = 0$ in condition (4), and adding we find

$$A + Bp = 1.$$

Case 1. p even. This is clearly impossible.

Case 2. p odd. For this to be possible, B and hence N must be odd. But if p is odd, it follows from condition (4) that $k_1 - k_2$ and $k_3 - k_4$ must have the same parity for $l_2 = 0$. Then $N = k_1 + k_2 + k_3 + k_4$ must be even, which is a contradiction.

Proof of theorem 2. Necessity: assume p odd. Setting $l_1 = l_2 = 1$, $l_3 = 0$ in condition (4) of the preceding proof, we obtain

$$A + Bp = 2$$

which implies that B and hence N must be even. But condition (4) implies that $k_1 - k_2$ and $k_3 - k_4$ must have opposite parity for p odd and $l_2 = 1$. Therefore N must be odd from condition (2), which is a contradiction.

Sufficiency. It suffices to find numbers $j_1, j_2, \ldots, m_4$ such that the conditions (1)–(4) are satisfied. Set

$$\boldsymbol{j} = (1, p, 1, 0) \qquad N = p + 2$$
$$\boldsymbol{k} = (1, p, 1, 0) \qquad p \text{ even}$$
$$\boldsymbol{m} = (1, 1, p/2, p/2).$$

Write N factors of $x_1 x_2 x_3$. To j_1 of the x_1 assign the exponent 1; to j_2 of the x_1 attach the exponent -1, to j_3 of x_1 assign the exponent p, and to the remaining $j_4 x_1$ assign the exponent $-p$. Assign exponents to the x_2 and x_3 in the same way.

Each factor then represents one step of a path from the origin to the point (l_1, l_2, l_3).

Proof of theorem 3. Necessity: suppose p to be even. Then if the point $(1, 1, 1)$ is accessible, the point $(1, 1, 0)$ is not, by theorem 1. This contradicts theorem 2.

Sufficiency. Set

$$\boldsymbol{j} = \boldsymbol{k} = \boldsymbol{m} = \left(\frac{3p+3}{2}, \frac{5p+1}{2}, p+1, p\right)$$
$$N = 6p + 3 \qquad p \text{ odd}.$$

Appendix 2. Functions of Darboux type

The choice of the asymptotic form

$$\langle R_N^2 \rangle = AN^{6/5}\left[1 + \frac{B}{N} + \mathrm{O}\left(\frac{1}{N^2}\right)\right]$$

is not as arbitrary as might first appear. Darboux (1878) has proved the following theorem (see also Domb 1971).

If $F(z)$ has an isolated singularity at $z = \alpha$ on the circle of convergence, and can therefore be written as

$$F(z) = (\alpha - z)^{-\gamma} G(z) + H(z)$$

where G and H are regular at $z = \alpha$, then the coefficients a_N of the Maclaurin expansion

$$F(z) = \sum a_N z^N$$

may be written asymptotically as

$$a_N = AN^{\gamma - 1}\left[1 + \frac{B}{N} + \mathrm{O}\left(\frac{1}{N^2}\right)\right].$$

The theorem is, in fact, valid for any function which is analytic save for a number of isolated singularities. γ in this case would be the index of the dominant singularity closest to the origin.

To illustrate the ideas involved we reproduce here the proof for the special case where γ is an integer. Write

$$F(z) = \frac{A_0}{(\alpha - z)^{\gamma}} + \frac{A_1}{(\alpha - z)^{\gamma - 1}} + \ldots + H(z).$$

Expanding both sides in Maclaurin series and equating coefficients of z^N:

$$\alpha^N a_N = \frac{A_0}{\alpha^\gamma}(N+1)(N+2)\ldots(N+\gamma-1)$$

$$= \frac{A_1}{\alpha^{\gamma-1}}(N+1)(N+2)\ldots(N+\gamma-2)+\ldots$$

which completes the proof.

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