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Self-avoiding walks on oriented square lattices

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Abstract. An analysis is undertaken of the self-avoiding walk problem on two distinct oriented square lattices. The importance of these two oriented cases to the problem on the unoriented square lattice is pointed out by means of a number of transformations showing the interdependence of various apparently different 'walk' problems on the oriented and unoriented square lattices.

The total number of self-avoiding walks, C_N, and their mean-square sizes, $\langle R_N^2\rangle$, are exactly enumerated on a computer up to 28 and 36 steps for the two oriented square lattices respectively.

Rigorous upper and lower bounds together with estimates are presented for the connective constant $\mu(\mu \equiv \lim_{N\to\infty} C_N^{1/N})$ for both the oriented square lattices.

An investigation of the data for the mean-square sizes strongly suggests that if the asymptotic form $\langle R_N^2\rangle = AN^\gamma + \ldots$ is assumed, then the effect of the two specific orientations dealt with is to change the constant A but not the critical exponent γ. The validity of the conjecture $\gamma = 1.5$ in two dimensions is discussed in the light of the new results. Estimates for the constant A are obtained for several 'restricted' cases with the assumption that $\gamma = 1.5$

Substantial support is provided, by means of our transformations and results, to the recently proposed view that the critical indices of the self-avoiding walks are not changed by the exclusion of nearest-neighbour contacts or by the introduction of 'weak' attractive nearest-neighbour forces.

1. Introduction

The self-avoiding walk problem on a crystal lattice is a well-established model of lattice statistics. Mathematically this problem is of great interest since it forms a well defined non-Markovian process.

Physically the problem is of considerable importance for it takes account in a realistic way of the 'excluded volume' effect of a polymer chain in dilute solutions (Domb 1963). The model is related to other problems in lattice statistics, namely the Ising problem of ferromagnetism (Domb 1970a, Fisher and Sykes 1959) and related topics.

The self-avoiding condition, whereby the walk does not involve double occupancy of any lattice site, introduces a long range interaction between the steps of the walk which has proved to be a particularly intractable problem. Although the problem is still far from being solved there is now a considerable amount of information regarding at least three main properties of self-avoiding walks which, in order of physical significance, are the following.

(i) The mean square end-to-end distance $\langle R^2\rangle$.
(ii) The distribution function for self-avoiding walks.
(iii) The total number of self-avoiding walks of N steps C_N.

Nevertheless the only definite mathematical information available is concerned with property (iii) (Hammersley 1957, Kesten 1963) and property (ii) (Fisher 1966, Chay 1972). It is true that most of the studies of this problem are computer-oriented, and it is probably as a result of these studies that a good deal of information is now available. This latter computer-oriented approach has followed two independent directions, namely the Monte Carlo and the exact enumeration methods.

In the present paper we shall follow the latter of these two methods and we enumerate all the possible self-avoiding walks up to a certain number of steps for two distinct (although related) orientations on the square lattice.

Section 2 has been devoted to explaining the motive behind our investigation and to describing a number of transformations of self-avoiding walks with attractive or repulsive forces between nearest-neighbour contacts on the oriented and unoriented square lattices. The interdependence of these problems suggests that the critical indices α and γ (see equations (1) and (2) below) are unchanged for a variety of apparently different problems and this is further discussed in §§ 5 and 6. The results of our enumeration are presented in § 3 (see table 1), up to 28 and 36 steps for the two oriented cases respectively. Upper and lower bounds together with estimates for the asymptotic behaviour of the total number of self-avoiding walks are determined in § 4 for both these oriented square lattices.

In particular it is argued that the conjectured asymptotic form for the total number of self-avoiding walks

$$C_N \simeq N^{\alpha}\mu^N \tag{1}$$

is valid for both the oriented cases. N is the number of steps, μ is the so-called connective constant (or attrition parameter) and the exponent α is a constant conjectured to depend on the 'dimensionality' of the lattice (Fisher and Sykes 1959).

Section 5 is devoted to an investigation of the mean square end-to-end distance $\langle R^2 \rangle$. It is shown that according to our transformation in § 2 the effect of the orientation (obtained by means of this transformation) on the shape of self-avoiding walks on the unoriented square lattice can be described as a repulsive or attractive potential (depending on the orientation) between nearest-neighbour contacts. In particular one of these orientations (UMS orientation, see § 2) acts via the transformation as a repulsive potential between nearest-neighbour contacts or, to use a different terminology, as a weighting function on the entire sample of self-avoiding walks on the unoriented square lattice. Thus it is argued (and we produce numerical results to justify this) that the mean square end-to-end distance for the unoriented square lattice lies between the corresponding quantities for the two unoriented square lattices described in § 2. In particular our numerical evidence shows that if we assume (as is usually done) the asymptotic form

$$\langle R_N^2 \rangle \simeq AN^{\gamma} \tag{2}$$

then the effect of these orientations is to change the constant A but not the critical exponent γ.

This is completely justified since we are using the same model (namely a specific traffic regulation) to describe two apparently different problems, ie a self-avoiding walk problem with successive steps of the walk at right angles and a self-avoiding walk problem with a repulsive potential between nearest-neighbour contacts. It is true that one should not expect the restriction of fixed angles between successive steps of the walk to change the critical exponent γ; therefore our transformation suggests that neither is the repulsive potential thus introduced strong enough to change γ.

Finally our conclusions are summarized in § 6.

2. Trivial and non-trivial traffic regulations

In this section we shall briefly discuss the random and self-avoiding walk problem on a square lattice with certain orientations.

Clearly, for certain orientations, any co-oriented walk is a self-avoiding walk, ie the self-avoidance condition is removed by the restrictions of the orientation. Let us consider in particular the orientation which allows the walk to proceed either upwards or to the right only. Hence, it follows that

$$C_N = 2^N \qquad \langle R_N^2 \rangle = (1/2^N) \sum_{n=0}^{N} \binom{N}{n} (N^2 - 2nN + 2n^2).$$

Thus we obtain

$$\tfrac{1}{2}N^2 \leqslant \langle R_N^2 \rangle \leqslant N^2$$

or

$$\langle R_N^2 \rangle \sim N^2.$$

Such orientations which remove the self-avoiding condition are much easier to solve (another less trivial example, but one that still gives results similar to those shown above, is obtained by not allowing the walks to progress in the $-Y$ direction), but they have a crucial effect on the asymptotic behaviour of the mean square end-to-end distance, $\langle R^2 \rangle$. One of the main questions to be answered in this paper is the following: do orientations which preserve the self-avoidance condition change the asymptotic behaviour of $\langle R^2 \rangle$ and in particular the critical exponent γ? The answer to this question is not by any means easy, but we conjecture that for certain orientations equation (2) is valid and in particular that the critical exponent γ is the same as in the unoriented case.

We have chosen for our study two particular orientations as shown in figures 1 and 2. In fact these orientations are related by the covering operation as shown by Kasteleyn (1963). Following Kasteleyn we shall refer to the oriented square lattice in figure 1 as the Manhattan-square lattice (MS) and to the oriented square lattice in figure 2 as the underlying lattice of the Manhattan-square lattice (UMS).

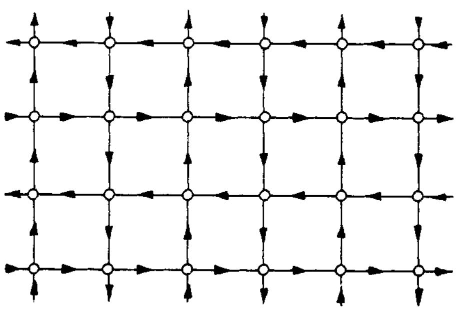

Figure 1. Square lattice oriented in accordance with the 'Manhattan' orientation (MS lattice).

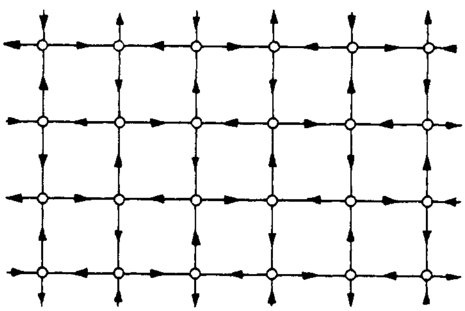

Figure 2. Square lattice oriented in accordance with the underlying orientation of the 'Manhattan' orientation (UMS lattice). Note that the Manhattan square lattice in figure 1 may be obtained from this lattice by means of the covering operation (Kasteleyn 1963).

The first striking observation regarding walks between these two oriented lattices arises from the fact that they (ie the above mentioned lattices) are related by means of the covering operation. Thus we may easily prove that there is a one-to-one correspondence between N-stepped 'trails' (ie walks not involving double occupancy of any step) on the UMS lattice and $(N-1)$-stepped self-avoiding walks on the MS lattice.

There is also a further one-to-one correspondence between N-stepped self-avoiding walks on the UMS lattice and $(N-1)$-stepped self-avoiding walks with no nearest-neighbour contacts on the MS lattice.

Similar relationships have been demonstrated by Watson (1970, 1974) for unoriented lattices related by the covering operation (Watson's publications were discovered by the present author immediately prior to the completion of this paper.)

Nevertheless the transformations described above establish the equivalence between 'walk' problems on the two oriented square lattices and although useful they are of limited importance. The following transformations (illustrated in figure 3) define relationships between 'walk' problems on oriented and unoriented square lattices and, in our opinion, they have far reaching consequences.

First, for the UMS lattice it can be easily shown that there is a one-to-one correspondence between N-stepped random walks on the unoriented square lattice and $2N$-stepped random (co-oriented) walks on the UMS lattice. This is shown by orienting (as with the UMS lattice) the lattice resulting from superposition of the square lattice over its dual (see figure 3). Therefore we may show that

$$\langle R_N^2 \rangle_{\mathrm{UMS}}^{\mathrm{r}} = b^2 N \tag{3}$$

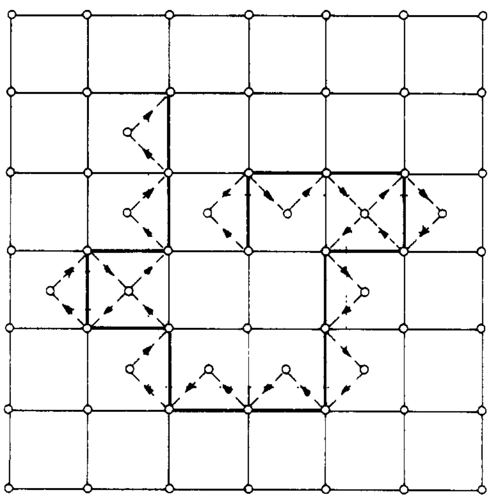

Figure 3. Example to illustrate the correspondence between walks on the oriented and unoriented square lattices. Heavy lines show a self-avoiding walk (of 15 steps) on the square lattice. Broken oriented lines represent the corresponding walk (of 30 steps) on a square lattice constructed as indicated by these lines and oriented as with the UMS lattice (figure 2). Note that the intersections along the oriented walk are the result of certain nearest-neighbour contacts along the unoriented self-avoiding walks (see also figure 5). Finally dotted lines represent the corresponding self-avoiding walk (of 39 steps) on the Manhattan square lattice.

where the superscript r refers to random walks and b is the lattice spacing of the UMS lattice. A similar result holds for the MS lattice.

The above result and the fact that the self-avoiding condition is maintained on these oriented lattices is an indication that the critical exponent may be the same as in the unoriented case. Another stronger indication is the following observation. For every $2N$-stepped self-avoiding walk on the UMS lattice there corresponds exactly one N-stepped self-avoiding walk on the unoriented square lattice. The reverse is not true (see example in figure 3). Thus since the self-avoidance condition tends to increase γ we may expect that

$$\gamma_{\mathrm{UMS}} \geqslant \gamma_{\mathrm{S}}. \tag{4}$$

Nevertheless numerical evidence shows (see §§ 3 and 5) that

$$\gamma_{\mathrm{UMS}} = \gamma_{\mathrm{S}}. \tag{5}$$

It follows from the above that

$$\mu_{\mathrm{UMS}} \leqslant \mu_{\mathrm{S}}^{1/2}. \tag{6}$$

Following similar considerations and using the covering property between the UMS and MS lattices we easily prove that, for every N-stepped self-avoiding walk on the square lattice, there corresponds exactly one $(2N-1)$-stepped self-avoiding walk on the MS lattice. The reverse is not true. Thus we obtain

$$\mu_{\mathrm{MS}} \geqslant \mu_{\mathrm{S}}^{1/2} \tag{7}$$

and we expect

$$\gamma_{\mathrm{MS}} \leqslant \gamma_{\mathrm{S}}. \tag{8}$$

3. The method of exact enumeration

As mentioned in the introduction one of the major attempts to investigate the self-avoiding walk problem on lattices consists in replacing the mathematical analysis of the problem by a digital computer algorithm. Two independent approaches have been followed, ie the Monte Carlo method (Wall and Erpenbeck 1959) and the exact enumeration method (Domb 1969). Both methods arrive independently at similar conclusions and there is now a good deal of information regarding various properties of self-avoiding walks. Our purpose in this paper is to compare these properties as they appear between the oriented and unoriented cases and to determine whether the specific traffic regulations (UMS and MS lattices) introduced in § 2 change the characteristics of these properties radically.

This comparison will be facilitated by employing the exact enumeration method since it seems to be better suited for this purpose.

In table 1 we present the results for the total number of self-avoiding walks C_N and the mean-square end-to-end distance, $\langle R_N^2\rangle$, for the following three cases.

(a) Square lattice (S) up to 18 steps (Domb 1963).
(b) Manhattan-square lattice (MS) up to 28 steps.
(c) The underlying lattice of the Manhattan-square lattice (UMS) up to 36 steps.

The work was executed on a PDP 10 computing machine. The program has been developed by the present writer and was written in ALGOL 60. The execution time for $N = 28$ and $N = 36$ for the MS and the UMS lattices respectively was in both cases nearly 4 h.

Previous results for the total number of self-avoiding walks, C_N, on the MS lattice by Barber (1970) up to 21 steps, together with the well-known results for the unoriented square lattice have served as a test of the accuracy of our program.

Table 1.

	S lattice		MS lattice		UMS lattice	
N	C_N	$\langle R_N^2 \rangle$	C_N	$\langle R_N^2 \rangle$	C_N	$\langle R_N^2 \rangle$
1	4	1·0000	2	1·0000	2	1·0000
2	12	2·6667	4	3·0000	4	2·0000
3	36	4·5556	8	5·0000	8	3·0000
4	100	7·0400	14	8·0000	12	5·3333
5	284	9·5634	26	10·8462	20	7·4000
6	780	12·5744	48	13·6667	32	10·0000
7	2172	15·5562	88	16·6364	52	12·6923
8	5916	19·0128	154	20·5714	84	15·6190
9	16268	22·4114	278	24·0216	136	18·6471
10	44100	26·2425	500	27·5760	220	21·7818
11	120292	30·0177	900	31·1511	356	25·0000
12	324932	34·1870	1576	35·7005	564	28·8794
13	881509	38·3043	2806	39·7855	904	32·5575
14	2374444	42·7864	4996	43·9023	1448	36·3425
15	6416596	47·2178	8894	48·0573	2320	40·2000
16	17245332	51·9925	15564	53·1380	3684	44·5081
17	46466676	56·7164	27538	57·7414	5872	48·7439
18	124658732	61·7665	48726	62·3746	9376	52·9625
19			86212	67·0452	14960	57·2770
20			150792	72·5750	23688	62·1101
21			265730	77·6521	37652	66·7886
22			468342	82·7530	59912	71·4555
23			825462	87·8873	95316	76·1833
24			1442866	93·8879	150744	81·4329
25			2535802	99·3382	239080	86·5250
26			4457332	104·8679	379528	91·5915
27			7835308	110·4280	602424	96·7111
28			13687192	116·7494	951788	102·3426
29					1507136	107·8105
30					2388252	113·2487
31					3784344	118·7321
32					5973988	124·7198
33					9447880	130·5386
34					14950796	136·3247
35					23658540	142·1511
36					37321752	148·4715

4. Bounds and asymptotic behaviour for the number of self-avoiding walks

In this section we shall derive upper and lower bounds for the asymptotic behaviour of the total number of self-avoiding walks on both the MS and UMS lattices. Estimates will also be given using the results shown in table 1.

First let us consider the MS lattice. For this lattice an exact solution was obtained by Kasteleyn (1963) for the different (albeit related) problem of Hamiltonian walks, ie self-avoiding walks filling the lattice (for further progress on this problem and its applications to the theory of polymers see Gordon *et al* 1975, Malakis 1975). Kasteleyn showed that the number of Hamiltonian walks on the MS lattice varies asymptotically as $(1{\cdot}338\ldots)^N$, where N is the total number of lattice sites. Later Barber and Ninham (1970) conjectured that the same number describes the asymptotic behaviour of the number of self-avoiding walks on the MS lattice. Nevertheless the same author (Barber 1970) realized that the limiting processes of the two problems are essentially different and by using the method of exact enumeration and the well-known ratio and Padé techniques he estimated that

$$\mu_{\mathrm{MS}} = 1{\cdot}733 \pm 0{\cdot}003 \tag{9}$$

and that the exponent α in equation (1) was

$$\alpha = 0{\cdot}33 \pm 0{\cdot}03. \tag{10}$$

A lower bound for these walks may easily be obtained by not allowing the walks to progress in the $-Y$ direction, thus obtaining for the generating function

$$G(x) = 1 + xG(x) + x^2G(x) \tag{11}$$

which produces the following lower bound:

$$\mu_{\mathrm{MS}} \geqslant \tfrac{1}{2}(1+5^{1/2}) = 1{\cdot}618\ldots. \tag{12}$$

An upper bound may be determined by considering walks with no square intersections. The oriented graph which eliminates the square intersections along the walks on the MS lattice is shown in figure 4(*a*). The dominant eigenvalue of the adjacency matrix of this graph provides the following upper bound:

$$\mu_{\mathrm{MS}} \leqslant 1{\cdot}839\ldots. \tag{13}$$

Let us next consider the UMS lattice. Following a similar procedure we find that

$$1{\cdot}414\ldots \leqslant \mu_{\mathrm{UMS}} \leqslant 1{\cdot}618\ldots. \tag{14}$$

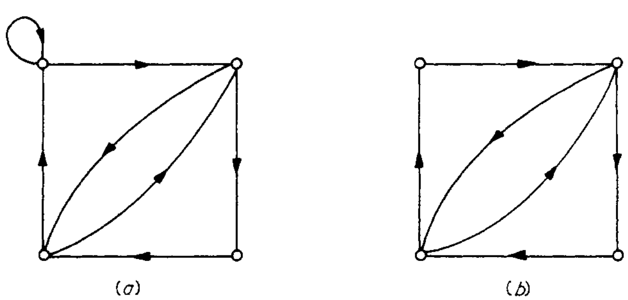

Figure 4. (*a*) The oriented graph which eliminates square intersections along the walks on the Manhattan square lattice. (*b*) The oriented graph which eliminates square intersections along the walks on the UMS lattice.

The oriented graph which eliminates the square intersections along the walk on the UMS lattice is shown in figure 4(*b*). Finally, using the results given in table I (columns 4 and 6) and the ratio method (Fisher 1967), we confirm the estimates (9) and (10) given by Barber, and we find that for the UMS lattice

$$\mu_{\mathrm{UMS}} = 1{\cdot}559 \pm 0{\cdot}003 \tag{15}$$

and for the exponent α

$$\alpha = 0{\cdot}32 \pm 0{\cdot}02. \tag{16}$$

Thus it appears that the formula $C_N \simeq N^{\alpha}\mu^N$ holds asymptotically for both the MS and UMS oriented lattices and, in particular, we note that the exponent α seems to retain its two-dimensional value, namely $\alpha = \frac{1}{3}$ (Fisher and Sykes 1959).

5. The mean-square end-to-end distance

It will easily be seen from the transformation described in § 2 (see also figure 3) that the UMS orientation shown in figure 2 defines a certain subclass of the total class of self-avoiding walks on the unoriented square lattice. More precisely the orientation acts as a weighting function on the total class of all the topologically distinct self-avoiding walks on the square lattice. The weights thus assigned are 0, $\frac{1}{2}$ and 1. In order to illustrate this, one example of each case is given in figure 5, where the length of the walks is taken to be eight. It is important to note that the weight 1 is assigned to self-avoiding walks with no nearest-neighbour contacts, whereas the weights $\frac{1}{2}$ and 0 are assigned to self-avoiding walks with *at least* one and two nearest-neighbour contacts respectively.

We would expect the mean-square end-to-end distance for these walks to lie between the corresponding quantities for simple self-avoiding walks and self-avoiding walks with no nearest-neighbour contacts at all. The results obtained below provide strong support for the above observation and throw considerable light on the problem as a whole. Similar considerations hold for the self-avoiding walk problem on the MS lattice, but these will be omitted for brevity.

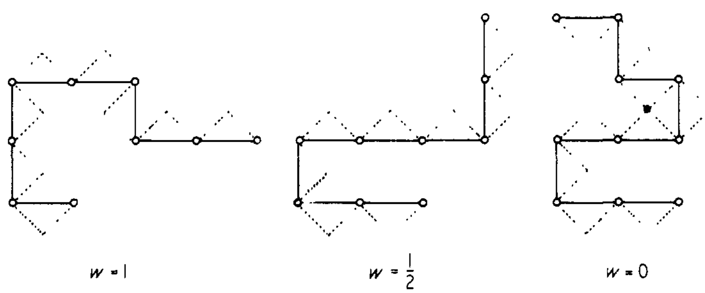

Figure 5. Three examples of self-avoiding walks on the unoriented square lattice to illustrate the relationship between self-avoiding walks on the unoriented square and the UMS lattices. Note that the weight $w = 1$ is assigned to self-avoiding walks with no nearest-neighbour contacts. The weight $w = \frac{1}{2}$ is assigned to self-avoiding walks with at least one nearest-neighbour contact. The meaning of the value $\frac{1}{2}$ is that half of the number of self-avoiding walks with a topology such as shown above (case two) is ruled out by the restrictions of the orientation. The last example ($w = 0$) clarifies the kind of topologies which are ruled out completely by the restrictions of the orientation.

Let a and b denote the lattice spacings of the square and UMS lattices respectively. Since $a^2 = 2b^2$ (see figure 3), it follows that the corresponding mean-square end-to-end distances are related by

$$\langle R_N^2\rangle_S^s = \tfrac{1}{2}\langle R_{2N}^2\rangle_{UMS} \tag{17}$$

where both $\langle R_N^2\rangle_S^s$ and $\langle R_{2N}^2\rangle_{UMS}$ are determined with their lattice spacings taken as unity and the superscript, s, is introduced to show that we are referring to a certain subclass of the total class of self-avoiding walks on the square lattice.

Thus, in order to determine the mean-square distance, $\langle R_N^2\rangle_S^s$, for the above-described subclass, one has to divide the corresponding quantity for $2N$ steps in the last column of table 1 by a factor of two. The resultant values are all higher than the corresponding values for the total class of self-avoiding walks in column 3 of table 1. Furthermore the ratio $\langle R_N^2\rangle_S^s/\langle R_N^2\rangle_S$ depends linearly on $1/N$ and tends to a limiting value. Thus if we define

$$a_N = \langle R_N^2\rangle_S^s/\langle R_N^2\rangle_S \tag{18}$$

then the linear projections defined by

$$a_N^* = (1/i)[(N+i)a_{N+i} - Na_N] \tag{19}$$

should provide successive estimates of the limiting value of a_N, $a = \lim_{N\to\infty} a_N$. Repeated application of equation (19) for $i = 2$ yields table 2 from which we may confidently estimate that

$$a = 1{\cdot}215 \pm 0{\cdot}005. \tag{20}$$

Similarly the total class of self-avoiding walks on the MS lattice defines a class of walks on the unoriented square lattice which includes all the self-avoiding walks on the unoriented square lattice together with self-intersecting walks on the same lattice. Following considerations similar to those outlined above we may define

$$b_N = \tfrac{1}{4}\langle R_{2N-1}^2\rangle_{MS}/\langle R_N^2\rangle_S. \tag{21}$$

Incidentally, there is a minor error in this calculation, in that the starting and ending points of the walks for the two cases (ie the self-avoiding walks on the MS lattice and the walks on the square lattice defined by the MS orientation) do not coincide; but this would make no difference to our calculations.

Table 3 shows that

$$b = \lim_{N\to\infty} b_N = 0{\cdot}66 \pm 0{\cdot}01. \tag{22}$$

Furthermore it is seen that the values of b_N constantly increase with N and since on physical grounds they would not exceed unity, we may safely conclude that they tend to a non-zero limiting value.

Now let us turn our attention to the asymptotic form, equation (2). If the mean-square end-to-end distances for all the three cases (S, M, UMS lattices) are given by equation (2) then the fact that a_N and b_N tend to the limiting values a and b respectively implies that

$$\gamma_{MS} = \gamma_S = \gamma_{UMS} = \gamma. \tag{23}$$

Consequently using the estimates (20) and (21) we find

$$A_S^s = (1{\cdot}215 \pm 0{\cdot}005)A_S \tag{24a}$$

$$A_{UMS} = (1/2^{\gamma-1})(1{\cdot}215 \pm 0{\cdot}005)A_S \tag{24b}$$

$$A_{MS} = 2^{2-\gamma}(0{\cdot}66 \pm 0{\cdot}01)A_S. \tag{24c}$$

Table 2. Estimates for the ratios $a_N = \langle R_N^2\rangle_S^s/\langle R_N^2\rangle_S$.

N	a_N	a_N^*	$(a_N^*)^*$	$((a_N^*)^*)^*$
1	1·0000			
		1·1464		
2	1·0000		1·2278	
		1·2186		1·3396
3	1·0976		1·2342	
		1·2007		1·2814
4	1·1093		1·3023	
		1·2264		1·0404
5	1·1388		1·2578	
		1·2413		1·1727
6	1·1483		1·1976	
		1·2369		1·3103
7	1·1681		1·2295	
		1·2288		1·1315
8	1·1705		1·2298	
		1·2350		1·1272
9	1·1816		1·2050	
		1·2290		1·2301
10	1·1834		1·2070	
		1·2290		1·2291
11	1·1902		1·2100	
		1·2250		1·2031
12	1·1910		1·2110	
		1·2258		1·2099
13	1·1956		1·2088	
		1·2229		1·2136
14	1·1960		1·2108	
		1·2234		
15	1·1992		1·2095	
		1·2213		
16	1·1994			
		1·2217		
17	1·2018			
18	1·2019			

The above equations ((23) and (24)) will be valid (provided that our estimates (20) and (21) are correct) even if the asymptotic form (2) is not, and the more general behaviour (25) is assumed.

$$\langle R_N^2\rangle = AN^{\gamma}+A'N^{\gamma'}+\dots \tag{25}$$

with $\dots < \gamma' < \gamma$. Thus, following Domb (1963), if we assume that

$$\langle R_N^2\rangle_S = 0{\cdot}755N^{3/2}+0{\cdot}24N \tag{26}$$

we find using equations (24) and (26) that

$$\langle R_N^2\rangle_S^s \simeq (0{\cdot}917\pm0{\cdot}003)N^{3/2} \tag{27a}$$

$$\langle R_N^2\rangle_{UMS} \simeq (0{\cdot}648\pm0{\cdot}002)N^{3/2} \tag{27b}$$

$$\langle R_N^2\rangle_{MS} \simeq (0{\cdot}705\pm0{\cdot}01)N^{3/2} \tag{27c}$$

Table 3. Estimates for the ratios $b_N = \frac{1}{4}\langle R^2_{2N-1}\rangle_{MS}/\langle R^2_N\rangle_S$.

N	b_N	b^*_N	$(b^*_N)^*$	$((b^*_N)^*)^*$
1	0·25000			
		0·76784		
2	0·46876		0·63166	
		0·71280		0·66561
3	0·59523		0·64009	
		0·67705		0·67186
4	0·59078		0·65430	
		0·67644		0·62448
5	0·62796		0·65598	
		0·66795		0·65240
6	0·61934		0·64237	
		0·66962		0·67215
7	0·63938		0·65478	
		0·66064		0·63367
8	0·63191		0·65088	
		0·66591		0·65632
9	0·64411		0·64951	
		0·65847		0·64901
10	0·63871		0·65209	
		0·66263		
11	0·64672		0·64941	
		0·65731		
12	0·64269			
		0·66043		
13	0·64835			
14	0·64523			

and for the class of intersecting walks on the square lattice defined by the Manhattan orientation

$$\langle R^2_N\rangle^{\text{int}}_{S} \simeq (0{\cdot}498 \pm 0{\cdot}007)N^{3/2}. \tag{27d}$$

These estimates are, however, based on our estimates (20) and (22) and on the asymptotic form (26) proposed by Domb (1963), and it would be interesting to test them by independently investigating each case without resorting to any comparison between the corresponding results on the unoriented square lattice. Following such an independent line we confirm that all the estimates thus obtained (with the assumption that $\gamma = 1{\cdot}5$), were found to lie in the range of those given above.

Turning our attention next to the value of the critical exponent γ and assuming the asymptotic form (2) we may define the successive estimates γ_N given by

$$\gamma_N = N[(\langle R^2_{N+1}\rangle/\langle R^2_N\rangle)-1] \tag{28}$$

or, when odd–even oscillations occur (for loose packed lattices), we may employ

$$\bar{\gamma}_N = \tfrac{1}{2}(\gamma_{N+1}+\gamma_N). \tag{29}$$

The values of $\bar{\gamma}_N$ for the three cases on the square unoriented lattice corresponding (*a*) to simple self-avoiding walks (branch A in figure 6), (*b*) to walks with possible intersections resulting from the transformation between MS and S lattices (branch B in figure 6)

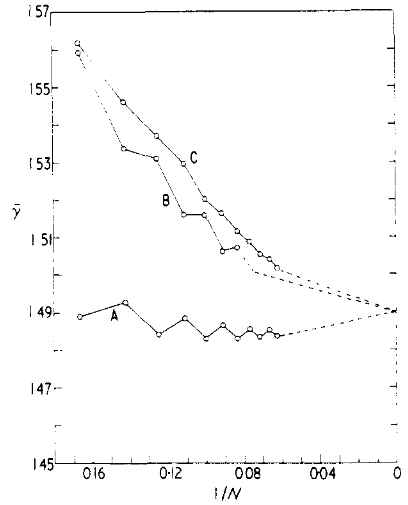

Figure 6. Plot of $\bar{\gamma}_N$ against $1/N$ for the three classes of walks on the square lattice explained in § 5 A, s lattice; B, MS lattice; C, UMS lattice.

and (*c*) to the 'weighted' self-avoiding walks resulting from the transformation between UMS and S lattices (branch C in figure 6) are tabulated in table 4. Although the strongest reason for proposing equality (23) for the critical exponent is the fact that the ratios a_N and b_N (defined by (18) and (21) respectively) tend to a limiting value quite regularly, nevertheless the variation of the corresponding values of $\bar{\gamma}_N$ further supports this conjecture. In particular, it may be argued that the critical exponent γ is overestimated by the conjectured value $\gamma = 1{\cdot}5$. This can be seen from figure 6 where all three branches (especially the top one) show a tendency to attain a value lower than 1·5. One would therefore suggest an estimate of the order of $\gamma = 1{\cdot}49 \pm 0{\cdot}01$ or possibly $\gamma = 1{\cdot}48 \pm 0{\cdot}02$.

Table 4. Estimates for $\bar{\gamma}_N = \frac{1}{2}(\gamma_N + \gamma_{N+1})$.

N	S lattice $\bar{\gamma}_N$	MS lattice $\bar{\gamma}_N$	UMS lattice $\bar{\gamma}_N$
1	1·5147	3·1692	1·7083
2	1·5264	1·9700	1·7179
3	1·5349	1·6886	1·6320
4	1·5040	1·6298	1·6038
5	1·4985	1·5735	1·5899
6	1·4891	1·5592	1·5617
7	1·4927	1·5337	1·5462
8	1·4843	1·5311	1·5370
9	1·4885	1·5161	1·5296
10	1·4832	1·5160	1·5203
11	1·4866	1·5067	1·5165
12	1·4832	1·5074	1·5115
13	1·4856		1·5089
14	1·4834		1·5056
15	1·4853		1·5041
16	1·4837		1·5017

On the other hand, the lowest branch in figure 6 shows a slight tendency to drift upwards, but not strongly enough to encourage the conjecture $\gamma = 1{\cdot}5$. Nevertheless this discrepancy has already been discussed by a number of authors (see, for example, Domb 1963, Hioe 1967). One could therefore scarcely disregard the long standing conjecture that $\gamma = 1{\cdot}5$, or the possibility of a slightly lower value.

6. Conclusions

The transformations carried out in § 2 and the numerical evidence presented in § 5 strongly suggest that there is a variety of apparently different 'walk' problems that give rise to the same values of the critical indices α and γ for the self-avoiding walk problem.

In particular the numerical evidence of § 5 greatly supports the view of Hioe (1967) (note that Fisher and Hiley (1961) had earlier suggested the opposite view) that the critical exponent remains unchanged when nearest-neighbour contacts are forbidden along a self-avoiding walk.

Our estimate (27*a*) for the subclass of self-avoiding walks on the square lattice (determined by the UMS orientation) lies between the estimate (26) given by Domb (1963) for simple self-avoiding walks and the estimate

$$\langle R_N^2\rangle_S^0 = 1{\cdot}25N^{3/2} \tag{30}$$

given by Hioe (1967) for self-avoiding walks with no nearest-neighbour contacts. The superscript, 0, means no 'nearest-neighbour contacts'.

Furthermore the interdependence between 'walk' problems on the three cases considered here (UMS, MS and S lattices) suggest that the 'trail' problem as well as the nearest-neighbour contact self-avoiding walk problem are equivalent regarding the values of α and γ.

Thus one can easily deduce from (27*b*) for the self-avoiding walk problem with no nearest-neighbour contacts on the MS lattice that

$$\langle R_N^2\rangle_{MS}^0 = (1{\cdot}296 \pm 0{\cdot}004)N^{3/2} \tag{31}$$

and for the 'trail' problem on the UMS lattice one finds from (27*c*) that

$$\langle R_N^2\rangle_{UMS}^t = (0{\cdot}3525 \pm 0{\cdot}005)N^{3/2}. \tag{32}$$

Thus it is clear that in all cases attractive forces decrease the value of the constant A whereas repulsive forces increase its value.

Furthermore, it now seems possible to hypothesize that the 'trail' problem will give rise to the same values of α and γ as the self-avoiding walk problem on the same lattice. One could possibly go a step further and conjecture that by restricting the walks to visit a lattice site at most m times a significant change on the critical exponent γ will not be produced whenever m is finite and $N \to \infty$.

Although there seems to be no rigorous way to verify these generalizations, their validity could probably be supported by Monte Carlo enumerations of very long walks. Of course the exact enumeration method cannot provide any such information since it is clear that the passage to the asymptotic behaviour will be very slow.

Finally it may be noted that our results and conclusions are relevant to the view recently expressed by Domb (1970b), to the effect that it is possible that for a single polymer chain there is no single θ-temperature at which the critical exponent γ is 1 for all N, whereas for a fixed value of N there is no doubt that such a θ-temperature exists.

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