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The trail problem on the square lattice

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Abstract. The trail problem on the square lattice is studied by the method of exact enumeration and its relation to the self-avoiding walk problem is pointed out. The number of N-stepped trails and their mean-square sizes are enumerated on a computer up to $N = 17$. An asymptotic analysis of the numerical data suggests that certain critical exponents obey the same values for both the trail and the self-avoiding walk problem on the square lattice.

1. Introduction

The problem to be discussed in this paper is closely related to the well known model of self-avoiding walks (SAW) on a crystal lattice; the latter being of considerable physical importance for it takes account in a realistic way of the 'excluded volume' effect of a polymer chain in dilute solutions (Domb 1963).

A SAW does not involve double occupancy of any (lattice) site, whereas in a *trail* no (lattice) edge occurs (or is visited) more than once. In a previous paper (Malakis 1975) it was pointed out that there is a one-to-one correspondence between trails on a closed oriented lattice (for definitions see Essam and Fisher 1970) and SAW on its covering lattice. On the one-dimensional lattice the trail and the SAW problems are equivalent by definition. Furthermore, on unoriented lattices of coordination number $z = 3$ (i.e. the honeycomb lattice) there is a striking similarity between the trail and the SAW problems. Indeed, in this case, if the formation of loops at the end points of the walks is forbidden, then these two problems become identical.

The above mentioned relationships would suggest that the trail problem obeys the same critical exponents as the SAW problem. However, for unoriented lattices with $z \geq 4$ there is no simple relation between SAW and trails on the same lattice; or trails on a lattice and SAW on its covering lattice. The most one can say in such cases is: 'to every trail on a lattice there corresponds a SAW on its covering lattice but not *vice versa*'.

Consider in particular the unoriented square lattice (s lattice). In this case the trail problem is essentially different from the SAW problem and any conclusion concerning critical behaviour should be drawn with caution. Nevertheless, an equivalence between SAW on the 'Manhattan-oriented' square lattice (MS lattice) and certain 'intersecting walks' on the s lattice (see Malakis 1975) has lead the present writer to conjecture that critical behaviour is the same for both the trail and the SAW problem on the s lattice.

The present paper is intended to study (numerically) the trail problem on the s lattice and in particular to compare critical behaviour between SAW and trails. Using the method of 'exact enumeration on a computer' (Domb 1969) we have determined the total number of N-stepped trails on the s lattice, C_N^t, and their mean-square end-to-end distances, $\langle R_N^2\rangle^t$, up to $N=17$ (see table 1). The program has been developed by the present writer and was written in ALGOL 60.

Section 2 has been devoted to a detailed analysis of C_N^t, while § 3 undertakes a similar analysis for $\langle R_N^2\rangle^t$. Finally, our conclusions are summarized in § 4 where an argument is presented to point out that although critical indices may not be altered by 'weak nearest-neighbour forces' in one and two dimensions this may not be true for three-dimensional lattices.

Table 1. The trail problem on the square lattice.

N	C_N^t	$\langle R_N^2\rangle^t$
4	108	6·518519
5	316	8·696203
6	916	11·021834
7	2628	13·517504
8	7500	16·140800
9	21268	18·921384
10	60092	21·824935
11	168984	24·877764
12	474284	28·032774
13	1326152	31·340570
14	3703376	34·740619
15	10312836	38·281823
16	28687804	41·913553
17	79629072	45·681001

2. Asymptotic analysis of the number of trails

Hammersley (1957) has proved the existence of the connective constant μ for the SAW problem on lattices satisfying certain very general conditions. The existence of such a constant for the trail problem can be easily established by a subadditivity argument similar with that employed by Hammersley (1957).

Throughout our treatment we shall assume the existence of μ for the trail problem. Furthermore, by analogy with the SAW problem we may assume that the number of trails on a lattice C_N^t is given by the asymptotic formula (1). Accordingly we shall use well established methods (from the theory of SAW; see Domb 1969) to estimate the connective constant μ and the critical exponent α for the trail problem on the s lattice:

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

Consider the successive ratios $\mu_N = C_{N+1}/C_N$, shown in table 2. If the formula (1) were exact (for small values of N), then the linear projections μ_N^* defined by analogy with (2) should provide rapidly converging estimates of μ:

$$x_N^* = (1/i)[(N+i)x_{N+i} - Nx_N]. \tag{2}$$

Table 2 also shows the values of the estimates μ_N^*, obtained from (2) where $i=1$, and $\bar{\mu}_N^*$ where $i=2$. The variation of these estimates suggests the following:

$$\mu = 2{\cdot}715 \mp 0{\cdot}005. \tag{3}$$

Table 2. Estimates for the connective constant of the trail problem.

N	μ_N	μ_N^*	$\bar{\mu}_N^*$
4	2·9259		
		2·7899	
5	2·8987		2·7551
		2·7203	
6	2·8690		2·7418
		2·7632	
7	2·8539		2·7359
		2·7087	
8	2·8357		2·7260
		2·7433	
9	2·8255		2·7175
		2·6917	
10	2·8121		2·7221
		2·7526	
11	2·8067		2·7162
		2·6799	
12	2·7961		2·7150
		2·7501	
13	2·7926		2·7163
		2·6825	
14	2·7847		2·7115
		2·7404	
15	2·7818		2·7127
		2·6850	
16	2·7757		

On the basis of (3) the following conjecture might be made:

$$\mu = \mathrm{e} = 2{\cdot}7182 \ldots . \tag{4}$$

A similar conjecture was made in the early history of the SAW problem. Lehman and Weiss (1958) conjectured that the connective constant for the SAW problem on the s lattice was given by (4). Today after extensive enumerations of SAW on the s lattice (up to $N = 26$, Sykes *et al* 1972d) there is no doubt that their conjecture is invalid, although this has not as yet been rigorously proved (Beyer and Wells 1972).

Now let us suppose that the value of the critical exponent α is known, then the estimates μ'_N defined by (5) would be expected to provide more accurate information for the connective constant. But even if the value of α, used in (5), is in error these estimates will eventually converge to the limiting value μ:

$$\mu'_N = N\mu_N/(N+\alpha). \tag{5}$$

On the basis of the evidence provided by Watson (1970, 1974) and Malakis (1975), it seems reasonable to expect that the critical exponent α for the trail problem will be the same as (or very close to) the value of α for the SAW problem. Accordingly, following the literature, we may assume that $\alpha \simeq \frac{1}{3}$ (Fisher and Sykes 1959). The variation of the estimates μ'_N against $1/N$ ($N = 6, 8, \ldots, 16$) for $\alpha = 0{\cdot}32$, $\alpha = 0{\cdot}333\ldots$ and $\alpha = 0{\cdot}34$ is shown in figure 1. The linear projections $(\mu'_N)^*$, obtained by analogy with (2) where $i = 2$, suggest an estimate closer to the value $2{\cdot}713$ rather than the value $2{\cdot}7182\ldots$.

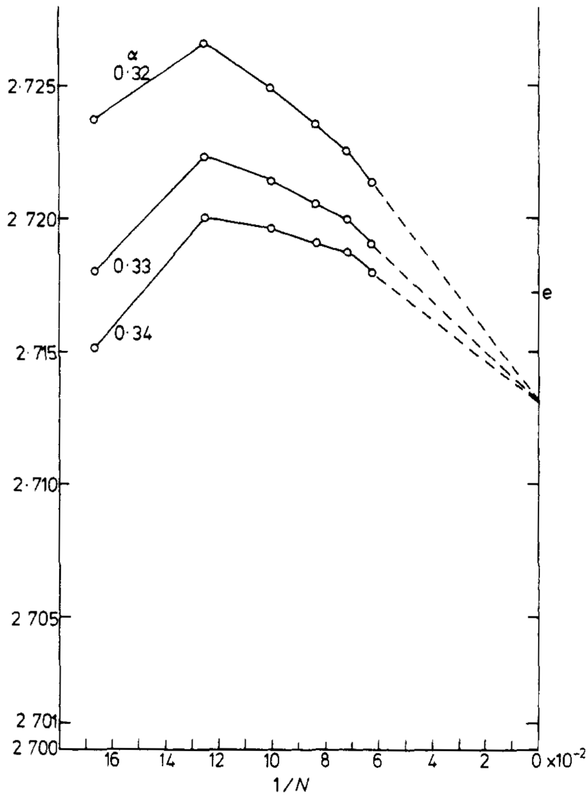

Figure 1. Plot of the estimates μ'_N against $1/N$ for three values of the critical exponent α.

On the other hand, knowledge of the value of the connective constant would provide us with the estimates α_N, given by (6), for the critical exponent α:

$$\alpha_N = N(\mu_N - \mu)/\mu. \tag{6}$$

The values of these estimates, obtained using the values $\mu = e = 2{\cdot}7182\ldots$ and $\mu = 2{\cdot}713$, are shown in table 3. In both cases the estimates α_N are higher than the conjectured value $\alpha = \frac{1}{3}$. However, we observe that the estimates $\alpha_N(\mu = e)$, i.e. obtained using the value $\mu = e$, are all closer to the value $\alpha = \frac{1}{3}$ than the corresponding values $\alpha_N(\mu = 2{\cdot}713)$.

Furthermore, the behaviour of these estimates is smoother for the trail problem than for the SAW problem. To illustrate this, we have also included in table 3 the estimates α_N corresponding to the SAW problem, obtained by utilizing the estimate $\mu = 2{\cdot}6385$ given by Sykes *et al* 1972c. To account for the characteristic even–odd oscillation, observed for loose-packed lattices, we shall further form the estimates $\bar{\alpha}_N = (\alpha_N + \alpha_{N-1})/2$. Table 4 shows the values of $\bar{\alpha}_N$ ($N = 8, 9, \ldots, 16$) corresponding to: (a) the trail problem using the value $\mu = e$; (b) the trail problem using $\mu = 2{\cdot}713$; and (c) the SAW problem using $\mu = 2{\cdot}6385$.

Finally, we have attempted to investigate the conjecture $\mu = e$ by employing the 'ferromagnetic' and 'antiferromagnetic' type of approximations used by Guttman *et al* (1968, see also Sykes *et al* 1972c). These approximations were developed from the

Table 3. Estimates for the critical exponent α.

	Trail problem		SAW problem
N	$\alpha_N(\mu=\mathrm{e})$	$\alpha_N(\mu=2{\cdot}713)$	$\alpha_N(\mu=2{\cdot}6385)$
4	0·3055	0·3139	0·3055
5	0·3319	0·3422	0·2046
6	0·3327	0·3450	0·3323
7	0·3492	0·3635	0·2262
8	0·3457	0·3618	0·3376
9	0·3549	0·3732	0·2468
10	0·3451	0·3653	0·3381
11	0·3577	0·3799	0·2614
12	0·3436	0·3676	0·3384
13	0·3553	0·3814	0·2715
14	0·3421	0·3700	0·3388
15	0·3503	0·3804	0·2792
16	0·3380	0·3698	0·3393

Table 4. Estimates for the critical exponent α.

	Trail problem		SAW problem
N	$\bar{\alpha}_N(\mu=\mathrm{e})$	$\bar{\alpha}_N(\mu=2{\cdot}713)$	$\bar{\alpha}_N(\mu=2{\cdot}6385)$
8	0·3474	0·3627	0·2819
9	0·3503	0·3675	0·2922
10	0·3500	0·3693	0·2925
11	0·3514	0·3726	0·3000
12	0·3507	0·3738	0·3000
13	0·3494	0·3745	0·3050
14	0·3487	0·3757	0·3052
15	0·3462	0·3752	0·3090
16	0·3442	0·3751	0·3093

analysis of Ising series (Sykes *et al* 1972a,b) and may be defined by (7) and (8) respectively:

$$\mu'_N=\mu(1+x/N^2) \tag{7}$$

$$\mu'_N=\mu(1+(-1)^N x/N^\theta). \tag{8}$$

By solving (7) or (8) for μ and x using pairs of the estimates μ'_N (given by (5)) one obtains a sequence of estimates for μ. Alternate pairs of μ'_N are usually employed in the 'ferromagnetic' approximation, whereas successive pairs of μ'_N may be employed when using the 'antiferromagnetic' approximation since the latter takes account of the characteristic even–odd oscillation. Although various values of α and θ were used in determining these approximations, these were chosen close to the values $\alpha=\frac{1}{3}$ and $\theta=1{\cdot}86$ (see Sykes *et al* 1972c, Martin *et al* 1967). This kind of analysis suggested that μ is indeed very close to the conjectured value $\mu=\mathrm{e}$, but the parameter x in (7) and (8) was found to be ill-defined.

In the light of the material presented in this section the following remarks might be made. Firstly, the behaviour of the various estimates, such as μ_N and α_N, appears to be smoother for the trail problem than for the SAW problem. Therefore, it is of some importance to carry out further enumerations for this particular case. Secondly, if the conjecture $\mu = \mathrm{e}$ is valid, or if the value of μ lies very close to the conjectured value e, then one would argue that the estimates presented in tables 3 and 4 strongly support the view that the critical exponent α is the same for both the trail and the SAW problem on the s lattice. Furthermore, the variation of the estimates $\bar{\alpha}_N(\mu = \mathrm{e})$, presented in table 4, supports the conjectured value $\alpha = \frac{1}{3}$.

Finally, if further enumerations show that the value of the connective constant for the trail problem lies closer to 2·713 than to the value 2·7182 . . . , and if the constancy observed in the estimates $\bar{\alpha}_N(\mu = 2{\cdot}713)$—see table 4—is maintained, then one would have to accept that certain conclusions drawn hitherto for the critical exponent α may not be valid. In particular this would cast doubts on the validity of the conjecture that α depends only on dimensionality (Fisher and Sykes 1959, Domb 1969) and also on the recent conjecture that α is not changed by 'weak attractive forces' (Watson 1974, Malakis 1975).

3. Analysis of mean-square sizes

The primary purpose of this section is to present numerical evidence utilizing the results obtained by the method of exact enumeration (table 1). In accordance with our earlier discussion we shall assume that the asymptotic behaviour of $\langle R_N^2\rangle^t$ (i.e. mean-square end-to-end distance for trails) will be similar to the asymptotic behaviour of $\langle R_N^2\rangle^s$ (i.e. mean-square end-to-end distance for SAW). Accordingly the asymptotic form (9) will be employed (see Domb 1969):

$$\langle R_N^2\rangle^t \simeq AN^{\gamma}. \tag{9}$$

If (9) is valid, then the successive estimates γ_N, defined by (10), should converge to their limiting value γ:

$$\gamma_N = N[(\langle R_{N+1}^2\rangle^t/\langle R_N^2\rangle^t) - 1]. \tag{10}$$

Table 5 shows the values of the estimates γ_N and $\bar{\gamma}_N$ (defined by $\bar{\gamma}_N = \frac{1}{2}(\gamma_{N+1} + \gamma_N)$) tabulated together with the linear projections $\bar{\gamma}_N^*$ and $\bar{\gamma}_N^{**}$ (obtained by analogy with (2) for $i = 1$ and $i = 2$ respectively).

In our opinion table 5 provides the most convincing evidence that the critical exponent γ is the same for both the trail and the SAW problem on the S lattice. Furthermore the variation between the different estimates shown in table 5 strongly supports the conjecture made by Domb (1963) that $\gamma = \frac{3}{2}$ in two dimensions.

If the critical exponent γ is the same for trails and SAW, then the ratios r_N, defined by (11), should tend to a non-zero limiting value (for the values of $\langle R_N^2\rangle^s$; see Domb 1963, Malakis 1975):

$$r_N = \langle R_N^2\rangle^t/\langle R_N^2\rangle^s. \tag{11}$$

The values of r_N ($N = 4, 5, \ldots, 17$) are tabulated in table 6; the last two columns of table 6 are obtained by repeated application of (2), where $i = 2$. Examination of the

Table 5. Estimates for the critical exponent γ derived from the trail problem.

N	γ_N	$\bar{\gamma}_N$	$\bar{\gamma}_N^*$	$\bar{\gamma}_N^{**}$
4	1·33632			
		1·33673	1·39242	
5	1·33714			1·40214
		1·34787	1·41187	
6	1·35859			1·41945
		1·35853	1·42704	
7	1·35847			1·44285
		1·36832	1·45867	
8	1·37817			1·46559
		1·37961	1·47251	
9	1·38106			1·46613
		1·38994	1·45975	
10	1·39882			1·47551
		1·39692	1·49127	
11	1·39502			1·49426
		1·40549	1·49725	
12	1·41597			1·49123
		1·41314	1·48520	
13	1·41031			1·49654
		1·41868	1·50787	
14	1·42706			1·50809
		1·42505	1·50832	
15	1·42305			
		1·43061		
16	1·43816			

Table 6. Comparison between mean-square sizes for the trail and the SAW problems.

N	r_N	r_N^*	$(r_N^*)^*$
4	0·92592		
5	0·90932		
6	0·87653	0·77773	
7	0·86895	0·76801	
8	0·84894	0·76619	0·73158
9	0·84428	0·75793	0·72265
10	0·83166	0·76254	0·74790
11	0·82877	0·75900	0·76382
12	0·81998	0·76159	0·75688
13	0·81820	0·76001	0·76591
14	0·81195	0·75377	0·77686
15	0·81075	0·76232	0·77696
16	0·80615	0·76550	0·77755
17	0·80543	0·76552	0·78956

extrapolated results suggests that r_N tends to a non-zero limiting value and this would, of course, imply that the critical exponent γ is the same for both trails and SAW on the s lattice (provided that the trends towards a non-zero limiting value will persist for large values of N).

Finally, on the basis of the various estimates in table 6, we shall estimate:

$$r = \lim_{N\to\infty} r_N = 0{\cdot}76 \mp 0{\cdot}015. \tag{12}$$

Thus, using the asymptotic formula proposed by Domb (1963) for $\langle R_N^2\rangle^s$, we obtain:

$$\langle R_N^2\rangle^t = (0{\cdot}574 \mp 0{\cdot}012)N^{3/2}. \tag{13}$$

4. Conclusions

The numerical evidence of the last two sections greatly supports the view that the critical exponents α and γ are the same for both the trail and the SAW problem on the s lattice. This is, no doubt, true (although a rigorous proof is required) for the honeycomb lattice since in this case these two problems are almost identical. Thus, it would appear reasonable to expect that the above described equivalence (regarding critical behaviour) may be valid for all two-dimensional lattices.

It was conjectured in a previous paper (Malakis 1975) that by restricting the walks to visit a (lattice) site not more than k times, a significant change on the critical exponents α and γ (and in particular on γ) will not be produced whenever k is finite and $N\to\infty$. We shall designate these walks 'k-tolerant walks', whereas the term 'k-tolerant trails' could be used for walks which may visit a (lattice) edge at most k times.

However, let us point out that although the conjecture advanced above is likely to be true for the k-tolerant walk problem in one and two dimensions, it may not be true (even for small values of k) in three dimensions. There are several reasons why this distinction should be made between one- and two-dimensional lattices on the one hand, and three-dimensional lattices on the other. To mention only two of these we shall recall some known results of the theory of random walks on lattices.

It is well known that random walks on three-dimensional lattices have a finite chance of escaping from the origin for ever, while on one- and two-dimensional lattices they return to the origin infinitely often. Also it should be pointed out that Montroll and Weiss (1965) have shown that if S_N denotes the average number of distinct lattice sites visited during an N-stepped random walk, then S_N satisfies the following:

$$S_N = \begin{cases} (8/\pi)^{1/2}N^{1/2} & \text{in one dimension} \\ \pi N/\ln N & \text{in two dimensions} \\ N/P(0,1) & \text{in three dimensions} \end{cases} \tag{14}$$

where $P(0, 1)$ is a constant whose value depends on the particular three-dimensional lattice and is related to Polya's probability of return to the origin f by $P(0, 1) = 1/(1-f)$. As regards the SAW problem $S_N = N$, whereas for the k-tolerant walk problem one would expect $S_N = N/c$, where $c \leqslant k$.

Since N/S_N for the random walk problem tends to infinity for one- and two-dimensional lattices, while it tends to a constant for three-dimensional lattices, it follows that our conjecture concerning the k-tolerant walk problem is not likely to be true in three dimensions while its validity for the one- and two-dimensional lattices cannot be rejected on such grounds. We note that N/S_N would be interpreted as the 'mean' repeated occupancy over all visited points bearing in mind, however, that the repeated occupancy of a lattice site depends on its location with respect to the origin.

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