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LETTER TO THE EDITOR

Asymptotic properties of lattice trails

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Abstract. The trail problem, a variant of the self-avoiding walk in which excluded volume is associated with lattice bonds rather than sites, is studied numerically in two and three dimensions. Monte Carlo and exact series methods are used, but the results obtained lack the consistency of similar results for self-avoiding walks. The evidence in support of the two models belonging to the same universality class is suggestive though not entirely convincing, but slowly decaying corrections to scaling could account for apparent exponent differences.

The self-avoiding walk, a well explored model for linear polymers, has spawned a number of variants that are no less intractable theoretically than the original. One such model is the trail (Malakis 1976), a random walk in which the excluded volume constraint applies to the bonds of the lattice rather than to the sites. Unlike the ordinary self-avoiding walk (SAW) where a site may be visited only once, the trail may revisit a site several times provided different bonds are traversed on each visit; for a lattice with coordination number q, up to $\frac{1}{2}q$ visits to any site are allowed. Additional models in the same family include k-tolerant walks (Malakis 1976) which allow sites to be visited up to k times but with no restriction on bond usage, and v-vertex trails (Shapir and Oono 1984) which are trails that are allowed to visit a site only v ($<q/2$) times; further models with combinations of these and other characteristics (e.g. loops smaller than a given size permitted) are readily devised, but none yield to analytic solution, and thus are of little help with the longstanding question of how exactly the non-Markovian self-avoidance condition alters the asymptotic behaviour of the random walk.

Each model relaxes the strength of the excluded volume relative to the SAW and it is tempting to think of them as interpolating between the SAW and the simple random walk (RW). SAWs and RWs exhibit very different kinds of asymptotic length dependence; the mean-square end-to-end distance of the SAW is given by $R_N^2 \sim AN^{2\nu}$ (N is the number of steps), with $\nu = 0.75$ for $d = 2$ (Nienhuis 1982) and $\simeq 0.592$ for $d = 3$ (Rapaport 1985a), whereas for the strictly Markovian RW $\nu = 0.5$, independent of lattice dimensionality. The question is whether the asymptotic behaviour of the other models resembles that of the SAW or whether the exponent ν has a value intermediate between ν_{SAW} and ν_{RW}.

A heuristic argument was given recently based on an analogy between a walk permitted a finite number of visits to each lattice site and a spin model with an extended but still finite interaction range (Guttmann *et al* 1984). In the latter, the critical exponents remain unchanged (a manifestation of universality), and the same could be expected to hold true for k-tolerant walks. Certain walk models have been examined

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close to the upper critical dimensionality of the SAW ($d_c = 4$), and it was again concluded that the same critical behaviour is obtained (Shapir and Oono 1984). The validity of this argument is apparently confined to $d \simeq 4$ where, it will be recalled, $\nu_{SAW} = \nu_{RW}$ due to the irrelevance of excluded volume in determining critical exponents. Other arguments have indicated that the situation may be more complicated. In particular, it has been suggested (Malakis 1976) that k-tolerant walks and SAWs share the same exponents for $d = 2$, but not for $d = 3$ because of differences in the properties of the RW (the relevance of the RW is not at all obvious since it is subject to no *a priori* restrictions on the number of revisits). Yet another argument applied to k-tolerant walks (Turban 1983) results in an exponent that varies with k below a certain k-dependent critical dimension.

Evidence that can be used to confirm or refute these arguments can only be based on numerical studies of the models themselves since, at the time of writing, no analytic solutions exist. In one such study carried out recently (Guttmann *et al* 1984) it was found that the proposed k-dependent exponent mentioned above failed to materialise. There are certain difficulties associated with such a programme however. One potential obstacle is that, contrary to the expectations of universality, the exponents of the various models *may* actually differ, but by only small amounts; available numerical techniques are of limited accuracy and may therefore be incapable of helping decide whether different models share common exponent values. Furthermore, given that the excluded volume effect is weakened in each of the models, it is quite likely that the onset of asymptoticity will be postponed to an extent that the typical walk lengths achievable in exact enumeration and Monte Carlo calculations are inadequate for these problems. These caveats have to be borne in mind when interpreting numerical results.

In this letter we describe the results of Monte Carlo (MC) and exact series calculations for one of the models—the trail problem—in both two and three dimensions. The key result is of course the exponent ν; the MC results will be shown to be of almost the same quality as those obtained in a recent MC study of the SAW (Rapaport 1985a, b), but it is by no means apparent that the exponents are the same for the two models in three dimensions. The series calculations turn out to be of little help in resolving the issue.

Monte Carlo simulations of trails on the square (SQ) and simple cubic (SC) lattices were carried out using techniques developed for the earlier SAW simulations. The only change required to the computational algorithm was to handle the altered nature of the excluded volume condition, a relatively minor modification. The trails generated ranged in length up to $N = 2400$; for each length approximately 50 000 distinct realisations were obtained, and the averaged values of mean-square end-to-end distance, R_N^2, and radius of gyration, S_N^2, are shown in table 1. The results of a least-squares fit to the data are given in table 2; the fits are to $R_N^2 \sim A_R N^{2\nu_R}$ and $S_N^2 \sim A_S N^{2\nu_S}$, and are carried out on the logarithms of the quantities concerned. The relative deviations included in table 1 are an indication of the close fits provided by these asymptotic expressions; the deviations are less than the statistical uncertainty of the MC results (the average spread obtained by grouping the measurements into eight blocks is close to 1.2% for both $d = 2$ and 3).

A closer look at table 2 reveals that in two dimensions the exponents ν_R and ν_S differ by approximately four times their statistical error, whereas for the SAW (Rapaport 1985b) the corresponding difference is less than the error; the errors themselves are of similar magnitude for both models. The value of ν_R for the trail, namely 0.7471, is

Table 1. Monte Carlo estimates of R_N^2 and S_N^2, and the deviations from asymptotic fit.

		R_N^2		S_N^2	
	N	mean	deviation	mean	deviation
SQ	160	1216.1	0.0001	174.19	0.0030
	320	3408.8	−0.0048	484.60	−0.0040
	640	9718.6	0.0072	1365.93	0.0020
	1200	24 673.4	−0.0003	3456.00	−0.0040
	2400	69 370.5	−0.0022	9750.69	0.0030
SC	120	252.0	0.0061	40.87	0.0059
	300	718.4	−0.0068	116.62	−0.0048
	600	1608.7	−0.0031	259.89	−0.0046
	1200	3601.3	0.0003	580.48	−0.0022
	2400	8060.0	0.0035	1303.44	0.0056

Table 2. Exponent and amplitude estimates based on fits to the MC results.

	SQ	SC
ν_R	0.7471 ± 0.0009	0.5788 ± 0.0010
ν_S	0.7432 ± 0.0008	0.5779 ± 0.0010
A_R	0.619 ± 0.008	0.981 ± 0.012
A_S	0.0920 ± 0.0009	0.1606 ± 0.0021

very close to the unbiased MC estimate for the SAW of 0.7479, a value subsequently replaced by the exact 0.75 with little degradation in the quality of the fit. In the case of the SAW ν_R and ν_S are essentially equal numerically, whereas the trail exponent ν_S lies significantly below ν_R (the qualifier 'significantly' is to be understood relative to the error estimates). It goes without saying that the errors present in the linear fit could easily conceal a certain amount of residual curvature due to a lack of complete convergence; this is an obvious (but not substantiable) explanation for the differences between the exponent estimates.

In three dimensions the difference between ν_R and ν_S lies within the error limits, although the errors themselves are approximately three times those of the SAW, as are the mean deviations from the asymptotic fits (Rapaport 1985a). The trail exponents lie about 2% below those of the SAW, a difference markedly greater than the statistical errors. Exponent equality cannot be ruled out, however, just for the reason given in the previous paragraph. The presence of this difference between the numerical results for trail and SAW should serve as a warning: if trails of the lengths considered here cannot be relied upon to yield the correct exponent there is little hope of reaching meaningful conclusions on the basis of much shorter trails, such as those to be used in the series analysis below. The foregoing statement is equally applicable to the other models mentioned earlier.

In the case of the SAW, series analysis has proved capable of giving a reasonable picture of the asymptotic N dependence, even though an element of uncertainty is introduced into the extrapolation by the absence of knowledge concerning the scaling corrections (Rapaport 1985a). To test the performance of the method for the trail problem we carried out an exact enumeration of trails with up to eleven steps on the FCC lattice. The counts c_N and conformational properties R_N^2 and S_N^2 are listed in table 3. The series for R_N^2 and S_N^2 are only one term shorter than the corresponding SAW series (Majid *et al* 1983, Rapaport 1985a).

Table 3. Exact enumeration results for trails on the FCC lattice.

N	c_N	$c_N R_N^2$	$(N+1)^2 c_N S_N^2$
1	12	12	12
2	132	288	552
3	1 452	4 908	15 600
4	15 924	73 104	349 176
5	173 940	1 012 980	6 788 580
6	1 895 820	13 408 464	120 076 224
7	20 631 372	171 955 932	1 984 031 328
8	224 238 132	2 154 751 440	31 134 855 984
9	2 434 736 556	26 526 854 028	469 241 620 620
10	26 414 247 492	322 030 865 424	6 845 665 570 824
11	286 368 796 668	3865 319 008 524	97 231 358 604 144

The series were analysed using the same methods as for the SAW. The Neville table for the connective constant μ computed from c_N is shown in table 4 (the assumed asymptotic form is $c_N \sim B\mu^N N^{\gamma-1}$). The values are close to 10.77, a result that is itself not too different from $q-1$ $(=11)$; $q-1$ is the value of μ for a random walk in which the only restriction is that immediate reversals of direction are prohibited. This proximity of μ values establishes the mildness of the excluded volume effect for trails on the FCC lattice; by way of contrast the SAW has $\mu \simeq 10.037$.

Table 4. Neville table extrapolation for the connective constant μ; m is the degree of the polynomial (in N^{-1}) to which the entry corresponds.

n \ m	0	1	2	3
8	10.869	10.772	10.743	10.668
9	10.858	10.770	10.761	10.798
10	10.849	10.769	10.764	10.770
11	10.841	10.767	10.758	10.742

Neville tables for the conformational exponents ν_R and ν_S are shown in table 5. Taken at face value the analysis suggests that both exponent values are near 0.54, but a slow drift to some higher value (e.g. to the MC prediction) cannot be excluded, in much the same way that the SAW Nevill tables suggested a value close to 0.60 but also indicated a gradual downward drift (Rapaport 1985a). The obvious conclusion is that series expansions for the trail model, even more so than for the SAW, are too short to provide an unambiguous answer as to the nature of the critical behaviour.

This would not be the first occasion that numerical analysis of critical phenomena has produced incorrect results; models that contain a seemingly irrelevant (from the

Table 5. Neville table analysis of the exponents ν_R and ν_S.

	n \ m	0	1	2	3
	7	0.5352	0.5346	0.5430	0.5611
R_N^2	8	0.5353	0.5359	0.5398	0.5344
	9	0.5355	0.5366	0.5391	0.5379
	10	0.5357	0.5377	0.5421	0.5489
	7	0.5534	0.5443	0.5455	0.5555
S_N^2	8	0.5522	0.5439	0.5426	0.5378
	9	0.5513	0.5435	0.5420	0.5408
	10	0.5505	0.5435	0.5437	0.5477

point of view of universality) parameter appear to have exponents that change as the parameter is altered, an effect that is demonstrably spurious (e.g., the dilute Ising model—Rapaport 1972). The reason for this effect is fully understood: varying the parameter alters the amplitudes of the scaling correction terms without modifying the principal exponent; if, however, the corrections become significantly large, the numerical analysis techniques see only an 'effective' exponent that includes contributions from the correction terms, with no possibility of isolating the leading order term. Since trails (together with k-tolerant walks, etc) can be regarded as perturbed forms of the SAW (with the parameter characterising the strength of the perturbation), it is reasonable to conclude that a similar effect occurs in the case of the trail exponents, and that the true critical properties are obscured by the presence of non-negligible correction terms.

Note added. A recent series study of the trail problem (Guttmann 1985) which examined the c_N expansions in two and three dimensions, and the R_N^2 expansion for the triangular lattice, arrived at a similar conclusion, namely that the trail appears to belong to the SAW universality class but is a considerably more difficult problem to handle numerically.

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