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LETTER TO THE EDITOR

On the universality class of self-avoiding walks

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Abstract. It is shown that, within a two-parameter cell-to-bond position space renormalisation group (PSRG) theory, self-avoiding walks and trails on the square lattice obey the same 'end-to-end distance' critical exponent ν. A critical examination of this result and recent speculations on this problem suggests that one should not draw qualitative predictions based on numerical estimates of the one-parameter PSRG theory.

The self-avoiding walk (SAW) problem was formulated as a model for the excluded volume effect of a polymer chain (Fisher and Sykes 1959, Domb 1963, McKenzie 1967). It is related to other lattice problems such as the Ising model of ferromagnetism (Domb 1970, McKenzie 1967, Whittington 1982) and the n-component spin model (de Gennes 1972). Thus, self-avoiding walks (SAWs) have been extensively studied (see McKenzie 1967, Whittington 1982 and references therein) and a variety of applications have been discussed.

Very recently, there has been renewed interest in this subject along several lines and two of them will be mentioned here. First, a considerable amount of work has been done in the study of the SAW problem on oriented (and directed) lattices (Malakis 1975, 1984, Guttmann 1983, Chakrabarti and Manna 1983, Cardy 1983, Redner and Majid 1983, Grassberger 1982, Prentis 1984). To justify the study of such oriented walk problems several arguments, appealing to anisotropy that may exist in some physical systems, have been presented (Chakrabarti and Manna 1983). However, another view (Malakis 1975, 1984, Guttmann 1983) is that the study of such problems may also help in a better understanding of the ordinary non-oriented problems.

A different route that several papers have followed is to consider the effect of loop formation on the statistical properties of polymers (Malakis 1976, Chen 1981, Oono 1979, 1981, Family 1982, Shapir and Oono 1984). In this case, polymer chains are modelled in terms of lattice walks that can have rings, doubly occupied bonds etc. Simple generalisations of the SAW problem such as the k-tolerant walk (and trail) models, introduced in 1976 (Malakis 1976), are often used as models for real polymers.

Here we address the SAW problem (or 1-tolerant walk problem) and the trail problem (or 1-tolerant trail problem) on the square lattice. The connection of these problems brings together the two lines of research mentioned above. The terms to be used in this paper are the following: RWs (random walks), SAWs (RWs that do not involve double occupancy of any lattice site), NAWs (neighbour-avoiding walks, i.e. SAWs that contain no nearest-neighbour contacts) and trails (i.e. lattice walks in which no lattice bond occurs more than once). The lattice used is the square (s) lattice and its two well known orientations which define the so-called Manhattan square (MS) lattice

(Kasteleyn 1963, Malakis 1975) and its underlying (UMS) lattice (Malakis 1984) also called 'L' lattice (Guttmann 1983). Both orientations are shown in figure 1.

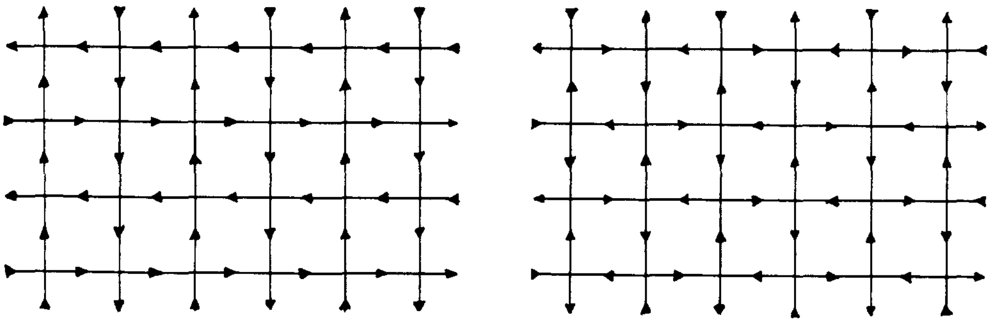

Figure 1. (*a*) The Manhattan square (MS) lattice. (*b*) The underlying of the Manhattan square (UMS) or L lattice.

We concentrate on an earlier conjecture (Malakis 1976) that predicts that SAWS and trails on the ordinary (non-oriented) S lattice obey the same critical exponent ν defined by:

$$\langle R_N^2 \rangle \sim N^{2\nu}. \tag{1}$$

As with similar cases in lattice statistics, it is difficult to prove or disprove such a prediction. Most of the existing evidence favours this prediction (Malakis 1976, Oono 1979, Shapir and Oono 1984) and its validity has been supported on field-theoretic grounds. However, Li *et al* (1984) question this and suggest that the value of the critical exponent for trails may be located between the values corresponding to RWS ($\nu = 0.5$) and to SAWS ($\nu \sim 0.75$). They find using a one-parameter $b \times b$ cell-to-bond PSRG transformation, the estimates $0.6549(b = 4)$ and $0.6866(b = 5)$ for trails, whereas for SAWS they find $0.7307(b = 4)$ and $0.7361(b = 5)$. It is difficult to see how from such estimates one could draw qualitative predictions since the convergence of the corresponding sequences appears very different, but it could also be erratic for a particular transformation, something that often happens in similar cases.

In the light of the speculations above, it seems interesting to point out that, contrary to the suggestion of Li *et al*, one can show that, within a two-parameter 3×3 cell-to-bond transformation the two problems belong to the same universality class and therefore obey the same critical exponent. To do so we first recall that according to an exact relation (Malakis 1975) trails on the UMS lattice and SAWS on the MS lattice *do belong* to the same universality class. Furthermore, very recently Prentis (1984) has shown that, within a two-parameter 3×3 cell-to-bond PSRG transformation, SAWS on the MS lattice and SAWS on the S lattice are in the same universality class. Therefore, within this theory, SAWS on the S lattice and trails on the UMS lattice are also in the same class. It follows that, if one can show that trails on the UMS lattice and trails on the S lattice are in the same class, then our conjecture is also true within this theory.

We proceed to show that the two-parameter 3×3 cell-to-bond PSRG transformation predicts the same class for trails on both UMS and S lattices. The details of the method can be found in Prentis (1984) and Malakis (1984). If the orientation of the UMS lattice is used then the 3×3 transformation equations for trails are:

$$K'p' = F(K, p, 1-p)/3 \tag{2}$$

$$K'(1-p') = F(K, 1-p, p)/3 \tag{3}$$

where p has the meaning of the probability that a step of the trail preserves the bond orientation of the UMS lattice, K is the fugacity and $F(K, X, Y)$ is determined by enumeration of the trails in a 3×3 cell:

$$\begin{aligned}F(K, X, Y) = {} & K^3(2X^2Y+XY^2)+K^4(6X^3Y+6XY^3)\\ & +K^5(4X^5+2X^4Y+10X^3Y^2+2X^2Y^3+4XY^4+2Y^5)\\ & +K^6(4X^6+6X^4Y^2+6X^2Y^4+4Y^6)\\ & +K^7(6X^6Y+6X^4Y^3+2X^3Y^4+6X^2Y^5)+K^8(4X^7Y+8X^5Y^3\\ & +8X^3Y^5+4XY^7)+K^9(4X^9+2X^8Y+2X^7Y^2+4X^6Y^3\\ & +12X^5Y^4+8X^4Y^5+2X^3Y^6+4X^2Y^7+4XY^8+2Y^9)\\ & +K^{10}(4X^{10}+2X^8Y^2+14X^6Y^4+10X^4Y^6+2X^2Y^8+4Y^{10})\\ & +K^{11}(6X^5Y^6).\end{aligned} \tag{4}$$

The flow pattern of the transformation is shown in figure 2. There exists a critical surface connecting the two problems, i.e. the trail problem on the UMS lattice ($p=0$

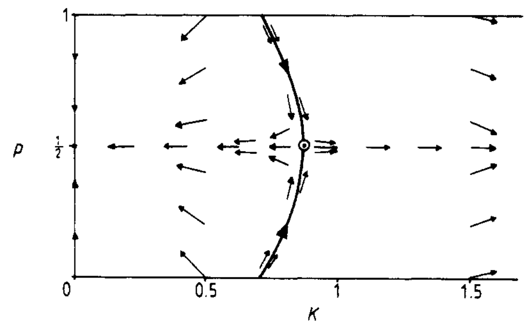

Figure 2. Flow diagram from the two-parameter 3×3 PSRG transformation as applied to trails on the UMS ($p=1, 0$) and S ($p=1/2$) lattices. The critical surface defines an equivalence class including both problems.

or $p=1$) and the trail problem on the S lattice ($p=1/2$). There exists only one fixed point on the critical surface given by:

$$p^* = 1/2, \qquad K^* = 0.869\ldots. \tag{5}$$

The points $K_c = 0.707\ldots$, $p=1$ and $K_c=0.707\ldots$, $p=0$ on the critical surface correspond to trails on the UMS lattice and approach the fixed point (5) upon repeating the transformation. Thus, the two problems are in the same universality class and the finite 3×3 transformation estimates the critical exponent via the relevant eigenvalue ($\lambda_K = 4.668\ldots$):

$$\nu = \ln(3)/\ln(\lambda_K) = 0.713\ldots. \tag{6}$$

It is interesting to recall here that the corresponding estimate of the same type of transformations for SAWs on the S lattice using the MS orientation (Prentis 1984) and the UMS orientation (Malakis 1984) is

$$\nu = 0.7283\ldots. \qquad (7)$$

The difference is not surprising and it should not be taken as an indication that something is wrong, it is only a consequence of the finite cell used. If the one-parameter theory is used for trails on the UMS lattice then a value different from that in (6) would be obtained. This was also observed by Prentis (1984) for the SAW problem on the MS lattice, there the one-parameter theory yields $\nu = 0.706\ldots$ whereas the two-parameter theory yields $\nu = 0.728\ldots$.

The isomorphic relation between trails on the UMS lattice and SAWs on the MS lattice, implies that both estimates (6) and (7) are 3×3 estimates of the two-parameter theory for trails on the UMS lattice. Yet they are different and it may be that this is partially due to the diagonal boundary conditions (Kasteleyn 1963, Malakis 1975) that should be applied on one of the two lattices to obtain the isomorphism of the two problems. The difference should vanish with increasing size of the cell in the PSRG transformations. However, the above emphasise the danger in using numerical estimates of the PSRG theory in order to make qualitative predictions. On the other hand, it is possible to make such predictions within the two-parameter theory since the critical surface defines an equivalence class. There seems to be no way to test uniquely the validity of the two-parameter theory predictions, but the test examples considered in a previous paper (Malakis 1984) provide strong support for the method.

We now present an argument which shows that the conjecture studied here is closely related to the universality hypothesis. According to this hypothesis (Whittington 1982) SAWs on all lattices of the same dimensionality are in the same universality class. The hypothesis can be extended to other problems such as the trail problem, the NAW problem etc. For RWs it is well known that all fundamental properties depend on dimensionality alone and this is, of course, a positive piece of evidence in favour of the universality hypothesis. It is not possible to extend the hypothesis to arbitrary oriented lattices, since there are notable exceptions (Malakis 1975), but it may be possible to do so for some 'isotropic' orientations and the MS and UMS cases are, we think, the typical examples. For these lattices we have the same positive evidence from the RW problem. The isomorphisms described in Malakis (1975) show that RWs on S, MS and UMS lattices are completely equivalent problems, something which is not true for arbitrary orientations.

Thus, if we restrict our argument to two dimensions, the hypothesis could be stated as follows: 'Each non-trivial walk problem in two dimensions such as the SAW, the NAW and the trail problem has its own universality class that includes all two-dimensional lattices and all two-dimensional 'isotropic' oriented lattices'. If the above is true, then the exact one-to-one correspondence between trails on the UMS and SAWs on the MS lattices identifies the classes for trails and SAWs. Similarly the one-to-one correspondence between SAWs on the UMS and NAWs on the MS lattices identifies the classes for SAWs and NAWs (this can be also derived from Watson's work (1974)) and the three problems (trail, SAW and NAW) should obey the same critical exponent.

Very recently, Shapir and Oono (1984) have presented arguments (based on field-theories and the ε-expansion) to support a much more general conclusion including k-tolerant walks and extending to three-dimensional lattices as well. However, when this k-tolerant walk conjecture was originally stated (Malakis 1976) a clear distinction was made between two and three dimensions and we still think that the three-dimensional case should be studied with caution. In three dimensions there exist no isomorphic relations between walk problems on lattices of the same structure and the arguments of the present paper do not apply. Furthermore, the 'mean occupancy' for RWS in three dimensions is finite (see for example, Malakis 1976, Montroll and Weiss 1965), whereas it is zero in two dimensions and this observation is a clear indication that the k-tolerant walk or trail problem may be more sensitive in three dimensions. In fact an extensive Monte Carlo study (Malakis and Hatzopoulos 1984) of the trail problem on a diamond lattice shows a clear difference between trails and SAWS on this lattice.

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