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LETTER TO THE EDITOR

Lower-dimensional defect transitions in self-avoiding walks and percolation

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Abstract. We study self-avoiding walks and percolation on d-dimensional lattices, focusing on the existence of transitions associated with a defect of dimensionality $d^* < d$. Such transitions are established for walks in all dimensions $d \geqslant 2$, in contrast to percolation for which they are absent if $d^* = 1$. An apparent contradiction with scaling arguments is resolved. A simple renormalisation group approximation yields phase diagrams consistent with these results and provides numerical estimates for crossover exponents and the splitting between 'special' and homogeneous critical points.

The critical phenomena specifically associated with spatial inhomogeneities near a surface (or other extended defects) have been studied extensively for over a decade (Wolfram *et al* 1971, Mills 1971, Lubensky and Rubin 1975). However, much recent activity has been stimulated by the scaling arguments of Bray and Moore (1977), who considered an n-component spin model, and (a) formulated a necessary condition for the existence of a distinct 'surface phase', i.e. a phase in which order exists locally without bulk ordering, as well as (b) proposed that all 'surface' critical exponents can be determined from the bulk exponents. In this note we address only the first question of whether or not a 'surface' transition occurs†.

More specifically, we consider the single self–avoiding walk and the percolation problem. The former may be considered as a model of a solution of linear polymers in the dilute regime (de Gennes 1979 and references therein), while percolation may reasonably model the process of gelation (Stauffer 1979 and references therein). When a surface is introduced in these problems, it has a natural interpretation as a container wall, and a surface phase corresponds to an adsorbed polymer chain or gel adhering to the wall. These problems have been studied in recent years using renormalisation group (De'Bell 1979, 1980), series expansions (De'Bell and Essam 1980) and Monte Carlo (Clerc *et al* 1981) techniques. However, all previous results have been consistent with the general condition proposed by Bray and Moore (1977), and no surprises have appeared. In contrast, we consider, following Bariev (1979) (see also Clerc *et al* 1981), a d^*-dimensional defect in an otherwise uniform, infinite system of d dimensions ($d > d^*$). In such a system, the analogue of the Bray–Moore criterion would be that the existence of a surface phase requires $(d - d^*)\nu \leqslant 1$, where ν is the exponent for the radius of gyration for self-avoiding walks or for the connectedness length in percolation, respectively. It will be seen below that $d^* = 1$ is a particularly interesting case: such a

† However, it now appears that (b) is inconsistent with ε expansions (Reeve and Guttmann 1980, Diehl and Dietrich 1980), and series results (Barber *et al* 1978).

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system might be realised physically by immersing a fine thread or wire in a dilute polymer solution or in the sol phase of gelatin. A bilipid membrane permeable to polymers might provide an example of the case $d^* = 2$.

Consider first a walk on a hypercubic lattice of d dimensions. Let each link of the chain have a fugacity z in the homogeneous (or bulk) part of the lattice, but z^* if it lies on the defect (of d^* dimensions). For a pure, bulk walk, consider the generating function $Z_d = \Sigma^d z^n$, where the summation Σ^d runs over all walks that start from a given site and n is the length of the walk. Then Z_d corresponds to the susceptibility, χ, of the n-component spin model in the limit $n \to 0$ (de Gennes 1972), and thus the bulk critical point, z_c, is determined by the radius of convergence of Z_d. Analogously, in our case, we study the generating functions

$$Z^* = \Sigma^{\mathrm{I}} z^m z^{*n} \qquad \text{and} \qquad Z^{**} = \Sigma^{\mathrm{II}} z^m z^{*n} \tag{1}$$

that correspond to the surface susceptibilities χ_1 and χ_{11} (Binder and Hohenberg 1972) of the spin model in the limit $n \to 0$ (Barber *et al* 1978). Thus the summation I runs over all walks starting from a given defect site, while m, n are the number of links in the walk lying in the bulk and defect, respectively. Likewise the summation II has the additional constraint that the end point must also lie on the defect. A divergence of Z^* and Z^{**} at $z < z_c$ corresponds physically to the formation of infinite walks adhering to the defect (with their lateral size probably finite). From arguments given below, Z^* clearly has divergent singularities for real z and z^*, and in this note, we assume that there are no other singularities of Z^* closer to the origin; as a result, the critical line is the locus of the divergences of Z^*.

Thus we are interested in the critical line $z^* = z_c^*(z)$ in the unit square in the (z, z^*) plane. Two points on this line A, B (see figure 1) may be located trivially: if $z = 0$, both Z^* and Z^{**} reduce to the d^*-dimensional homogeneous, bulk generating function Z_{d^*}, thus locating A at $(0, z_c^*)$; if $z = z^*$, the bulk critical point is recovered, implying B at (z_c, z_c). There are two additional exact features: (i) the line $z^* = z_c^*(z)$ cannot have a (bounded) positive slope, and (ii) it cannot extend to the right of $z = z_c$. (Thus a portion of the critical line is given by $z = z_c$, $z^* \leqslant z_c$.) The result (i) is due to the monotone increasing nature of Z^* in z and z^*, and (ii) is a direct consequence of the extension to general d of the theorem of Whittington (1975) which proves that the effective coordination number of a walk is the same for the walks in the full space as for those confined to a half space (homogeneous case). The only step required between this theorem and (ii) is that of realising that Z^* contains a subset of walks confined to a half space lying wholly in the homogeneous region.

We now demonstrate that $z_c^*(z)$ lies below the point A for $z > 0$ (see figure 1). It suffices to consider simply a subset of walks contributing to Z^{**} (and thus also to Z^*) constructed as follows: first take each walk entirely on the defect contributing to Z_{d^*}, and allow for the possibility that each z^* link can be replaced by a 'bridge' of bulk or homogeneous links (a minimum of three links are needed on a hypercubic lattice)†. Two successive 'bridges' can be accommodated by swinging them on either 'side' of the defect. Thus we obtain

$$Z^{**} > \Sigma^{d^*} w^n \qquad \text{with} \quad w = z^* + [2(d - d^*) - 1]z^3. \tag{2}$$

† In this discussion, we consider a simple layer defect (hyperplane) of d^* dimensions, although a similar argument should be possible for more general cases such as a defect of several such layers.

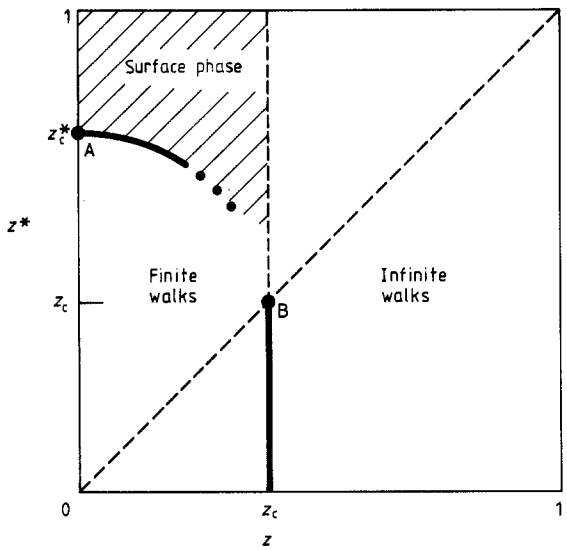

Figure 1. Schematic defect phase diagram for the self-avoiding walk problem. Points A and B correspond to the transition for bulk, homogeneous d^*- and d-dimensional lattices, respectively. In the shaded area marked 'surface phase', there are infinite walks adhering to the defect with no infinite walks far from the defect (in the bulk).

Consequently, Z^{**} will diverge for $w > z_c^*(0)$, and we have established the bound

$$z_c^*(z) \leqslant z_c^*(0) - [2(d-d^*)-1]z^3. \tag{3}$$

This upper bound can clearly be improved by taking longer bridges, etc. The important point is that it shows the existence of defect transitions even for $z^* < z_c^*$ for all $d > d^*$ in the case of walks (see figure 1). In order to obtain the form of the critical line, we also need an upper bound on Z^{**}. This is easy to do if $d^* = 1$: first, let $\tilde{Z}$ be a generating function similar to Z^{**} but with the additional constraint that no defect *link* is allowed to be included in the walks. (Defect *sites*, however, are allowed.) Then, by allowing one factor of $\tilde{Z}$ to be inserted at every terminal of a sequence of n steps forming a linear chain on the defect, we may place an upper bound on a *portion* of the walks contributing to Z^{**}. We say 'portion' since this prescription does not properly account for walks that double back across the defect. However, these can also be taken care of if we redefine $\tilde{Z}$ appropriately and insert one factor of $\tilde{Z}$ between each link *along* the chain conformation. This refinement only enters $\tilde{Z}$ at $O(z^4)$, and so we have

$$\tilde{Z} = 1 + 2(d-1)z^3 + O(z^4), \tag{4}$$

and thence

$$Z^{**} < \sum_{n=0}^{\infty} z^{*n}\tilde{Z}^{n+1} = \frac{\tilde{Z}}{1 - z^*\tilde{Z}}. \tag{5}$$

Clearly $\tilde{Z}$ itself is finite for $z < z_c$, and thus Z^{**} remains finite for $z^* < 1/\tilde{Z}$. This implies $z_c^*(z) \geqslant 1/\tilde{Z}$, and consequently the result for the vicinity of A is

$$z_c^*(z) \geqslant 1 - 2(d-1)z^3 \qquad (d^* = 1,\ z \to 0). \tag{6}$$

Let us now consider percolation. In this case the analogues of the surface susceptibilities χ_1, χ_{11} are the mean size of finite clusters S^* and S^{**} (De'Bell and Essam 1980), where S^* is defined for clusters attached to a given defect site and S^{**} is the mean size of the portions of such clusters that lie within the defect 'layer'. In parallel to the previous discussion, the singularity of S^* and S^{**} defines a critical line $p_c^*(p)$ where p is the bond probability in the homogeneous, bulk region of the lattice while p^* is that for the bonds in the defect.

In this case, Clerc *et al* (1981) recently argued that there could be no defect-induced transitions for $d^* = 1$, for any d. Their argument depends upon making p^* close to unity so that there are only isolated bonds missing in the defect. Thus, the probability that there are 'bridges' over these bonds is supposed independent, leading to the conclusion that connectivity could not extend to infinity. This conclusion is most plausible for small p. However, for any $p^* < 1$, missing defect bonds may occur either singly or multiply (i.e. contiguously), but we may consider any multiple missing bonds as one unit, and consider the probabilities that the end points of these units are connected. As $p \to 0$, these probabilities are dominated by p^n where n is the length of the shortest path spanning the unit, and thus $n \geqslant 3$. Moreover, since these paths do not have common bonds, the units are independent in this limit. Thus it follows that the connectivity cannot extend to infinity asymptotically for small p, for all $p^* < 1$. (The lack of rigour in these arguments lies in the failure to account for longer bridges that 'jump over' a number of sequences of missing defect bonds; but for p small, say $p < p_c/10$, such configurations should be negligible.)

If $d^* > 1$, we know that $p_c^* < 1$, and there is always a surface phase. In addition, the critical line $p_c^*(p)$ satisfies an inequality

$$p_c^*(p) \leqslant \frac{p_c^*(0) - [1 - (1-p^3)^{2(d-d^*)}]}{(1-p^3)^{2(d-d^*)}}. \tag{7}$$

This can be seen as follows: we can obtain a lower bound on connectivity by choosing to regard the two ends of a defect bond as connected only if either the defect bond itself is occupied or if there is a path through the bulk, homogeneous region of no more than three bonds. This restriction can only increase the value of p and p^* needed for percolation. Thus, the pair connectedness for defect sites are independent provided such pairs do not have a site in common. If there is a site in common, it is also clear that the probability that, say, two pairs are both connected, is not less than the product of the probabilities of each pair being connected. Thus, the 'independence' assumption always gives a lower bound on connectivity, and if $\tilde{w}$ is the probability that a pair of neighbour sites are connected (according to the present criterion), we have infinitely extending connectivity whenever $\tilde{w} > p_c^*$. Since $\tilde{w} = p^* + (1-p^*)[1-(1-p^3)^{2(d-d^*)}]$, we obtain (7).

In order to put these results in a more general perspective, recall the arguments of Bray and Moore (1977). In a Ginzburg–Landau–Wilson Hamiltonian, they introduced a 'surface' (or defect) perturbation term

$$H_s = \tfrac{1}{2}c \int \mathrm{d}^d \boldsymbol{x}\, \delta(z) \sum_{i=1}^{n} \varphi_i^2(\boldsymbol{x}). \tag{8}$$

They showed that, under a scale change $\boldsymbol{x} \to b\boldsymbol{x}'$, the coupling c transforms as

$$c' = b^{d-1-(1-\alpha)/\nu} = b^{(1-\nu)/\nu} c \tag{9}$$

(the latter equality following by use of hyperscaling). From this they concluded that $\nu > 1$ implies that no surface phase exists, and that if there exists a surface phase then the crossover exponent is $\varphi = 1 - \nu$. Bariev (1979) considered a more general case of a $d^*(< d)$-dimensional defect, where (7) is replaced by

$$c' = b^{d^*-(1-\alpha)/\nu} c = b^{[1-(d-d^*)\nu]/\nu} c. \tag{10}$$

Although Bariev was interested only in the case of marginality (where $(d-d^*)\nu = 1$), which leads to non-universal behaviour, we can equally well consider other cases. In particular, the logic of Bray and Moore (1977) would yield the statement: $(d-d^*)\nu > 1$ implies that no surface phase exists, but if there is a surface phase, $\varphi = 1-(d-d^*)\nu$.

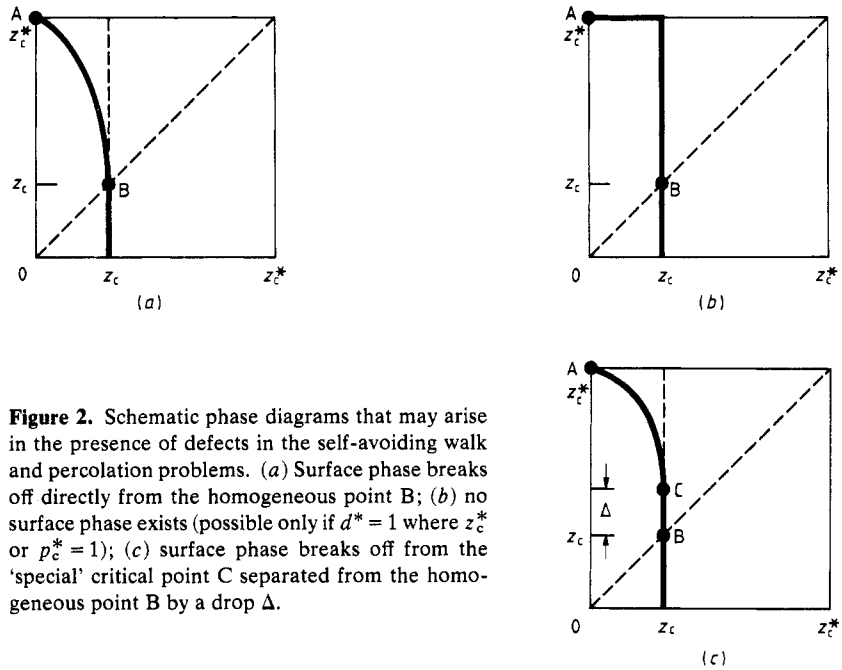

Figure 2. Schematic phase diagrams that may arise in the presence of defects in the self-avoiding walk and percolation problems. (*a*) Surface phase breaks off directly from the homogeneous point B; (*b*) no surface phase exists (possible only if $d^* = 1$ where z_c^* or $p_c^* = 1$); (*c*) surface phase breaks off from the 'special' critical point C separated from the homogeneous point B by a drop Δ.

However, we can see that this conclusion is, in fact, inadequate. In terms of phase diagrams, this logic allows only for those of figure 2(*a*) and (*b*), where (*b*) would be obtained if $(d-d^*)\nu > 1$. In table 1, we list the estimates of $(d-d^*)\nu$ for walks (Flory 1971) and percolation (den Nijs 1979, Nakanishi and Stanley 1980, and references therein). Although percolation does not fall into the n-component spin hierarchy, a perturbation of the type given in (8) can still be considered as a model for a defect (Carton 1980). From this table, we note at once that, for walks with $d^* = 1$, $d > 2$, the inequality $(d-d^*)\nu > 1$ is always valid even though we have just proved that surface phases exist. So, what should the phase diagrams look like in these cases? We note that the above argument deals only with the effect of the defect perturbation locally for strengths near $c = 0$. Thus, even if c is an irrelevant parameter as when $(d-d^*)\nu > 1$, there is a possibility that a surface phase breaks off at a *finite* value of c as illustrated in figure 2(*c*).

Therefore, our results together with the scaling arguments predict, for walks, the phase diagram of figure 2(*c*) if $(d-d^*)\nu > 1$ and that of figure 2(*a*) otherwise. For

Table 1. Numerical estimates of $(d-d^*)\nu$ for self-avoiding walks (upper) and percolation (lower). For walks, $\nu = 0.75$ ($d = 2$) and $\nu = 0.6$ ($d = 3$) are used (Flory 1971); in percolation, we use $\nu = \frac{4}{3}$ (a conjecture due to den Nijs (1979)) for $d = 2$, and a table from Nakanishi and Stanley (1980) for $d > 2$.

d	$d^* = 1$	2	3	4	5
2	0.75				
	1.33				
3	1.2	0.6			
	1.70	0.85			
4	1.5	1.0†	0.5		
	1.92	1.28	0.64		
5	2.0	1.5	1.0†	0.5	
	2.08	1.56	1.04	0.52	
6	2.5	2.0	1.5	1.0†	0.5
	2.5	2.0	1.5	1.0†	0.5

† Case of a marginal operator similar to that discussed by Bariev (1979).

percolation, the special case of $d^* = 1$ yields the diagram of figure 2(b) with no surface phase, while for $d^* > 1$, that of figure 2(c) is predicted if $(d-d^*)\nu > 1$ and (a) otherwise. Thus we have shown that the criterion $(d-d^*)\nu \leqslant 1$ is not a necessary condition for the existence of a surface phase, nor even necessary for the phase boundary to lie below point A (figure 1). Unfortunately, quite strictly, it is not a sufficient one either (Bray and Moore 1977).

A remaining problem is to estimate numerically the threshold displacement Δ in figure 2(c) and the crossover exponent φ associated with point C. We have extended a cell renormalisation technique developed for homogeneous walks (de Queiroz and Chaves 1980, Family 1980, 1981, Redner and Reynolds 1981) for the cases $d = 2, 3$ and $d^* = 1, 2$. This approach has the advantage of extreme simplicity and surprisingly good numerical accuracy compared with other more elaborate methods (Watts 1974, 1975, McKenzie 1976, Le Guillou and Zinn-Justin 1980 and references therein) that are believed to be more reliable. These latter methods, however, become either very complex or unreliable when applied to spatially inhomogeneous systems such as those with a defect or surface. In contrast, our approach retains its simplicity, and as seen below, yields phase boundaries in agreement with all the expected features discussed previously.

In this renormalisation group, we seek to conserve Z^* (and Z^{**}) approximately by using two different types of cells. A 'defect cell' is used to renormalise z^* (for that part of the walk lying along the defect) and a 'bulk cell' to renormalise z (for the remainder of the walk). The renormalised links $z^{*\prime}$ and z' are calculated by summing the weights of the subwalks within the cell that start from a corner site and span the cell along the direction in which the renormalised links are to lie (figure 3). (A similar method was used for percolation by De'Bell (1979, 1980).) In the particular example of the square lattice with 2×2 cells, this procedure yields the recursion relations

$$z^{*\prime} = z^{*2} + z^*(z^3 + z^2) + z^3, \tag{11}$$

$$z' = z^4 + 2z^3 + z^2. \tag{12}$$

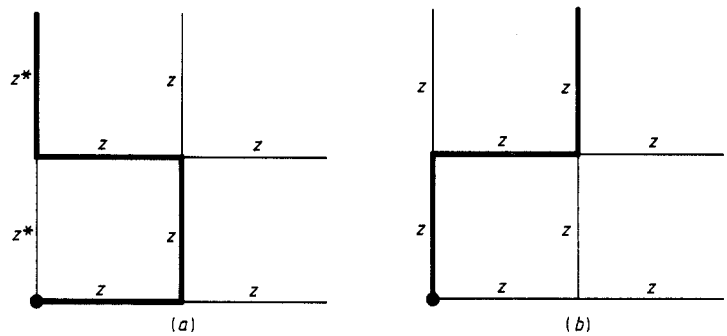

Figure 3. (*a*) A cell used to renormalise z^*; (*b*) similarly for z. Walks within the cell starting from the corner site (marked by a heavy dot) and spanning vertically are summed over to obtain recursion relations (11) and (12) (typical walks included in the summation are illustrated by bold lines).

These generate discrete flows as usual and indicate a phase diagram of the type shown in figure 2(*a*) in agreement with the previous discussion. The numerical results are: the homogeneous point B lies at ($z = 0.47$, $z^* = 0.47$), with $\nu = 0.72$, and $\varphi = 0.23$. These values should be compared with the current 'best' estimates of B at (0.379, 0.379) (Watts 1975) with $\nu = 0.75$ and $\varphi = 1 - \nu$ ($= 0.25$) (Watts 1974, McKenzie 1976), which agree with Flory (1971).

It is trivial to extend this approach to other lattices and dimensions. One finds that the analogous treatment for the simple cubic lattice with a planar defect ($d = 3$, $d^* = 2$) again yields a phase boundary of type figure 2(*a*). The numerical results for B are (0.30, 0.30), $\nu = 0.59$, and $\varphi = 0.47$; the latter two values are not too far from the best accepted values $\nu = 0.588$, $\varphi = 1 - \nu$ (Le Guillou and Zinn-Justin 1980). However, the interesting case is that of $d = 3$, $d^* = 1$, and there we obtain a phase diagram of the type in figure 2(*c*) just as predicted in the previous discussion. This arises in the recursion relation by the motion of a fixed point that was below the line $z^* = z$ to a position above $z^* = z$. The threshold displacement Δ (see figure 2(*c*)) is estimated to be about 0.08, or 27 per cent of z_c in this approximation; the crossover exponent at C is estimated to be $\varphi = 0.065$.

De'Bell (1979, 1980) applied a similar method to percolation with $d = 2$, $d^* = 1$ and $d = 3$, $d^* = 2$, where $d = 2$, $d^* = 1$ resulted in a phase diagram of type figure 2(*b*). We find that the case $d = 3$, $d^* = 1$ also yields a diagram similar to figure 2(*b*), thus agreeing with the expected results in these cases.

In summary, we have shown that a naive interpretation of the local stability criterion with respect to the existence of a surface phase is misleading by giving explicit examples of self-avoiding walks in systems with a linear defect. In particular, the inequality $(d - d^*)\nu \leqslant 1$ is neither a sufficient (Bray and Moore 1977) nor a necessary condition for the existence of a surface phase. We have corroborated the arguments by using a very simple renormalisation approach which agrees fully with the predictions, and which gives explicit numerical estimates for various quantities of interest.

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