Renormalisation group for percolation using correlation parameters

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Abstract. We have applied position-space RG methods to the problem of percolation of correlated sites on the square and simple cubic lattices. Our approach uses a cell-to-site transformation and superposition approximation to renormalise the site probabilities and a set of correlation parameters. In two dimensions we find two non-trivial fixed points, for random percolation and Ising-correlated percolation respectively. In three dimensions only a single non-trivial physically accessible fixed point is found, controlling the percolation of random sites. In contrast to the two-dimensional case a fixed point for positive values of correlation is found to have complex eigenvalues, and does not correspond to a physical percolation point. The finding of a single universality class for correlated percolation in three dimensions is in agreement with the known behaviour of Ising-correlated percolation.

1. Introduction

As its name suggests, correlated percolation (CP) is a variant of the standard percolation problem, in that the lattice elements—sites or bonds—are correlated as opposed to independent random variables. In an earlier letter (Tuthill and Klein 1982) we described a method for studying two-dimensional site CP in which the parameters in position-space renormalisation group (PSRG) are the site–site correlations themselves. In this paper we discuss that approach in more detail, and describe the results of calculations on a three-dimensional (simple cubic) lattice.

Motivation for our PSRG approach is found first in the nearest-neighbour Ising ferromagnet if (say) 'down' spins are regarded as occupied sites and the remainder as empty. It is well known from the work of Coniglio *et al* (1977) that the Ising critical point $T = T_c$, $H = 0$ (T = temperature, H = magnetic field) on planar lattices is a percolation threshold; a line $H_p(T)$ of percolation points extends from the critical point to infinite temperature, as shown in figure 1(a). In three dimensions, on the other hand, Monte Carlo results (Müller-Krumbhaar 1974) indicate that $H_p(T)$ does not terminate at the Ising critical point, but instead (cf figure 1(b)) reaches $H = 0$ at a temperature below T_c—the so-called Müller-Krumbhaar (MK) point—on the first-order phase transition line. Recently (Klein *et al* 1978, Coniglio and Klein 1980) PSRG techniques have been applied to this subject, exploiting a connection between percolation and the q-state Potts model in the $q \to 1$ limit (Kasteleyn and Fortuin
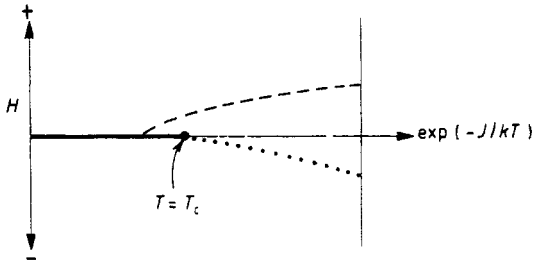
Figure 1. Correlated percolation of aligned spins in the Ising ferromagnet with nearest-neighbour interactions (J = interaction strength) in the plane of $\exp(-J/kT)$ against magnetic field H. Shown are the lines of percolation points for two-dimensional (dotted) and three-dimensional (broken) systems; percolation of 'down' spins takes place for temperatures and fields below these lines. In the two-dimensional case the line of percolation points ends at the Ising critical point $H = 0$, $T = T_c$.

1969). This 'Potts lattice gas' approach gives satisfactory results in two dimensions, showing that in fact the Ising critical point is a higher-order critical point for percolation. The same method when applied in three dimensions, however, gives a duplicate of the 2D results and is clearly incorrect.

The Potts lattice gas approach fails in three dimensions first for technical reasons, since it gives recursion relations for temperature and field which are identical to those of the Ising model, and free of the Potts coupling constant. Thus only the critical point—and not the MK point—can be singled out on the $H = 0$ axis. There exists a more fundamental difficulty, however, for any renormalisation procedure using the variables H and T. This is due to the fact that the MK point is a critical end-point for percolation, appearing when H changes sign and a new thermodynamically stable phase intrudes. In the RG such an end-point should generally be signalled by a separatrix (or critical surface) leaving the physically accessible region of parameter space. A flow diagram in the H,T plane with this geometry is not possible, since every point at finite H and T corresponds to a single physically accessible equilibrium state.

We circumvent this problem as follows. We replace H as an RG parameter by the more customary (for percolation problems) quantity p, the probability that a site is occupied. This likelihood is simply related to the reduced magnetisation M, the conjugate of H, by $p = (M + 1)/2$. The temperature, or nearest-neighbour coupling, is then replaced by a nearest-neighbour correlation parameter t, defined through the relation

$$t = [1 - \langle s_i s_j \rangle]/[4p(1-p)], \tag{1}$$

where s_i and s_j are nearest-neighbour spins. Thus $t = 1$ corresponds to the case of no correlation ($T \to \infty$, or pure random percolation) while $0 < t < 1$ for finite temperatures. Introduction of p, t parameters means that RG flows are not necessarily restricted to thermodynamically stable regions of the phase diagram; that is, the metastable region is not *a priori* excluded. We anticipate that the percolation line (if it can be located) will not be forced to end at the higher-order critical point, but may extend into this metastable area. We do not expect a two-parameter percolation RG to locate so subtle a feature as a first-order thermal transition when, as in this case, it is not made obvious

by symmetry considerations. The behaviour of the RG in the metastable region, and the character of the percolation line in the three dimensions, are topics of central interest in this work.

A second reason for introducing an RG scheme parametrised by densities, not fields, is the existence of CP problems which are difficult, if not impossible, to describe using a Hamiltonian or global statistical weight. Such problems are best introduced by an example. In a model proposed by Edwards and Anderson (1975) for an Ising spin glass in two dimensions, one considers a square lattice populated by Ising spins which are connected by nearest-neighbour bonds of uniform size but random sign. If the fraction p_b of ferromagnetic bonds is reduced from unity, the $T = 0$ magnetisation decreases continuously, reaching zero at a value of p_b near 0.9. It has been conjectured (Domany 1979) that this value corresponds to the percolation threshold for 'unfrustrated plaquettes'—elementary squares of bonds with an even number of antiferromagnetic segments. Regarding such plaquettes as occupied sites on the dual lattice, it is clear that one is dealing with site CP in which correlations are induced by the bond geometry. It is plausible that one could map such a problem onto an Ising model (plaquette → site → spin). Unfortunately, to choose properly the multi-spin interactions that would reproduce the existing site correlations is not straightforward. A method which focuses directly on those local configurations seems preferable. The application of our PSRG methods to this specific problem has been discussed in earlier work (Tuthill 1982).

This paper is organised as follows. In the next section we sketch the cell-to-site PSRG which is to be used. In the absence of a Hamiltonian we need to find a statistical weight for each configuration. This is constructed from correlation parameters through a modified superposition approximation. The expected role of scaling powers in this scheme is also discussed.

Two-dimensional results are reviewed in § 3. We employ two levels of approximation, the first based on the possible configurations of two adjacent sites, and the second treating correlations within a four-site cluster. Both approaches suggest that there exist only two universality classes for site CP. A fixed point with random percolation exponents controls problems with weak correlation, while for more strongly correlated sites—e.g., down-spins at the Ising critical point—a higher-order percolation point may appear.

In § 4 the two-site approach is applied to the simple cubic lattice. The strong-correlation fixed point of two dimensions is retained, but the eigenvalues at this point are complex. We argue that the unphysical nature of this scale-invariant point (much the same as the extension of a separatrix into an inaccessible regime) indicates that the equilibrium branch of the percolation curve penetrates into the metastable region. We close in § 4 with a discussion of this PSRG and the metastability problem.

2. The cell-to-site PSRG

PSRG methods for random site percolation have been extensively described by other authors (Reynolds *et al* 1977, 1978). In brief, a multi-site cell of the original lattice is replaced by an empty or occupied site of the new (rescaled) lattice according to a rule chosen with a view to the physics. i.e., if a cell is connected from side to side by a path over nearest-neighbour occupied sites, then the renormalised site is considered to be occupied. The specifics of various connectivity rules have been discussed by

Reynolds *et al.* The likelihood that a renormalised site is occupied is the net probability of all internal configurations of empty and occupied sites for which the cell is connected.

Rescaling in site CP is performed in a similar way, with the exceptions that (i) a multi-cell cluster must be considered, since multi-site correlations are rescaled, and (ii) the probability for each internal configuration must be chosen with the correlations in mind. The first change means simply that extending this approach to large cells, or treating correlations involving very many spins, would soon make the calculation intractable. Point (ii) involves a different limitation, since in fact one must approximate the likelihood of a configuration from correlations involving fewer sites. The procedure for 'building up' the weight from short-range correlations will be described below.

A natural first approach to treating correlations is to introduce independent probabilities u_i for the various configurations of two nearest-neighbour sites:

$$u_1 = \langle \circ\circ \rangle, \qquad u_2 = \langle \times\circ \rangle = \langle \times\circ \rangle, \qquad u_3 = \langle \times\times \rangle \tag{2}$$

where $\circ$ denotes an empty and $\times$ an occupied site. Since $u_1 + 2u_2 + u_3 = 1$, in fact only two parameters are needed in the PSRG at this level. It is convenient to choose them as described in the previous section, namely p and t:

$$p = u_2 + u_3, \qquad t = u_2[(u_2 + u_3)(u_1 + u_2)]^{-1}. \tag{3}$$

Clearly $0 < t < 1/\max(p, 1-p)$ if the u's are positive. A tendency for occupied (or empty) sites to cluster together is reflected by a value of t less than one. We also note that t is not defined in the $p \to 1$ or $p \to 0$ limits, although the basic quantities $\{u_i\}$ keep their meaning.

To generate rescaling transformations we use a cluster of two neighbouring cells, with each cell 2×2 on the square lattice or $2 \times 2 \times 2$ on the simple cubic. The renormalised site occupancy is defined by

$$p' = \Sigma' \text{ (configuration weights)} \tag{4}$$

where Σ' is a sum over only those configurations in which the (say) right cell is rescaled to an occupied site, via whatever connectivity rule is in use. The recursion relation for t is then

$$t' = [p'(1-p')]^{-1} \Sigma'' \text{ (configuration weights)} \tag{5}$$

where now Σ'' is over all configurations rescaling to '$\times\circ$'.

There is of course substantial freedom in the choice of a method for weighting cluster configurations. We describe next an approach which is a compromise between simplicity and physical plausibility. Each occupied or empty lattice site acquires a factor p or $1-p$, while for each nearest-neighbour pair in the cluster one includes a term $u_1/(1-p)^2$, $u_2/[p(1-p)]$ or u_3/p^2 as appropriate. The expression that results at this stage, however, gives a poor estimate for the likelihood of a closed loop of occupied or empty sites. In particular, a plaquette of four occupied sites would have a weight of $(1-t+tp)^4 = [u_3/(u_2+u_3)]^4$, which is a constant in the $u_2 \to 0$ (or $t \to 0$) limit, independent of u_3. This limit should simply correspond to a situation in which large regions of occupied sites coexist with large regions of empty sites, in such a way that the intervening boundaries contain a vanishingly small fraction of the total system. In this light, a more reasonable weight for the fully occupied cluster as u_2 goes to zero would simply be p, the likelihood of finding a single site occupied. This can be arranged by including a term p^2/u_3 (or $(1-p)^2/u_1$) for each plaquette consisting solely

of occupied (or empty) sites. In three dimensions an additional factor of u_3/p^2 or $u_1/(1-p)^2$ is needed for each fully occupied or empty cube.

The relative probability, approximated in this way, is illustrated in figure 2 using sample configurations of clusters on both the square and simple cubic lattices.
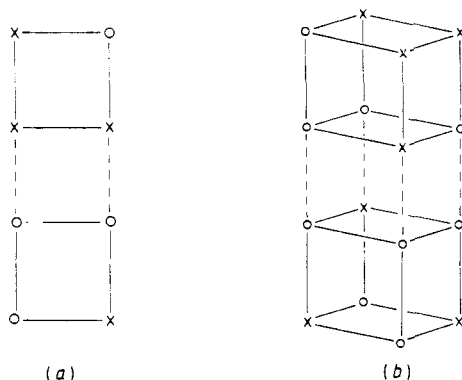

Figure 2. Typical two-cell clusters on the square and simple cubic lattices, both mapping to the renormalised site configuration '×○'. The relative statistical weight of (a) is $(u_1u_3)^2u_2^6p^{-6}(1-p)^{-6}$, and that of (b) is $u_1^8u_2^{17}u_3^3p^{-16}(1-p)^{-24}$.

The weights formed as described above satisfy the following criteria. (a) They correctly reduce to the product of independent site probabilities in the limit that $t = 1$ (limit of pure random percolation). (b) They are non-singular in the $p = 0$ or $p = 1$ limits when $t < 1$; only the configuration with all sites empty or occupied, respectively, has non-vanishing probability. (c) As remarked above, in the $t = 0$ limit the likelihood of finding a cluster with all sites occupied is simply p, and that for all sites empty, $1 - p$. Partially occupied configurations have vanishing probability as $t = 0$.

The p and t recursion relations therefore consist of sums of terms, each of which is a product of powers of the u_i, p, $1 - p$ and t. Enumeration of all the terms could be done by hand for the eight sites of the two-dimensional problem, but for the simple cubic lattice (16-site cluster) a computer was of course necessary. Fixed points of the recursion relations were found numerically by Newton's method.

A second approach, which was applied only in two dimensions, has as its starting point the correlations within a four-site plaquette. Independent probabilities w_1–w_6 are defined for the distinct configurations (reduced by reflections and rotations) of a square of four lattice sites:

$$w_1 = \left\langle {\scriptstyle \bigcirc\bigcirc \atop \scriptstyle \bigcirc\bigcirc} \right\rangle \qquad\qquad w_4 = \left\langle {\scriptstyle \bigcirc\times \atop \scriptstyle \times\bigcirc} \right\rangle \left\langle {\scriptstyle \times\bigcirc \atop \scriptstyle \bigcirc\times} \right\rangle$$

$$w_2 = \left\langle {\scriptstyle \times\bigcirc \atop \scriptstyle \bigcirc\bigcirc} \right\rangle = \left\langle {\scriptstyle \bigcirc\times \atop \scriptstyle \bigcirc\bigcirc} \right\rangle = \ldots \text{etc} \qquad\qquad w_5 = \left\langle {\scriptstyle \times\times \atop \scriptstyle \times\bigcirc} \right\rangle = \left\langle {\scriptstyle \times\bigcirc \atop \scriptstyle \times\times} \right\rangle = \ldots \text{etc}$$

$$w_3 = \left\langle {\scriptstyle \bigcirc\times \atop \scriptstyle \bigcirc\times} \right\rangle = \left\langle {\scriptstyle \times\times \atop \scriptstyle \bigcirc\bigcirc} \right\rangle = \ldots \text{etc} \qquad\qquad w_6 = \left\langle {\scriptstyle \times\times \atop \scriptstyle \times\times} \right\rangle. \qquad\qquad (6)$$

With the normalisation condition

$$w_1 + 4w_2 + 4w_3 + 2w_4 + 4w_5 + w_6 = 1 \qquad\qquad (7)$$

five parameters are involved in the renormalisation. The two-site probabilities u_i are of course expressible in terms of the w_j:

$$u_1 = w_1 + 2w_2 + w_3, \qquad u_2 = w_2 + w_3 + w_4 + w_5, \qquad u_3 = w_3 + 2w_5 + w_6. \qquad (8)$$

For rescaling by a factor of two, we use a square cluster of sixteen sites (four cells) and again weight individual configurations by a superposition approximation. Each plaquette (excepting the centre) is given a weight w_i, while each bond shared by these cells acquires a factor $1/u_j$. The recursion relations are stored and studied numerically in the same manner as in the two-site three-dimensional case.

3. Two-dimensional results

We next review the square lattice results, which are qualitatively similar in both the two- and four-site approximations. The PSRG trajectories have only two ordinary fixed points, excluding those trivial ones corresponding to the fully occupied or completely empty lattice. The first is situated at zero correlation, has a single relevant eigenvalue, and dominates the percolation properties of weakly correlated sites. We refer to it as the random percolation fixed point R, and note that it was first found by Reynolds *et al*. A second fixed point, denoted I and unstable with respect to the first, is located at strong positive correlation and is characterised by two relevant eigenvalues.

In table 1 are listed sample locations of R and I, together with their relevant eigenvalues λ_i and scaling powers y_i, where $y = \ln \lambda / \ln 2$. For the specific cases shown we have used an R_1-type connectivity rule, in which cells must be spanned in a chosen direction. (In the two-site approximation, this is parallel to the long axis of the cluster; in the four-site case, to preserve reflection symmetry, cells of type w_3 are considered spanned if the occupied sites are shared with a neighbouring cell.) We point out that the basic geometry of the phase diagram is relatively insensitive to the particular connectivity rule used, although precise details do vary slightly. The R_1 rule is a convenient choice since it closely reproduces the random-site percolation threshold $p = 0.593$ for the square lattice, known from numerical studies.

We show in figure 3 the flow diagram derived for the two-site case of table 1. Rather than plotting p against t, which introduces (arbitrarily located) fixed points

Table 1. Fixed-point parameters for two- and three-dimensional correlated percolation.

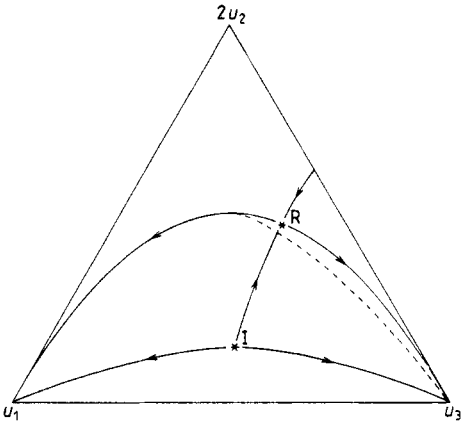| Fixed point		R	I
2-site, 2D	u_1-u_3	0.146, 0.236, 0.382	0.417, 0.073, 0.438
	p, t	0.618, 1.0	0.511, 0.291
	λ_1, λ_2	1.528, —	1.974, 1.546
	y_1, y_2	0.612, —	0.629, 0.981
4-site, 2D	w_1-w_6	0.0213, 0.0344, 0.0557, 0.0557, 0.0902, 0.146	0.143, 0.0346, 0.0385, 0.00908, 0.0515, 0.341
	p, t	0.618, 1.0	0.616, 0.565
	λ_1, λ_2	1.528, —	1.400, 1.082
	y_1, y_2	0.612, —	0.485, 0.114
2-site, 3D	u_1-u_3	0.473, 0.215, 0.097	0.436, 0.112, 0.340
	p, t	0.312, 1.0	0.452, 0.451
	λ_1, λ_2	2.051, —	$2.850 + i0.725$
	y_1, y_2	0.965, —	—

Figure 3. Renormalisation flow diagram for the square lattice correlated percolation problem using the two-site approximation. R is the random percolation fixed point, and is stable against weak positive or negative correlation between adjacent sites. I is a doubly unstable strong-correlation fixed point, characteristic of Ising-correlated percolation. Shown dotted is the curve $u_1(u_2)$ for unfrustrated plaquettes.
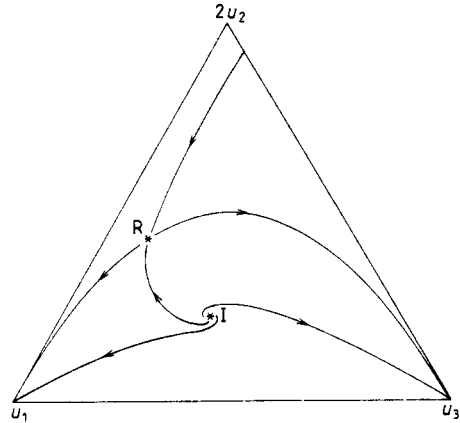
Figure 4. Renormalisation flows for the three-dimensional (simple cubic lattice) correlated percolation problem. The random percolation fixed point R controls all percolation transitions, since the fixed point I has complex eigenvalues and is physically inaccessible.

on the $p = 1$ and $p = 0$ lines, we use a composition triangle with vertices u_1, u_3 and $2u_2$. In this representation the line of no correlation ($t = 1$) appears as the curve $u_1 = (u_1 + u_2)^2$, which is also the separatrix linking R with the u_1 and u_3 vertices. The curve $u_1(u_2)$ for unfrustrated plaquettes in the $\pm J$ Ising model is seen to cross the critical separatrix leading to R, indicating that their percolation properties are in the same universality class as uncorrelated sites.

The strong-correlation fixed point I is a higher-order percolation point, and we identify it with the thermal critical point of the two-dimensional Ising ferromagnet. The location of I for the two-site approximation in fact agrees quite closely with the exact critical values p_c and t_c for a magnetic system:

$$p_c = 0.5, \qquad t_c = 1 - 2^{-1/2} = 0.2929 \ldots \qquad (9), (10)$$

The latter expression arises from equation (3) and the exact result (Kaufman 1949, Kaufman and Onsager 1949, Montroll *et al* 1963) that the nearest-neighbour correlation function $\langle s_i s_j \rangle$ takes the value $2^{-1/2}$ at criticality. This correspondence is sensitive to the particular choice of the superposition approximation, but less so to the type of connectivity rule. A striking feature of the phase diagram shown is the existence of a fixed line at $u_2 = 0$, or maximum positive correlation. This is a consequence of our choice of the configuration weights to meet criterion (c) above. It gives rise to a 'mixed phase' regime below the u_1–I–u_3 separatrix, where PSRG trajectories flow toward the base of the composition triangle.

The results of the four-site approximation (table 1) are less easily displayed, since the trajectories lie in a space of five RG parameters. The fixed point I remains a higher-order percolation point with two relevant eigenvalues and a separatrix leading to R. As it is the attractor in a three-dimensional critical subspace, I is not expected to have values of p and t corresponding to those of the Ising model at criticality.

In both approximations the single relevant eigenvalue at R gives a connectedness length exponent for percolation ν_p of 1.635 (cf Reynolds *et al* 1980). The scaling powers at I, on the other hand, should be compared with those of the Ising model. In the two-site approximation the scaling fields are essentially $p - p^*$ and $t - t^*$ (with eigenvalues λ_1 and λ_2, respectively). We expect the first to scale like the magnetisation, while the latter is proportional to the nearest-neighbour correlation function, or internal energy:

$$t - t^* \sim (T - T_c)^{1-\alpha}, \qquad p - p^* \sim (T - T_c). \qquad (11), (12)$$

Thermal (M, T) and percolation (p, t) exponents are then expected to obey the relations

$$y_p = y_M, \qquad y_t = d - y_T. \qquad (13), (14)$$

The exact two-dimensional values for y_M and y_T are 0.125 and 1.0, respectively. Thus our results in the two-site approximation are quite good for y_t, but poor in the case of y_p.

For the four-site approximation, we point out that a four-spin Ising correlation function should scale like $(T - T_c)^{-\alpha}$ near criticality; since $\alpha = 0$ in two dimensions, the appearance of a scaling power near zero (rather than near unity) is consistent with the picture established so far.

4. The two-site approach for the simple cubic lattice

In three dimensions (simple cubic lattice) the two-site approach produces a flow diagram roughly similar to the 2D case. Figure 4 shows the situation under a connectivity rule in which a cubic cell is occupied if there exist spanning paths between opposite faces in at least two directions. In table 1 are listed the fixed point parameters, relevant eigenvalues, and scaling powers. The random percolation fixed point R (on the $t = 1$ curve) occurs at $p^* = 0.312$, as compared with the 'exact' (from numerical simulations) value $p = 0.311$. The percolation exponent ν_p arising from the single relevant eigenvalue at R is given in this scheme as 0.965, while estimates (cf the review of Essam 1980) from other methods lie in the range 0.8–0.9.

A mixed-phase region for small values of u_2 is again apparent, as is a strong correlation fixed point (I) unstable in all directions. However, the eigenvalues of the linearised recursion relations at I are complex, so that we cannot regard it as a physically accessible scale-invariant point. Indeed, for systems initially close to I, the large-scale connectedness would be an oscillating function of the site concentration, since the separatrices spiral outward from I.

In this approach, which makes use of uncontrolled approximations, we cannot completely rule out the possibility that such behaviour is simply an artifact of the method, and unrelated to the physics. One can, however, vary the steps in the method that are largely arbitrary, and note their influence on the results. With this in mind we adopted several alternative versions of the connectivity rule, e.g., spanning paths to include one specified direction, or spanning in at least two directions, one of which is specified. Complex eigenvalues at the fixed point I are a persistent feature of all the rules tested. It is reassuring to find further that such behaviour is *not* present under the majority rule. This preserves the symmetry between empty and occupied

sites, and therefore would be expected to locate the thermal critical point—not a percolation threshold.

Complex relevant eigenvalues are not unknown in RG studies of phase transitions (Boyanovsky and Cardy 1982, Weinrib and Halperin 1983). By relevant we mean, as in Weinrib and Halperin, that the real part is greater than one and the trajectories spiral outward from the fixed point. The meaning of these eigenvalues is by no means clear, but certain tentative conclusions are possible.

Since our recursion relations and fixed points are real, complex eigenvalues imply complex scaling fields. An additional characteristic of the recursion relations is that the RG flows from the unstable fixed point I define a separatrix which ends at $p = 0$ or 1 and t finite—a fixed-point location which is quite arbitrary and depends heavily on the exact definition of the RG transformation. This is similar to the behaviour of RG flows which have been speculated to indicate a smeared transition, in the work of Weinrib and Halperin.

We conclude tentatively that the choice of p and t as renormalisation variables, and the addition of the superposition approximation, has allowed this RG method to penetrate into the metastable state. Near the coexistence curve (for shallow quenches) the critical droplet needed to nucleate the metastable phase is large (Langer 1967) and small cluster methods such as those employed in this work cannot 'see' the critical droplet. As the system is quenched deeper the critical droplet size decreases until it can be detected by a small cluster approximation. This gives rise to a separatrix, on one side of which the system appears stable (in this RG approximation) and on the other side unstable.

Whether a configuration of spins contains a critical droplet of finite size will depend quite heavily on the exact way in which configurations are weighted, i.e., on how one handles the ground state. As noted above, this is not a well defined procedure in our method. Hence the separatrix defined by the unstable fixed point with relevant complex eigenvalues should not be considered as defining a sharp transition line, but instead a smeared region in which the system crosses over from metastable to unstable in a given formulation of the RG. This resembles somewhat the situation in Weinrib and Halperin, which they speculate may be associated with a smeared transition. Investigations currently under way are directed at a clearer understanding of this situation.

Acknowledgments

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