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Essential Singularities at First-Order Phase Transitions*

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Renormalization group ideas are applied to the problem of first-order phase transitions in Ising-like models. They support the existence of essential singularities as the coexistence region is approached, at all temperatures below the critical temperature.

The renormalization group (RG) has been developed as a tool for describing the behavior of systems which involve, in an essential way, the cooperative behavior of a large number of degrees of freedom. In the context of phase transitions, one thinks conventionally of applications to second-order phase transitions, where (essentially) infinite-range fluctuations appear as precursors of the transition between the ordered and disordered states. There do exist many applications of the RG to the ordered state[1] where, e.g., in the Ising model or equivalent field models, one can study the problem of the first-order transition between the two ordered states. These applications have until now considered only the effect of fluctuations away from a system which is in a *single* ordered phase. However, the existence of other types of fluctuations in the coexistence region of the two ordered phases of Ising-like models has already been recognized by several authors.[2] These other fluctuations correspond to configurations in which large regions of the *different* phases coexist. Such fluctuations permit the restoration of the convexity of the free energy to mean-field approximations[3] through the existence of solitonlike solutions in spontaneously broken field theories. The most concrete realization of this problem is seen in the formulation of cluster or droplet models of condensation[2] (see the work of Langer[4] and of Fisher[4] in particular for an introduction to this subject). This model predicts infinitely differentiable singularities.[4,5] Together with the proof[6] that all derivatives with respect to H of the free energy of the two-dimensional Ising model are finite at $H=0$, the axiomatic work of Lanford and Ruelle[7] also provides strong support for such singularities.

In this article we apply RG ideas to this problem. We formulate our approach in terms of Ising-like models on a lattice, with the Hamiltonian

$$\mathcal{H}/kT = -K\sum_{\langle ij\rangle} S_i S_j - H\sum_i S_i + \text{O.T.}, \tag{1}$$

where $\langle ij\rangle$ specifies a nearest-neighbor sum, K is the conventional nearest-neighbor coupling ($K=J/kT$), H represents an external field, and O.T. stands for any other types of interactions which may or may not be required to be included in $\mathcal{H}$. We are interested in the partition function $Z=\sum \exp(-\mathcal{H}/kT)$, and other quantities such as the spontaneous magnetization $M=\sum S_i \exp(-\mathcal{H}/kT)/Z$, in the coexistence region where H (and all other spin-ordering fields in O.T.) tends to zero at all

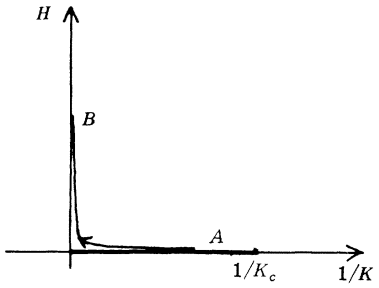

FIG. 1. The simplest phase diagram for the system described by Eq. (1). The RG trajectory shows how a point A near the coexistence region passes by the fixed point $H=0=1/K$ on its way to the point B where the low-temperature, high-field approximation can be applied.

temperatures below the critical temperature ($K > K_c$). We assume here the simplest possible phase diagram for (1)—a critical point and line of first-order (in H) phase transitions down to $T = 0$ as in Fig. 1.

For arbitrarily small H, the existence of fluctuations with large regions of the different phases prevents a straightforward application of conventional perturbation theories. We propose a conventional RG solution; the physical system at point A in Fig. 1 is reformulated in terms of a system at point B, whose behavior *can* be analyzed by the well-known high-field, low-temperature series approximation.

The projection in the subspace H, K^{-1} of the RG flow from A to B is shown qualitatively in Fig. 1. Its form is dictated by the following observations. For $H=0$, we expect to have three fixed points at $K=0$, $K=K_c$, and $K=\infty$. (We imagine a projection of the flow into the H, K plane in which the entire critical sheet is collapsed on to the point K_c). The existence of the critical fixed point is established within the approximation schemes[8-11] which have been developed so far. The high-temperature series approximation in conjunction with the decimation scheme[8] establishes conclusively the existence of the fixed point at $K=0$ and provides a systematic expansion about it. The $K=\infty$ fixed point also exists in all the approximate RG schemes although no method has yet been developed to provide a systematic expansion about the $K=\infty$ fixed point.[12]

Our main contention is that there is first a transient region in which the system moves under the RG transformation from $T<T_c$ towards the fixed point at $T=0$, which is approached arbitrarily closely if H is sufficiently small. Thus, it is the eigenvalues of the $T=0$, $H=0$ fixed point which control singularities on the coexistence curve. The linearized recursion formulas about the fixed point may be written (we discuss their origin later)

$$K' = b^{d-1}K, \tag{2a}$$

$$H' = b^d H, \tag{2b}$$

where b is the change in length scale of the RG transformation and d is the dimension of space. We expect these relations to be valid up to corrections of the type $\exp(-K+\alpha H)$ where $\alpha \sim O(b)$. So, as long as K is large and $\alpha H < K$, the expansion about the $K=\infty$ fixed point should be permissible.

After l iterations (neglecting the initial transient iterations), we have $K^{(l)} = b^{l(d-1)}K$, $H^{(l)} = b^{ld}H$. At what value of l should we stop the iteration of the RG transformation? We argue, on physical grounds akin to those applied in the droplet model, that one should iterate to a value l^* which just approaches the range of validity of the linearization about the $K=\infty$ fixed point, namely $\alpha H^{(l^*)} = K^{(l^*)}$. An $H^{(l)}$ of this order damps out all clusters of the "wrong" phase, in the sense that the "critical cluster" in the droplet model is the size of the new lattice spacing. Eliminating l^*, we obtain

$$K^{(l^*)} = K^d/(\alpha H)^{d-1}. \tag{3}$$

Since K is large initially, $K^{(l^*)}$ (and hence $H^{(l^*)}$) is extremely large. Therefore we expect to be able to apply the low-temperature, high-field expansion to the system $K^{(l^*)}, H^{(l^*)}$ and hence obtain a perturbation expansion for the thermodynamic quantities of the original system as a power series in $\exp(-K^{(l^*)})$ and $\exp(-H^{(l^*)})$, i.e., in powers of

$$\exp(-K^d/H^{d-1}). \tag{4}$$

These terms produce the essential singularities; they are infinitely differentiable at $H=0^+$, but clearly not analytic.

An additional attractive feature of the result (4) is that in the limit $T \to 0$, with the "physical" J and external field held constant (the $1/kT$ factors are extracted), the expression (4) tends to 0, i.e., *at* $T=0$ there is *no* singularity as $H \to 0$; this is desirable because there are no fluctuations to produce singularities at $T=0$.

Ideally, one would like to be able to set up Eqs. (2a) and (2b) as the first terms in a systematic expansion about the $T=0$ fixed point; this work is in progress. Even without the existence of a sys-

tematic expansion, the following arguments dictate their forms:

(i) We know from symmetry that the recursion formulas linearized for small H will be of the form $K' = f(K)$, $H' = g(K)H$ [or a similar form if O.T. in Eq. (1) must be included in the RG transformation].

(ii) The form (2b) for the H equation (linearized about the $T = 0$ fixed point) is necessary for the existence of a spontaneous magnetization[13]; it must hold for all systems where the phase separation problem exists.

(iii) In order to establish (2a) we need consider only the subspace of interactions even in the spin, where we can exploit dual transformations in d dimensions.[14] An Ising model at low temperatures (and $H = 0$) duals into a high-temperature model of interactions of Ising spins on the boundaries of $(d-1)$-dimensional cubes. Decimation on the latter model and inversion of the dual transformation induces the result (2a), up to exponentially small corrections.

(iv) The result (2a) is also exhibited in a fairly straightforward way in the Niemeijer and van Leeuwen approach.[9] [At the first nontrivial order, the new nearest-neighbor interaction is K $\times$(number of bonds connecting the two cell blocks) for K large, i.e., $K' = b^{d-1}K$ as required]. The recursion formula (20) of Migdal's paper[11] also displays Eq. (2a). We have not analyzed Kadanoff's method[10] systematically for high K. A different approach to first-order phase transitions which does not produce the result (2a) has been suggested by Subbarao.[15]

We make the following remarks:

(i) Note that (2a) is also correct in one dimension. The exact recursion formula by decimation is $\tanh K' = (\tanh K)^b$ which gives for K large, $K' = K - \frac{1}{2}\ln b$, up to exponentially small corrections. In fact one can combine this exact result with (2a) to show the lowest order of an ϵ expansion in $1 + \epsilon$ dimensions.[16]

(ii) One puzzling feature which we do not understand is that the result (2a) is produced only if the new lattice is *not* rotated with respect to the old. An example of this puzzle is provided by the results of van Leeuwen's work in Ref. 13. This aspect requires further clarification.

(iii) For $d > 4$, the critical behavior of the system (1) is described by mean-field theory. One might have been led to conjecture that mean-field critical behavior might also be accompanied by mean-field behavior in the coexistence region, in the sense that the free energy might be continuable into the coexistence region, to describe metastable states.[17] This conjecture is not supported by expression (4), which shows the existence of the essential singularity in any space dimension d (> 1).

(iv) In addition to the term (3), there are also contributions to the free energy at each iteration of the RG transformation. Within model analyses these contributions are of the form

$$\exp(-K^{(l)})\cosh\alpha H^{(l)}. \tag{5}$$

Both these contributions and the recursion relations [Eqs. (2a) and (2b)] change character simultaneously at l^* (allowing a well-defined summation to $l = \infty$, in principle). The sum of the terms (5) up to l^* gives a form of the free energy which is similar to that of the droplet model. In fact l^* is just that value of l for which the critical cluster size $L_c \sim K/H$ is of order 1. However, there is no asymmetry in expression (5) corresponding to that of the droplet model, where approximations for the free energy involve summing over clusters of the opposite phase in a background parallel to H (or analyzing the sum of clusters, up to the critical size L_c, of the "right" phase in the "wrong" background).

Finally once a systematic low-temperature expansion is found for the RG approach, one can calculate systematically the behavior near the coexistence curve.

Despite the qualitative nature of much of the above discussion, it is clear that it opens the way for a new application of the renormalization group to a problem of considerable interest.

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[16]If the limit $\epsilon \to 0$ is continuous, the recursion formula should have the form $K' = b^{\epsilon}K - \frac{1}{2}\ln b + O(\epsilon, \exp(-K))$. This exhibits a critical fixed point $K^* = 1/2\epsilon$ with $\nu = 1/\epsilon$, as in Ref. 11. (The eigenvector in $1+\epsilon$ dimensions is almost certainly not pure nearest-neighbor coupling, but corrections to the eigenvector do not change the eigenvalue at lowest order.)

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Renormalization Group Results for Lattice-Gas Phase Boundaries in Two Dimensions*

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Lattice-gas phase boundaries have been calculated for the simple quadratic and honeycomb lattices from the corresponding antiferromagnetic critical curves. Results were obtained using nonlinear renormalization group methods with periodic cell clusters. The result for the simple quadratic lattice is in excellent agreement with the existing temperature-series result.

The recent discovery that some order-disorder transitions in certain superionic conductors are pure Ising like[1] has revived interest in lattice-gas theories.[2,3] Many recent experiments have been reported which measured the order parameters as a function of the temperature.[4-7] There is a definite need for better theoretical predictions of the phase boundaries—i.e., the critical concentration versus the temperature. Here we wish to report the phase boundaries for the lattice gas obtained, for the first time, by using the method of the renormalization group.[8,9] We report results for the simple quadratic (sq) and honeycomb (hc) lattices. The sq lattice is chosen for a direct comparison with the excellent results of Bienenstock using the high-temperature series.[10,11] The other two-dimensional lattice is interesting because of its applicability to the superionic conductor β-alumina.[6-12] Several experiments are currently under way to measure order-disorder phase boundaries.[7,13,14]

The critical curve for the lattice gas is obtained by first determining the critical curve of the antiferromagnetic Ising model with a magnetic field,[15-17]

$$H_I = -K_1 \sum_j \sigma_j - K_2 \sum_{\langle ij \rangle} \sigma_i \sigma_j . \qquad (1)$$

We use the nonlinear renormalization group approach of Niemeijer and van Leeuwen.[8] As suggested first by Nauenberg and Nienhuis,[9] the free energy $F_I(K_1, K_2)$ is obtained as an infinite series, which converges rapidly. We also use their method of cell clusters, with periodic boundary