PHYSICAL REVIEW LETTERS

VOLUME 35 25 AUGUST 1975 NUMBER 8

First-Order Phase Transitions in Renormalization-Group Theory

B. Nienhuis* and M. Nauenberg†
Natural Sciences, University of California, Santa Cruz, California 95064
(Received 20 March 1975)

Conditions are given for the renormalization-group transformations of the Hamiltonian of a thermodynamic system which lead to a discontinuity in an order parameter.

In renormalization-group applications to statistical mechanics, the singularities of thermodynamic functions associated with phase transitions are located on critical surfaces determined by the fixed points of the renormalization transformation.[1] While the properties of the fixed points which give rise to second-order phase transitions and critical phenomena, e.g., infinite correlation length, are well understood, the corresponding properties associated with first-order phase transitions, e.g., discontinuous change in an order parameter, have remained largely unexplored. In a recent review article,[2] Aharony refers to renormalization transformations leading to these discontinuities as mappings into a "no man's land" of first-order phase transitions,[3] while in other reviews[1] the problem is ignored altogether. The purpose of this note is to give sufficient conditions on the fixed points and eigenvalues of renormalization transformations for the Hamiltonian of a thermodynamic system which give rise to a discontinuous order parameter for temperatures T below a critical temperature T_c. Some of these conditions can be shown to be generally valid for renormalization-group transformations of Ising-spin models which preserve the symmetry of the ground-state spin configuration. However certain assumptions that we make about the general properties of the renormalization mappings have been verified only in approximate numerical calculations for several first-order phase transitions which occur for a square-lattice Ising model.

Let the Hamiltonian of the thermodynamic system under consideration depend on a set of fields K_α, $\alpha = 1, 2, \ldots$, and on the field H which is conjugate to an order parameter M. A first-order phase transition for temperatures T below a critical temperature T_c can be described by a discontinuity of M as a function of H which can be taken to occur at $H=0$. Assume there exists a renormalization-group transformation of this Hamiltonian to new fields $K_\alpha'(K,H)$ and $H'(K,H)$ which are analytic functions of K and H. Since the origin and the sign of H for small values of H must be preserved by this transformation, it follows that $H'(K,0)=0$ while $\partial H'(K,0)/\partial H \neq 0$. As is well known,[1] in renormalization-group theory the critical behavior of such a system is determined by a fixed point at $K_\alpha = K_\alpha^*$ and $H=0$, with a relevant eigenvalue $\lambda_H^* = \partial H'(K^*,0)/\partial H$ associated with the ordering field H, and with one or more relevant eigenvalues obtained by diagonalizing the matrix $T_{\alpha\beta} = \partial K_\alpha'(K^*,0)/\partial K_\beta$. These eigenvalues determine the universal critical exponents of the thermodynamic functions with power-law singularities located on the critical surface associated with this fixed point, i.e., the subspace of points K_α, $H=0$, which are mapped by successive renormalization transformations arbitrarily close to this fixed point.

We now state further conditions on these renormalization transformations and on the order parameter M which are sufficient for the occurrence of a discontinuity ΔM in M for temperatures T below the critical temperature T_c:

(a) There exists another fixed point at $K_\alpha = K_\alpha^{**}$ and $H=0$ such that points K_α and $H=0$ which belong to a domain $\mathfrak{D}$ (corresponding to $T < T_c$) bounded on one side by the critical surface are mapped by successive renormalization transformations into this fixed point. We shall refer to it as the *discontinuity fixed point.*

(b) At this fixed point, the eigenvalue $\lambda_H^{**} = \partial H'(K^{**}, 0)/\partial H$ associated with the ordering field H is given by $\lambda_H^{**} = L$, where L is the change in the scale of volume under the renormalization transformations. For discrete lattices L is the number of spins in a Kadanoff cell.

(c) The limit ΔM^{**} of the discontinuity $\Delta M(K)$ of the order parameter as K approaches K^{**} does not vanish.

We first prove that condition (b) is necessary for a discontinuity $\Delta M(K)$ at $H=0$ for $K_\alpha \in \mathfrak{D}$, by applying the inhomogeneous scaling equation for the free energy $f(K,H)$ of the system.[4] We have

$$f(K,H) = g_L(K,H) + L^{-1} f(K',H'), \qquad (1)$$

where $g_L(K,H)$ is the self-energy per spin of the Kadanoff cell and is assumed to be analytic at $H=0$. Hence $\Delta M(K) \equiv M_+(K) - M_-(K)$, where

$$M_\pm(K) = \lim_{H\to 0^\pm} \partial f(K,H)/\partial H,$$

satisfies the equation[5]

$$\Delta M(K) = R(K)\,\Delta M(K'), \qquad (2)$$

where $R(K) = L^{-1}\partial H'(K,H)/\partial H$ at $H=0$.

By considering Eq. (2) at the discontinuity fixed point we obtain $R(K^{**}) = 1$ provided that $\Delta M(K^{**}) \neq 0$. This proves that condition (b) is necessary.[6] Note that condition (b) also implies that $\partial g_L(K^{**}, 0)/\partial H = 0$ in order that $M_\pm$ not be logarithmically divergent at the discontinuity fixed point. To show that these conditions are also sufficient to obtain $\Delta M(K) \neq 0$ for $K_\alpha \in \mathfrak{D}$ we apply the renormalization transformations successively to Eq. (2) and obtain

$$\Delta M(K) = \prod_{n=0}^{\infty} R(K^{(n)})\,\Delta M^{**}, \qquad (3)$$

where $K_\alpha^{(n)}$ is the mapping of K_α after the nth renormalization transformation and $K_\alpha^{(0)} = K_\alpha$.

A sufficient condition that the infinite product in Eq. (3) be finite is

$$\rho = \lim_{n\to\infty} [R(K^{(n+1)}) - 1]/[R(K^{(n)}) - 1] < 1.$$

In the case that K_α^{**} is finite we find that $\rho = \lambda_1^{**}$, where λ_1^{**} is the largest eigenvalue at the discontinuity fixed point for mappings restricted to $\mathfrak{D}$. Since this fixed point is stable with respect to $\mathfrak{D}$ we have $\lambda_1^{**} < 1$. A similar proof applies if K_α^{**} is infinite, and asymptotically the mapping is linear in K_α, i.e., $K_\alpha' \simeq \sum_\beta T_{\alpha\beta}^{**} K_\beta$ which implies in this case that $\lambda_1^{**} > 1$. Assuming that $R - 1 \sim O(K^{-\epsilon})$ $(K_\alpha \to \infty)$, where $\epsilon > 0$, we find that $\rho = (\lambda_1^{**})^{-\epsilon} < 1$.

The K_α dependence of the discontinuity $\Delta M(K)$ is given by Eq. (3) entirely in terms of the successive renormalization transformations of K_α and the ordering field H in the limit $H=0$. For $K_\alpha \notin \mathfrak{D}$, e.g., $T > T_c$, $H=0$, these transformations will map K_α towards a different fixed point. In general we expect that $R < 1$ at such a fixed point, and Eq. (2) then implies that $\Delta M(K) = 0$.

In the limit that $K_\alpha \in \mathfrak{D}$ approaches the critical fixed point, Eq. (2) becomes

$$\Delta M(K) \cong \lambda_H^{*}\Delta M(K')/L, \qquad (4)$$

where

$$K_\alpha' \cong K_\alpha^{*} + \sum_{\beta=1} T_{\alpha\beta}(K_\beta - K_\beta').$$

If the matrix $T_{\alpha\beta}$ has only one relevant (thermal) eigenvalue λ_T^{*} with a corresponding left eigenvector φ_T, Eq. (4) implies the well-known scaling power-law singularity[1]

$$\Delta M(K) \sim |u_T|^\beta, \qquad (5)$$

where $u_T = \sum_\alpha \varphi_{T\alpha}(K_\alpha - K_\alpha^{*})$ and the critical exponent $\beta = (\ln L - \ln\lambda_H^{*})/\ln\lambda_T^{*}$. This result is applicable also if $T_{\alpha\beta}$ has several relevant eigenvalues $\lambda_1 < \lambda_2 < \lambda_3 \ldots$ with left eigenvectors $\varphi_{i\alpha}$. The condition that $K_\alpha \in \mathfrak{D}$ requires that $u_i = c_i \times |u_1|^{\Delta_i}$, where $u_i = \sum_\alpha \varphi_{i\alpha}(K_\alpha - K_\alpha^{*})$, $\Delta_i = \ln\lambda_i/\ln\lambda_1 > 1$, and c_i is a constant, with $i = 2, 3, \ldots$. In this case we set $u_T = u_1$ and $\lambda_T^{*} = \lambda_1$ in Eq. (5). In the case that $K_\alpha \in \mathfrak{D}$ approaches the critical surface away from the fixed point K_α^{*}, these results are readily extended by substituting for u_T in Eq. (5) the corresponding scaling field ζ_T which depends nonlinearly on K_α.[4,7]

Conditions (b) and (c) can also be readily verified by examining the properties of the renormalization-group transformations of general Ising-spin models in the limit of zero temperature.[8] It is essential that these transformations preserve the ground-state spin configuration. This is valid for the construction method proposed by Niemeijer and van Leeuwen[9] provided that the Kadanoff cells are suitably chosen[10] and that periodic boundaries are applied in the cluster approximation.[4,8]

Let us assume that there are two ordered spin configurations denoted by + and − which have the same energy in a subspace of the coupling constants K_α. The energy per spin of each configuration is $f^{(\pm)}(K)=\sum_\alpha f_\alpha^{(\pm)}K_\alpha$, where $f_\alpha^{(\pm)}$ are constants and the condition for degeneracy becomes $\sum_\alpha(f_\alpha^+ - f_\alpha^-)K_\alpha=0$. If the renormalization transformation preserves the spin ordering, the scaling equation, Eq. (1), applies to $f^{(+)}(K)$ and $f^{(-)}(K)$ separately with $g(K)=\sum g_\alpha K_\alpha$. Hence the field $H=\sum\{f_\alpha^{(+)} - f_\alpha^{(-)}\}K_\alpha$ scales according to

$$H' = LH \tag{6}$$

which verifies condition (b) with H as the ordering field. For somewhat more general renormalization transformations proposed by Wilson[11] and by Kadanoff and Houghton[12] which depend on undetermined parameters, one can readily derive conditions[13] on these parameters which leave the ground-state spin configuration invariant and map the subspace for zero temperature into itself. However, we cannot show by purely theoretical arguments that some of the detailed properties which we have assumed for renormalization-group transformations, e.g., condition (a), are valid for all Ising-spin transformations.[13] Even the existence of critical fixed points has been demonstrated to date in these models only in approximate calculations.

We have also been able to verify all the conditions discussed in this paper in numerical calculations for the square-lattice Ising-spin model, by applying the cell-cluster approximation of Niemeijer and van Leeuwen to four cells.[8] This restricts the space of coupling constants K_α to the subspace of nearest- and next-nearest-neighbor spin couplings K_1 and K_2, three- and four-spin couplings K_3 and K_4, and a magnetic field $\mathcal{K}$. In this subspace there occur a variety of first-order phase transitions. We have considered in particular[8] first-order phase transitions in the ferromagnetic domain $K_1>0$, $K_2>0$, and $\mathcal{K}=0$, and in the tricritical domain $K_1<0$, $K_2>0$, and $\mathcal{K}\neq 0$. In each of these cases we found the discontinuity fixed point at zero temperature with $\lambda_H{}^{**}=L$. The discontinuous order parameter for the ferromagnetic transition is basically the magnetization $\mathfrak{M}$, while for the tricritical transition it is a linear combination of $\mathfrak{M}$ and the nearest-neighbor spin correlation $\mathfrak{N}$. Similar results were also obtained in the domain $K_2>0$, $K_1=0$, and $\mathcal{K}=0$ for $\mathfrak{N}$ as a function of K_1.

---

*Present address: Institute for Theoretical Physics, University of Utrecht, Utrecht, The Netherlands.

†Work supported by a grant from the National Science Foundation.

[1]For recent reviews and references to the literature see K. G. Wilson and J. Kogut, Phys. Rep. 12C, 77 (1974); and M. E. Fisher, Rev. Mod. Phys. 46, 597 (1974).

[2]A. Aharony, in "Phase Transitions and Critical Phenomena," edited by C. Domb and M. S. Green (Academic, New York, to be published), Vol. 6.

[3]For another viewpoint, see G. R. Golner, Phys. Rev. B 8, 3419 (1973).

[4]M. Nauenberg and B. Nienhuis, Phys. Rev. Lett. 33, 344, 1598 (1974).

[5]For simplicity we have considered here the case that there is only one independent discontinuous order parameter M; i.e., the parameter M can be chosen such that $\partial f(K,H)/\partial K_\alpha$ is continuous at $H=0$. This requires that H be taken proportional to the nonlinear scaling field associated with the eigenvalue $\lambda_H{}^*$. More generally, if there are more independent discontinuities ΔM_α associated with ordering fields H_α, Eq. (2) becomes a matrix equation

$$\Delta M_\alpha(K,H_\alpha=0)=\sum_\beta R_{\alpha\beta}(K)\Delta M_\beta(K',0),$$

where $R_{\alpha\beta}(K)=L^{-1}\partial H_\alpha'(K,0)/\partial H_\beta$, and our results can be readily generalized.

[6]The mathematical possibility exists that condition (c) is not valid, which requires that $\lambda_H{}^{**}>L$ [instead of condition (b)] for $\Delta M(K)\neq 0$. However we doubt that this case is of physical interest.

[7]F. J. Wegner, Phys. Rev. B 5, 4529 (1972).

[8]B. Nienhuis and M. Nauenberg, Phys. Rev. B 11, 4152 (1975), and to be published.

[9]Th. Niemeijer and J. M. J. van Leeuwen, Phys. Rev. Lett. 31, 1412 (1973), and Physica (Utrecht) 71, 17 (1974).

[10]J. M. J. van Leeuwen, to be published.

[11]K. G. Wilson, in "Field Theory and Critical Phenomena," Cargese Lecture Notes, 1973, edited by E. Brézin and J. Charap (to be published).

[12]L. P. Kadanoff and A. Houghton, Phys. Rev. B 11, 377 (1975).

[13]It has been shown by K. Subbarao (to be published) that for the Kadanoff-Wilson renormalization transformation matrix which is linear in the Ising spins the single parameter of this transformation can be chosen so that the eigenvalue condition (b) is satisfied on each flow line mapping onto a line of fixed points. However, this renormalization group does not have a critical fixed point.