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Renormalization-Group Approach to the Solution of General Ising Models*

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It is shown how the renormalization-group ideas of Wilson can be applied to obtain the complete thermodynamic functions for general Ising models. The most singular term near the critical transition is given explicitly in terms of the renormalization-group transformations. As an example an approximate numerical solution is given to the original Ising model.

The fundamental renormalization-group approach of Wilson[1] based on Kadanoff's intuitive deduction[2] of Widom's scaling law[3] has led to considerable progress in understanding critical transitions. In particular the well-known scaling behavior and the universality of critical exponents is obtained from the existence of a fixed point and the analyticity of the renormalization transformations. The values of these exponents were first calculated by Wilson and Fisher[4] in the ϵ expansion which exhibited the role of lattice dimensionality, and have been obtained also by other methods. Recently Niemeijer and van Leeuwen[5] have shown how to implement more directly Kadanoff's ideas using the Wilson approach to evaluate the critical exponents and the transition temperature for Ising models. In this note we want to show how to extend this method to obtain the complete thermodynamic function for the general Ising model in terms of the renormalization-group transformations. The essential point is to use the fact that the partition function of the Ising-spin system is form invariant under the renormalization-group transformation only up to a factor $\exp[Ng_N(K)]$ [see Eq. (2)], where $g_N(K)$ is a function of the spin interaction parameter K for N spins and is completely determined by this transformation. We will show that the partition function can be evaluated in terms of $g_N(K)$ for any desired range of values of K for which the nonlinear renormalization-group mappings are determined, including the singular behavior on the critical surface. Near the critical surface we obtain the well-known power-law or logarithmic singularities, but including explicitly an expression for the coefficient of these singularities. As an example, we have solved numerically our equations for the case of a square lattice in a four-cell approximation, and obtained the free energy, the energy, and the specific heat as a function of the nearest-neighbor spin coupling.

The renormalization-group transformation for N spins

$$K_\alpha' = F_\alpha(K) \tag{1}$$

in the parameter space K of the generalized Ising-spin lattice and the function $g_N(K)$ are determined by the invariance requirement

$$\exp[H_{N/L}(K', S') + Ng_N(K)] = \sum_{\{\sigma\}} \exp[H_N(K, S)], \tag{2}$$

where the summation is carried out over all possible configurations σ for fixed values of the cell spins s_i', and

$$H_N(K, S) = \sum_a K_a \prod_{i \in a} S_i, \quad S_i = \pm 1, \tag{3}$$

is the generalized Ising-spin Hamiltonian ($kT = 1$), summed over sets a of spins as defined by Niemeijer and van Leeuwen, but excluding the empty set.[5] This accounts for the explicit appearance of the function $g_N(K)$ on the left-hand side of Eq. (2) which plays a special role in our approach.

An important property of the renormalization-group mapping, Eq. (1), is the existence of a fixed point $K_\alpha{}^* = F_\alpha(K^*)$ where $F(K^*)$ is analytic. Hence, to first order in $K_\alpha - K_\alpha{}^*$ we have

$$K_\alpha' - K_\alpha{}^* = \sum_\beta T_{\alpha\beta}(K_\beta - K_\beta{}^*), \tag{4}$$

where the matrix $T_{\alpha\beta} = \partial F_\alpha / \partial K_\beta$, evaluated at the fixed point $K_\alpha{}^*$, has right eigenvectors $\varphi_{\alpha i}$ with eigenvalues λ_i. The condition for critical behavior is the existence of eigenvalues $\lambda_i > 1$, $i = 1, 2 \ldots j$, while $\lambda_{i+j} < 1$ for $j = 1, 2, \ldots$. In this case there exists a critical surface where each point maps into the fixed point $K_\alpha{}^*$. In practice the renormalization-group transformations can be calculated approximately by keeping only a finite number of spins.[5]

In the thermodynamic limit $N \to \infty$, the free energy per spin $f(K)$ is given by

$$f(K) = \lim_{N \to \infty} N^{-1} \ln \sum_{\{s\}} \exp[H_N(K)] \tag{5}$$

and, according to Eq. (2), it satisfies the scaling condition

$$f(K') = L[f(K) - g(K)], \tag{6}$$

where L is the number of spins in a cell. Applying the renormalization transformation, Eq. (1), to this scaling equation n times, we obtain

$$f(K) = \sum_{m=0}^{n} L^{-m} g(K^{(m)}) + h_n(K), \tag{7}$$

where

$$h_n(K) = f(K^{(n)})/L^n \tag{8}$$

and

$$K_\alpha{}^{(n+1)} = F_\alpha(K^{(n)}), \quad K_\alpha{}^{(0)} = K_\alpha.$$

In the limit $n \to \infty$, we find that $h_n(K) \to 0$, and Eq. (7) then gives an infinite-series solution of the scaling equation,[6] Eq. (6). However, in the presence of symmetry-breaking fields, e.g., a magnetic field H, the limit of $\partial h_n(K)/\partial H$ is finite below the critical temperature T_c for $H = 0^\pm$, and gives the spontaneous magnetization.[7]

It can be readily seen that since $g(K)$ is not a constant, $f(K)$ must be singular on the critical surface, because a value of K which is not on this surface will map along a trajectory which cannot cross or be mapped onto this surface. As K approaches close to the critical surface, the mapping is essentially along this surface towards the fixed point K^* up to large values of n, but then it turns sharply away from this surface and maps towards a characteristic surface associated with the eigenvalues $\lambda_i > 1$. At the fixed point K^* we have simply[8]

$$f(K^*) = [L/(L-1)]g(K^*). \tag{9}$$

Near the fixed point we can sum approximately the infinite series, Eq. (7), to obtain an explicit expansion for $f(K)$ near its singularity. For this purpose we introduce a set of variables ζ_i associated with each eigenvalue $\lambda_i \neq 0, 1$ which determines K by a nonlinear transformation,[9]

$$K_\alpha = G_\alpha(\zeta_1, \zeta_2, \ldots), \tag{10}$$

such that the mapping of K_α, Eq. (1), is given by

$$K_\alpha' = G_\alpha(\lambda_1 \zeta_1, \lambda_2 \zeta_2, \ldots). \tag{11}$$

The critical point $K_\alpha{}^*$ corresponds to $\zeta_i = 0$ for all i and the critical surface is obtained by setting $\zeta_i = 0$ for i such that $\lambda_i > 1$. In terms of these variables we have, according to Eqs. (7), (10), and (11),

$$f(\zeta) = \sum_{n=0}^{\infty} L^{-n} g(\lambda_1{}^n \zeta_1, \lambda_2{}^n \zeta_2, \ldots). \tag{12}$$

As an illustration, we consider planar Ising models where ζ_1 and ζ_2 are the temperature and magnetic field variables near the critical transition where $\lambda_1 = L^{1/2}$ and $\lambda_2 = L^{15/16}$, while $\lambda_i < 1$ for $i \neq 1, 2$. In this case we consider the second derivative of $f(\zeta)$ with respect to ζ_1 and ζ_2, setting $\zeta_i = 0$ for $i \neq 1, 2$.

$$f_{ii}(\zeta) = \sum_{n=0}^{\infty} (\lambda_i{}^2/L)^n g_{ii}(\lambda_1{}^n \zeta_1, \lambda_2{}^n \zeta_2, \ldots), \tag{13}$$

where

$$f_{ii}(\zeta) \equiv \partial^2 f(\zeta)/\partial \zeta_i{}^2, \quad g_{ii} \equiv \partial^2 g(\zeta)/\partial \zeta_i{}^2. \tag{14}$$

The series given by Eq. (13) becomes clearly divergent when ζ_1 and ζ_2 vanish. For example, in the limit $\zeta_1 \to 0^\pm$, $\zeta_2 = 0$, where $\zeta_1 \propto (T - T_c)$ and $\zeta_2 \to H$, we obtain

$$f_{ii}(\zeta) = \frac{L g_{ii}(0)}{\lambda_i{}^2 - L} \left\{ \left| \frac{\chi_i{}^\pm}{\zeta_1} \right|^{(2 \ln \lambda_i - \ln L)/\ln \lambda_1} - 1 \right\}, \tag{15}$$

where

$$g_{ii}(0)=\sum_{\alpha\beta}\left\{\frac{\partial g}{\partial K_\gamma}\sum_k\frac{\varphi_{\gamma k}\varphi_{k\delta}^{-1}}{(\lambda_i^2-\lambda_k)}\frac{\partial^2 F_\delta}{\partial K_\alpha\partial K_\beta}+\frac{\partial^2 g}{\partial K_\alpha\partial K_\beta}\right\}\varphi_{\alpha i}\varphi_{\beta i}. \tag{16}$$

The coefficients $\chi_i^{\pm}$ are determined by the two solutions of the equation

$$\sum_{n=1}^{\infty}\left\{\left[g_{ii}\left(\frac{\chi}{\lambda_1^n}\right)-g_{ii}(0)\right]\left(\frac{L}{\lambda_i^2}\right)^n+\sum_{n=0}^{\infty}g_{ii}(\lambda_1^n\chi)\left(\frac{\lambda_i^2}{L}\right)^n\right\}=0 \tag{17}$$

for positive and negative values of χ.

Equation (15) gives the well-known power-law singularity associated with scaling with a coefficient determined by Eqs. (16) and (17), which is in general discontinuous across the critical surface.

For $\lambda_1^2=L$ and $i=j=1$, Eq. (15) becomes[9]

$$f_{11}(\zeta)=-\frac{g_{11}(0)}{\ln\lambda_1}\ln|\zeta_1| \tag{18}$$

corresponding to the well-known logarithmic singularity of Onsager's solution.[10] This result can also be verified by direct substitution in Eq. (6). To obtain the regular part $f_r(\zeta)$ of $f(\zeta)$ near the fixed point, we expand $g(\zeta)$ in a power series in ζ_i

$$g(\zeta)=\sum\frac{g_{i_1 i_2\ldots}}{i_1!\,i_2!\ldots}\zeta_1^{i_1}\zeta_2^{i_2}\ldots . \tag{19}$$

Substituting in Eq. (6), we obtain

$$f_r(\zeta)=\sum\frac{g_{i_1 i_2\ldots}}{i_1!i_2!}\frac{L}{L-\lambda_1^{i_1}\lambda_2^{i_2}\ldots}\zeta_1^{i_1}\zeta_2^{i_2}, \tag{20}$$

where terms in the sum with vanishing denominator, as in the case $\lambda_1^2=L$, are deleted.[11] Near the fixed points $K^*=0$ (high temperatures) and $K^*=\infty$ (low temperatures) we expect no singularities in f, and the series in Eq. (20) gives the complete expansion of the free energy.

In practice, the series solution for the free energy, Eq. (7), can be calculated numerically[12] for arbitrary values of K after the renormalization-group transformations, Eq. (1), for a finite number of spins N have been obtained. For high and low temperatures this solution approaches the exact asymptotic limits of f provided that periodic boundary conditions are imposed and that the cell clusters maintain the lattice symmetry. As an example, we have calculated the values of $f(K)$, $\partial f(K)/\partial K_1$, and $K_1^2\,\partial^2 f(K)/\partial K_1^2$ corresponding to the free energy, energy, and specific heat, respectively, for a square lattice along the Ising nearest-neighbor axis $-K_1$, in a four-cell cluster approximation, $N=16$, which is the smallest cluster satisfying these requirements.[13] The results are shown in Fig. 1 where we have also drawn for comparison Onsager's exact solution.[10] The fixed point associated with the critical transition is found at $K_1^*=0.307$, $K_2^*=0.084$, and $K_3^*=-0.004$, where K_2 is the next to nearest-neighbor interaction, and K_3 is the four-spin interaction. The corresponding eigenvalues are $\lambda_1=1.914$, $\lambda_2=0.248$ and $\lambda_3=0.137$. The critical surface intersects the Ising axis at $K_1^c=0.420$

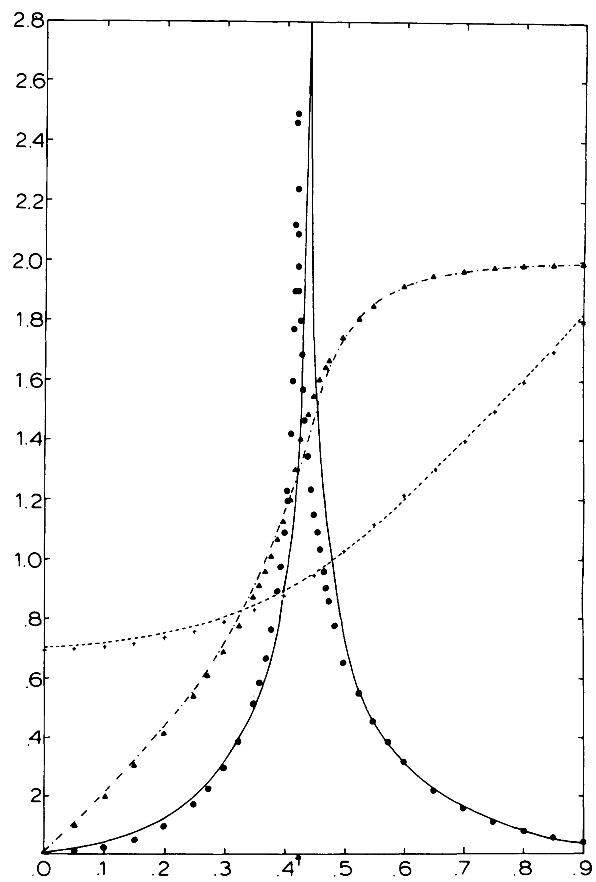

FIG. 1. Dashed curve, Onsager's free energy; crosses, $f(K_1)$, free energy, Eq. (7); dash-dotted curve, Onsager's energy; triangles, $\partial f(K_1)/\partial K_1$, energy from first derivative Eq. (7); solid curve, Onsager's specific heat; dots, $K_1^2\partial^2 f(K_1)/\partial K_1^2$, specific heat from second derivative Eq. (7).

while the Onsager value for the critical transition is $K^c = \frac{1}{2}\ln(\sqrt{2}+1) \cong 0.440\,69$. The properties of the renormalization-group mappings, Eq. (1), and transformations, Eqs. (10) and (11), have been investigated in detail for the square[13] and the triangular[14] lattices in collaboration with Professor J. A. Tjon, to whom we are indebted for numerous discussions.

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[6]K. Wilson (private communication) has informed us that in his original paper, Ref. 1, he had written out formulas for the free energy, but that he has not pursued the matter further. We would like to thank him for his comments on our manuscript. See also M. P. Nightingale and A. H. t'Hooft, to be published.

[7]For large n, $K_\alpha^{(n)}$ maps towards the fixed points $K^*=0$ or $K^*=\infty$ for values of T below or above T_c, respectively, and it is then straightforward to evaluate $h_n(K)$, Eq. (8). Note that $g(K^{(n)})$ is invariant to the change of the sign of the symmetry-breaking fields; hence $\partial g(K^{(n)})/\partial H = 0$ for $H=0$, and these terms do not contribute in the free-energy series, Eq. (7), to the spontaneous magnetization. Numerical values of the dependence of the magnetization and susceptibility on the temperature and the magnetic field have been calculated in a four-cluster approximation and will be published separately.

[8]This result can be verified readily for the fixed point $K=0$ where $f(0)=\ln 2$ for Ising models.

[9]Nonlinear transformations of this type were developed by Poincaré and play an important role in stability studies in mechanics; see, for example, C. L. Siegel and J. K. Moser, *Lectures on Celestial Mechanics* (Springer, Berlin, 1971). We are indebted to J. F. C. van Velsen for bringing this reference to our attention. The application of these transformations to critical phenomena was first made by F. J. Wegner, Phys. Rev. B $\underline{5}$, 4529 (1972).

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Photoemission Partial Yield Measurements of Unoccupied Intrinsic Surface States for Ge(111) and GaAs(110)*

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Energy-resolved photoemission-yield spectroscopy measurements are reported for transitions from $3d$ core levels to empty surface states and conduction-band states. Unoccupied surface-state bands are observed in the band gap with peaks about 0.2 and 0.9 eV above the valence-band maxima (E_V) of Ge(111) and GaAs(110), respectively. These surface-state bands cause the well-known Fermi-level (E_F) pinning at the surface ($E_F - E_V = 0$) for Ge(111) and the range of pinning ($E_F - E_V = 0$ to 0.6 eV) for doped GaAs(110).

Intrinsic surface states, both empty and filled, are well known to exist in or near the forbidden gap of Group-IV and -III-V semiconductors such as Ge and GaAs.[1-5] Previously, photoemission measurements have determined the density of filled surface states,[4-6] while optical[3] and elec-