where the exchange constant J_{mn} depends on the ion position R,

$$J_{mn}(R) = J_{mn}(R_0) + (\nabla J_{mn})_{R=R_0}\,\delta R, \qquad (3)$$

and so produces a coupling between spin system and phonons.[19] A quantitative comparison between theory and experiment will, however, only be possible following detailed calculations for the various modes.

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Corrections to Scaling Laws*

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The effects of higher-order contributions to the linearized renormalization group equations in critical phenomena are discussed. This analysis leads to three quite different results: (i) An exact scaling law for redefined fields is obtained. These redefined fields are normally analytic functions of the physical fields. Corrections to the standard power laws are derived from this scaling law. (ii) The theory explains why logarithmic terms can exist in the free energy. (iii) The case in which the energy scales like the dimensionality is analyzed to show that quite anomalous results may be obtained in this special situation.

I. INTRODUCTION

It has been shown by several authors[1-3] that a linearized form of the renormalization group equations leads to scaling laws for critical phenomena. In this paper we use the renormalization group equations to obtain corrections to the well-known[4] power laws for the singular part of the free energy and for the expectation values of different operators and susceptibilities.

The free energy of a magnetic system and of superfluid helium as a function of the symmetry breaking field h and $\tau \propto T - T_c$ is obtained as an expansion

$$F = g_0 + |g_E|^{2-\alpha} f^{\pm}\left(\frac{\beta h}{|g_E|^{\Delta}}\right) + \sum_i g_i |g_E|^{2-\alpha-\Delta_i} f_i^{\pm}\left(\frac{\beta h}{|g_E|^{\Delta}}\right) + \ldots \qquad (1.1)$$

in which the redefined fields g_0, g_E, and g_i are analytic functions of $\tau \propto T - T_c$ unless certain relations are fulfilled (see below). The function g_E vanishes for $\tau = 0$, $g_E = \tau + O(\tau^2)$. The first term g_0

is the regular part of the free energy, the term $|g_E|^{2-\alpha} f^{\pm}$ is the leading singular term. The functions $f^{\pm}, f_i^{\pm}$ depend on the sign of τ. The last term of Eq. (1.1) comes from the contributions of the "irrelevant" operators to the energy density. We note that the exponents Δ_i are negative (the gap exponent $\Delta = \beta + \gamma$ for the symmetry breaking field is positive, of course). The exponent Δ_i of the leading *correction* is approximately -0.5. For other second-order phase transitions one has to replace βh by a function g_h. Both g_h and g_E are analytic functions of βh and τ vanishing at criticality. The expansion (1.1) differs considerably from corrections to scaling laws obtained by other authors[5] since we take the "irrelevant" operators into account.

If certain relations between the critical exponents are fulfilled then logarithmic singularities arise. In particular if the critical exponent of the free energy $2-\alpha$ is an integer, then this theory predicts a contribution to the free energy proportional to $|\tau|^{2-\alpha} \ln|\tau|$. This behavior has been found for the eight-vertex model.[6] (For odd α the eight-vertex model does not show this singularity. It follows from symmetry arguments that this term vanishes for odd α in the eight-vertex model.)

The case in which the energy scales like the dimensionality leads to anomalous results. For this case we obtain an asymptotic series in τ for the free energy. The free energy of the F model can also be described by an asymptotic series[7] in τ. We attribute the different asymptotic behavior in the F model to the presence in this case of two operators which scale like r^{-d}.

In Sec. II we outline briefly some basic ideas of renormalization group theory and state our basic equations and assumptions. In Sec. III we review the derivation of the scaling laws from the linearized renormalization group equations. Since the energy is not an exact eigenoperator of the linearized equation one obtains already in this order corrections to the power laws. In Secs. IV and V we consider the nonlinear equations which lead to a scaling law in terms of the redefined fields. From this scaling law we deduce the corrections described by Eq. (1.1). In Sec. VI we discuss some logarithmic contributions. In Sec. VII we discuss some properties arising from operators which scale like r^{-d}. These operators may lead to fixed lines which may produce a breakdown of universality (eight-vertex model[6,8]). We also discuss the case of an energy density scaling like r^{-d} which leads to a singularity of the free energy in infinite order and compare with the free energy of the F model.

II. RENORMALIZATION GROUP THEORY

We briefly outline the basic ideas of renormalization group theory leading to Eqs. (2.8) and (2.12). We consider a d dimensional system with N degrees of freedom $z_1 \cdots z_N$ in a box of length L. The system is described by the operator

$$H_0(N) = H_0(z_1 \ldots z_N) = -\beta\mathcal{H}, \tag{2.1}$$

in which $\mathcal{H}$ is the Hamilton operator and $\beta = (k_B T)^{-1}$ with Boltzmann constant k_B and temperature T. We assume that $H_0(N)$ is translational invariant (apart from the boundary conditions). Now we extend the system in all linear dimensions by a scale factor e^l. Then we obtain a system with Ne^{dl} degrees of freedom in a box of length Le^l described by

$$H_0(Ne^{dl}) = H_0(z_1 \cdots z_{N\exp(dl)}) . \tag{2.2}$$

We transform to a new set of variables[9] $z_1' \cdots z'_{N\exp(dl)}$ and average over all variables z_k' with $k > N$ by taking the trace of $\exp[H_0(Ne^{dl})]$ over all these variables. We denote the result by

$$\exp[H_l(N)] = \exp[H_l(z_1' \cdots z_N')] = \mathrm{Tr}' \exp[H_0(z_1' \ldots z'_{N\exp(dl)})] . \tag{2.3}$$

If we have chosen the variables z_k' in an appropriate way then $H_l(N)$ is translational invariant also. We denote the total operation of extending the system and eliminating degrees of freedom by R^l,

$$H_l(N) = R^l(H_0(N)) . \tag{2.4}$$

According to our definition the partition function $Z = \mathrm{Tr}\exp(H)$ obeys

$$Z(H_l(N)) = Z(H_0(Ne^{dl})) \tag{2.5}$$

and we obtain (in the thermodynamic limit $N \to \infty$)

$$\ln Z(H_l(N)) = e^{dl} \ln Z(H_0(N)) . \tag{2.6}$$

Denoting the free energy by $\mathfrak{F}$ and introducing the dimensionless free energy

$$F = -\beta\mathfrak{F} = \ln Z , \tag{2.7}$$

one obtains

$$F(R^l(H)) = e^{dl} F(H) . \tag{2.8}$$

We may denote $R^l(R^l(H))$ by $R^{2l}(H)$ since the system is extended by a scale factor e^{2l} and then reduced to a system with N degrees of freedom. In general R^l generates a semigroup consisting of the elements R^{nl} (with n a non-negative integer). In the following we assume that we may define an operator R^δ for infinitesimal δ.[10] Then R^l is defined for any l, and we avoid unconveniently complicated equations. For our further calculations we make three basic assumptions: Firstly, we assume that there exists an eigensolution

$$H^* = R^\delta(H^*) , \tag{2.9}$$

which is called a fixed point. Secondly, we assume

$$R^l(H^* + \sum_i \tilde{\mu}_i \tilde{O}_i) = H^* + \sum_j \tilde{c}_j\{\tilde{\mu}\}\tilde{O}_j \tag{2.10}$$

for a complete set of operators $\tilde{O}_j$. Moreover we assume that $\tilde{c}_j\{\tilde{\mu}\}$ has a power expansion in $\tilde{\mu}$ around the origin

$$\tilde{c}_j\{\tilde{\mu}\} = \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{i_1 \cdots i_n} \tilde{a}_{ji_1 \cdots i_n} \tilde{\mu}_{i_1} \cdots \tilde{\mu}_{i_n} . \tag{2.11}$$

The functions $\tilde{c}$ and the coefficients $\tilde{a}$ depend on l. For infinitesimal δ we write

$$R^\delta(H^* + \sum_i \tilde{\mu}_i \tilde{O}_i) = H^* + \sum_i \tilde{\mu}_i \tilde{O}_i + \delta \sum_j \tilde{c}'_j\{\tilde{\mu}\}\tilde{O}_j \ , \tag{2.12}$$

with $\tilde{c}'_j = \partial \tilde{c}_j / \partial l \mid_{l=0}$. Thirdly, we will assume certain properties[11] for the matrix $\tilde{a}'_{ji} = \partial \tilde{a}_{ji}/\partial l$ which we will state in Secs. III and V. Starting from these assumptions we will discuss some singularities of critical systems.

III. FIRST-ORDER THEORY: SCALING LAWS

In this section we derive the scaling laws from the linearized form of Eq. (2.12) for infintesimal δ:

$$R^\delta(H^* + \sum_i \tilde{\mu}_i \tilde{O}_i) = H^* + \sum_i \tilde{\mu}_i \tilde{O}_i + \delta \sum_{ij} \tilde{a}'_{ji} \tilde{\mu}_i \tilde{O}_j \ . \tag{3.1}$$

We assume that the matrix $\tilde{a}'_{ji}$ can be diagonalized[11]

$$R^\delta(H^* + \sum_i \mu_i O_i) = H^* + \sum_i \mu_i(1 + \delta y_i) O_i \ , \tag{3.2}$$

where the coefficients y_i are the eigenvalues of $\tilde{a}'$ and the O_i are the eigenoperators of the Eq. (3.1). We mention that the density $O_i(r)$ scales like r^{-x_i}, where $x_i + y_i = d$.[12] From Eq. (3.2), we obtain

$$R^l(H^* + \sum_i \mu_i O_i) = H^* + \sum_i \mu_i e^{y_i l} O_i \ ; \tag{3.3}$$

and from Eqs. (3.3) and (2.8), one obtains the scaling law

$$F\{\mu_i\} = e^{-dl} F\{\mu_i e^{y_i l}\} \ . \tag{3.4}$$

The operators O_i with $y_i > 0$ are called relevant, since an application of R^l leads to an increase of μ_i leading away from H^*, whereas the operators with $y_i < 0$ are called irrelevant since the application of R^l leads to a decrease of μ_i (the limiting case $y_i = 0$ will be discussed in Sec. VII). If the repeated application of R on a Hamiltonian H_c converges to the fixed point H^*,

$$\lim_{l \to \infty} R^l(H_c) = H^* \ , \tag{3.5}$$

then we say we are at criticality. Within the linearized approximation the Hamiltonian

$$H_c = H^* + \sum_i \mu_{ic} O_i \ , \tag{3.6}$$

with $\mu_{ic} = 0$ for all relevant operators, defines criticality. Normally there is only a small number of relevant operators. Several of these (magnetization, anisotropy, etc.) break the symmetry of the Hamiltonian. For the symmetry-conserving Hamiltonian the fields μ_i of the symmetry-breaking operators vanish. For second-order phase transitions[13] there are only two relevant operators which conserve the symmetry, the operator $O_0 = 1$ and an operator we call O_E.

The operator 1 and its field μ_0 are extremely easy to treat since

$$F(\mu_0, \mu_1, \cdots) = \mu_0 + F(0, \mu_1, \cdots) \tag{3.7}$$

and $y_0 = d$. Although 1 is a relevant operator, it is not necessary to fulfill $\mu_{0c} = 0$ at criticality because of Eq. (3.7). We call μ_0 the regular part of F and $F(0, \mu_1, \cdots)$ the singular part of F. Let us expand H^* and $\mathcal{H}$ in the operators O_i:

$$H^* = \sum \mu_i^* O_i \ , \tag{3.8}$$

$$-\mathcal{H} = \sum \mu_i^0 \ O_i \ . \tag{3.9}$$

Then we obtain

$$H_0 = H^* + \sum \mu_i O_i \ , \tag{3.10}$$

with

$$\mu_i = \beta \mu_i^0 - \mu_i^* \ . \tag{3.11}$$

Since criticality is defined by the condition that the fields of all relevant operators but the operator 1 vanish, the field μ_E has to vanish at criticality. This defines the critical temperature

$$k_B T_c = \mu_E^0 / \mu_E^* \ . \tag{3.12}$$

We now define τ, α, l, and Δ_i by[14]

$$\tau = \mu_E = \mu_E^0(\beta - \beta_c) \ , \tag{3.13}$$

$$2 - \alpha = d / y_E \ , \tag{3.14}$$

$$e^{-dl} = |\tau|^{2-\alpha} \ , \tag{3.15}$$

$$\Delta_i = y_i / y_E \ . \tag{3.16}$$

Then we obtain, from Eqs. (3.4) and (3.7),

$$F = \mu_0 + |\tau|^{2-\alpha} f^{\pm}_{\text{sing}}\{\mu_i |\tau|^{-\Delta_i}\} \ . \tag{3.17}$$

The function $f^{\pm}_{\text{sing}}$ depends only on the reduced fields $q_i = \mu_i |\tau|^{-\Delta_i}$ $(i \neq 0, E)$ and on the sign of τ, since $q_E = \text{sgn}\,\tau$,

$$f^{\pm}_{\text{sing}}\{q_i\} = F(\mu_0 = 0, \mu_E = \pm 1, q_i). \tag{3.18}$$

From Eq. (3.17) one obtains

$$\langle O_i \rangle = |\tau|^{\beta_i} \frac{\partial f^{\pm}_{\text{sing}}}{\partial q_i} \tag{3.19}$$

and

$$\frac{\partial \langle O_i \rangle}{\partial \mu_j} = \frac{\partial \langle O_j \rangle}{\partial \mu_i} = |\tau|^{-\gamma_{ij}} \frac{\partial^2 f_{\text{sing}}}{\partial q_i \partial q_j} \ , \tag{3.20}$$

with

$$\beta_i = 2 - \alpha - \Delta_i \ , \tag{3.21}$$

$$\gamma_{ij} = \Delta_i + \Delta_j - 2 + \alpha \ , \tag{3.22}$$

which leads to the scaling law

$$\alpha+\beta_i+\beta_j+\gamma_{ij}=2\ . \tag{3.23}$$

Since the reduced fields q_i depend on the temperature one obtains corrections to the power laws $\langle O\rangle\propto|\tau|^{\beta}$ and $\partial\langle O\rangle/\partial\mu\propto|\tau|^{-\gamma}$ for fixed $\mathcal{H}$. If we assume that f_{sing} can be expanded in powers of the q_i for irrelevant operators O_i, then one obtains

$$\langle O_i\rangle=|\tau|^{\beta_i}\frac{\partial f^{\pm}_{\text{sing}}(0)}{\partial q_i}+\sum_j|\tau|^{\beta_i-\Delta_j}\mu_j\frac{\partial^2 f^{\pm}_{\text{sing}}(0)}{\partial q_i\partial q_j}+\cdots\ . \tag{3.24}$$

For irrelevant operators one has $\Delta_j<0$, hence the leading term is proportional to $|\tau|^{\beta_i}$. However if Δ_j is close to zero, then the correction might be important although the operator O_j is "irrelevant." From expansions of the critical exponents in $\epsilon=4-d$ one obtains the estimation $\Delta_j=-0.5$ for the leading correction term $[\Delta_{2S}=-\frac{1}{2}\epsilon+O(\epsilon^2)$ from Ref. 15] in three dimensions. This agrees exactly with the result of Wortis[16] who predicted from empirical analysis of susceptibility series a behavior $\chi=|\tau|^{-\gamma}(k_0+k_1|\tau|^{p})$ for Ising models with spin S with constant γ and $p=0.5$ for all S.

We obtain the energy of the system from

$$-\langle H\rangle=\frac{dF}{d\beta}=\mu_E^0(2-\alpha)\tau|\tau|^{-\alpha}f^{\pm}_{\text{sing}}+\sum_i\tau|\tau|^{-\alpha-\Delta_i}(\mu_i^0\mu_E-\Delta_i\mu_E^0\mu_i)\frac{\partial f^{\pm}_{\text{sing}}}{\partial q_i}\ . \tag{3.25}$$

From this one obtains the energy at criticality

$$-\langle H\rangle_c=\mu_0^0\ . \tag{3.26}$$

Deviations from $-\langle H\rangle-\mu_0^0\propto\tau|\tau|^{\alpha}$ come explicitly from the sum in Eq. (3.25) and from the dependence of $f^{\pm}_{\text{sing}}$ on the temperature-dependent fields q_i.

IV. HIGHER-ORDER CONTRIBUTIONS

In Sec. III we derived the scaling laws from the linearized renormalization group equations. In this section we take into account higher-order terms in μ. In the basis of the operators O_i, Eq. (2.12) reads

$$\begin{aligned}R^{\delta}(H^*+\textstyle\sum_i\mu_iO_i)&=H^*+\textstyle\sum_i\mu_iO_i+\delta\sum_j c_j'\{\mu\}O_j\\&=H^*+\textstyle\sum_i(1+\delta y_i)\mu_iO_i+\delta\displaystyle\sum_{n=2}^{\infty}\frac{1}{n!}\sum_{jI}a'_{jI}\mu_IO_j\ ,\end{aligned} \tag{4.1}$$

with the notation I for $i_1, i_2, \ldots, i_n$ and

$$\mu_I=\mu_{i_1}\cdots\mu_{i_n}\ . \tag{4.2}$$

In Sec. III we obtained the Hamiltonian $H^*+\sum\mu_iO_i$ with the transformation property (3.3) which led to the scaling law (3.4). This does no longer hold if we take into account the higher-order terms in μ [Eq. (4.1)]. To overcome this we try to define an operator $H\{g_i\}$ parametrized by scaling fields g_i so that

$$R^l(H\{g_i\})=H\{g_ie^{y_il}\} \tag{4.3}$$

still holds. H does not depend linearly on g, but we expect

$$H\{g_i\}=H^*+\sum_j\mu_j\{g_i\}O_j \tag{4.4}$$

in which the real fields μ_j are nonlinear functions of the "scaling fields" g_i with an expansion

$$\mu_j\{g_i\}=\sum_{n=1}^{\infty}\frac{1}{n!}\sum_I b_{jI}g_I\ , \tag{4.5}$$

$$g_I=g_{i_1}\cdots g_{i_n}\ . \tag{4.6}$$

To first order we expect from Eq. (3.3) $\mu_j=g_j+O(g^2)$, that is $b_{ji}=\delta_{ji}$. We postpone the calculation of the coefficients b from the coefficients a' to Sec. V and discuss the consequence of Eqs. (4.3) and (4.4). From Eq. (4.3) we again obtain the scaling law

$$F\{g_i\}=e^{-dl}F\{g_ie^{y_il}\}\ , \tag{4.7}$$

which is exact for the Hamiltonian (4.4).

Since the fields μ_j are nonlinear functions of the scaling fields g_i one obtains power laws for the field-dependent operators $\partial H/\partial g$:

$$\frac{\partial F}{\partial g_i}=\left\langle\frac{\partial H\{g\}}{\partial g_i}\right\rangle=\left\langle O_i+\sum_{j,i_1}b_{jii_1}g_{i_1}O_j+\cdots\right\rangle. \tag{4.8}$$

Therefore, we obtain deviations from the power law $\langle O_i\rangle\propto|\tau|^{\beta_i}$, which comes from the correction terms $bg\langle O\rangle$ and higher-order terms. We may convert expression (4.5) into an expansion for the scaling fields

$$g_j=\mu_j-\tfrac{1}{2}\sum b_{ji_1i_2}\mu_{i_1}\mu_{i_2}+\cdots\ . \tag{4.9}$$

These scaling fields are (normally) analytic functions of the fields μ. Suppose we may vary two physical parameters, the temperature and the symmetry breaking field h:

$$H=-\beta\mathcal{H}-\beta hM\ . \tag{4.10}$$

With the expansion for the order parameter

$$-M=\sum\mu_i^hO_i\ , \tag{4.11}$$

we obtain [compare Eq. (3.11)]

$$\mu_i=\beta\mu_i^0+\beta h\mu_i^h-\mu_i^*\ . \tag{4.12}$$

Therefore, the fields μ_i are linear functions of τ and βh. Then all redefined fields g_i are analytic functions of τ and βh. If the operators O_E and O_h are the only relevant operators and if we assume that we may expand in powers of all the other (irrelevant) fields g_i, then we obtain the free energy

$$F=g_0+|g_E|^{2-\alpha}f^{\pm}\left(\frac{g_h}{|g_E|^{\Delta}}\right)+\sum_i g_i|g_E|^{2-\alpha-\Delta_i}f_i^{\pm}\left(\frac{g_h}{|g_E|^{\Delta}}\right)+\frac{1}{2}\sum_{ij}g_ig_j|g_E|^{2-\alpha-\Delta_i-\Delta_j}f^{\pm}_{ij}\left(\frac{g_h}{|g_E|^{\Delta}}\right)+\cdots\ , \tag{4.13}$$

in which $f^{\pm}$ is the function $f^{\pm}_{\text{sing}}$, $f^{\pm}_i$ the first derivative of $f^{\pm}_{\text{sing}}$ with respect to q_i and $f^{\pm}_{ij}$ the second derivative. The function and derivatives are evaluated at all $q_i = 0$ except $q_h = g_h |g_E|^{-\Delta}$. The fields g_h and g_E vanish at criticality. From Wilson's approximation[2] and from the exact recursion relations obtained by changing the momentum cut off one finds that the magnetic field h for a ferromagnet and the symmetry breaking field for superfluid helium transform into themselves. In these cases one obtains

$$g_h = \beta h \tag{4.14}$$

and all the other fields (g_0, g_E, g_i) depend only on τ.

V. HAMILTONIAN $H\{g\}$

In this section we will calculate the operator $H\{g\}$. We will find that in some cases $H\{g\}$ cannot be represented by a power series in the fields g. But it can be written in the form (4.4) and (4.5) if we allow the coefficients b to be polynomials of finite order in l. These polynomials can equally well be replaced by polynomials in $\ln|g|$. Writing down the equations for b we take into account the explicit dependence of b on l by carrying also terms $\partial b/\partial l$. From Eqs. (4.3) and (4.4), we obtain

$$\begin{aligned}\frac{\partial}{\partial l} R^l(H\{g_i\}) &= \frac{\partial}{\partial l} H\{g_i e^{y_i l}\} \\ &= \sum_{n=1}^{\infty} \frac{1}{n!} \sum_{jI} g_I e^{y_I l} \left(\frac{\partial b_{jI}}{\partial l} + y_I b_{jI}\right) O_j \\ &= \frac{\partial}{\partial \delta} R^\delta(H\{g_i e^{y_i l}\}) = \sum \frac{1}{n!} \sum_{jI} a'_{jI} \mu_I \{g_i e^{y_i l}\} O_j ,\end{aligned} \tag{5.1}$$

with

$$y_I = y_{i_1} + \cdots + y_{i_n} . \tag{5.2}$$

We used the group property $R^{l+\delta} = R^\delta R^l$. Substituting $\mu_j \{g_i e^{y_i l}\}$ into Eq. (5.1) and comparing the coefficients of g_I, we obtain the equation for b_{jI}:

$$\frac{\partial b_{jI}}{\partial l} + \sum_{j'} (y_I \delta_{jj'} - a'_{jj'}) b_{j'I} = f_{jI} . \tag{5.3}$$

The inhomogeneity f depends on the coefficients a' and the functions $b_{j' i_1 \cdots i_m}$ with $m < n$. One obtains

$$f_{ji} = 0 , \tag{5.4}$$

$$f_{ji_1i_2} = \sum_{j_1j_2} b_{j_1i_1} b_{j_2i_2} a'_{j\,j_1j_2} , \tag{5.5}$$

$$\begin{aligned} f_{ji_1i_2i_3} &= \sum_{j_1j_2j_3} b_{j_1i_1} b_{j_2i_2} b_{j_3i_3} a'_{jj_1j_2j_3} \\ &\quad + \sum_{j_1j_2} (b_{j_1i_1} b_{j_2i_2i_3} + b_{j_1i_2} b_{j_1i_2i_3} \\ &\quad + b_{j_1i_3} b_{j_2i_1i_2}) a'_{jj_1j_2} , \quad \text{etc.} \end{aligned} \tag{5.6}$$

We first consider the case where a'_{ji} is diagonal,

$$a'_{ji} = y_i \delta_{ji} . \tag{5.7}$$

Then Eq. (5.3) becomes

$$\frac{\partial b_{jI}}{\partial l} + (y_I - y_j) b_{jI} = f_{jI} \tag{5.8}$$

and we may choose $b_{ji} = \delta_{ji}$ as before. Then Eqs. (5.5) and (5.6) become

$$f_{ji_1i_2} = a'_{ji_1i_2} , \tag{5.9}$$

$$\begin{aligned} f_{ji_1i_2i_3} = a'_{ji_1i_2i_3} + \sum_{j_1} & (b_{j_1i_2i_3} a'_{ji_1j_1} + b_{j_1i_1i_3} a'_{ji_2j_1} \\ & + b_{j_1i_1i_2} a'_{ji_3j_1}). \end{aligned} \tag{5.10}$$

If $y_I \neq y_j$, then Eq. (5.8) has the solution

$$b_{jI} = \frac{f_{jI}}{\gamma_I - \gamma_j} - \frac{\partial f_{jI}/\partial l}{(y_I - y_j)^2} + \frac{\partial^2 f_{jI}/\partial l^2}{(y_I - y_j)^3} - \cdots . \tag{5.11}$$

Hence b_{jI} is a constant if f_{jI} is a constant. However, in the exceptional case $y_I = y_j$ one obtains l dependent coefficients b_{jI} (unless f_{jI} vanishes) which lead to logarithmic terms:

$$b_{jI}(l) = \int_0^l f_{jI}(l')\, dl' + \text{const.} \tag{5.12}$$

From Eqs. (5.11) and (5.12) we find that the coefficients b are polynomials of finite order in l.

A matrix $\bar{a}'_{j'i}$ of finite order[11] can always be transformed by a similarity transformation into the form

$$\begin{aligned} & a'_{ji} = 0 \quad \text{for } i < j , \\ & a'_{ii} = y_i , \\ & a'_{ji} = 0 \quad \text{if } i > j \text{ and } y_i \neq y_j . \end{aligned} \tag{5.13}$$

Therefore, the only nondiagonal terms are those with $i > j$ and $y_i = y_j$. Then for $n = 1$ the solution

$$b = e^{(a' - y) l} \tag{5.14}$$

leads to polynomials $b_{ji}(l)$ of finite order in l. For $n > l$ one obtains for $y_I = y_j$

$$b_{jI}(l) = \sum_i \int_0^l b_{ji}(l') f_{iI}(l')\, dl' + \text{const} \tag{5.15}$$

and for $y_I \neq y_j$

$$b_{jI}(l) = \sum_i \left((y_I - a')^{-1}_{ji} f_{iI}(l) - (y_I - a')^{-2}_{ji} \frac{\partial f_{iI}}{\partial l} + \cdots \right). \tag{5.16}$$

Again the coefficients b_{jI} are finite polynomials in l. We observe that we may replace l in the polynomials by $l + l_0$, where l is a constant. Defining

$$l_0 = l_0\{g_i\} = \sum S_i \ln|g_i| \tag{5.17}$$

with constants S_i which obey

$$\sum S_i y_i = 1 , \tag{5.18}$$

we obtain

$$l_0\{g_i e^{y_i l}\}=l_0\{g_i\}+l\ . \tag{5.19}$$

Therefore, H has an expansion in the scaling fields g_i and $l_0\{g_i\}$:

$$H\{g\}=H^*+\sum_{n=1}^{\infty}\frac{1}{n!}\sum_{jI}b_{jI}(l_0\{g\})g_I O_j\ . \tag{5.20}$$

From Eq. (3.7) which is exact in any order in μ it follows that a'_{jI} vanishes for $n>1$ if one of the indices i is equal to 0. From Wilson's approximation[2] as well as from the exact recursion relations obtained by changing the momentum cut off one finds that the homogeneous magnetization transforms into itself. Therefore a'_{jI} vanishes for $n>1$ if one of the indices i corresponds to the homogeneous magnetization $S_{q=0}$. Therefore,

$$a'_{jI}=b_{jI}=0 \text{ if } n>1 \text{ and } O_i=1 \text{ or } S_{q=0} \text{ for one } i\in I\ . \tag{5.21}$$

VI. LOGARITHMIC SINGULARITIES

In this section we discuss logarithmic singularities in the specific heat using the results of Sec. V and compare with the Ising model and the eight-vertex model. We restrict ourselves to the operators O_0 and O_E. We find from Eq. (5.21) that the only nonvanishing coefficients for $n=2$ are $a'_{0,EE}$ and $a'_{E,EE}$. For the two-dimensional Ising model[17] one has $y_0=2$ and $y_E=1$ and, since the operator O_E is odd under the Kramers-Wannier transformation, one obtains solutions

$$b_{0,EE}=a'_{0,EE}{}^{l} \quad\text{and}\quad b_{E,EE}=0\ . \tag{6.1}$$

We choose $l_0=\ln|g_E|$ and obtain

$$F(0,g_E)=g_E^2F(0,\pm 1)-\tfrac{1}{2}g_E^2a'_{0,EE}\ln|g_E|\ , \tag{6.2}$$

which leads to the logarithmic singularity in the specific heat. Now we take into account all coefficients a'_{jI} with $i,j=0,E$. The only nonvanishing coefficients are $a'_{0,0}=y_0$, $a'_{0,E\cdots E}$ for $n\geq 2$, and $a'_{E,E\cdots E}$. Denoting n indices E by n, we obtain, from Eqs. (4.1) and (4.5),

$$c'_0(\mu_0,\mu_E)=y_0\mu_0+\sum_{n=2}^{\infty}\frac{1}{n!}a'_{0,n}\mu_E^n\ , \tag{6.3}$$

$$c'_E(\mu_E)=\sum_{n=1}^{\infty}\frac{1}{n!}a'_{E,n}\mu_E^n\ , \tag{6.4}$$

$$\mu_0(g_0,g_E)=g_0+\sum_{n=2}^{\infty}\frac{1}{n!}b_{0,n}g_E^n\ , \tag{6.5}$$

$$\mu_E(g_E)=\sum_{n=1}^{\infty}\frac{1}{n!}b_{E,n}g_E^n\ . \tag{6.6}$$

Neglecting the l dependence of b Eq. (5.1) can be written

$$\sum_i\frac{\partial\mu_j\{g\}}{\partial g_i}y_ig_i=c'_j\{\mu\}\ . \tag{6.7}$$

For $j=E$ we obtain

$$\frac{\partial\mu_E}{\partial g_E}y_Eg_E=c'_E(\mu_E)\ , \tag{6.8}$$

which can be easily integrated

$$\ln g_E=y_E\int\frac{d\mu_E}{c'_E(\mu_E)}=\ln\mu_E-\frac{a'_{E2}}{2y_E}\mu_E+\left(\frac{a'^2_{E2}}{8y_E^2}-\frac{a'_{E3}}{12y_E}\right)\mu_E^2-\cdots \tag{6.9}$$

and converted into a series expansion for μ_E:

$$\mu_E=g_E+\frac{a'_{E2}}{2y_E}g_E^2+\left(\frac{a'_{E3}}{12y_E}+\frac{a'^2_{E2}}{4y_E^2}\right)g_E^3+\cdots\ . \tag{6.10}$$

For $j=0$ Eq. (6.7) reads

$$y_0g_0+\frac{\partial\mu_0}{\partial g_E}y_Eg_E=y_0\mu_0+c'_0(0,\mu_E)\ . \tag{6.11}$$

We may expand

$$c'_0(\mu_0=0,\mu_E)=\sum\frac{1}{n!}f_{0,n}g_E^n=\tfrac{1}{2}a'_{02}g_E^2+\left(\frac{a'_{02}a'_{E2}}{2y_E}+\tfrac{1}{6}a'_{03}\right)g_E^3+\cdots\ . \tag{6.12}$$

Then we obtain

$$(ny_E-y_0)b_{0n}=f_{0n}\quad\text{for } ny_E\neq y_0\ , \tag{6.13}$$

whereas for $ny_E=y_0$, we obtain

$$y_Eb_{0n}=f_{0n}\ln|g_E|\ . \tag{6.14}$$

With $y_0/y_E=2-\alpha$, we obtain

$$F(\mu_E)=|g_E|^{2-\alpha}F_\pm-\mu_0(0,g_E)\ , \tag{6.15}$$

where $F(\mu_E)$ is the free energy of $H=H^*+\mu_EO_E$ and

$$F_\pm=F[\mu_E(g_E=\pm 1)]-\mu_0(0,g_E=\pm 1)\ . \tag{6.16}$$

If $2-\alpha$ is not an integer then one obtains a singularity proportional to $|\mu_E|^{2-\alpha}$. If $n=2-\alpha$ is an integer then b_{0n} leads to the singularity

$$F_{\text{sing}}=-f_{0n}y_E^{-1}g_E^n\ln|g_E|\ . \tag{6.17}$$

These logarithmic singularities were observed in the eight-vertex model[6] for even $2-\alpha$. Because of the symmetry under the Kramers-Wannier transformation[18] f_{0n} vanishes for odd n. The amplitude f_{0n}/y_E of the singularity is the same above and below the critical point as already observed by Widom,[19] Griffiths,[20] and Kadanoff.[1]

VII. LIMIT CASE $y=0$

It is beyond the scope of this paper to discuss all the properties of operators with vanishing exponent y. (These operators scale like r^{-d}.) We mention the following four types of operators with $y=0$: (a) The stress tensor scales like r^{-d} (Kawasaki[21]).

(b) If the Hamiltonian H^* is a function of continuous variables z and the trace, Eq. (2.3) is the multiple integral $\prod\int dz_k$, then a scale transformation $z\to\alpha z$ does not change the partition function Z (besides a trivial factor). An infinitesimal scale transformation $\alpha=1+\epsilon$ changes H^* by $\epsilon\delta H^*$ with

$$\delta H^*=\sum_k z_k\partial H^*/\partial z_k . \tag{7.1}$$

Therefore, the index y of the operator δH^* vanishes. (c) An operator $O_u(r)$ which scales like r^{-d} might break universality (Kadanoff[22]). An example is the eight-vertex model.[6,8] If the equation

$$R^6(H\{g_i=\delta_{iu}g_u\})=H\{g_i=\delta_{iu}g_u\} \tag{7.2}$$

holds for any g_u, then there is a whole line of fixed points $H^*(g_u)$. To fulfill Eq. (7.2) it is necessary to have $y_u=0$. This condition is not sufficient, since Eq. (7.2) has to hold for a whole line. (d) If there is an operator O_u with vanishing exponent y_u which is not of one of the above mentioned types then it might lead to a bifurcation point of fixed points as a function of dimensionality. This has been demonstrated by Wilson and Fisher for the break away of the fixed point for a whole class of second order phase transitions at dimensionality 4 from the Gaussian fixed point.[23] Such an operator is a limit case of relevant and irrelevant operators. The limit

$$\lim_{l\to\infty} R^l(H^*+\mu_u O_u) \tag{7.3}$$

may or may not converge to H^*. If, for example, $f_{u,uu}=a'_{u,uu}\neq 0$, then we obtain

$$R^6(H^*+\mu_u O_u)=H^*+(\mu_u+\tfrac{1}{2}\delta a'_{u,uu}\mu_u^2)O_u . \tag{7.4}$$

For $\mathrm{sgn}(\mu_u)=-\mathrm{sgn}(a'_{u,uu})$ the limit (7.3) converges to H^*, whereas for $\mathrm{sgn}(\mu_u)=\mathrm{sgn}(a'_{u,uu})$ the limit (7.3) does not converge to H^*.

Now we discuss the behavior of the free energy if the most singular operator with the symmetry of the Hamiltonian (besides O_0) O_E has a vanishing exponent y_E. Considering only the operator O_0 and O_E, we obtain, from Eq. (2.12),

$$R^6(H^*+\mu_E O_E)=H^*+\mu_E O_E+\delta(c'_0(\mu_E)+c'_E(\mu_E)O_E) . \tag{7.5}$$

Substituting into Eq. (2.8) yields the differential equation

$$dF=\frac{\partial F}{\partial\mu_E}c'_E(\mu_E)+c'_0(\mu_E) . \tag{7.6}$$

The homogeneous equation

$$dF_0=\frac{\partial F_0}{\partial\mu_E}c'_E(\mu_E) \tag{7.7}$$

has the solution

$$F_0=\exp(-p_1/\mu_E)\mu_E^{-p_0}P(\mu_E) , \tag{7.8}$$

in which P is a polynomial

$$P(\mu_E)=1+d[2a'^2_{E3}/(9a'^3_{E2})-a'_{E4}/(6a'^2_{E2})]\mu_E+\cdots \tag{7.9}$$

and

$$p_1=2d/a'_{E2} ,\quad p_0=2da'_{E3}/(3a'^2_{E2}) . \tag{7.10}$$

The solution of Eq. (7.13) is

$$F(\mu_E)=-F_0(\mu_E)\int^{\mu_E}d\mu\, F_0^{-1}(\mu)c'_0(\mu)/c'_E(\mu) . \tag{7.11}$$

This integral leads to an asymptotic expansion in μ_E. In particular, for

$$c'_E(\mu_E)=\tfrac{1}{2}a'_{E2}\mu_E^2 ,\quad c'_0(\mu_E)=\tfrac{1}{2}a'_{02}\mu_E^2 , \tag{7.12}$$

one obtains

$$F(\mu_E)=da'_{02}a'^{-2}_{E2}\sum_{n=2}^{\infty}(n-1)!\,(\mu_E/p_1)^n+c_\pm\exp(-p_1/\mu_E). \tag{7.13}$$

If a'_{E2} vanishes but $a'_{E3}\neq 0$, then one obtains Eq. (7.18) with

$$F_0(\mu_E)=\exp(-p_2\mu_E^{-2}+p_1\mu_E^{-1})\mu_E^{-p_0}P(\mu_E) , \tag{7.14}$$

in which P is a polynomial different from that in Eq. (7.9) and

$$\begin{aligned}&p_2=3d/a'_{E3} ,\quad p_1=3da'_{E4}/(2a'^2_{E3}) ,\\ &p_0=d[3a'_{E5}/(10a'^2_{E3})-3a'_{E4}/(8a'^3_{E3})] .\end{aligned} \tag{7.15}$$

In particular, for

$$c'_E(\mu_E)=\tfrac{1}{6}a'_{E3}\mu_E^3 ,\quad c'_0(\mu_E)=\tfrac{1}{2}a'_{02}\mu_E^2 , \tag{7.16}$$

one obtains

$$F(\mu_E)=\frac{3a'_{02}}{2a'_{E3}}\sum_{n=1}^{\infty}(n-1)!\,(\mu_E^2/p_2)^n+c_\pm\exp(-p_2\mu_E^{-2}) . \tag{7.17}$$

The exponent y_E for the operator O_E in the F model vanishes. Lieb[7] has obtained an asymptotic series for the free energy of the F model around the critical temperature. Approximating the coefficients B and E in Eq. (16) of Ref. 7 by their asymptotic values

$$B_{2n}\approx(-1)^{n+1}\frac{2(2n)!}{(2\pi)^{2n}},\quad E_{2n}\approx(-1)^n\frac{4^{n+1}(2n)!}{\pi^{2n+1}} ; \tag{7.18}$$

and neglecting 1 against E_{2n}, the expansion for the free energy of the F model reads

$$F\propto\sum(2n-1)!(c\mu_E)^n , \tag{7.19}$$

in which c is a constant. Therefore, this expansion is neither of the type (7.13) nor (7.17). We attribute this discrepancy to the occurrence of a second operator O_u with vanishing exponent y.

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New Variational Method for the Antiferromagnetic Ground State*

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A new method is developed to treat the problem of the antiferromagnetic ground state. Starting with an approximate perturbation theory, a functional form for the ground-state wave function is found. This functional form is used as the basis for a variational calculation. The present calculation is specialized to the case of spin $\frac{1}{2}$ but can be generalized to higher spin. From this calculation the ground-state energy and spin deviation are found for several lattices. An advantage of this method is that it yields an explicit wave function for the ground-state quantities. A comparison between this method and previous techniques is also presented.

INTRODUCTION

Several methods have been developed to treat the problem of the ground state of an antiferromagnet. Spin-wave theory[1] was one of the earliest of these. A calculation by Marshall[2] in which he enumerates all states of a local cluster and performs a variational calculation has given good results. A similar