Critical behavior of spin-one three-dimensional Ising model with single-ion anisotropy

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The low-density linked-cluster expansion of the free energy of the ferromagnetic Ising model with single-ion anisotropy, i.e., the $\Delta \sum_i S_{zi}^2$ term, is given by $-\beta f(\beta J, \beta\Delta, \beta h) = \frac{1}{2}qJ + h - \Delta + \sum_{l=1}^{\infty} (u^{12}\mu)^l L_l(u, \eta)$, with $u = \exp(-J/k_B T)$, $\mu = \exp(-2mh/k_B T)$, and $\eta = \exp(\Delta/k_B T)$. This is a low-temperature expansion with each spin S_i having magnitude one. The sixth-order series available in the literature is analyzed by evaluating the zeros of $\tilde{L}_l = u^{12l}L_l$ as a function of Δ, and from that the critical temperature is deduced. The knowledge of the critical temperature as a function of the anisotropy leads to the second-order part of the phase boundary of βJ with $\beta\Delta$ which estimates a tricritical value of Δ. The asymptotic behavior of $\tilde{L}_l$ is studied and from that the critical exponent δ of the M-h isotherm as $h \to 0$ is found. It is observed that the anisotropy determines the transition temperature, but the exponent δ is independent of the same as expected from the universality hypothesis.

I. INTRODUCTION

In the theory of critical phenomena in the Ising model, it is of interest to examine the universality of the critical exponents when a particular coupling constant, which could be varied in relation to the exchange, is introduced. Saul, Wortis, and Stauffer[1] have studied the Ising model for a face-centered cubic lattice to which a single-ion anisotropy term has been added. The model considered is described by the Hamiltonian.

$$H = -J \sum_{\langle i,j \rangle} S_{zi}S_{zj} + \Delta \sum_i S_{zi}^2 - h \sum_i S_{zi} \quad . \tag{1}$$

It represents a special case of the Blume-Emery-Griffiths-Potts model, described often in the literature as the Blume-Capel model. By adding a constant term in the Hamiltonian, the single-ion anisotropy term can be written as $S_z^2 - \frac{1}{3}S(S+1)$, and this anisotropy vanishes for $S = \frac{1}{2}$. Therefore, we are interested in the spin-1 Ising model, $S = 1$ for each spin.

For $S = 1$, the Hamiltonian (1) represents an interesting system as it involves three distinct phases. At low temperatures for small anisotropy, there is a ferromagnetically ordered phase. The S_{zi}^2 term distinguishes between the 0 and ± 1 states but cannot separate the ± 1 states. There are two other types of phases; one paramagnetic phase with all the $S_{zi} = 0, \pm 1$ states equally populated; another with only $S_{zi} = \pm 1$ states or only the $S_{zi} = 0$ states preferentially populated (which is lower depends on the sign of Δ). Accordingly distinct boundaries must exist separating the three phases. As the ratio Δ/J is varied, the system traces through the three phases, and a tricritical point is expected to occur where the three phases coexist. We note that for $\Delta = -\infty$, the $S_{zi} = 0$ state is suppressed, and the model (1) reduces to the $S = \frac{1}{2}$ Ising model. For $\Delta = +\infty$, the $S_{zi} = \pm 1$ states are suppressed, and we have only the $S_z = 0$ states so that the model is spin-zero nonmagnetic at all temperatures. For intermediate values of $\beta\Delta$, another paramagnetic phase exists in which all the $S_{zi} = 0, \pm 1$ states are populated in the ground state of the system, i.e., [with $\eta = \exp(\Delta/k_B T) \equiv \exp(\rho\Delta)$]

$$\Delta > 0, \quad \lim_{T \to 0} \eta = \infty, \quad S_{zi} = 0 \quad ,$$

spin-zero ground state, and

$$\Delta < 0, \quad \lim_{T \to 0} \eta = 0, \quad S_{zi} = \pm 1 \quad ,$$

paramagnetic ground state (ferromagnetic with exchange).

Saul *et al.*[1] employed the method of series expansion and obtained the boundaries of the first- and second-order transitions. The second-order ϵ expansion in the renormalization group has also been applied to this problem,[2,3] but this method is designed only to predict the universal scale-invariant behavior, and the transition temperature which depends on the structure of the Hamiltonian cannot be computed.

The ratio method[4] of calculating the transition temperature is suitable only for the high-temperature expansion of the free energy. When the ratios of the coefficients of the successive terms are plotted against the inverse of the term number, it normally leads to a linear plot only for high-temperature series from which the limit that gives the transition temperature can be easily found. However, for the low-temperature series, the ratio plot does not lead to a linear function. Accordingly, the ratio plot is not applicable to the low-temperature expansion with which we shall be concerned in the present problem. Saul *et al.* noted this difficulty while checking such ratio plots for the low-temperature expansion and were forced to resort to a second check with the Padé method. The low-density and the low-temperature linked-cluster expansion of the free energy has been obtained for a number of Ising lattices by Sykes *et al.*[4] for $S=\frac{1}{2}$, whereas the authors of Ref. 1 give the low-temperature sixth-order series for $S=1$ analyzed in the present work. Majumdar has developed[5] a new method to calculate the transition temperature from the zeros of the polynomials in $u=\exp(-4J/k_BT)$, these polynomials being coefficients in the series expansion in the variable $\mu=\exp(-2mh/k_BT)$. For low-temperature series, where the ratio method does not work, either the Padé or the Majumdar method must be used. The latter method is used so that we can test its success for the Hamiltonian (1).

We also calculate the critical exponent δ as a function of the anisotropy Δ, and thus extend the work of Saul *et al.* in this direction.

Our method of calculation is as follows: We obtain the zeros of the high-field polynomials in the low-temperature expansion of the free energy in a ferromagnetic face-centered cubic lattice for the Hamiltonian (1). As Majumdar found,[5] a particular limit point of the zeros yields the transition temperature. This calculation is done as a function of the anisotropy parameter, and from that the tricritical point is determined. The values of the polynomials at the transition point are computed for various values of the anisotropy parameter near the tricritical point, and from that an effort is made to estimate the universal parameter δ, the exponent of the magnetization $h \sim M^\delta$, for small field h. We are able to obtain the phase boundary of one of the phases (see Fig. 2) and check the universality.

II. PHASE DIAGRAM

The low-temperature linked-cluster expansion provides the free energy,

$$-\beta f(u,\mu,\eta)=\tfrac{1}{2}qJ+h-\Delta+\sum_{l=1}^{\infty}\mu^l u^{12l}L_l(u,\eta) \quad , \tag{2a}$$

where

$$L_l(u,\eta)=\sum_{m=0}^{l}L_{lm}(u)\eta^m \quad . \tag{2b}$$

Here in accordance with Eq. (1),

$$\beta=1/k_BT,\quad \mu=\exp(-\beta h) \quad ,$$

$$\eta=\exp(\beta\Delta),\quad u=\exp(-\beta J) \quad ,$$

and q is the coordination number of the lattice. $L_l(u,\eta)$ is a polynomial in u^{-1} and η, calculated by Saul, Wortis, and Stauffer for l up to 6 for $S=1$ (their Table II). The polynomial L_{lm} for $S=1$ is zero unless l and m are both even or both odd. There is a direct correspondence with the polynomials of Sykes *et al.*[4] for $S=\frac{1}{2}$. The quantities $u^{6l}L_{ll}(u)$ are in fact their polynomials. The lattice constants necessary for $l\leq 5$ have been published by Sykes *et al.* The six point clusters appear first in $L_{66}(u)$ where these are decorated only with type-1 particles. Such contributions for $S=1$ can be taken quite generally from the $S=\frac{1}{2}$ Ising polynomials. Indeed the arbitrary-spin polynomials can be calculated from $S=\frac{1}{2}$ embeddings. For $\Delta=-\infty$, $\eta=0$, the $S=1$ results reduce to the $S=\frac{1}{2}$ Ising results. For $\Delta=0$, $\eta=1$, one obtains the $S=1$ polynomials given by Fox and Gaunt.[4] Majumdar's method[5] is to examine the coefficients of the infinite series in μ in Eq. (2a). At low temperatures, when there is spontaneous magnetization, there must be[6] a singularity at $\mu=1$ ($h=0$). A sufficient condition for such a singularity is that all the coefficients of the power series in μ are of the same sign. Whether all the coefficients are of the same sign or not can be found by locating the zeros of $L_l(u,\eta)$ and one looks at the distribution of the roots of $L_l(u,\eta)$ in the u plane. These roots in the u plane are functions of η; this is a new feature of the present problem, compared to the previous one studied by Majumdar.[5]

The first polynomial sum for $l=2$ is of trivial nature with the root given by

$$u=-6\eta^2(1-\tfrac{13}{2}\eta^2)^{-1} \quad . \tag{3}$$

The root is $\frac{12}{11}$ for $\Delta=0$ and approaches $\frac{12}{13}$ as η goes to infinity. The remaining polynomial sums up to $l=6$ are solved on a computer with double-precision arithmetic. Because of the factor u^{12l}, there is a multiple zero at the origin in the u plane, this is of no interest. The first real zero of the polynomial sums occurs in the interval $0<u<1$, and is denoted by $u_l^{(1)}(\eta)$. These values of $u_l^{(1)}(\eta)$ are plotted in Fig. 1 as a function of η, the convergence of $u_l^{(1)}(\eta)$ as $l\rightarrow\infty$ is determined by a least-squares fit with the expression,

$$u_l^{(1)}(\eta)=u_\infty^c(\eta)+c_1 l^{-a} \quad . \tag{4}$$

All the coefficients of the various powers of μ in the series (2a) are then positive in $0<u<u_\infty^c(\eta)$. The significance of the exponent a has been discussed by Majumdar.[5] In a recent work using the scaling an-

satz, Gaunt[7] has connected the index a to the gap index. We do not use the scaling results but utilize the least-squares method. The Eq. (4) is obviously an assumption neglecting powers in $1/l$ higher than $(1/l)^a$, such as $(1/l)^{2a}$, etc. The least-squares fit assumes the corrections to be negligible for small l and cannot be used as evidence that a is not universal, although we find that a does depend on η. The quantity $u_\infty^c(\eta)$ is the $l\to\infty$ limit of $u_l^{(1)}(\eta)$ and determines the transition temperature. The behavior of k_BT/J with Δ/J thus deduced is shown in Fig. 2. Note that we have started from the low-temperature magnetized phase, and are deducing the critical temperature by Eq. (4). We observe that the transition temperature smoothly changes with η, until near $\eta\sim 6.0$ there is a dramatic fall. If a tricritical point occurs, it may be expected near $\eta=6.0$, as found in Ref. 1. Note that we have only analyzed one phase; that is what the series enables us to do. We have not analyzed the other phases as in Saul, Wortis, and Stauffer,[1] but their more complete analysis indicates that a tricritical point does occur. Our result of locating the tricritical point by observing the changes in T_c is weaker, and perhaps the change in δ to be discussed in Sec. III is a better motivated and more accurate method of locating the tricritical point.

At the point $\eta=6.0$, our parameters are

$$u_l^{(1)}(6)=0.2761+0.8214l^{-0.32} \tag{5}$$

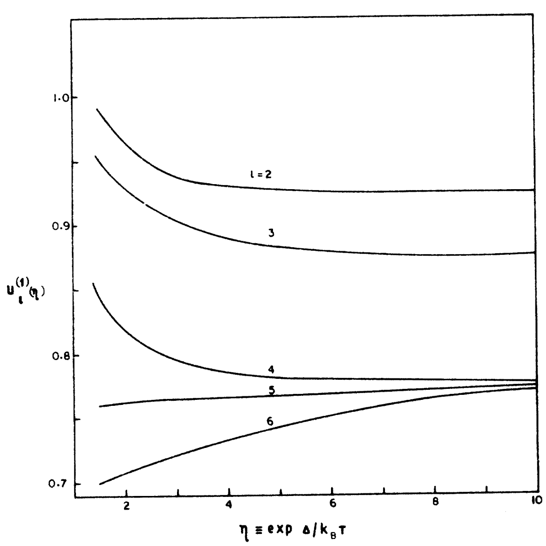

FIG. 1. First zeros of the polynomials $\tilde{L}_l$ as a function of the anisotropy parameter. It may be noted that the tricritical behavior is not shown by the polynomials individually but is rather a matter of collective phenomenon obtained in the limit $l\to\infty$.

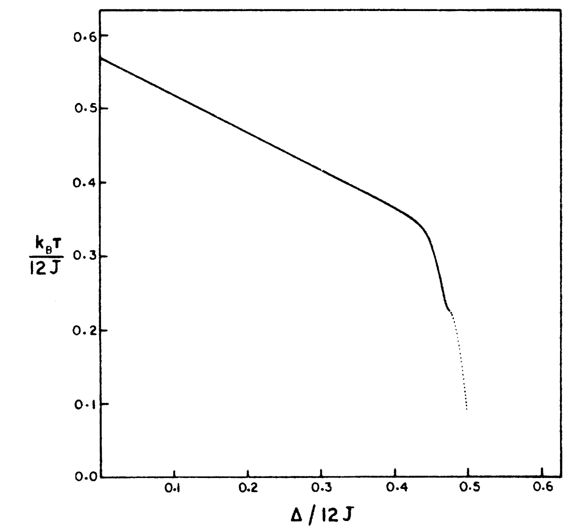

FIG. 2. Tricritical phase diagram of the fcc ferromagnetic Ising model with single-ion anisotropy. The dashed line indicates the area where the transition is first order whereas the continuous curve gives the boundary of the second-order phase transition. For large values of Δ, the transition temperature approaches zero. The point where the continuous curve just starts bending near $\eta=6$ is the tricritical point.

So we obtain,

$$\begin{aligned}&\exp(-4J/k_BT_t)=u_t=0.2761\ ,\\&\exp(\Delta_t/k_BT_t)=\eta_t=6.0\ ,\\&(\Delta/k_BT)_t=1.79,\ \ (\Delta/4J)_t=1.392\ ,\\&(k_BT/4J)_t=0.777\ ,\end{aligned} \tag{6}$$

whereas the corresponding values of the tricritical point by Saul *et al.* are

$$\begin{aligned}&u_t=0.2795,\ \ \eta_t=6.07,\ \ (\Delta/k_BT)_t=1.8\ ,\\&(\Delta/4J)_t=1.4148,\ \ (k_BT/4J)_t=0.784\ .\end{aligned} \tag{7}$$

The two calculations are very close to each other. In expression (5) the least-squares fit is quite satisfactory since the total mean-square deviation does not exceed 10^{-4} in any of the computations, which are performed as a function of η. In making the phase diagram of Fig. 2 we made use of the correspondence of the $S=1$ polynomials for $\Delta=0$. The correspondence of $S=\frac{1}{2}$ with those of $S=1$ has also been checked. Although the least-squares fit to Eq. (4) is an approximation, the shape of the phase boundary shown in Fig. 2 is such that the determination of the tricritical point from the almost vertical tangent is not likely to be affected seriously.

There is a considerable reduction in u_∞^c as one introduces the anisotropy. Compared to the $\Delta=0$

value of $u_\infty^c \sim 0.55$, (as determined by the present method) the values of $u_\infty^c(\eta)$ are much smaller, for example, $0.3858(\eta=3.42)$, 0.3752(3.66), 0.3529(4.08), 0.2108(5.02), 0.2910(5.70), and 0.2761(6.0). At the tricritical point u_t our value is about half of the value at zero anisotropy. Thus the transition temperature is very sensitive to small changes in the anisotropy. The larger the single-ion anisotropy, the lower the transition temperature.

III. UNIVERSAL EXPONENT δ

The important observation for determining the universal parameter δ in that the polynomials at the critical temperature diminish according to a power law

$$u_c^{12l}L_l = c_0 l^{-s} \ . \tag{8}$$

Then we can write, by asymptotic considerations,

$$-\beta f - \tfrac{1}{2}qJ - h + \Delta \simeq c_0 \sum_l \mu^l l^{-s} \ . \tag{9}$$

We now let $h \to 0+$ or $\mu \to 1$ and approach the singularity. It turns out that s is greater than one, and we know[8]

$$\phi(x,s) = \sum_{n=1}^{\infty} x^n n^{-s} = \Gamma(1-s)(-\ln x)^{s-1} + \sum_{n=0}^{\infty} \zeta(s-n)(\ln x)^n/n! \ , \tag{10}$$

where $\Gamma(x)$ is the Γ function and $\zeta(x)$ is the Riemann ζ function. The first term in the expansion will have a singularity if s is nonintegral. Therefore to attain the singular part f_s of the free energy, we are interested only in this part. Hence

$$\beta f_s \simeq -c_0\Gamma(1-s)(-\ln\mu)^{s-1} \ . \tag{11}$$

The singular part of the magnetization appears to be

$$M = -\partial f_s/\partial h = c_0(s-1)\Gamma(1-s)(h/k_BT_c)^{s-2} \ . \tag{12}$$

Comparing with the standard isotherm $h \sim M^\delta$, we obtain

$$\delta^{-1} = s-2 \ . \tag{13}$$

It is well known that the mean-field theory gives $\delta=3$, and the three-dimensional spherical model gives $\delta=5$ exactly.[9,10] The value predicted on the basis of Padé approximations in a spin-$\frac{1}{2}$ Ising ferromagnet is $\delta=5$. Majumdar's method outlined in the equations above also give $\delta \simeq 5$ for the spin-$\frac{1}{2}$ Ising ferromagnet. The second-order ϵ expansion in the renormalization-group approach gives $\delta=4.42$. Majumdar and Rao[5] obtained $\delta=3.9$ for the Lennard-Jones fluid; this value of δ is smaller than the spin-$\frac{1}{2}$ Ising value. Experimentally the value of δ in Ni is 4.2 ± 0.1 and in Gd it is 4.0 ± 0.1. In the liquid-gas transition and in some binary mixtures, the values are known, e.g., 4.2 in CO_2, 4.4 ± 0.4 in Xe, 4 in $CCl_4-C_7F_{14}$. Equation (13) has therefore yielded values roughly consistent with other theoretical estimates and experimental determinations.

Recent calculations[3] using the renormalization group in the Blume-Capel model give $\delta=4.605$ for the critical and 8.29 for the tricritical point in three-dimensional systems. The values of δ obtained by Saul, Wortis, and Stauffer[1] lie between 4.5 and 6.3. In particular their value 6.3 deviates from the value 8.29 at the tricritical point.

In order to apply the method outlined in the Eqs. (8)–(13), we redefine our polynomials as

$$\tilde{L}_l(u,\eta) = u^{12l}L_l(u,\eta) \ . \tag{14}$$

Then $\tilde{L}_l$ are evaluated at (u_∞^c,η). It is then found that

$$\begin{aligned}
\tilde{L}_l(0.38582, 3.42) &= 2.4\times10^{-8}l^{-2.21} + 2.3\times10^{-9}(l^{-2.21})^2 \ ,\\
\tilde{L}_l(0.37516, 3.66) &= 5.8\times10^{-9}l^{-2.21} + 1.1\times10^{-11}(l^{-2.21})^2 \ ,\\
\tilde{L}_l(0.35287, 4.08) &= 4.0\times10^{-9}l^{-2.19} + 1.2\times10^{-11}(l^{-2.19})^2 \ ,\\
\tilde{L}_l(0.31049, 5.02) &= 3.4\times10^{-10}l^{-2.22} + 4.0\times10^{-12}(l^{-2.22})^2 \ ,\\
\tilde{L}_l(0.27614, 6.00) &= 2.8\times10^{-11}l^{-2.11} + 3.8\times10^{-15}(l^{-2.11})^2 \ .
\end{aligned} \tag{15}$$

In the limit of large l, the second term becomes negligible compared to the first. So the values of s appear to be about 2.21, 2.21, 2.19, 2.22, and 2.11 for the anisotropy parameters quoted in $\tilde{L}_l$. The final value $\eta=6$ corresponds to the tricritical point. The values of δ^{-1} are thus 0.21, 0.21, 0.19, 0.22, and 0.11. A careful examination of Eq. (15) shows that we are quite far from the asymptotic region required by Eq. (8). The scatter in the first few members gives an idea of the accuracy of the δ thus determined. Yet these values are within the range expected from the renormalization-group calculations. It is clear that the values of the critical exponent are relatively insensitive to variations in anisotropy except when we go very near the tricritical point.

IV. CONCLUSION

We have been able to trace one phase boundary βJ, with $\beta\Delta$ for the Hamiltonian (1), starting from the low-temperature side. We have also obtained the critical exponent δ of the magnetization with the field tending to zero. Our computation shows that the transition temperature is strongly dependent on the anisotropy and the critical index δ is more or less independent of the same (except near the tricritical point). Within a certain range we are thus able to check numerically the idea of universality.

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