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Specific-Heat Scaling Functions for Ising and Heisenberg Models and Comparison with Experiments on Nickel*

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We calculate the scaled constant-magnetization and constant magnetic field specific heats $[C_M(\epsilon,M) - C_M(\epsilon,0)]/M^{-\alpha/\beta}$ and $[C_H(\epsilon,H) - C_H(\epsilon,0)]/H^{-\alpha/\beta\delta}$ as functions of the scaled variable $x \equiv \epsilon/M^{1/\beta}$ and $y \equiv \epsilon/H^{1/\beta\delta}$, respectively. [where $\epsilon \equiv (T - T_c)/T_c$ and T_c is the critical temperature] ,for the spin-½ Ising model (bcc lattice) and the spin-½, ∞ Heisenberg models (fcc lattice). Our calculations are based on previously calculated scaling functions for the $M(H,T)$ equation of state. We also calculate the amplitudes of the zero-field specific heat for $T > T_c$ and $T < T_c$. Thus, we obtain the functions $C_M(\epsilon,M)$ and $C_H(\epsilon,H)$, though for the Heisenberg models we cannot obtain the finite nonzero constant $C_M(0,0) = C_H(0,0)$. We compare our calculated functions with the data of Connelly, Loomis, and Mapother on nickel.

I. INTRODUCTION

Recently measurements of specific heat in a field have been made on the ferromagnet nickel,[1] and these data were shown[1] to obey the scaling hypothesis.[2-4] That is, data from different isotherms (T = const) and "isochamps" (H = const), when appropriately scaled, were observed to collapse onto a single curve.[3] The scaling scheme used was to reduce the observed relation between the *three* variables specific heat $C_{\mathcal{H}}$, magnetic field $\mathcal{H}$, and temperature T to a relation between the *two* variables $\mathcal{T}' \equiv (C_{\mathcal{H}} - C_0)\mathcal{H}^{\alpha/\beta\delta}$ and $\mathcal{Y} \equiv \epsilon\mathcal{H}^{-1/\beta\delta}$, where $\epsilon \equiv (T - T_c)/T_c$ (with T_c the critical temperature) and α, β, δ are the usual critical-point exponents. (The reason for the prime on the variable $\mathcal{T}'$ will become apparent in Sec. II.)

The functional relation between $\mathcal{T}'$ and $\mathcal{Y}$, however, remained unknown. Ho[5] obtained for Ni a scaling function $\mathcal{T}'(\mathcal{Y})$ by using the Maxwell relation between the entropy $\mathcal{S}$, field $\mathcal{H}$, magnetization $\mathfrak{M}$, and temperature T,

$$\left(\frac{\partial \mathcal{S}}{\partial \mathfrak{M}}\right)_T = -\left(\frac{\partial \mathcal{H}}{\partial T}\right)_{\mathfrak{M}}, \tag{1.1}$$

on an empirical fit to available $\mathcal{H}$-$\mathfrak{M}$-T data.[6] The empirical fit consisted in assuming the $\mathcal{H}$-$\mathfrak{M}$-T data to be well represented by the "linear model" in the parametric representation.[7] It is a one-parameter fit, where the parameter is the slope of the $m(\theta)$ line, in the notation of Ref. 7. It is important to point out that the "linear model" is not a model in the sense of a microscopic Hamiltonian, but rather is a useful way of presenting $\mathcal{H}$-$\mathfrak{M}$-T data, once the data have been obtained either experimentally or by calculations on a microscopic Hamiltonian.

We present here the first calculations of scaling functions for specific heats *based on microscopic Hamiltonians*; our work requires *no* adjustable parameters. These calculations became possible after the magnetic equations of state $\mathcal{H}(T, \mathfrak{M})$ for these Hamiltonians were obtained by Milošević and Stanley,[8] and Karo,[9] through analysis of high-temperature expansions.

A major virtue of the present results is that they are arrived at without recourse to the very lengthy and tedious process of obtaining and analyzing high-temperature series expansions for the specific heat. Such series are usually extremely irregular and therefore much less reliable than series of the same order for the magnetic equation of state.

In Sec. II we show how knowledge of the magnetic equation of state $\mathcal{H}(T, \mathfrak{M})$ can be used to obtain the scaling functions for the specific heats. In Sec. III, we discuss the normalization scheme used in this work. In Sec. IV, we present our results for the scaling functions for specific heats at constant field and at constant magnetization and compare them with Ni data. Finally, Sec. V shows how one can then use the knowledge of the scaling functions to obtain the amplitudes of the singularities in the zero-field specific heat.

II. METHOD

In critical phenomena work it is usual to reduce the variables to dimensionless quantities which are zero at the critical point. Thus we define the variables $H \equiv \mathcal{H}(kT_c/m)^{-1}$ (here k is Boltzmann's constant, m is the magnetic moment per site), $M \equiv \mathfrak{M}/Nm$ (N is the number of sites), and $\epsilon \equiv (T - T_c)T_c$. In these variables, the Maxwell relation, Eq. (1.1), becomes

$$\left(\frac{\partial S}{\partial M}\right)_\epsilon = -\left(\frac{\partial H}{\partial \epsilon}\right)_M, \tag{2.1}$$

where $S \equiv \mathcal{S}/R$ is the entropy in units of R, the universal gas constant. We may use this relation to obtain information about the entropic equation of state $S=S(\epsilon, M)$, and therefore about the specific heats as well.

From Eq. (2.1) it is clear that from the equation of state $H(\epsilon, M)$ one may learn only about the M-dependent part of the entropy,

$$\Delta S(\epsilon, M)\equiv S(\epsilon, M)-S(\epsilon, 0)\ , \qquad (2.2)$$

since the addition of an M-*in*dependent term to S will not show up in the left-hand side of Eq. (2.1). (In Sec. V we will see that if the zero-field specific heat has a singularity, we can learn the amplitude of that singularity as well.)

We consider three models, the spin-$\frac{1}{2}$ and spin-infinity Heisenberg models, and the spin-$\frac{1}{2}$ Ising model. All three models have equations of state[8,9] which obey the static scaling hypothesis,[2] i.e., near the critical point they can be cast in a form

$$H=M^{\delta}h(x)\ , \qquad (2.3)$$

with

$$x\equiv \epsilon M^{-1/\beta}\ . \qquad (2.4)$$

From Eqs. (2.1) and (2.3) it can be shown[10] that $\Delta S(\epsilon, M)$ also obeys the static scaling formulation, that is, it can be written

$$\Delta S=M^{z}s(x)\ , \qquad (2.5)$$

where z and $s(x)$ are to be determined using the Maxwell relation, Eq. (2.1).

Differentiating the scaling forms, Eqs. (2.3) and (2.5), with respect to ϵ and M, respectively, and using (2.1), we find

$$M^{z-1}[zs(x)-xs'(x)/\beta]=-M^{\delta-1/\beta}h'(x)\ , \qquad (2.6)$$

where the prime denotes differentiation with respect to the argument. Since the Maxwell relation is everywhere valid, we may equate powers of M, and find

$$z=1+\delta-1/\beta\ . \qquad (2.7)$$

Thus from (2.6) and (2.7), $s(x)$ must obey the differential equation

$$xs'(x)-\beta zs(x)=\beta h'(x)\ . \qquad (2.8)$$

While we could integrate this differential equation for $s(x)$, and thus obtain the scaling function for the entropy [cf. Eq. (2.5)], our primary interest is the specific heat. Differentiating both sides of (2.5) with respect to ϵ we find, for $\Delta C_M\equiv C_M(\epsilon, M)-C_M(\epsilon, 0)$,

$$\Delta C_M=\left(\frac{\partial \Delta S}{\partial \epsilon}\right)_M=M^{z-1/\beta}s'(x)\ . \qquad (2.9)$$

Thus the specific heat is itself a scaled function near the critical point, with scaling function $s'(x)$. A differential equation for $s'(x)$ can be promptly obtained from Eq. (2.8) by differentiation with respect to x,

$$xs''(x)+\alpha s'(x)=\beta h''(x)\ , \qquad (2.10)$$

where use has been made of the exponent relation[2]

$$\alpha=2-\beta(\delta+1) \qquad (2.11)$$

for the exponent α of the zero-field specific heat. The same relation yields together with Eq. (2.7),

$$z=(1-\alpha)/\beta\ , \qquad (2.12)$$

and thus the power of M in Eq. (2.9) is $-\alpha/\beta$.

The general solution to the differential equation [Eq. (2.10)] is

$$s'(x)=\pm\ |x|^{-\alpha}\int_{x_\pm}^{x}|x|^{\alpha-1}\beta h''(x)dx+C_\pm\ |x|^{-\alpha}\ , \qquad (2.13)$$

where the upper and lower signs correspond to positive and negative x, respectively. The lower limits on the integral, $x_\pm$, and the constants $C_\pm$ are used to match the boundary conditions imposed on $s'(x)$. These conditions are that the difference of specific heats ΔC_M vanish on the $H=0$ line, for x both positive and negative. For $x<0$, we may choose the lower limit $x_-=-x_0$, with the constant C_- set equal to zero. For $x>0$, the lower limit x_+ may be chosen as $+\infty$, with the constant C_+ also set to zero. This choice of lower limits is not unique, but any other choice of $x_\pm$ would necessitate nonzero $C_\pm$, in order to satisfy the boundary conditions. Such nonzero values of $C_\pm$ would then be strictly equivalent to our choice of $x_\pm$ with zero constants $C_\pm$.

The value of $s'(x)$ at $x=0$ can be obtained without recourse to the integration of Eq. (2.13). We may obtain the value $s'(0)$ by considering Eq. (2.10). Near $x=0$, $C_M(\epsilon, M)$ is nonsingular if $M\neq 0$, and can be replaced by its value at $\epsilon=0$, while $C_M(\epsilon, 0)$ is singular, behaving as $|\epsilon|^{-\alpha}$. Thus s' itself must contain a term in $|x|^{-\alpha}$, while s'' will behave as $|x|^{-\alpha-1}$. There are two cases to consider, $\alpha<0$ and $\alpha>0$. If $\alpha<0$, as for the Heisenberg models, $s'(0)$ will be finite and $xs''(x)$ will go to zero as x tends to zero. Thus Eq. (2.10) tells us that

$$s'(0)=\beta h''(0)/\alpha<0\ . \qquad (2.14)$$

When $\alpha>0$, as is the case for the Ising model, *both* $s'(x)$ and $xs''(x)$ become infinite as x tends to zero, although the left-hand side of Eq. (2.10) remains finite. Actually $s'(0)\to-\infty$, since by (2.9) $s'(x)\propto\Delta C_M$ and $C_M(\epsilon, 0)\to+\infty$, while $C_M(\epsilon, M)$ remains finite.

Once the scaling function $s'(x)$ for the specific heat C_M has been found, we use the thermodynamic identity

$$C_H-C_M=T\left(\frac{\partial H}{\partial T}\right)_M^2\chi_T\ , \qquad (2.15)$$

where χ_T is the isothermal susceptibility, to calculate the scaling function for the constant-H specific heat, which we call $t'(y)$. Thus,

$$C_H(\epsilon, H) - C_H(\epsilon, 0) = H^p\, t'(y)\,, \tag{2.16}$$

$$y \equiv \epsilon H^{-1/\beta\delta}\,, \tag{2.17}$$

where p can be shown[2] to be equal to $-\alpha/\beta\delta$. Equation (2.15) applied to Eq. (2.16) yields an equation for $t'(y)$,

$$t'(y) = h(x)^{\alpha/\beta\delta}\left(s'(x) + \frac{\beta h'^2(x)}{\beta\delta\, h(x) - xh'(x)}\right)\,, \tag{2.18a}$$

where $x = x(y)$ implicitly, using the relation

$$y = xh(x)^{-1/\beta\delta}\,, \tag{2.18b}$$

obtained by combining Eqs. (2.3), (2.4), and (2.11).

The reason the present scaling function $t'(y)$ is expressed as a derivative is because if we chose to express the scaled entropy as a function of (ϵ, H) instead of (ϵ, M), it would read

$$S(\epsilon, H) - S(\epsilon, 0) = H^{(1-\alpha)/\beta\delta}\, t(y)\,, \tag{2.19}$$

from which Eq. (2.16) follows immediately.

We now turn to a normalization scheme found useful in this work.

III. NORMALIZATION

In order to compare the equations of state of different physical systems which are presumed to be similar in some sense, or to compare a model with a real system, a certain amount of variable transformation becomes necessary. Thus, we replaced the temperature T by a reduced temperature $\epsilon \equiv (T - T_c)/T_c$, divided the magnetization $\mathfrak{M}$ by the magnetic moment per site and by the number N of sites, thus obtaining the variable $M \equiv \mathfrak{M}/Nm$, and we divided the magnetic field $\mathcal{H}$ by kT_c/m since that is the combination in which $\mathcal{H}$ participates in the Hamiltonian, obtaining then the variable $H \equiv m\mathcal{H}/kT_c$. A choice of normalization for $\mathcal{H}$, $\mathfrak{M}$, and T, however, implies a normalization for all other thermodynamic quantities, since they all derive from the same free energy. It is straightforward to show that, in this convention, the entropy $\mathcal{S}$ becomes $S \equiv \mathcal{S}/R$, where R is the universal gas constant, and the specific heat $\mathcal{C}$ becomes the variable $C \equiv \mathcal{C}/R$.

Despite this normalization by constants characteristic of each system, different systems are observed to have differing amplitudes (as well as exponents) on the various special critical loci (critical isochore, critical isotherm, and phase boundary). The elimination of the amplitude dependence of the special loci can be dealt with by the simple normalization

$$\bar{H} \equiv H/[h(0)x_0^{-\beta\delta}] \tag{3.1}$$

and

$$\bar{M} \equiv M/x_0^{-\beta}\,, \tag{3.2}$$

which have the effect of normalizing to unity, in the variables $\bar{H}$, $\bar{M}$, ϵ, the amplitudes of both the phase boundary and the critical isotherm.[11] In the x, $h(x)$ language, this redefines the scaling variables

$$\bar{H} = \bar{M}^{\delta}\bar{h}(\bar{x})\,, \tag{3.3}$$

where

$$\bar{h}(\bar{x}) \equiv h(\bar{x}x_0)/h(0) \tag{3.4}$$

and

$$\bar{x} \equiv x/x_0\,. \tag{3.5}$$

The choice of a normalization for H and M, however, implies again a scale for all other quantities. For example, from Eq. (2.1) it follows that a new entropy $\bar{S}$ is given by

$$\bar{S} = Sx_0^{\beta(\delta+1)}/h(0)\,, \tag{3.6}$$

and thus the scaling function $s(x)$ is replaced by

$$\bar{s}(\bar{x}) = s(\bar{x}x_0)x_0/h(0)\,, \tag{3.7}$$

while the specific heat normalizes as

$$\bar{C}_{\bar{M}} = C_M x_0^{\beta(\delta+1)}/h(0) \tag{3.8}$$

and its scaling function $s'(x)$ becomes

$$\bar{s}'(\bar{x}) = s'(\bar{x}x_0)x_0^2/h(0)\,. \tag{3.9}$$

Equations (2.10) and (2.13) must remain the same in the barred variables, except for the lower limit $\bar{x}_-$ on the integral for $\bar{x} < 0$, which becomes -1. Thus

$$\bar{s}'(\bar{x}) = \pm\,|\bar{x}|^{-\alpha} \int_{\substack{-1\\+\infty}}^{\bar{x}} |\bar{x}|^{\alpha-1}\beta\bar{h}''(\bar{x})\,d\bar{x} \tag{3.10}$$

is the expression for the scaling function being sought.

Concerning the scaling function for $\bar{C}_{\bar{H}}$, Eqs. (2.18), (3.4), and (3.5) yield the normalization

$$\bar{t}'(\bar{y}) = t'(\bar{y}y_0)/t_0\,, \tag{3.11}$$

$$\bar{y} = y/y_0\,, \tag{3.12}$$

with

$$t_0' \equiv x_0^2 h(0)^{-\alpha/\beta\delta-1} \tag{3.13}$$

and

$$y_0 = h(0)^{-1/\beta\delta}x_0\,. \tag{3.14}$$

Equation (2.18) is the same in the barred variables.

IV. SCALING FUNCTIONS FOR $\bar{C}_{\bar{M}}$ AND $\bar{C}_{\bar{H}}$

Table I gives the scaled equations of state[8,9] for the spin $= \infty$ and spin-$\frac{1}{2}$ Heisenberg models and for the spin-$\frac{1}{2}$ Ising model. Using these functions

TABLE I. Scaling functions for the equation of state $H(T, M)$ [cf. Eq. (2.3)] from Refs. 8 and 9. The scaling function for the Ising model had been previously calculated by Gaunt and Domb (Ref. 12) but in a different form.

Model	Small x	Large x	Parameters used	
(a) Heisenberg spin $=\infty$ (fcc)	$h(x) = \frac{0.8x_1}{c^\delta}\left(1 - \frac{z}{z_0}\right)^q$ $\times \frac{3 - 22.169z + 23.71z^2 + 9.512z^3}{1 - 7.823z + 10.745z^2 + 1.697z^3}$, $c(xc^{1/\beta} + 1) = 0.8x_1$, $z = x_1/(c^{1/\beta}x + 1)$, $-x_0 \le x \le 22$	$h(x) = 3.584x^\gamma \frac{1 + 0.4291x^{2\beta}}{1 - 0.6223x^{2\beta}}$, $22 \le x \le \infty$	$\beta = 0.380$ $\gamma = 1.379$ $x_0 = 0.5890$ $h(0) = 2.1284$ $x_1 = 0.1573$ $q = 1.33$	$\delta = 4.63$ $\alpha = -0.130$ $z_0 = 0.1577$
(b) Heisenberg spin $=\frac{1}{2}$ (fcc)	$h(x) = [(c^{1/\beta}x + 1)/c^\delta] \tanh^{-1}[cg(z)]$, $g(z) = \left(1 - \frac{z}{z_0}\right)^q$ $\times \frac{1 + 3.789z + 1.671z^2 + 3.612z^3}{1 + 3.775z + 4.622z^2 + 14.397z^3}$, $z \equiv x_1/(c^{1/\beta}x + 1)$, $-x_0 \le x \le 1.3$	$h(x) = x^\gamma \frac{0.9328 + 0.2805x^{-2\beta}}{1 - 0.2472x^{-2\beta}}$, $1.3 \le x \le \infty$	$\beta = 0.385$ $\gamma = 1.429$ $x_0 = 0.256\,51$ $h(0) = 0.206\,30$ $c = 0.4$ $x_1 = 0.2492$ $q = 1.29$	$\delta = 4.71$ $\alpha = -0.198$ $z_0 = 0.255\,26$
(c) Ising spin $=\frac{1}{2}$ (bcc)	$h(x) = [(c^{1/\beta}x + 1)/c^\delta] \tanh^{-1}[c\tau(\nu)]$, $\tau(\nu) = \left(1 - \frac{\nu}{\nu_0}\right)^q$ $\times \frac{1 - 4.566\nu + 5.406\nu^2 + 5.842\nu^3 + 0.3907\nu^4}{1 - 5.936\nu + 17.603\nu^2 - 37.098\nu^3 + 25.811\nu^4}$, $\nu \equiv \tanh[x_1/(c^{1/\beta}x + 1)]$, $-x_0 \le x \le 1$	$h(x) = x^\gamma \frac{1.0097 + 1.0189x^{-2\beta} + 0.4945x^{-4\beta} + 0.1696x^{-6\beta}}{1 + 0.4388x^{-2\beta}}$, $1 \le x \le \infty$	$\beta = \frac{5}{16}$ $\gamma = \frac{5}{4}$ $x_0 = 0.303\,80$ $h(0) = 0.424\,71$ $c = 0.6$ $x_1 = 0.157\,43$ $q = 1.076$	$\delta = 5$ $\alpha = \frac{1}{8}$ $\nu_0 = 0.1658$

a numerical integration of Eq. (3.10) was carried out to obtain the $\overline{C}_{\overline{M}}$ scaling functions $\overline{s}'(\overline{x})$. Our results are shown in Fig. 1. Equation (2.18) in the normalized (barred) variables was then used to obtain the $\overline{C}_{\overline{H}}$ scaling functions $\overline{t}'(\overline{y})$. Figure 2 shows the results of this calculation. The Ni data of Ref. 1 are compared with the spin $=\infty$ Heisenberg-model scaling function in Fig. 2(a). The agreement may be considered good in light of the fact that Ni is neither an insulating ferromag-

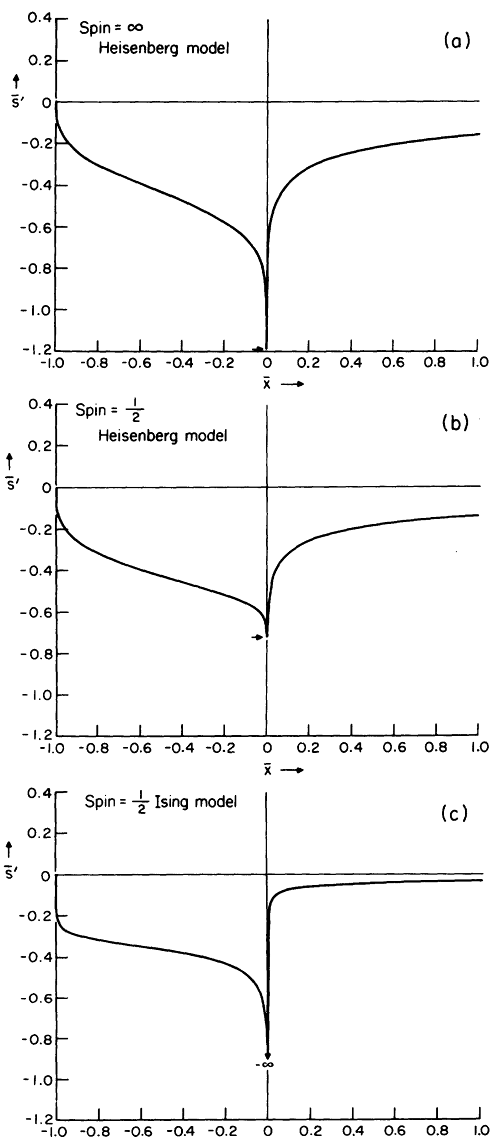

FIG. 1. Scaling functions for the constant magnetization specific heat C_M [cf. Eqs. (2.9) and (3.7)] for (a) Heisenberg spin $=\infty$ (fcc lattice), (b) Heisenberg spin $=\frac{1}{2}$ (fcc lattice), and (c) Ising spin $=\frac{1}{2}$ (bcc lattice). Cusp at $x=0$ in (a) and (b) represents a negative exponent α, while infinity at $x=0$ in (c) represents $\alpha>0$.

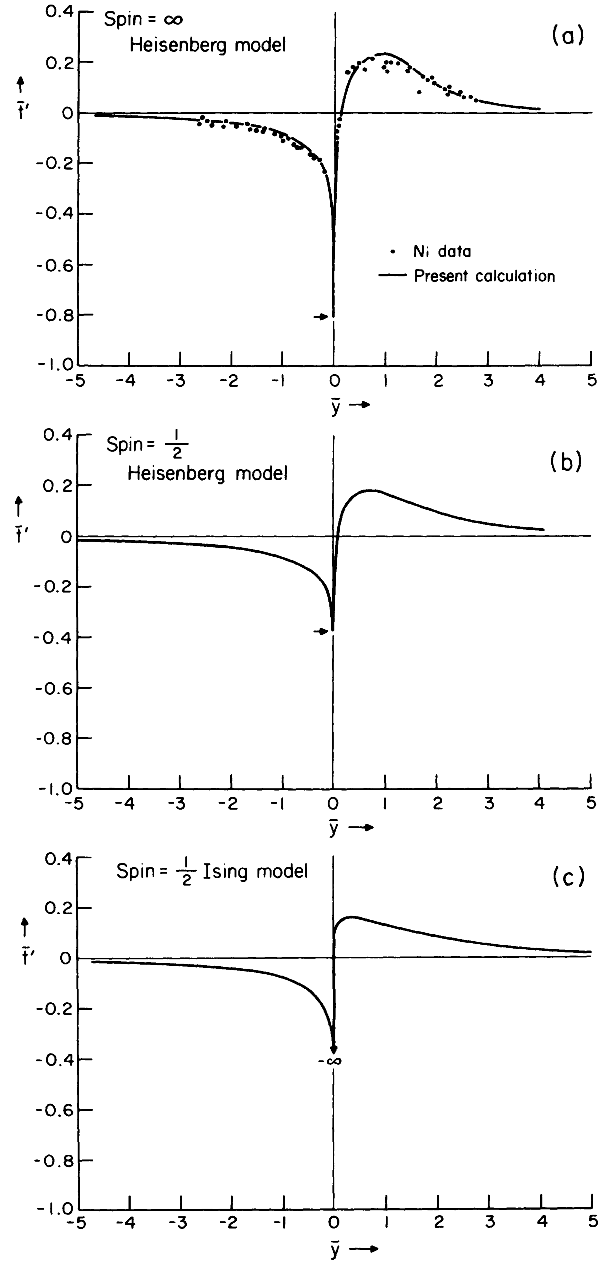

FIG. 2. Scaling function for the constant-field specific heat C_H[cf. Eqs. (2.18), (3.11), and (3.12)] for (a) Heisenberg spin $=\infty$ (fcc), (b) Heisenberg spin $=\frac{1}{2}$ (fcc), and (c) Ising spin $=\frac{1}{2}$ (bcc). Points in (a) are data for Ni, from Ref. 1. Parameters used for Ni are $h(0)=0.29063$, $x_0=0.39400$ (Ref. 6).

net, nor has it a large spin. In fact, the data for Ni lie somewhere in between the curves for spin $=\frac{1}{2}$ and spin $=\infty$.

A prominent feature of the three models is an infinite slope in $\overline{s}'(\overline{x})$ at $\overline{x}=-1$. This has its origin in the nonintegral power q of the singularity at the phase boundary (cf. Table I). The origin and con-

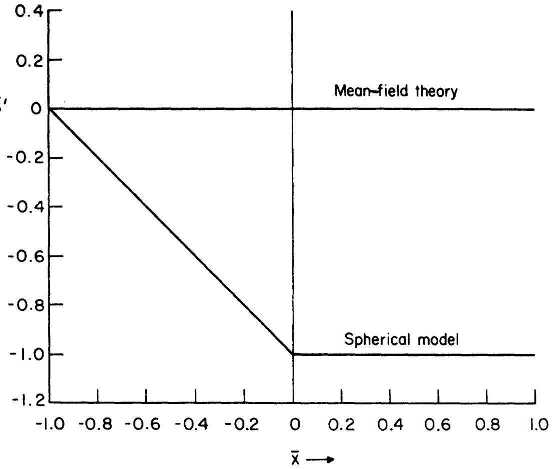

FIG. 3. Scaling functions for the constant-M specific heat for the mean-field theory and the spherical model [cf. Eqs. (2.9), (3.7), (4.3), and (4.5)]. Discontinuity in slope at $x=0$ for the spherical model represents a negative integer value for $\alpha(-1)$.

sequences of nonintegral q have been discussed elsewhere.[8,13] In addition to computing the specific-heat scaling functions for these three models, we also used Eqs. (3.10) and (2.18) (in normalized variables) to calculate the mean-field and spherical-model scaling functions for comparison. For the mean-field scaled equation of state we used[14]

$$\bar{h}(\bar{x}) = 1+\bar{x}\ , \tag{4.1}$$

while for the spherical model we used[15]

$$\bar{h}(\bar{x}) = (1+\bar{x})^2\ . \tag{4.2}$$

In these simple cases Eq. (3.10) can be integrated in closed form. It is then straightforward to show that the specific-heat scaling functions are

$$\bar{s}'(\bar{x}) \equiv 0\ , \tag{4.3}$$

$$\bar{t}'(\bar{y}) = 1/(3+\bar{x}) - \tfrac{1}{2}[1-\theta(\bar{y})]\ , \tag{4.4a}$$

with $\bar{y}$ implicit in $\bar{x}$ through

$$\bar{y}(\bar{x}) = \bar{x}/(1+\bar{x})^{2/3} \tag{4.4b}$$

for the mean-field theory (cf. Fig. 3). Here $\theta(x)$ is the unit step function, $\theta(x)=0$ for $x<0$ and 1 for $x>0$. Similarly,

$$\bar{s}'(\bar{x}) = -1-\bar{x}[1-\theta(\bar{x})]\ , \tag{4.5}$$

$$\bar{t}'(\bar{y}) = (1+\bar{x})^{-4/5}\left(\bar{s}'(\bar{x}) + \frac{4(1+\bar{x})^2}{5+6\bar{x}+\bar{x}^2}\right)\ , \tag{4.6a}$$

with $\bar{y}$ implicit in $\bar{x}$ through

$$\bar{y}(\bar{x}) = \bar{x}/(1+\bar{x})^{4/5} \tag{4.6b}$$

for the spherical model (cf. Fig. 4).

V. AMPLITUDES OF THE ZERO-FIELD SPECIFIC HEAT

We have also estimated the amplitudes $A_\pm$ of the zero-field specific heat,[16]

$$C_M(\epsilon, 0) - C_M(0,0) \cong A_\pm |\epsilon|^{-\alpha} \quad (\alpha<0) \tag{5.1}$$

and

$$C_M(\epsilon, 0) \cong A_\pm |\epsilon|^{-\alpha} \quad (\alpha>0)\ , \tag{5.2}$$

where the upper sign is for $x>0$ and the lower for $x<0$, by the following argument. If $H\neq 0$, then upon crossing the $x=0$ line there should be no singularity in the specific heat. Thus any singularity in $\Delta C_M M^{\alpha/\beta}$ (Fig. 1) arises solely from the singularity in the zero-field specific heat. The amplitude of this singularity can then be obtained as the amplitude of the singularity in the scaling functions $s'(x)$. We divide our argument into two cases.

A. $\alpha < 0$ (e.g., Heisenberg Models)

The amplitude is defined by Eq. (5.1). In the case $\alpha<0$, we have found that $s'(x)$ is finite and negative (Fig. 1). Thus $C_M(\epsilon, M) \leq C_M(\epsilon, 0)$ for all M. Therefore $C_M(0,0)$ cannot be zero, or else $C_M(0, M)$ would be negative, which is unacceptable. In addition, we find from $s'(x)$ that

$$s'(x) > s'(0) \tag{5.3}$$

or, put in terms of specific heats,

$$C_M(\epsilon, M) - C_M(\epsilon, 0) > C_M(0, M) - C_M(0,0)\ . \tag{5.4}$$

But sufficiently near $\epsilon=0$, we can replace the nonsingular $C_M(\epsilon, M)$ by its value at $\epsilon=0$, so that Eq. (5.4) reads

$$C_M(\epsilon, 0) < C_M(0,0) \tag{5.5}$$

and hence the amplitude defined in Eq. (5.1) is negative.

Writing then

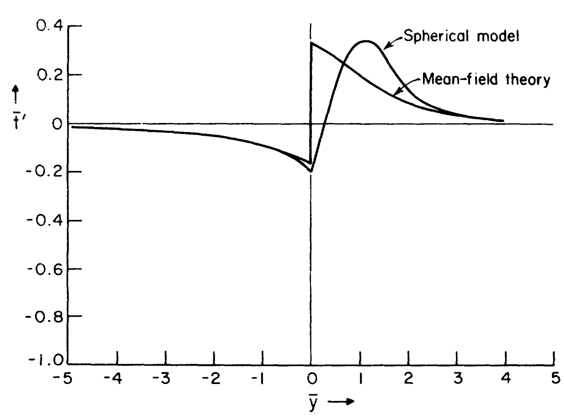

FIG. 4. Scaling functions for the constant-H specific heat for the mean-field theory and the spherical model [cf. Eqs. (4.4) and (4.6)].

TABLE II. Amplitudes $\bar{A}_\pm$ of zero-field specific heats, in normalized units [cf. Eqs. (5.1) and (5.2)]. Domb and Bowers (Ref. 17) obtained a value of $\bar{A}_+ = -1.6$ for the spin $=\infty$ Heisenberg model, using $\alpha = -\frac{1}{16}$ (unspecified lattice).

	Heisenberg spin $=\infty$ (fcc)	Heisenberg spin $=\frac{1}{2}$ (fcc)	Ising spin $=\frac{1}{2}$ (bcc)	Nickel (Ref. 1)
$\bar{A}_+$	-1.05 ± 0.10	-0.66 ± 0.01	0.453 ± 0.001	$-0.9337^{+0.404}_{-0.217}$
$\bar{A}_-$	-0.72 ± 0.10	-0.25 ± 0.01	0.144 ± 0.001	$-0.8217^{+0.356}_{-0.192}$

$$C_M(\epsilon, 0) = A_\pm \, |\epsilon|^{-\alpha} + C_M(0,0) , \tag{5.6}$$

we have

$$\Delta C_M = C_M(\epsilon, M) - C_M(\epsilon, 0)$$

$$= C_M(\epsilon, M) - A_\pm \, |\epsilon|^{-\alpha} - C_M(0,0) \tag{5.7}$$

$$\cong C_M(0, M) - C_M(0,0) - A_\pm \, |\epsilon|^{-\alpha} , \tag{5.8}$$

where the approximation has been made because the last term in the above equation varies so much more rapidly than $C_M(\epsilon, M)$ near $\epsilon = 0$. This allows us to consider

$$\Delta C_M(\epsilon, M) - \Delta C_M(0, M) = -A_\pm \, |\epsilon|^{-\alpha} \tag{5.9}$$

or

$$s'(x) - s'(0) = -A_\pm \, |x|^{-\alpha} \tag{5.10}$$

and thus

$$\bar{s}'(\bar{x}) - \bar{s}'(0) = -\bar{A}_\pm \, |\bar{x}|^{-\alpha} . \tag{5.11}$$

Equation (5.11) thus allows an estimate for $\bar{A}_\pm$ (cf. Table II).

B. $\alpha > 0$ (e.g., Ising model)

From Eq. (5.2) we infer that

$$C_M(\epsilon, 0)/M^{-\alpha/\beta} = A_\pm \, |x|^{-\alpha} \tag{5.12}$$

sufficiently near $x = 0$. Since this is the only divergence possible in $s'(x)$, we can write

$$s'(x) \cong -A_\pm \, |x|^{-\alpha} + \text{const} \tag{5.13}$$

sufficiently near $x = 0$. But then $xs''(x) = \alpha A_\pm \, |x|^{-\alpha}$ and Eq. (2.10) implies

$$s'(x) = \beta[h''(0)/\alpha] - A_\pm \, |x|^{-\alpha} . \tag{5.14}$$

We can then estimate $\bar{A}_\pm$ by the amplitude of the difference

$$\bar{s}'(\bar{x}) - \beta \bar{h}''(0)/\alpha = -\bar{A}_\pm \, |\bar{x}|^{-\alpha} . \tag{5.15}$$

Table II contains the results of our estimates.

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[8]S. Milošević and H. E. Stanley, Phys. Rev. B **6**, 986 (1972); Phys. Rev. B **6**, 1002 (1972). That the functions $h(x)$ should be given by different expressions in different domains of x presents no problems of analyticity, as the functional forms of Table I are merely *numerical* fits obtained by Padé approximants to series expansions. Therefore, the expressions for $h(x)$ in Table I are *not* the "true" closed-form scaled equations of state for the models indicated.

[9]Large-x scaled equation of state for Heisenberg spin $= \infty$ has been recalculated by D. Karo (unpublished); see also S. Milošević D. Karo, R. Krasnow, and H. E. Stanley, Invited Talk, 1973 Internation Congress on Magnetism, Moscow (unpublished).

[10]If $H(\epsilon, M)$ is a generalized homogeneous function (GHF) (cf. Refs. 2a and 2c) as Eq. (2.3) implies, then so is the derivative $(\partial H/\partial \epsilon)_M$. Therefore, by Eqs. (2.1) and (2.2), $(\partial \Delta S/\partial M)_\epsilon$ is a GHF. This in turn implies that ΔS is a GHF plus an unspecified function of ϵ alone, $f(\epsilon)$. But at $M = 0$, ΔS is by definition (2.2) also zero. Since a GHF is zero or infinity at the origin (and the entropy is finite), it follows that $f(\epsilon) = 0$, and therefore ΔS is entirely a GHF. This is the content of Eq. (2.5).

[11]If a system scales, a normalization of ϵ by a third constant cannot be used to make *any* other amplitude come out to unity. The reason is that if the system scales, then the relation between the three variables H, M, and ϵ reduces to a relation between only *two* scaled variables such as H/M^δ and $\epsilon/M^{1/\beta}$. Thus we really only have the freedom to normalize two variables.

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[14]See, e.g., Eq. (6.29) of Ref. 4.

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[16]Because the power q in $h(x)$ (cf. Table I) is different from unity, the right-hand side of Eq. (2.15) is zero at $x = -x_0$. This in turn implies that $C_H = C_M$ on the coexistence curve $H = 0$, so that the amplitudes $A_\pm$ can be defined with respect to C_M. (Note this is a different statement from the usual $C_{H=0} = C_{M=0}$ for $T < T_c$.)

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