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Low-Temperature Critical Exponents from High-Temperature Series: The Ising Model*

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First, a new method proposed by Baker and Rushbrooke is used to study the simple ferromagnetic Ising model *at* and *below* the Curie temperature. Of course, the properties of the Ising model are already well known, so that the main aim here is to assess the potential and reliability of the new method, since it has wide applicability to other models which have not been otherwise studied. Between 8 and 16 coefficients of exact *high-temperature* expansions for fixed values of the magnetization are derived for various two- and three-dimensional lattices. A Padé-approximant analysis of these expansions at the critical isotherm and magnetic phase boundary enables us to estimate the critical exponents β, γ', and δ, and plot the spontaneous magnetization. The results are in good agreement with previous calculations. Secondly, an analysis of the exact series expansions provides no support for the conjecture that the phase boundary is a line of essential singularities. However, the same expansions strongly suggest the existence of a "spinodal" curve, whose properties are in reasonable agreement with the predictions of various heuristic arguments (based essentially upon analyticity at the phase boundary and one-phase homogeneity in the critical region). Finally, structure and a mild extension of the proven analyticity of the free energy are used to show the $\Delta\leq\Delta', \gamma\leq\gamma'$.

1. INTRODUCTION AND SUMMARY

RECENTLY, a new method was proposed and used to study the Heisenberg model at and below its Curie temperature $T=T_C$.[1] The method which is applicable to a wide range of models for which the one-phase region is thought to be analytic is based upon exact high-temperature expansions for fixed values of the magnetization M. One aim of the present paper is to assess this method by applying it to the spin-$\frac{1}{2}$ Ising ferromagnet with nearest-neighbor interactions, since its behavior is fairly reliably known in advance.[2–4] In Sec. 2, between 8 and 16 coefficients are derived for various two- and three-dimensional lattices. Padé approximants[3,4] are used in Sec. 3 to determine the behavior of these expansions at the critical isotherm and magnetic phase boundary for values of M not too close to the critical value. Extrapolation to $M=0$ yields estimates for the critical exponents β, γ', and δ, in reasonably good agreement with the exact values (where available) and those derived from exact low-temperature or high-field expansions. In addition, spontaneous magnetization curves have been constructed for $1-T/T_C\gtrsim 2\times10^{-2}$ and are in satisfactory agreement with the exact results in two dimensions, and those calculated from exact low-temperature series in three dimensions.

More specifically, our estimates of the critical exponents lie close to the values[5] $\beta=\frac{5}{16}$, $\delta=5$, $\gamma'=1\frac{1}{4}$ in three dimensions, and $\beta=\frac{1}{8}$, $\delta=15$ in two dimensions. (The Padé approximants have not converged sufficiently for us to estimate γ' in two dimensions.) However, the confidence limits for the three-dimensional lattices are not sufficiently small for us to exclude the slightly larger values of $\delta=5\frac{1}{5}$ and $\gamma'=1\frac{5}{16}$, which have been proposed.[6,7]

We have also investigated (in Sec. 5) what conditions are imposed on the values of critical exponents by the known structure[8,9] of the Ising-model free energy and a slight conjectural extension of its known analyticity properties[10,11] in temperature and magnetic field. In particular, we conclude $\Delta\leq\Delta'$. We show that there follows a family of inequalities relating high-temperature exponents, low-temperature ones, and those on the critical isotherm. One further consequence of our analysis (which assumes the existence of the magnetization, susceptibility, etc., on the phase boundary) is that the phase boundary, at least near the critical point, is free of singularities except at the critical point itself.

It has been suggested[12] that the boundary separating the one- and two-phase regions is a line of essential singularities. We find in Sec. 4 that the Padé approximants to the high-temperature expansions at fixed M, and also the high-field expansions at fixed T, show no sign of them. However, both types of expansion appear to have singularities whose nature and locations are

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consistent with the existence of a "spinodal" curve,[13] i.e., a curve lying inside the two-phase region along which the susceptibility is infinite. It should perhaps be emphasized that analytic continuation into the two-phase region and the existence of a spinodal curve do not necessarily require analyticity along the phase boundary. Even if the phase boundary were non-analytic, one could merely consider, say, the real part of the complex susceptibility. (The imaginary part "grows" from the phase boundary.) It would be nice to be able to identify analytic continuation with metastability and regard the spinodal curve as the limit of metastability. However, no such identification is known.[13]

We also show in Sec. 4 that if one is prepared to assume the existence of a Taylor-series expansion in powers of the magnetic field H about the phase boundary, then the asymptotic forms of the coefficients determined by Essam and Hunter[14] lead to a spinodal curve whose location agrees (to within the accuracy limits of our calculations) with that obtained from the exact high-temperature and high-field expansions. This provides further evidence for analyticity all along the phase boundary. In addition, it appears that the asymptotic shape of the spinodal curve and phase boundary are described by the same exponent β, although strict asymptotic tangency (equality of critical exponents *and* amplitudes) is ruled out. Similar arguments starting from the usual homogeneity properties[15,16] or the magnetic equation of state[17] are also outlined in this section.

2. SERIES EXPANSIONS

In the thermodynamic limit, the configurational partition function for a regular lattice of coordination number q has the high-temperature expansion[2]

$$\ln\Lambda(\tau,v)=\ln[2(1+\tau)^{-1}(1+v)^{-q/2}]+\sum_{n=1}^{\infty}\varphi_n(\tau)v^n. \quad (2.1)$$

Here

$$\varphi_n(\tau)=\sum_{k=0}^{n}t_k(n)\tau^{2k} \quad (2.2)$$

is a polynomial in τ^2 of degree n, and v and τ are related to the temperature T and magnetic field H by

$$v=\tanh(J/k_BT), \quad \tau=\tanh(mH/k_BT). \quad (2.3)$$

[In (2.3), J is the exchange integral, m is the magnetic moment per spin, and k_B is Boltzmann's constant.] The coefficient $t_k(n)$ arises from configurations of n lines having $2k$ "odd" vertices. (An "odd" vertex is one upon which an odd number of lines are incident.) The φ polynomials have been calculated by Sykes and co-workers (unpublished work) for the square (sq), triangular (t), diamond (d), simple cubic (sc), body-centered cubic (bcc), and face-centered cubic (fcc) lattices through v^N, where $N=15$, 10, 16, 12, 12, and 8, respectively.

From these polynomials we have calculated the series

$$\tau(M,v)=M\sum_{n=0}^{\infty}\psi_n(M)v^n, \quad \psi_0=1 \quad (2.4)$$

through the same order in v. Here, M is the magnetization and

$$\psi_n(M)=\sum_{k=0}^{n}m_k(n)M^{2k}, \quad n=1,2,\ldots \quad (2.5)$$

is a polynomial in M^2 of degree n. As mentioned in Sec. 1, (2.4) is fundamental to our subsequent analysis. Accordingly, we have listed the ψ polynomials in the Appendix.

The ψ polynomials were derived from the φ polynomials by following the simple steps outlined below. First, one calculates the magnetization

$$M=1+(1-\tau^2)[\partial(\ln\Lambda)/\partial\tau]_v. \quad (2.6)$$

Substituting (2.1) and (2.2) into (2.6) gives an expansion for M/τ in powers of v through v^N, where the nth coefficient is a polynomial in τ^2 of degree n. This series is easily rearranged into the form

$$M(v,\tau)=\sum_{n=0}^{\infty}g_n(v)\tau^{2n+1}, \quad (2.7)$$

where $g_n(v)$ is a power series in v whose leading nonzero coefficient is of order v^n and which is known through order v^N. Reverting (2.7) yields

$$\tau(v,M)=\sum_{n=0}^{\infty}h_n(v)M^{2n+1}, \quad (2.8)$$

where $h_n(v)$ is another series of precisely the same form as $g_n(v)$. [This double-series reversion is readily accomplished by an iterative procedure. The iteration procedure consists of starting with $\tau=M/g_0(v)$ and substituting this series in M into all the known terms of (2.7) except the linear term which is used to solve for the next iterate. The accuracy increases by one order of M^2 per iteration and rapidly yields the reverted series to the required order. For the Heisenberg model[1] the reversion was accomplished by the direct use of Lagrange's formula, which is easier to the order required there but harder for the order required here.] Finally, rearrangement of (2.8) yields the desired form (2.4). These manipulations were performed, for convenience and reliability, on an electronic computer. A

[13] See B. Chu, F. J. Schoenes, and M. E. Fisher (unpublished), and references therein, where our "spinodal" curve is referred to as a "pseudo-spinodal" curve. For a more detailed discussion than that presented below of the background and controversy surrounding the spinodal curve, the reader is referred to this paper.
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simple but effective check on the calculations is provided by noticing that

$$\psi_n(1)=0 \quad (n=1,2,3,\ldots)$$
$$=1 \quad (n=0), \tag{2.9}$$

since if $M=1$, then $\tau=1$ for all v.

The "judicious" choice of τ, rather than $L\equiv mH/k_BT$, as the magnetic field variable should be noted. Expanding τ in powers of L and substituting into (2.7) gives an expansion for $M(v,L)$ of precisely the same form as (2.7) but with L replacing τ. However, the leading term of $g_n(v)$ is now of order v^0. As before, reversion followed by rearrangement yields an expansion [this time for $L(M,v)$] of the form (2.4) but with $\psi_n(M)$ a power series in M^2 rather than a polynomial in M^2. Consequently, it is no longer possible to fix M and evaluate the coefficients exactly. On the other hand, the choice of temperature variable is not so crucial. As can be seen from (2.4), it makes no difference whether one uses v or J/k_BT; in both cases, the coefficients are polynomials in M^2.

Our subsequent analysis is based upon expansions in powers of v for fixed values of M of the functions

$$\tau(M,v), \quad [\partial(\ln\tau)/\partial \ln M]_v, \quad [\partial(\ln\tau)/\partial v]_M. \tag{2.10}$$

The expansions have been computed from the basic series (2.4) in the following way: Suppose $M=\mathfrak{M}$ is the fixed value of M; then

$$\tau(M,v)|_{\mathfrak{M}}\equiv\tau_{\mathfrak{M}}(v)=\sum_{n=0}^{\infty}\mathfrak{M}\psi_n(\mathfrak{M})v^n, \tag{2.11}$$

$$[\partial(\ln\tau)/\partial \ln M]_v| \equiv\tilde{\delta}_{\mathfrak{M}}(v)=1+\sum_{n=1}^{\infty}\mathfrak{M}\psi_n'(\mathfrak{M})v^n/\sum_{n=0}^{\infty}\psi_n(\mathfrak{M})v^n, \tag{2.12}$$

and

$$[\partial(\ln\tau)/\partial v]_M|_{\mathfrak{M}}=\left(\frac{\partial \ln(\tau/M)}{\partial v}\right)_M\Big|_{\mathfrak{M}}=(d/dv)[\ln\tau_{\mathfrak{M}}(v)]. \tag{2.13}$$

The prime in (2.12) means the polynomials $\psi_n(M)$ are differentiated with respect to M before setting $M=\mathfrak{M}$.

Finally, we will use the following values of v_c:

$$v_c(\text{fcc})=0.10175, \quad v_c(\text{d})=0.35383,$$
$$v_c(\text{bcc})=0.15614, \quad v_c(\text{t})=0.2679492\cdots, \tag{2.14}$$
$$v_c(\text{sc})=0.21814, \quad v_c(\text{sq})=0.4142136\cdots.$$

In two dimensions, the values[4] are exact. The estimates for the three-dimensional lattices are from Essam and Hunter,[14] and are probably correct to 3 parts in 10^4.

3. SERIES ANALYSIS

The v expansions (2.11)–(2.13) have been analyzed by the Padé-approximant technique for fixed values of M ranging typically from 0.975 down to about 0.6 in three dimensions and about 0.8 in two dimensions. The expansions are too short to give good convergence properties for smaller values of M. However, even for such relatively large values of M, one is already chose to the critical point. For example, on the phase boundary of a two-dimensional lattice the usual asymptotic form shows that $M=0.8$ corresponds to $1-T/T_C\simeq4\times10^{-2}$. As will be shown in Sec. 4, the spinodal curve in this region lies very closely behind the phase boundary, which fact contributes significantly to the relatively slow convergence for smaller values of M.

Detailed results will only be presented for the bcc and sq lattices. (The results for different lattices of a given dimension are very similar to one another.)

Exponent δ

Along the critical isotherm we have

$$\tau\approx DM^\delta \quad (v=v_c,\ M\to 0+) \tag{3.1}$$

to leading asymptotic order, so that

$$\left(\frac{\partial \ln\tau}{\partial \ln M}\right)_v\Big|_{v=v_c,M=0+}=\delta, \tag{3.2}$$

where the order of the subscripts prescribes setting $v=v_c$ before allowing M to approach zero.

For $M\neq0$, we have

$$\left(\frac{\partial \ln\tau}{\partial \ln M}\right)_v\Big|_{v_c,M}=\delta^*(M), \tag{3.3}$$

where we have used an asterisk to denote a quantity which approaches a critical exponent as one of the independent variables approaches its critical value, the other having been fixed at its critical value. Evidently,

$$\delta^*(M)\to\delta \quad \text{as} \quad M\to0+, \tag{3.4}$$

but the manner of approach is determined by the (unknown) higher-order asymptotic behavior of (3.1).

By forming Padé approximants to the $\tilde{\delta}_M(v)$ series (2.12) and evaluating these at $v=v_c$, we have estimated $[\partial(\ln\tau)/\partial(\ln M)]_v|_{M,v_c}$, where the order of the subscripts is the reverse of that in (3.3). Of course, at the critical point the order is crucial, for according to (2.12), $[\partial(\ln\tau)/\partial(\ln M)]_v|_{M=0,v_c}\equiv1$, whereas by (3.4) $[\partial(\ln\tau)/\partial(\ln M)]_v|_{v_c,M=0}=\delta$. Away from the critical point, however, the order of evaluation should not be important, and so ideally we expect

$$[\partial(\ln\tau)/\partial(\ln M)]_v|_{M,v_c}=\delta^*(M), \quad M>0$$
$$\equiv1, \quad M=0. \tag{3.5}$$

The approximants to the $\tilde{\delta}_M(v)$ series are also evaluated at a series of points between $v=0$ and v_c, so by comparing the values of approximants of different orders at corresponding points one may assess how well they have converged in the neighborhood of v_c. Then, from the higher-order approximants, $\delta^*(M)$ is estimated together with reasonable confidence limits.

In practice, the following behavior is found. For values of M larger than or equal to about 0.65 in three dimensions and 0.9 in two dimensions, the approximants converge rapidly to $\delta^*(M)$. Then there is a second region, for which values of M the approximants appear moderately converged, followed by a third region (for small values of M), where once again convergence is apparently very good. In the second and third regions, $\delta^*(M)$ appears to be decreasing smoothly to unity. Such behavior must inevitably result from an attempt to represent a function of the form (3.5) by Padé approximants based upon a relatively few series coefficients. In actual fact, true convergence has been achieved only for values of M quite far from the critical point (that is, in the first region).

Converged values of δ^* for fixed M are listed in the first two columns of Tables I and II for the bcc and sq lattices, respectively. To estimate δ, one must extrapolate from these values right down to $M=0$. Fortunately, there is a more suitable extrapolation variable than M. To see this, let us estimate, with the aid of (3.1), the value of τ on the critical isotherm corresponding to the smallest value of M for which δ^* has converged. For the bcc lattice[5] ($\delta\simeq5$, $D\simeq0.35$), $\tau\simeq0.04$ when $M=0.65$, while for the sq lattice[5] ($\delta\simeq15$, $D\simeq0.43$), $\tau\simeq0.09$ when $M=0.9$. Consequently, if δ^* were plotted versus τ (rather than M), the range of extrapolation would be considerably reduced.

To calculate the value of τ for a given value of M on the critical isotherm, the coefficients of the $\tau_M(v)$ series (2.11) are computed and Padé approximants are formed and evaluated at a series of points from $v=0$ through $v=v_c$. From the values at v_c the desired value of τ is estimated, while values at intermediate points enable one to assess convergence, as before. Converged values of τ obtained in this way are listed in the third columns of Tables I and II.

In Fig. 1 (curve a), values of δ^* are plotted versus τ. For $\tau\gtrsim0.23$ the curve is accurately linear; in fact, the error bars do not preclude this linearity continuing right down to $\tau=0$. If it does continue, then $\delta\simeq5.4$, which is a little larger than expected.[5,6] It is to be noted, however, that the last four points do have a definite downward trend below this line. We have shown in Fig. 1 what we consider to be reasonable upper and lower bounds on δ^* for $\tau\lesssim0.23$. We conclude that

$$5.0\lesssim\delta\lesssim5.4 \quad (\text{bcc}). \tag{3.6}$$

TABLE I. Corresponding values of M, δ^*, and τ along the critical isotherm for the bcc lattice.

M	δ^*	τ
0.975	10.650±0.001	0.7480
0.95	9.453±0.001	0.5767
0.90	7.947±0.001	0.3618
0.85	7.051±0.002	0.2362
0.80	6.48 ±0.05	0.1570
0.75	6.07 ±0.06	0.1048
0.70	5.8 ±0.25	0.0697±0.0001
0.65	5.55 ±0.2	0.0457±0.0001
0.60		0.0294±0.0002
0.55		0.0183±0.0002
0.50		0.012 ±0.0025

TABLE II. Corresponding values of M, δ^*, and τ along the critical isotherm for the sq lattice.

M	δ^*	τ
0.975	24.340±0.003	0.4887±0.0001
0.96	21.66 ±0.02	0.3426±0.0001
0.95	20.41 ±0.07	0.2749±0.0002
0.94	19.44 ±0.09	0.2227±0.0002
0.92	18.0 ±0.15	0.1488±0.0001
0.90	17.05 ±0.08	0.1010±0.0003
0.85		0.040 ±0.004
0.80		0.015 ±0.003

The plots for the other three-dimensional lattices strengthen the above conclusions. For example, for the d and sc lattices, the linear portion for large τ extrapolates to around 5.7 at $\tau=0$, which value is definitely too large to be identified with δ. As before, the last few values of δ^* dip down indictating a value of δ somewhere in a range roughly as wide as that in (3.6) and centered around

$$5.2 \ (\text{sc}), \quad 5.0 \ (\text{d, fcc}). \tag{3.7}$$

The values in (3.6) and (3.7) are in good agreement with previous estimates[5,6] of δ for three-dimensional lattices.

The corresponding plot for the sq lattices is given in Fig. 2 (curve a). Its qualitative behavior is identical to that observed for the three-dimensional lattices. The plot is accurately linear for $\tau\gtrsim0.2$, extrapolating to about 15.3 at $\tau=0$. However, the actual estimates of δ^* for $\tau\lesssim0.2$ decrease slightly more rapidly and appear to be approaching what is almost certainly the exact value $\delta=15$. Conversely, one may infer

$$\delta=15.0\pm0.3 \ (\text{sq}), \tag{3.8}$$

in excellent agreement with previous estimates[5,6] of δ for a two-dimensional lattice. The corresponding plot for the t lattice is consistent with the same behavior and confirms (3.8) but with somewhat lower accuracy.

Although the extrapolation procedure just discussed appears to work reasonably well, we could make much better use of the points closest to the critical point if only the behavior of $\delta^*(\tau)$ for small τ were known. At the end of this subsection we will present arguments which suggest that

$$\delta^*=\delta+c\tau^{1-1/\delta}, \quad v=v_c, \ \tau\to0+ \tag{3.9}$$

where c is a positive constant. According to (3.9), the curvature exhibited by curve a in Figs. 1 and 2 for small τ should be removed by plotting δ^* versus $\tau^{1-1/\delta}$. [Of course, in the region (τ large) where δ^* increases linearly with τ, the plots versus $\tau^{1-1/\delta}$ will increase faster than linearly.] Self-consistency requires that after assuming

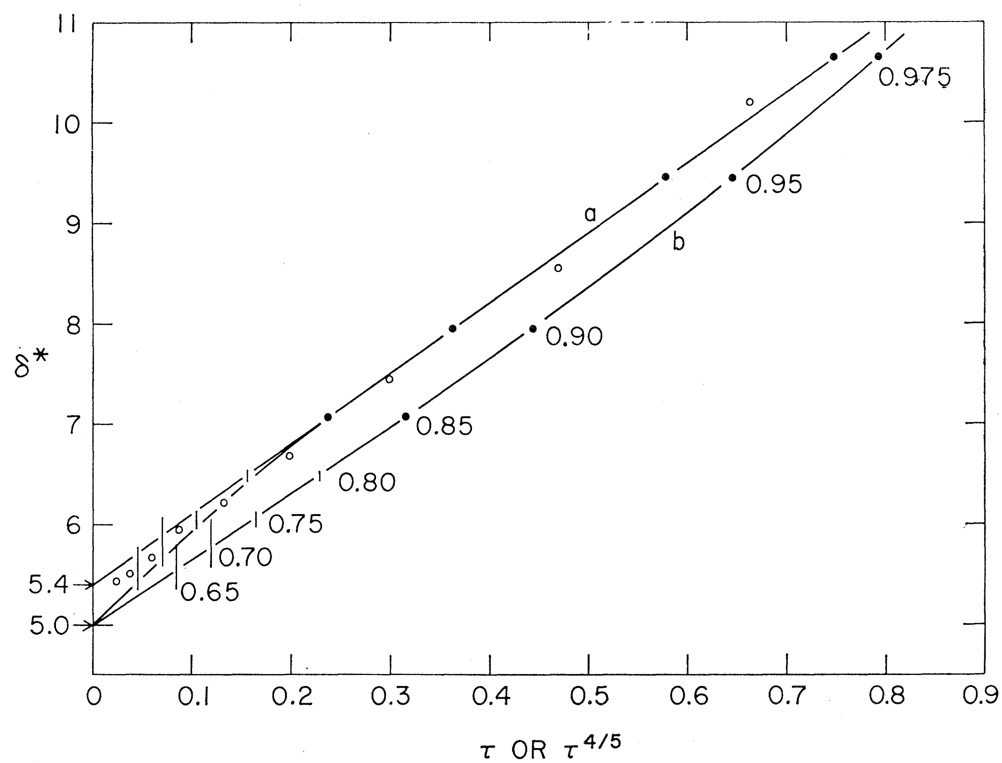

FIG. 1. Plot of δ^* versus τ (curve a), and versus $\tau^{1-1/\delta}$ (curve b) assuming $\delta=5$, for the bcc lattice. Each point is accompanied by the corresponding value of M. The open circles are approximations to curve a obtained by estimating the slope of curve a, Fig. 4, at various values of τ.

a value for δ, the δ^*-versus-$\tau^{1-1/\delta}$ plots must approach the *assumed* value of δ.

When δ^* is plotted versus $\tau^{4/5}$ for the bcc lattice (see Fig. 1, curve b), the central values are accurately linearly for $\tau\lesssim 0.23$ and extrapolate to $\delta=5.0$ as they must for self-consistency. On the other hand, a plot of δ^* versus $\tau^{4.2/5.2}$ is almost indistinguishable from curve b, so that the central values of δ^* still extrapolate to around 5.0 instead of 5.2. Thus, for the bcc (and fcc) lattice, $\delta=5.0$ is definitely the preferred value. However, taking account of the uncertainties in the values of δ^* closest to $\tau=0$, we finally estimate

$$\delta=5.0\pm0.2 \quad (\text{bcc, fcc}). \qquad (3.10)$$

For the sc lattice, a slightly larger value is indicated, namely,

$$\delta=5.2\pm0.2 \quad (\text{sc}), \qquad (3.11)$$

while the data for the d lattice are consistent with either (3.10) or (3.11), preferring neither one above the other.

Similarly, in two dimensions, plotting δ^* against $\tau^{14/15}$ (see Fig. 2, curve b, for the sq lattice) has the expected effect of straightening out the δ^*-versus-τ curve, the new plot extrapolating to $\delta=15.0$ as it must for self-consistency.

Instead of plotting δ^* against $\tau^{1-1/\delta}$, one could equivalently plot δ^* against $M^{\delta-1}$, since by (3.9) and (3.1)

$$\delta^*=\delta+cD^{1-1/\delta}M^{\delta-1}, \quad v=v_c,\ M\to 0+. \qquad (3.12)$$

In Fig. 3, for example, δ^* is plotted versus M^4 for the bcc lattice, thus confirming the earlier estimate (3.10) but with lower accuracy. In theory, the plots versus $M^{\delta-1}$ are preferable to those versus $\tau^{1-1/\delta}$, in that the values of M are exact and, therefore, uncertainties enter only through δ^*. However, the uncertainties in τ are very small (see Tables I and II), and in addition the linearity versus $\tau^{1-1/\delta}$ is found to extend over a greater range of M values than does the linearity versus $M^{\delta-1}$. In practice, therefore, the plots of δ^* versus $\tau^{1-1/\delta}$ seem preferable to those versus $M^{\delta-1}$.

We have studied the exponent δ in one other way. According to (3.1), a plot of τ versus M on log-log graph paper should be asymptotically linear for small values of M with slope δ. Using the estimates in Table I for the bcc lattice, we obtain the plot shown in Fig. 4, curve a. Comparing curve a with curve b, which has been constructed with slope 5, one sees that the slope of curve a is indeed approaching a value consistent with $\delta=5$. To analyze curve a more carefully we have calculated the slopes of successive linear segments connecting pairs of adjacent points. The slope associated with any particular pair of points should approximately equal δ^* at the value of τ which is the average

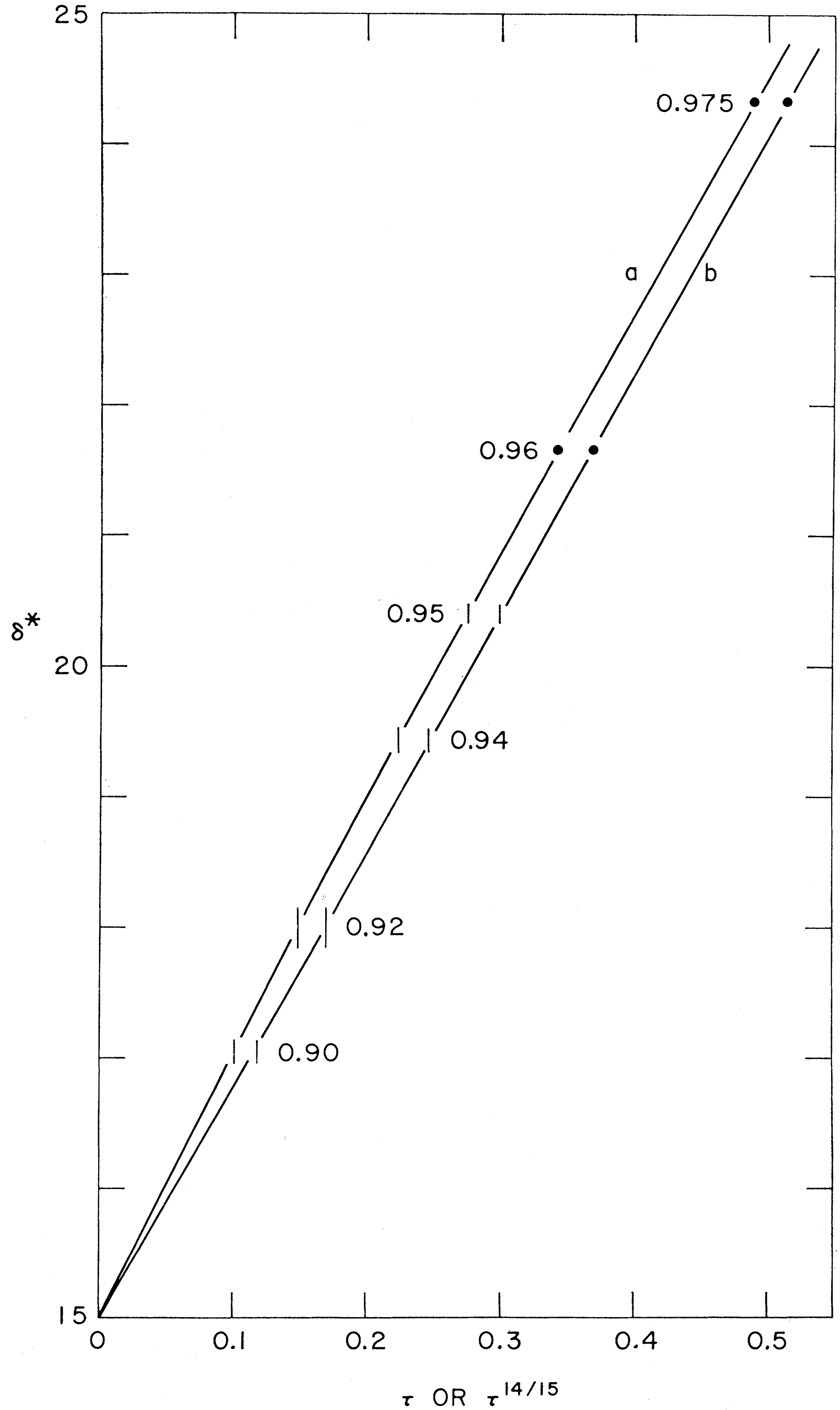

FIG. 2. Plot of δ^* versus τ (curve a), and versus $\tau^{1-1/\delta}$ (curve b) assuming $\delta=15$, for the sq lattice. Each point is accompanied by the corresponding value of M.

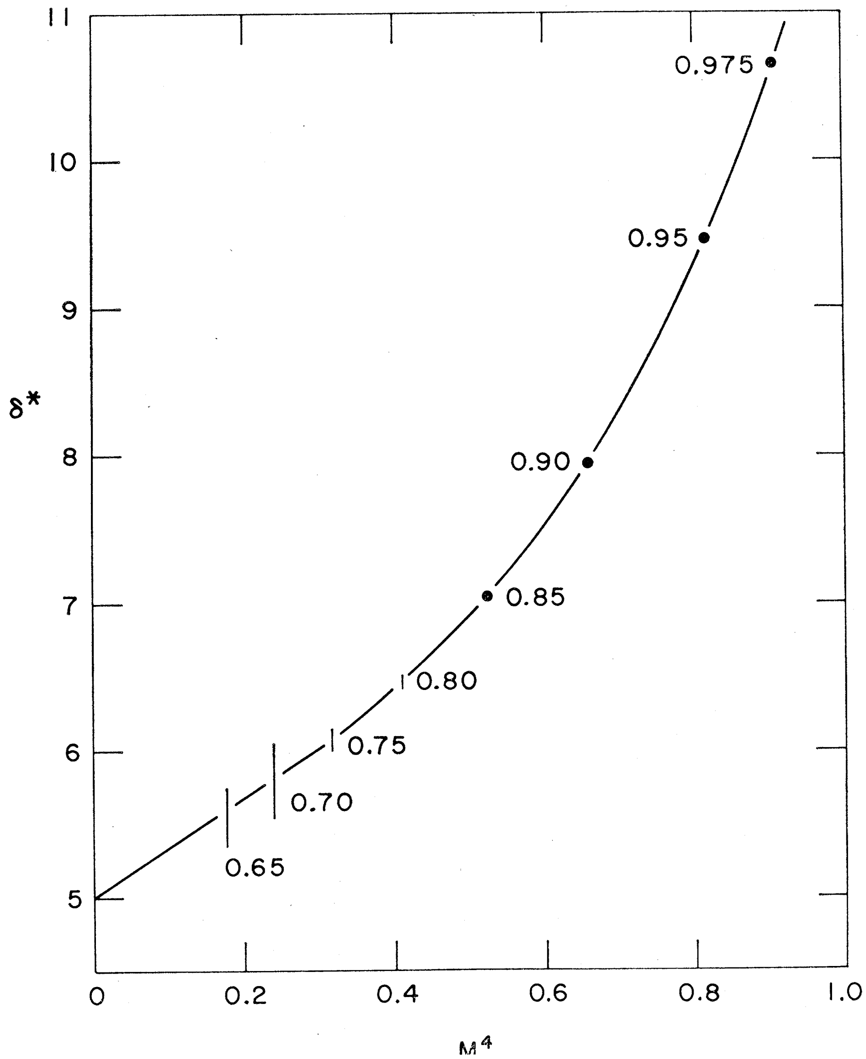

FIG. 3. Plot of δ^* versus $M^{\delta-1}$ assuming $\delta=5$ for the bcc lattice. Each point is accompanied by the corresponding value of M.

of the τ values at each end point. These approximations to δ^* are plotted versus τ in Fig. 1 (see the open circles), and are seen to be in excellent agreement with the previous results. Comparable results are obtained for the other two- and three-dimensional lattices.

To conclude this section let us return to the assumption (3.9), which appears to work so well, and see if there is any evidence for it.

First, we note that it is valid in the mean-field approximation with

$$\delta=3, \quad c=(6/5)\times 3^{2/3}. \tag{3.13}$$

Second, as mentioned after (3.4), it implies the leading correction term to (3.1). Specifically, we find

$$\tau\approx DM^{\delta}(1+dM^{\delta-1}+\cdots), \tag{3.14}$$

or, equivalently,

$$M\approx D^{-1/\delta}\tau^{1/\delta}(1-e\tau^{1-1/\delta}+\cdots), \tag{3.15}$$

where d and e are positive constants. Equation (3.15) may be compared with the asymptotic forms suggested previously by Gaunt,[5] namely,

$$M\approx D^{-1/\delta}\tau^{1/\delta}(1-e'\tau+\cdots) \tag{3.16}$$

in two dimensions, and

$$M\approx D^{-1/\delta}\tau^{1/\delta}[1-e''\tau|\ln\tau|+\cdots] \tag{3.17}$$

in three dimensions, where e' and e'' are constants. Obviously, we do not have precise analytic agreement, but from a numerical point of view (3.16) will look very much like (3.15) when $\delta=15$, provided τ is not *very* close to zero, which it is not. Similarly, for the same region of τ, it is well known[6] that $|\ln\tau|$ appears to diverge like $\tau^{-\lambda}$, where $\lambda=0.2$–0.3, so that in three dimensions the $\tau^{4/5}$ term in (3.15) would appear deceptively like the $\tau|\ln\tau|$ term in (3.17). We conclude that if (3.15) is the correct behavior, there is no difficulty in understanding the previous results (3.16) and (3.17).

Third, we may examine the exact integral representa-

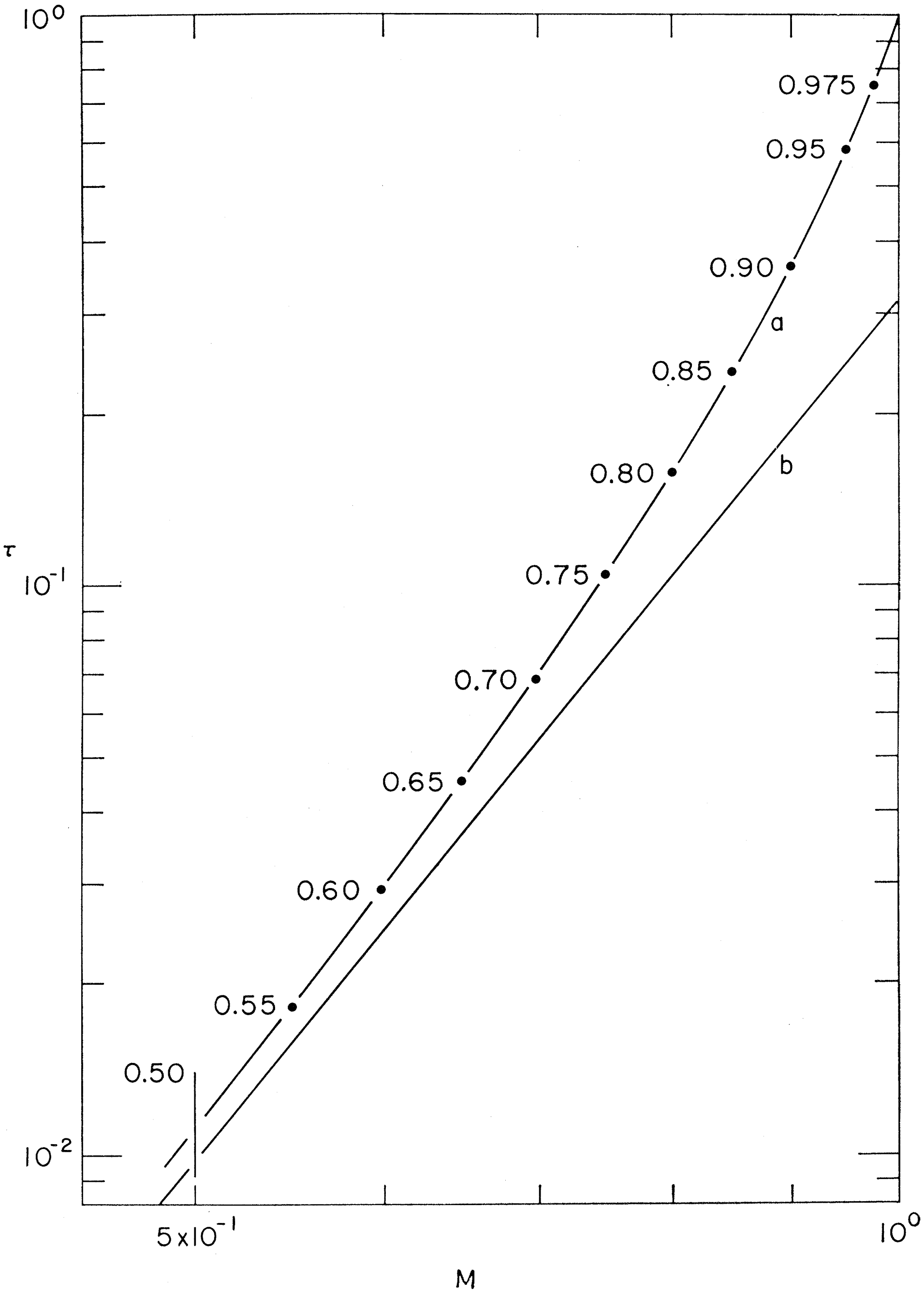

FIG. 4. Log-log plot (curve a) of τ versus M along the critical isotherm for the bcc lattice. Each point is accompanied by the corresponding value of M. The straight line b has slope 5.

tion due to Baker,[9] namely,

$$M=\tau+\tau(1-\tau^2)\int_0^\infty \frac{d\psi(\omega)}{1+\tau^2\omega}, \tag{3.18}$$

where $d\psi\geq 0$ [see also (5.7)]. To get (3.1), the leading asymptotic behavior of the integral must be $D^{-1/\delta}\times\tau^{-(1-1/\delta)}$. In view of the first term on the right-hand side of (3.18), it would not be surprising for a term of the same order to come out of the second term on the right-hand side of (3.18). This would mean the asymptotic behavior of the integral contains a constant term $-k$, say, so that

$$M\approx D^{-1/\delta}\tau^{1/\delta}-(k-1)\tau, \tag{3.19}$$

which is identical with the expected form (3.15) provided $k>1$. (If $k<1$, The constant e has the wrong sign.) Of course, there could be a term in the asymptotic form of the integral whose order lies between the constant term and the $\tau^{-(1-1/\delta)}$ term; for example,

$\tau^{-\lambda}$, where $0<\lambda<1-1/\delta$. However, this would lead to

$$\delta^*=\delta+c\tau^{(1-1/\delta)-\lambda}, \tag{3.20}$$

and a smaller exponent than $1-1/\delta$ in (3.9) would appear ruled out by the numerical evidence (see curve b of Figs. 1 and 2, for example). To get a larger exponent than $1-1/\delta$, on the other hand, would require $k=1$, and the cancellation of terms which this implies would also seem rather unlikely.

Magnetic Phase Boundary

The value of $v=v_{\rm pb}(M)$ on the magnetic phase boundary may be determined as a function of the magnetization M from any of the three expansions (2.11)–(2.13). To see this, let us consider the behavior of each function in the vicinity of the phase boundary. For $v>v_c$ and $\tau\gtrsim 0$, we will assume that

$$M(v,\tau)\simeq M_0(v)+M_1(v)\tau^{\iota}. \tag{3.21}$$

$M_0(v)$ is the phase boundary or spontaneous magnetization. For the Ising model there is little doubt that the new exponent ι equals unity, so that $M_1(v)$ is the reduced zero-field susceptibility below T_C. However, since ι is unknown for most models, we prefer to use the general expression and to try and estimate its value from the series expansions. (For certain models, notably the spherical model and the isotropic Heisenberg model in the noninteracting spin-wave approximation, it is known that $\iota=\frac{1}{2}$.[18]) Let us rewrite (3.21) as

$$\tau\simeq\left(\frac{M-M_0(v)}{M_1(v)}\right)^{\iota-1}, \tag{3.22}$$

and regard M and v as the independent variables. For fixed M, the phase boundary ($\tau=0$) is encountered when v has increased to the value $v_{\rm pb}$, at which point $M=M_0(v_{\rm pb})$. Expanding $M_0(v)$ and $M_1(v)$ about $v_{\rm pb}$ yields

$$M_0(v)=M+(dM_0/dv)|_{v_{\rm pb}}(v-v_{\rm pb})+O((v-v_{\rm pb})^2) \tag{3.23}$$

and

$$M_1(v)=M_1(v_{\rm pb})+O(v-v_{\rm pb}). \tag{3.24}$$

Substituting (3.23) and (3.24) into (3.22) gives

$$\tau_M(v)\simeq T(v_{\rm pb}-v)^{1/\iota}, \tag{3.25}$$

where the amplitude T is given by

$$T^{\iota}=(dM_0/dv)|_{v_{\rm pb}}/M_1(v_{\rm pb}). \tag{3.26}$$

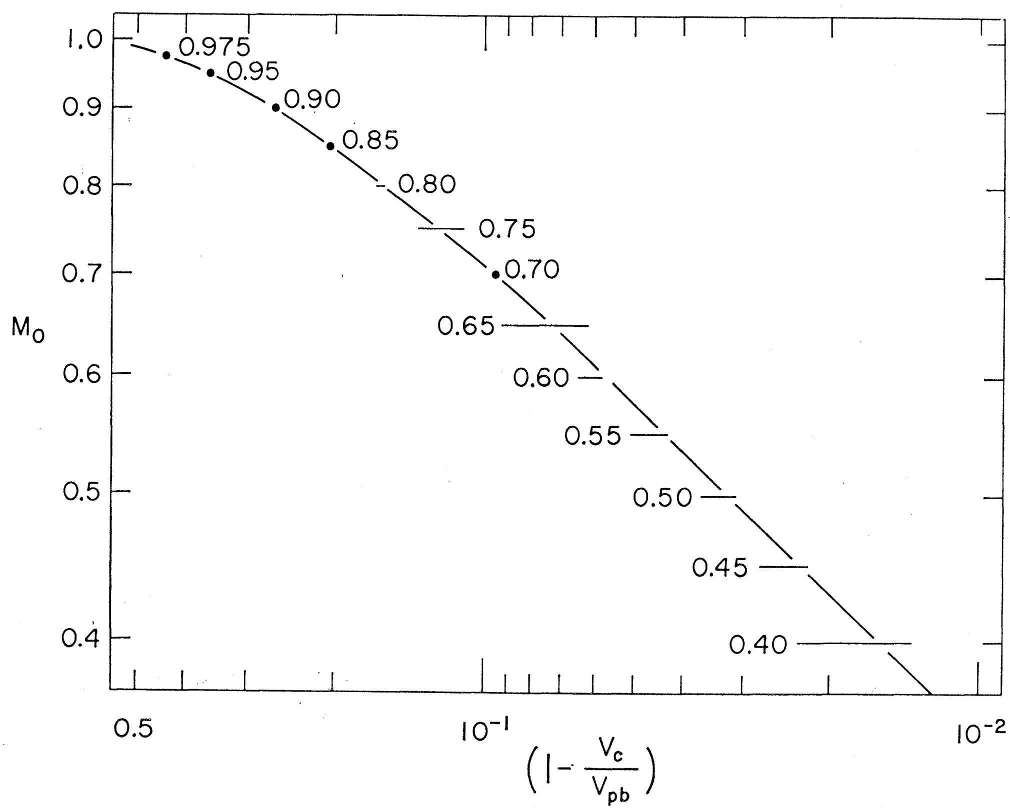

FIG. 5. Log-log plot of M_0 versus $(1-v_c/v_{\rm pb})$ along the phase boundary for the bcc lattice. Each point is accompanied by the corresponding value of M. The broken solid curve is calculated from the exact low-temperature series, assuming T_c and β are known.

[18] M. E. Fisher, J. Appl. Phys. 38, 981 (1967).

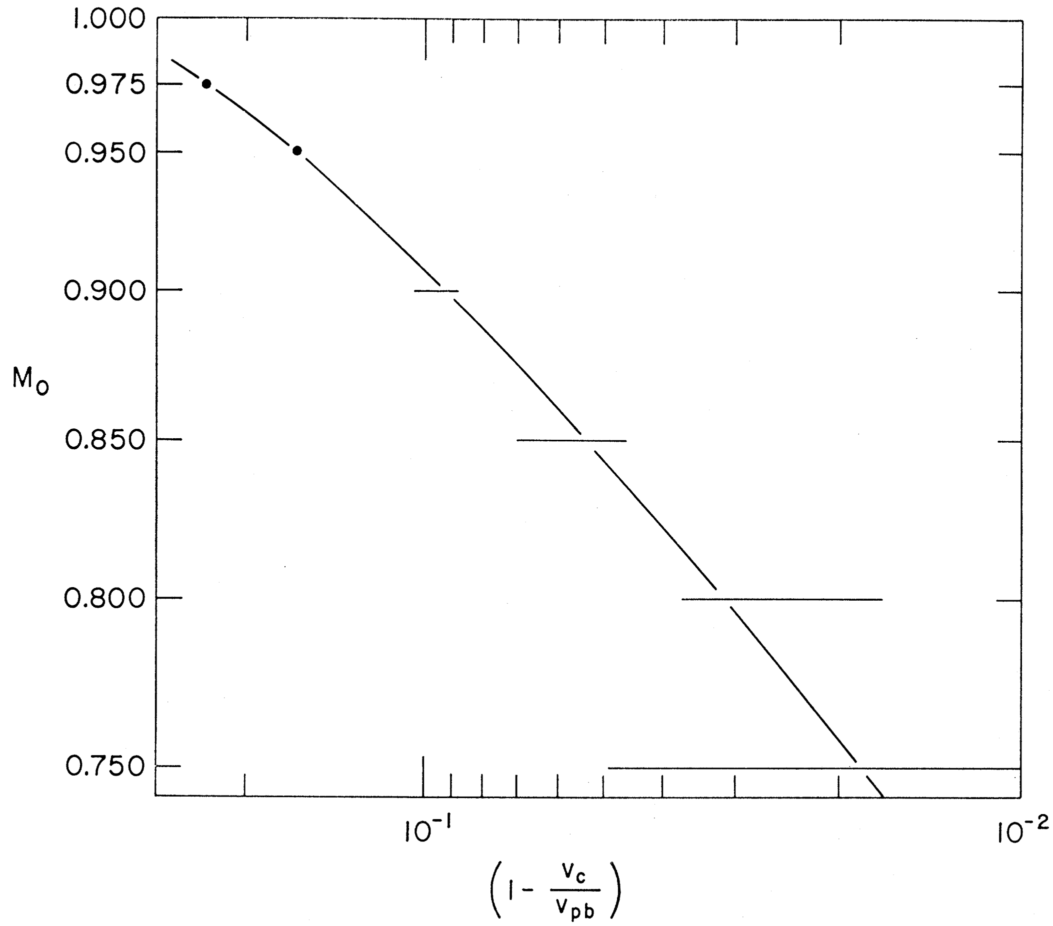

FIG. 6. Log-log plot of M_0 versus $(1-v_c/v_{\rm pb})$ along the phase boundary for the sq lattice. The broken solid curve is calculated from the exact solution.

Hence, from (3.25)

$$(d/dv)\ \ln\ \tau_M(v)\approx \iota^{-1}/(v-v_{\rm pb}). \qquad (3.27)$$

Returning to (3.21), one easily verifies

$$\tilde{\delta}_M(v)\simeq \iota^{-1}M[M-M_0(v)]^{-1},$$

and substitution from (3.23) gives

$$\tilde{\delta}_M(v)\approx D/(v-v_{\rm pb}), \qquad (3.28)$$

where

$$D^{-1}=-\iota[d(\ln M_0)/dv]|_{v_{\rm pb}}. \qquad (3.29)$$

It should be noted that (3.25), (3.27), and (3.28) are valid only if $M\neq 0$. When $M=0$, $\tilde{\delta}_{M=0}(v)\equiv 1$ according to (3.5), while from (2.11) it follows that

$$\tau_{M=0}(v)\equiv 0 \qquad (3.30)$$

and

$$(\tau/M)|_{M=0}\equiv \chi(v)^{-1}, \qquad (3.31)$$

where $\chi(v)$ is the reduced zero-field susceptibility above T_C. Using the usual asymptotic form[4] for $\chi(v)$, one finds

$$(d/dv)\ \ln\ \tau_M(v)\approx \gamma/(v-v_c),\quad M=0 \qquad (3.32)$$

in place of (3.27).

We see from (3.27) and (3.28) that $v_{\rm pb}(M)$ may be estimated by forming Padé approximants to either the (d/dv) ln $\tau_M(v)$ or the $\tilde{\delta}_M(v)$ series and picking out the appropriate zero of the denominator. Alternatively, if we assume $\iota=1$ in (3.25), an estimate of $v_{\rm pb}(M)$ may be obtained from the zeros of the numerators of the Padé approximants to the $\tau_M(v)$ series. In general, the best-converged approximants for large M are those formed from either the $\tau_M(v)$ or the $\tilde{\delta}_M(v)$ series. For smaller values of M, the (d/dv) ln $\tau_M(v)$ series tend to be the best, but if M is smaller than 0.55 (fcc), 0.40 (bcc, sc), 0.50 (d), 0.85 (t), and 0.75 (sq), none of the series has converged adequately. By studying all three methods, we have obtained the "best possible estimates" of $v_{\rm pb}$ for various values of $M=M_0$ on the phase boundary. Best estimates of $1-v_c/v_{\rm pb}$ are plotted versus M_0 on a log-log scale in Figs. 5 and 6 for the bcc and sq lattices, respectively. The broken solid curve in Fig. 6 is the phase boundary as calculated from the exact solution[19] for the sq lattice [see (3.35) and (3.39)]. The corresponding curve in Fig. 5 was

[19] C. N. Yang, Phys. Rev. **85**, 808 (1952).

calculated from the exact low-temperature series[20] for the spontaneous magnetization (by assuming $V_c=0.15614$ and $\beta=\frac{5}{16}$). We conclude that the high-temperature series are reasonably successful in locating the magnetic phase boundary.

Exponent ι

The exponent ι is defined in (3.21), and for the Ising model $\iota=1$ is almost certainly correct. According to (3.27), Padé approximants to the $(d/dv)\ln\tau_M(v)$ series should exhibit simple poles at $v_{\rm pb}$ with residues ι^{-1}, provided $M\neq 0$. By (3.31) the residue equals γ when $M=0$. Since we only have a finite number of coefficients, we expect the residues to appear reasonably converged for all M and increase smoothly from around 1 to the value γ as M decreases to zero. The results in Table III for the bcc and sq lattices show that this is precisely what happens in practice. Only for M greater than 0.85 (bcc) and 0.975 (sq) do the estimated error bars permit $\iota=1$ independent of M. For smaller values of M (except $M=0$) the rate of convergence is deceptively slow, so that the error bars estimated from the last few approximants are totally inadequate.

If the value of ι were unknown, the above results would be rather inconclusive. However, suppose there was evidence—as there is for the Heisenberg model—that 1 or $\frac{1}{2}$ was the most likely value. Then, the fact that the residue seems to *decrease* from γ to around 1 as M increases, rather than *increase* from γ to around 2, would point to $\iota=1$ in preference to $\frac{1}{2}$.

Exponent β

By definition, the plots of $\ln M_0$ versus $\ln(1-v_c/v_{\rm pb})$ should have an asymptotic slope of β. The maximum and minimum slopes allowed by the error bars on the last few points in Figs. 5 and 6 indicate

$$0.26\lesssim\beta\lesssim 0.40 \quad (\text{bcc}) \tag{3.33}$$

TABLE III. Estimates of ι^{-1} for various values of M. When $M=0$, ι^{-1} is identically equal to γ.

M	ι^{-1} (bcc)	ι^{-1} (sq)
0.975	0.9 ±0.4	1.04 ±0.05
0.95	1.0 ±0.2	1.09 ±0.04
0.90	1.005±0.005	1.16 ±0.02
0.85	1.015±0.015	1.238±0.004
0.80	1.026±0.004	1.32 ±0.01
0.75	1.036±0.009	1.40 ±0.04
0.70	1.04 ±0.08	1.47 ±0.07
0.65	1.084±0.005	1.51 ±0.06
0.60	1.10 ±0.03	1.56 ±0.07
0.55	1.11 ±0.03	1.60 ±0.09
0.50	1.11 ±0.03	1.63 ±0.09
0.40	1.16 ±0.05	1.7 ±0.2
0.30	1.2 ±0.1	1.71 ±0.01
0.20	1.22 ±0.01	1.74 ±0.01
0.10	1.241±0.003	1.746±0.003
0.00	1.250±0.003	1.750±0.001

[20] M. F. Sykes, J. W. Essam, and D. S. Gaunt, J. Math. Phys. **6**, 283 (1965).

and

$$0.07\lesssim\beta\lesssim 0.14 \quad (\text{sq}), \tag{3.34}$$

which bracket the known values[4] of $\frac{5}{16}$ and $\frac{1}{8}$, respectively. Similar results are obtained for the other two- and three-dimensional lattices.

A better method of estimating β is the following. Suppose

$$M_0(v)=B(v)(1-v_c/v)^\beta, \tag{3.35}$$

where $B(v)$ is an analytic function of v at v_c. Substituting into (3.29) gives

$$D^{-1}=-\iota\beta\left(\frac{v_c}{v_{\rm pb}^2}\right)\left(1-\frac{v_c}{v_{\rm pb}}\right)^{-1}-\iota\frac{B'(v_{\rm pb})}{B(v_{\rm pb})}, \tag{3.36}$$

where the prime denotes differentiation. Thus,

$$\beta^*=-\iota^{-1}D^{-1}(v_{\rm pb}^2/v_c)(1-v_c/v_{\rm pb}) \tag{3.37}$$

$$=\beta+\frac{v_{\rm pb}^2}{v_c}\frac{B'(v_{\rm pb})}{B(v_{\rm pb})}\left(1-\frac{v_c}{v_{\rm pb}}\right). \tag{3.38}$$

For the two-dimensional lattices, for which (3.35) is exact,[2]

$$B(v)=2^{-1/2}v_c^{-1/4}v^{-3/8}(1+v^2)^{1/4}(1-v_cv)^{1/8}\times(1+v_cv)^{1/8}(v+v_c)^{1/8} \quad (\text{sq}) \tag{3.39}$$

$$=2^{-1/2}v_c^{-1/8}v^{-1/4}(1+v^2)^{3/8}(1-v_cv)^{1/8}\times(1-v+v^2)^{-1/8} \quad (\text{t}), \tag{3.40}$$

so that the precise variation of β^* with $1-v_c/v_{\rm pb}$ may be calculated from (3.38). Close to the critical point, one finds

$$\beta^*\simeq\beta-b(1-v_c/v_{\rm pb})+\cdots \quad (v_{\rm pb}\gtrsim v_c), \tag{3.41}$$

with $\beta=\frac{1}{8}$ and

$$b=(1/32)(7\sqrt{2}-2)\simeq 0.2469 \quad (\text{sq}) \tag{3.42}$$

$$=(1/48)(7\sqrt{3}-3)\simeq 0.1901 \quad (\text{t}). \tag{3.43}$$

In three dimensions, it is possible that (3.35) is no longer correct, although (3.41) may remain valid.

One begins by forming Padé approximants to the $\tilde{\delta}_M(v)$ series and calculating the residue D corresponding to the pole at $v_{\rm pb}$ [see (3.28)]. Using D and $v_{\rm pb}$ deter-

TABLE IV. Corresponding values of M, $(1-v_c/v)$, $\iota\beta^*$, and β^* along the phase boundary for the bcc lattice.

M	$1-v_c/v_{\rm pb}$	$\iota\beta^*$	β^*
0.975	0.438±0.004	0.114±0.007	0.10 ±0.06
0.95	0.361±0.001	0.152±0.003	0.15 ±0.03
0.90	0.267±0.001	0.197±0.001	0.198±0.001
0.85	0.206±0.001	0.223±0.001	0.226±0.005
0.80	0.162±0.003	0.239±0.004	0.245±0.004
0.75	0.12 ±0.01	0.26 ±0.04	0.27 ±0.04
0.70	0.096±0.006	0.27 ±0.01	0.28 ±0.03
0.65	0.08 ±0.015	0.27 ±0.02	0.29 ±0.03
0.60	0.06 ±0.02	0.28 ±0.01	0.31 ±0.02
0.55	0.050±0.008	0.29 ±0.01	0.32 ±0.02
0.50	0.040±0.009	0.30 ±0.03	0.33 ±0.05

mined in this way, one then calculates $\iota\beta^*$ defined by (3.38). Corresponding values of M, $1-v_c/v_{\rm pb}$, and $\iota\beta^*$ are tabulated in the first three columns of Tables IV and V for the bcc and sq lattices, respectively. (The Padé approximants have not converged for smaller values of M.) Since ι should exactly equal unity, we first try plotting $\iota\beta^*$ against $1-v_c/v_{\rm pb}$. The plot for the bcc lattice in Fig. 7 extrapolates linearly to a value very close to $\frac{5}{16}$. For large values of $1-v_c/v_{\rm pb}$, there is possibly a slight downward curvature. Plots of almost comparable accuracy are obtained for the other three-dimensional lattices. On the other hand, the plot for the sq lattice in Fig. 8 is rather disquieting, for although the estimates of $\iota\beta^*$ seem fairly well determined, they lie well below the exact theoretical curve (solid line in Fig. 8) calculated from (3.38) and (3.39), and appear to extrapolate to around 0.10 rather than $\frac{1}{8}$.

Suppose now we make no assumption about the value of ι. For fixed M, the product of $\iota\beta^*$ (in Tables IV and V) and ι^{-1} (in Table III) should provide an estimate of β^* alone. This follows from (3.37), (3.27), and (3.28), since then

$$\iota\beta^*\iota^{-1}=-D^{-1}(v_{\rm pb}^2/v_c)(1-v_c/v_{\rm pb})(v-v_{\rm pb})(d/dv)\ln\tau_M(v)$$
$$=-\frac{1}{(v-v_{\rm pb})\tilde{\delta}_M(v)}\frac{v_{\rm pb}^2}{v_c}\left(1-\frac{v_c}{v_{\rm pb}}\right)(v-v_{\rm pb})\frac{d}{dv}\ln\tau_M(v)$$
$$=-\left(\frac{v_{\rm pb}^2}{v_c}\right)\left(1-\frac{v_c}{v_{\rm pb}}\right)\frac{(d/dv)\ln\tau_M(v)}{\tilde{\delta}_M(v)}. \qquad (3.44)$$

where we have assumed the Padé approximants to $\tilde{\delta}_M(v)$ and $(d/dv)\ln\tau_M(v)$ have poles at precisely the same value of $v_{\rm pb}$. Using the chain rule

$$\left(\frac{\partial\ln\tau}{\partial v}\right)_M\left(\frac{\partial v}{\partial\ln M}\right)_\tau\left(\frac{\partial\ln M}{\partial\ln\tau}\right)_v=-1, \qquad (3.45)$$

(3.44) becomes

$$\iota\beta^*\iota^{-1}=\left(\frac{v_{\rm pb}^2}{v_c}\right)\left(1-\frac{v_c}{v_{\rm pb}}\right)\left(\frac{\partial\ln M}{\partial v}\right)_\tau, \qquad (3.46)$$

where the last factor must be evaluated at the phase boundary. Calculating this term from (3.35) and substituting into (3.46) yields precisely the right-hand side of (3.38). Thus, $\iota\beta^*\iota^{-1}=\beta^*$ as expected. Values of β^* are listed in the fourth columns of Tables IV and V for the bcc and sq lattices, respectively. Because of the uncertainties in the values of ι^{-1}, the uncertainties in the values of β^* are larger than those in $\iota\beta^*$. Nevertheless, it is still possible to construct a line passing through all points of the β^*-versus-$(1-v_c/v_{\rm pb})$ plot for the bcc lattice, and having an intercept close to $\frac{5}{16}$. While such a plot is inferior to that in Fig. 7, the plot in Fig. 9 which is for the sq lattice is a distinct improvement over that in Fig. 8, since the central values now lie very close to the exact theoretical curve (broken

TABLE V. Corresponding values of M, $(1-v_c/v)$, $\iota\beta^*$, and β^* along the phase boundary for the sq lattice.

M	$1-v_c/v_{\rm pb}$	$\iota\beta^*$	β^*
0.975	0.236±0.003	0.059±0.004	0.061±0.008
0.95	0.168±0.008	0.073±0.006	0.080±0.009
0.90	0.100±0.003	0.084±0.002	0.097±0.004
0.85	0.066±0.004	0.089±0.001	0.110±0.002
0.80	0.035±0.015	0.09 ±0.02	0.12 ±0.03

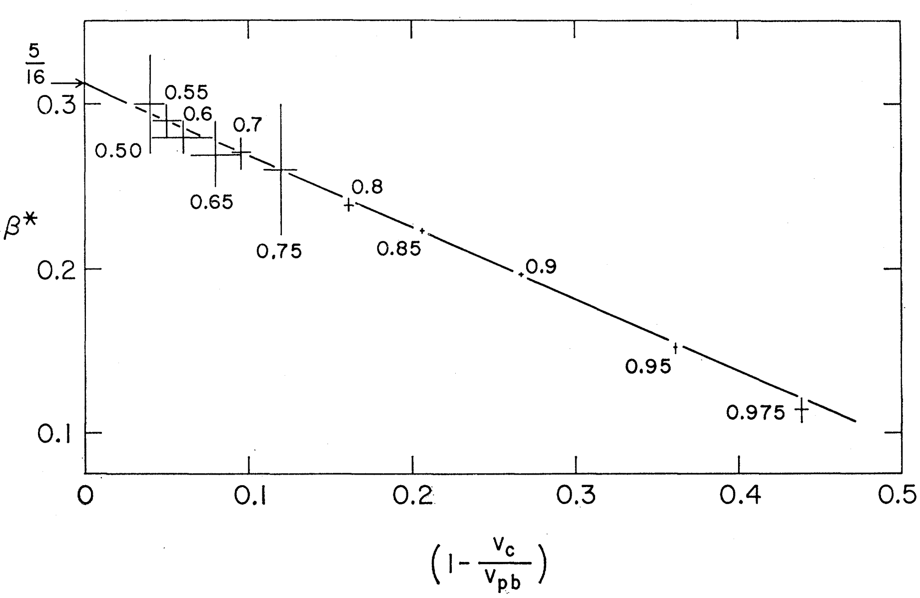

FIG. 7. Plot of $\iota\beta^*$ versus $(1-v_c/v_{\rm pb})$ for the bcc lattice. Each point is accompanied by the corresponding value of M.

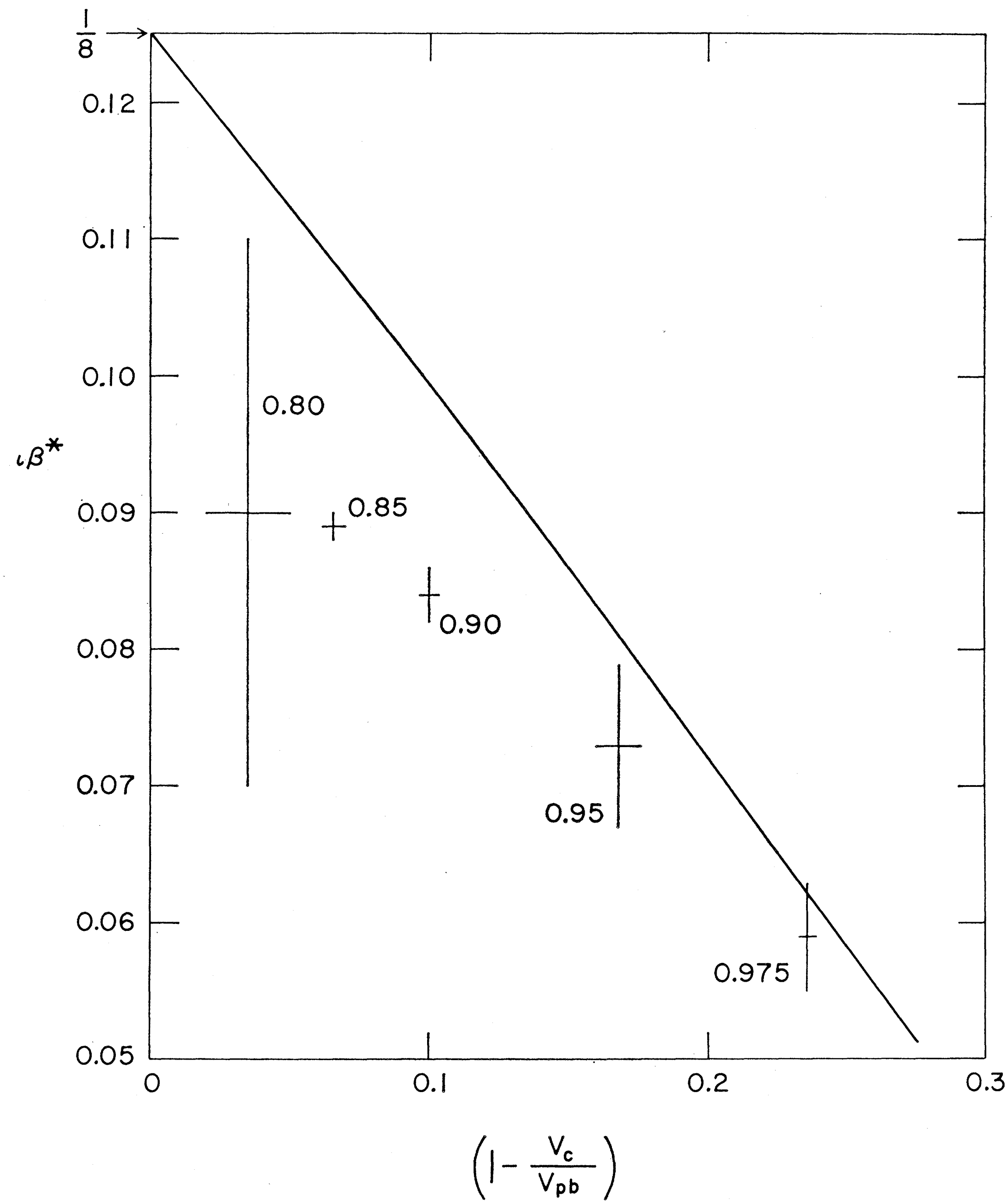

FIG. 8. Plot of $\iota\beta^*$ versus $(1-v_c/v_{pb})$ for the sq lattice. Each point is accompanied by the corresponding value of M. The solid curve is calculated from the exact solution.

solid line in Fig. 9). If the exact value of $\beta=\frac{1}{8}$ were unknown, one might estimate

$$\beta=0.127\pm0.009 \quad (\text{sq}). \tag{3.47}$$

The β^*-versus-$(1-v_c/v_{pb})$ plots can also be determined from the $\ln M$ versus $\ln(1-v_c/v_{pb})$ plots in precisely the same way that we obtained the δ^*-versus-τ plots from the $\ln\tau$-versus-$\ln M$ plots [see the last complete paragraph preceding (3.13)]. We give no further details since the plots are no more accurate than those in Figs. 7 and 9.

Finally, we note that according to (3.35) and (3.41)

$$\beta^*\simeq\beta-mM_0{}^{1/\beta}, \quad M_0\to 0+ \tag{3.48}$$

where m is a positive constant. The plots of β^* versus $M_0{}^{1/\beta}$, which must be self-consistent and asymptotically linear, will also be omitted, since they do not yield more

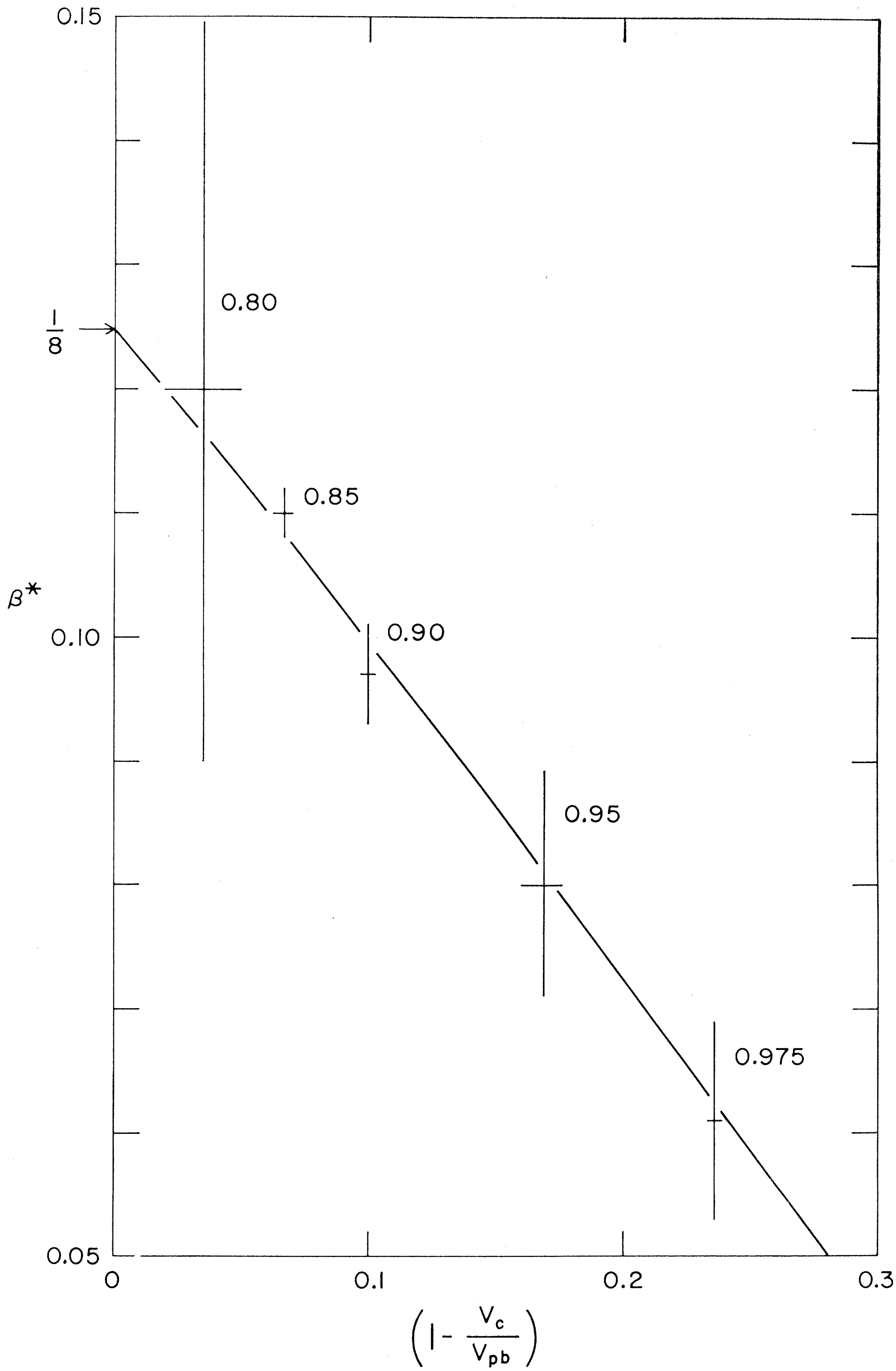

FIG. 9. Plot of β^* versus $(1-v_c/v_{pb})$ for the sq lattice. Each point is accompanied by the corresponding value of M. The solid curve is calculated from the exact solution.

accurate estimates for β despite having uncertainties in only one direction.

Exponent γ'

We will now assume $\iota=1$, so that $M_1(v)$ in (3.21) is the reduced susceptibility evaluated at the magnetic phase boundary. The exponent γ' is then defined by

$$M_1(v) \approx C'(1-v_c/v_{\rm pb})^{-\gamma'}, \quad v_{\rm pb} \to v_c+ \qquad (3.49)$$

where C' is a constant amplitude. According to (3.25) and (3.26),

$$\tau_M(v) \approx T(v_{\rm pb}-v), \quad v \to v_{\rm pb}^- \qquad (3.50)$$

where

$$T = (dM_0/dv)|_{v_{\rm pb}}/M_1(v_{\rm pb}). \qquad (3.51)$$

Substituting (3.49) and

$$M_0(v) \approx B(1-v_c/v)^{\beta}, \quad v \to v_c+ \qquad (3.52)$$

(where B is a constant amplitude) into (3.51), we get

$$T = \beta(B/C')(v_c/v_{\rm pb}^2)(1-v_c/v_{\rm pb})^{\beta+\gamma'-1}. \qquad (3.53)$$

While (3.50) shows that corresponding values of T and $v_{\rm pb}$ can be estimated from Padé approximants to the $\tau_M(v)$ series, (3.53) shows that a log-log plot of $(v_{\rm pb}^2/v_c)T$ versus $1-v_c/v_{\rm pb}$ should be asymptotically linear with slope $\Gamma \equiv \beta+\gamma'-1$. Since β has been determined previously, knowledge of Γ yields an estimate of γ'.

The plots for the bcc and sq lattices shown in Fig. 10 (curves a and b, respectively) appear to become parallel to curves c and d, which have slopes of $\frac{9}{16}$ and $\frac{7}{8}$, respectively. Since $\beta=\frac{5}{16}$ in three dimensions and $\frac{1}{8}$ in two dimensions, this means the asymptotic slopes of curves a and b are consistent with values for γ' of $1\frac{1}{4}$ and $1\frac{3}{4}$, respectively.[4] However, a slightly different value (for example, $1\frac{5}{16}$ in three dimensions[6,7]) cannot be ruled out.

The Γ^*-versus-$(1-v_c/v_{\rm pb})$ plot in Fig. 11 is for the bcc lattices and was calculated from a plot similar to curve a of Fig. 10 but which contains more closely spaced values of M. Unfortunately, the error bars are too large for us to determine accurately either the intercept on the Γ^* axis or the manner of approach. However, it is clear that the plot is consistent with either $\gamma'=1\frac{1}{4}$ or $1\frac{5}{16}$. For the sq lattice, the error bars are even larger and the corresponding plot is, therefore, omitted.

4. SPINODAL CURVE

The spinodal curve has already been discussed in the Introduction (see also Ref. 13). Let us begin this section, then, by supposing a spinodal curve exists. As we move along it towards the critical point, the susceptibility remains infinite while both the magnetization M_s and magnetic field variable τ_s approach their critical value zero. Asymptotically, we will write

$$M_s \approx B_s(1-T/T_C)^{\beta_s}, \quad T \to T_C^- \qquad (4.1)$$

and

$$\tau_s \approx -D_s(1-T/T_C)^{\Delta_s'}, \quad T \to T_C^- \qquad (4.2)$$

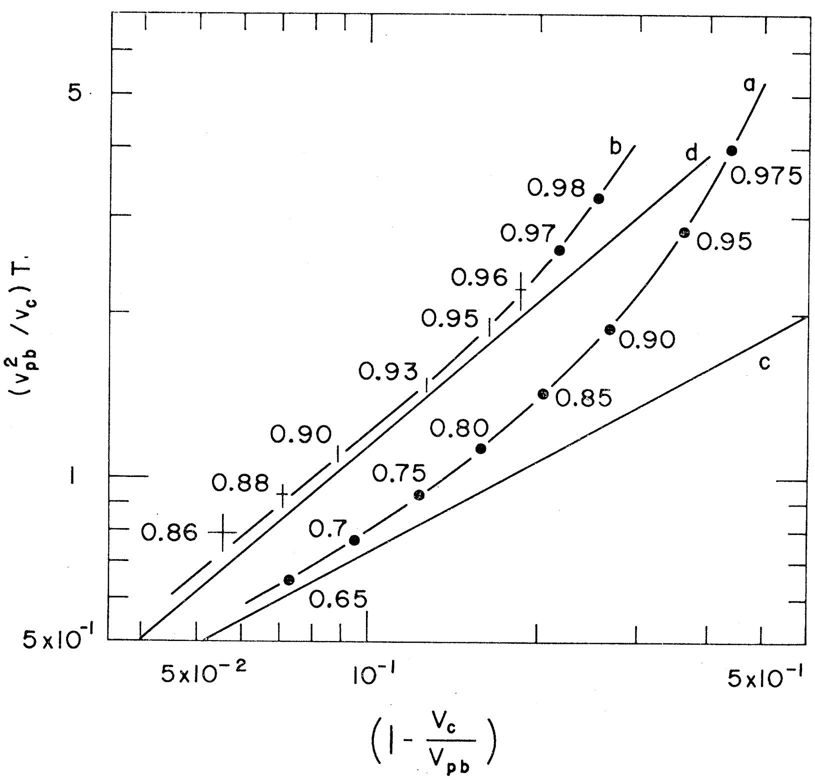

FIG. 10. Log-log plot of $(v_{\rm pb}^2/v_c)T$ versus $(1-v_c/v_{\rm pb})$ for the bcc and sq lattices (curves a and b, respectively). Each point is accompanied by the corresponding value of M. The straight lines c and d have slopes of $\frac{9}{16}$ and $\frac{7}{8}$, respectively.

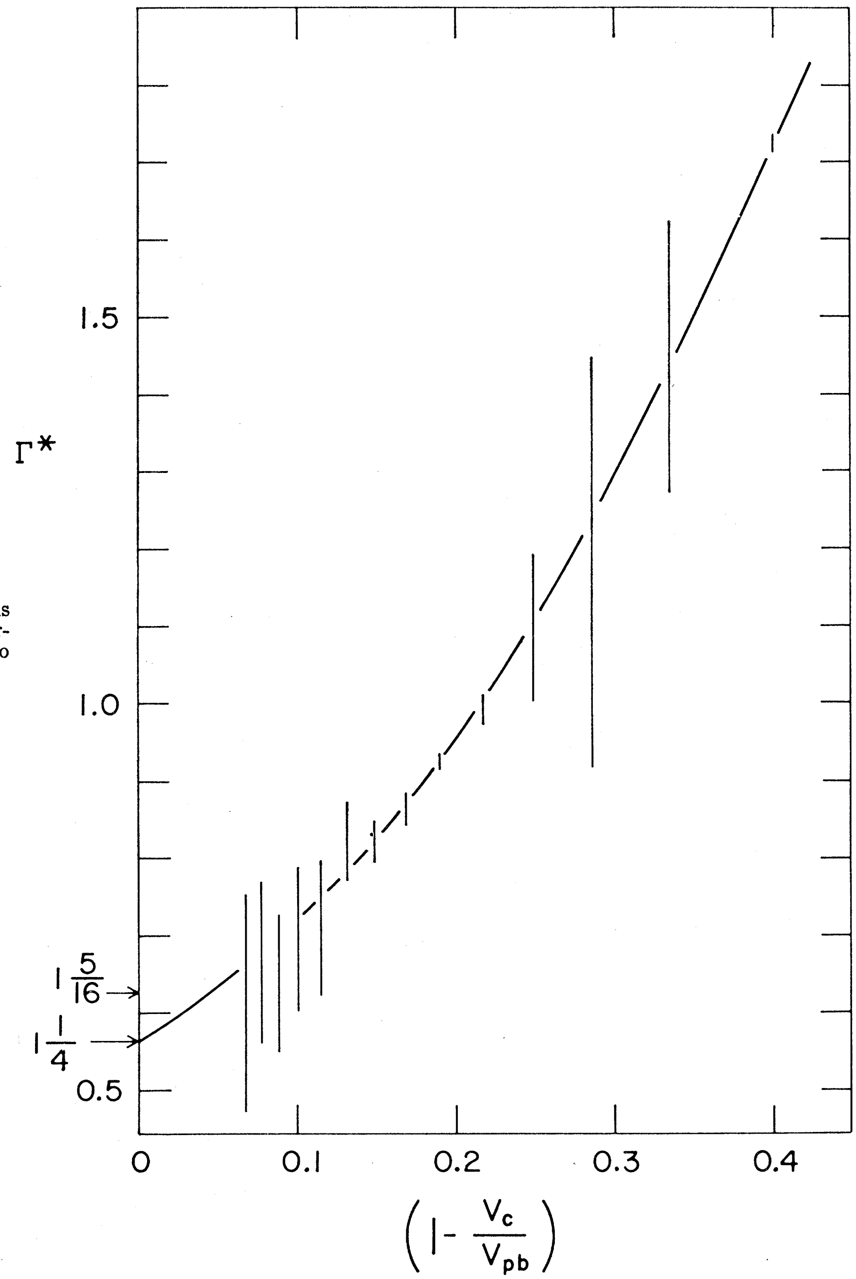

FIG. 11. Plot of $\Gamma^* \equiv (\beta+\gamma'-1)^*$ versus $(1-v_c/v_{pb})$ for the bcc lattice. The intercepts marked by arrows corresponding to $\gamma'=1\frac{1}{4}$ and $1\frac{5}{16}$ (assuming $\beta=\frac{5}{16}$).

where β_s and Δ_s' are new critical exponents, and B_s and D_s the corresponding amplitudes. Along the phase boundary, on the other hand, we have

$$M_0 \approx B_0(1-T/T_C)^\beta, \quad T \to T_C^- \tag{4.3}$$

and $\tau \equiv 0$.

As is well known, mean-field theory yields a single-phase solution which is analytic at the phase boundary. It is, therefore, easily continued into the two-phase region and predicts the existence of a spinodal curve. We begin by showing that in this approximation

$$\beta_s=\beta, \quad \Delta_s'=\Delta', \tag{4.4}$$

where $\Delta'=1\frac{1}{2}$ is the low-temperature "gap" exponent, and $\beta=\frac{1}{2}$. The amplitudes D_s, B_s, and B_0 are also readily calculated.

If one assumes the existence of a Taylor-series expansion in powers of mH/k_BT for fixed T about a point on the phase boundary, then the asymptotic behavior of the coefficients (as deduced by Essam and Hunter[14]) suggests the existence of a spinodal curve with the properties (4.4), and enables one to estimate B_s and D_s for various lattices. Alternatively, one can start from the equation of state for a ferromagnet in the critical region.[17] The equation has been expressed in various forms, the most convenient for us being that due to Domb,[21] namely,

$$\tau=(t-1)^{\Delta'}F^*(\omega)\,,\quad t=T_C/T>1 \tag{4.5}$$

with

$$\omega=M^{-1}(t-1)^{\beta}. \tag{4.6}$$

(There is also a high-temperature branch, which we will not need.) The equation of state can arise, in turn, from the homogeneity properties[15,16] of certain functions in the critical region. The connections between these various approaches are briefly discussed.

Finally, we study with the aid of Padé approximants the exact high-temperature expansions at fixed magnetization derived in this paper, as well as the exact high-field expansions at fixed temperature. If the phase boundary is a line of essential singularities, the Padé approximants certainly give no hint of this. However, they do indicate branch-point singularities which may be identified with a spinodal curve. It is possible to estimate M_s and τ_s at various points on the spinodal curve and these values are found to be consistent with those calculated from (4.1), (4.2), and (4.4) using the estimates of B_s and D_s we have derived from Essam and Hunter's work.

Mean-Field Theory

As pointed out by Domb,[22] a particularly useful way of writing the mean-field approximation for the spin-$\frac{1}{2}$ Ising model is

$$\tau=\frac{M-\tanh(tM)}{1-M\tanh(tM)}. \tag{4.7}$$

Expanding the tanh terms gives

$$\tau=-(t-1)M+[\tfrac{1}{3}t^3-t(t-1)]M^3+\cdots\,, \tag{4.8}$$

which for $T\leq T_C$ ($t\geq 1$) and $\tau=0$ yields

$$B_0=3^{1/2},\quad \beta=\tfrac{1}{2}. \tag{4.9}$$

Along the spinodal curve

$$\chi^{-1}=(\partial\tau/\partial M)_T=-(t-1)+[t^3-3t(t-1)]M^2+\cdots=0\,, \tag{4.10}$$

so that for $t\geq 1$, one finds

$$B_s=1\,,\quad \beta_s=\tfrac{1}{2}. \tag{4.11}$$

Substituting $M_s=(t-1)^{1/2}$ into (4.8), we get (4.2) with

$$D_s=\tfrac{2}{3}\,,\quad \Delta_s'=\Delta'=1\tfrac{1}{2}. \tag{4.12}$$

Thus, we have confirmed (4.4) and found

$$B_s=1\,,\quad D_s=\tfrac{2}{3}\,,\quad B_0/B_s=3^{1/2}. \tag{4.13}$$

[21] C. Domb, J. Appl. Phys. **39**, 620 (1968).
[22] C. Domb, Ann. Acad. Sci. Fennicoe **A6**, 167 (1966).

Essam and Hunter's Series

Consider a point on the phase boundary and let us *assume* the existence of an expansion for the magnetization at fixed $T<T_C$ as a power series in $mH/k_BT\equiv L$. Thus,

$$M=\sum_{n=1}^{\infty}\frac{f_n(T)L^{n-1}}{(n-1)!}\,, \tag{4.14}$$

where $f_n(T)$ is essentially the nth field derivative of the free energy evaluated at the phase boundary in the one-phase region. In particular, $f_1(T)$ is the spontaneous magnetization and $f_2(T)$ is the reduced zero-field susceptibility below T_C. After analyzing the low-temperature series for $f_1(T)$ through $f_6(T)$, Essam and Hunter[14] suggested

$$f_n(T)\approx C_n^-(1-T/T_C)^{\beta-(n-1)\Delta'},\quad T\to T_c- \tag{4.15}$$

for all n, where Δ' is the low-temperature "gap" exponent. Differentiating (4.14) with respect to L to give the reduced susceptibility χ and replacing the coefficients $f_n(T)$ by their asymptotic forms (4.15) yields

$$\chi(L)\approx\sum_{n=2}^{\infty}\frac{C_n^-(1-T/T_C)^{\beta-(n-1)\Delta'}L^{n-2}}{(n-2)!}\,, \tag{4.16}$$

which should be valid close to T_C. Regrouping (4.16) as an expansion in power of

$$\mathcal{L}\equiv(1-T/T_C)^{-\Delta'}L \tag{4.17}$$

gives for fixed $T\lesssim T_C$

$$\chi(\mathcal{L})\approx\left(1-\frac{T}{T_C}\right)^{-\gamma'}\sum_{n=0}^{\infty}\frac{C_{n+2}^-\mathcal{L}^n}{n!}\,, \tag{4.18}$$

where we have used $\gamma'=\Delta'-\beta$, which follows from (4.15) when $n=2$. Suppose the series on the right-hand side of (4.18) exists and has a finite radius of convergence determined by a singularity at

$$\mathcal{L}_s\equiv(1-T/T_C)^{-\Delta'}L_s=-D_s\,, \tag{4.19}$$

at which point $\chi(\mathcal{L})$ diverges to infinity. In this case, (4.2) follows immediately from (4.19) with $\Delta_s'=\Delta'$ as in (4.4).

Alternatively, substituting (4.15) into (4.14) and regrouping in powers of $\mathcal{L}$ gives

$$M(\mathcal{L})\approx\left(1-\frac{T}{T_C}\right)^{\beta}\sum_{n=0}^{\infty}\frac{C_{n+1}^-\mathcal{L}^n}{n!}. \tag{4.20}$$

At $\mathcal{L}=\mathcal{L}_s$, the series on the right-hand side of (4.20) is presumably singular although finite—equal to B_s, in fact. Thus we get (4.1) with $\beta_s=\beta$ as in (4.4).

Let us rewrite the series on the right-hand sides of (4.18) and (4.20) as

$$\hat{\chi}(\mathcal{L})\equiv\sum_{n=0}^{\infty}\frac{C_{n+2}^-\mathcal{L}^n}{n!} \tag{4.21}$$

and

$$\hat{M}(\mathcal{L})\equiv\sum_{n=0}^{\infty}\frac{C_{n+1}^{-}\mathcal{L}^n}{n!}. \tag{4.22}$$

Since Essam and Hunter have estimated the first few C_n^- from exact series expansions, we may attempt to verify directly the conjectured behavior of $\hat{\chi}(\mathcal{L})$ and $\hat{M}(\mathcal{L})$. One finds for the bcc lattice

$$\hat{\chi}(\mathcal{L})=0.1954-0.165\mathcal{L}+0.1848\mathcal{L}^2-0.218\mathcal{L}^3+0.279\mathcal{L}^4-\cdots, \tag{4.23}$$

$$\hat{M}(\mathcal{L})=1.5056+0.1954\mathcal{L}-0.0825\mathcal{L}^2+0.0616\mathcal{L}^3-0.0545\mathcal{L}^4+0.0558\mathcal{L}^5-\cdots, \tag{4.24}$$

and for the sq lattice

$$\hat{\chi}(\mathcal{L})=0.02568-0.01746\mathcal{L}+0.0174\mathcal{L}^2-0.028\mathcal{L}^3+\cdots, \tag{4.25}$$

$$\hat{M}(\mathcal{L})=1.22241+0.02568\mathcal{L}-0.00873\mathcal{L}^2+0.0058\mathcal{L}^3-0.007\mathcal{L}^4+\cdots. \tag{4.26}$$

Notice that the $\hat{\chi}(\mathcal{L})$ series alternate in sign, indicating that the closest singularity lies on the negative real $\mathcal{L}$ axis as demanded by (4.19). The ratios of successive coefficients in (4.23) and (4.25) are

$$-0.844,\quad -1.120,\quad -1.180,\quad -1.280,\quad \ldots \quad (\text{bcc}) \tag{4.27}$$

and

$$-0.680,\quad -0.997,\quad -1.609,\quad \ldots \quad (\text{sq}). \tag{4.28}$$

Plotting the sequence (4.27) versus $1/n$ indicates a limit around -1.39 ± 0.05, corresponding to

$$D_s=0.72\pm0.03 \quad (\text{bcc}). \tag{4.29}$$

This estimate is supported by the locations of the poles of the Padé approximants to the $(d/d\mathcal{L})\ln\hat{\chi}(\mathcal{L})$ series, namely,[23]

$$-0.72[1,0],\quad -0.76[2,0],\quad -0.76[1,1],\quad -0.67[3,0],\quad -0.66[1,2],\quad \ldots \quad (\text{bcc}), \tag{4.30}$$

where the [2,1] entry has been omitted since there is a pole-zero pair on the positive real axis closer to the origin. From (4.29) and (4.30), we obtain the final estimate

$$D_s\simeq 0.69_{-0.13}^{+0.07} \quad (\text{bcc}). \tag{4.31}$$

For the sq lattice, the ratios (4.28) are increasing quite rapidly and the only Padé-approximant entries are

$$-0.76[1,0],\quad -0.49[2,0],\quad -0.41[1,1],\quad \ldots \quad (\text{sq}). \tag{4.32}$$

It is, therefore, not really feasible to estimate D_s. Nevertheless, a value around

$$D_s\simeq 0.39\pm0.2 \quad (\text{sq}) \tag{4.33}$$

does not seem unreasonable. The estimates (4.31) and (4.33) are of the expected order of magnitude, the value for the three-dimensional lattice lying closest to the mean-field value of $\frac{2}{3}$ [see (4.13)], as might have been anticipated.

If we adopt the above values for D_s, then the amplitudes B_s may also be estimated by forming Padé approximants to the $\hat{M}(\mathcal{L})$ series in (4.24) and (4.26), and evaluating these at $\mathcal{L}_s=-D_s$. Fortunately, it turns out that $\hat{M}(\mathcal{L})$ varies quite slowly in the vicinity of $\mathcal{L}_s$ (particularly for the two-dimensional lattices), so that reasonably accurate estimates of B_s can be made despite the fairly large uncertainties in the estimates of D_s. Consider, for example, the sq lattice for which the uncertainty in D_s is the greatest. The complete Padé table is shown in Table VI. The entries not in parentheses were obtained by evaluating the approximants at $\mathcal{L}_s=-0.39$, while those in parentheses resulted from evaluation at $\mathcal{L}_s=-0.49$ (representing a deviation from the central estimate of one-half the estimated uncertainty). Thus, we are able to estimate

$$B_s\simeq 1.21\pm0.01 \quad (\text{sq}) \tag{4.34}$$

and

$$B_s\simeq 1.25\pm0.10 \quad (\text{bcc}). \tag{4.35}$$

Both these estimates are of the expected order of magnitude, the mean-field value being unity. Using the known values of B_0, namely,

$$B_0\simeq 1.22241 \quad (\text{sq}),\qquad \simeq 1.5056 \quad (\text{bcc}), \tag{4.36}$$

we get

$$B_0/B_s\simeq 1.01\pm0.01 \quad (\text{sq}) \tag{4.37}$$

$$\simeq 1.20\pm0.10 \quad (\text{bcc}), \tag{4.38}$$

compared with the mean-field value of $3^{1/2}$.

It appears from (4.37) that the spinodal curve and phase boundary might be asymptotically tangent at the critical point, that is, $B_0/B_s=1$. However, if the $\hat{M}(\mathcal{L})$ series [(4.24) and (4.26), for example] continue to alternate in sign, as seems likely, we must have $B_0>B_s$ for all lattices. This follows by observing that

TABLE VI. Estimates of B_s for the sq lattice obtained from the $[M,N]$ Padé approximants (Ref. 23) to the $\hat{M}(\mathcal{L})$ series, by evaluation at $\mathcal{L}=-0.39$ and -0.49 (in parentheses).

M \ N	0	1	2	3	4
0		1.2124 (1.2098)	1.2111 (1.2077)	1.2107 (1.2070)	1.2106 (1.2066)
1	1.2125 (1.2100)	1.2109 (1.2073)	1.2106 (1.2067)	1.2104 (1.2061)	
2	1.2111 (1.2078)	1.2106 (1.2067)	1.2103 (1.2055)		
3	1.2107 (1.2071)	1.2104 (1.2061)			
4	1.2106 (1.2067)				

[23] In the $[M,N]$ Padé approximant, M and N are the degrees of the denominator and numerator, respectively.

the leading coefficient of $\hat{M}(\mathfrak{L})$ is always B_0 and that for $\mathfrak{L}_s$ negative, all the remaining terms will be negative.

If the heuristic arguments presented above are correct, it appears that even though asymptotic tangency is unlikely, B_0/B_s-1 is so small that in the vicinity of the critical point the spinodal curve lies very close to the phase boundary—particularly for two-dimensional lattices. Specifically, we find from (4.1), (4.3), and (4.4),

$$\Delta v \equiv v_s - v_{pb} \approx KM^{1/\beta}, \tag{4.39}$$

where v_{pb} and v_s are the values of v on the phase-boundary and spinodal curve, respectively, for a given value of M, and K is a constant given by

$$K=(J/k_BT_c)(1-v_c^2)(B_s^{-1/\beta}-B_0^{-1/\beta}). \tag{4.40}$$

Substituting (4.34) to (4.36) yields

$$\Delta v \approx KM^{3.2}, \quad K=0.034\pm0.02 \quad (\text{bcc}) \tag{4.41}$$

and

$$\Delta v \approx KM^{8}, \quad K=0.006\pm0.005 \quad (\text{sq}). \tag{4.42}$$

When $M=0.7$, for example, these give

$$\Delta v \simeq 0.011\pm0.006 \quad (\text{bcc}) \tag{4.43}$$

$$\simeq 0.0004\pm0.0003 \quad (\text{sq}). \tag{4.44}$$

The asymptotic formula

$$\tau_s \approx -(D_s/B_s^{\delta})M_s^{\delta}, \tag{4.45}$$

giving the value of τ for a given value of M on the spinodal curve, can be derived from (4.1), (4.2), and (4.4). Substituting our estimates of B_s and D_s yields, for example,

$$\tau_s \simeq -0.026_{-0.012}^{0.018} \quad (M_s=0.65, \quad \text{bcc}) \tag{4.46}$$

and

$$\tau_s \simeq -0.0003\pm0.0002 \quad (M_s=0.75, \quad \text{sq}). \tag{4.47}$$

Equation-of-State and Homogeneity Arguments

The low-temperature branch of the equation of state has already been written down in (4.5) and (4.6). In this theory[17,21,22] the phase boundary corresponds to $\omega=\omega_0$, at which point $F^*(\omega_0)=0$, since here $\tau=0$ even though $M\neq0$. Furthermore, (4.3) follows from (4.6) with

$$B_0=\omega_0^{-1}. \tag{4.48}$$

Differentiating (4.5) with respect to M, one obtains

$$\chi^{-1}=(\partial\tau/\partial M)_t=-(t-1)^{\gamma'}\omega^2(dF^*/d\omega), \tag{4.49}$$

and since the susceptibility in the one-phase region is non-negative, $dF^*/d\omega$ must be negative. Thus, $F^*(\omega)$ decreases monotonically from infinity to zero as ω increases from zero to ω_0. Inside the two-phase region, $\omega>\omega_0$ and $F^*(\omega)\equiv0$.

The previous approach, using the results of Essam and Hunter, is closely related to the analyticity of $F^*(\omega)$ at $\omega=\omega_0$. Specifically, the existence of a Taylor-series expansion for $F^*(\omega)$ about ω_0 is easily shown to imply (4.14) with (4.15). Analyticity at ω_0 enables us to simply continue $F^*(\omega)$ for $\omega\leq\omega_0$ into the region $\omega>\omega_0$. Suppose the continuation exhibits a minimum at some point $\omega=\omega_s>\omega_0$. According to (4.49), the susceptibility is infinite at this point, which must correspond, therefore, to the spinodal curve. Thus (4.1) and (4.2) follow from (4.6) and (4.5), respectively, with

$$B_s=\omega_s^{-1} \tag{4.50}$$

and

$$D_s=|F^*(\omega_s)|. \tag{4.51}$$

From (4.48) and (4.50),

$$B_0/B_s=\omega_s/\omega_0. \tag{4.52}$$

It follows from (4.49) and (4.15) that

$$(dF^*/d\omega)|_{\omega=\omega_0}=-1/(\omega_0^2C_2^-)\neq0, \tag{4.53}$$

so that if $F^*(\omega)$ is analytic at ω_0, we must have $\omega_s>\omega_0$, and, hence, $B_0>B_s$. Thus, asymptotic tangency of the phase boundary and spinodal curve is definitely ruled out if ω_0 is an analytic point of $F^*(\omega)$.

To illustrate this approach, consider the mean-field approximation. Domb[21] has shown that (4.5) and (4.6) are valid with $\Delta'=1\frac{1}{2}$, $\beta=\frac{1}{2}$, and

$$F^*(\omega)=\omega^{-3}(\tfrac{1}{3}-\omega^2). \tag{4.54}$$

Clearly, $F^*(\omega)$ is infinite at $\omega=0$ and decreases montonically to zero at $\omega=\omega_0=3^{-1/2}$. It exhibits a minimum beyond ω_0 at $\omega_s=1$, at which point $F^*(\omega_s)=-\frac{2}{3}$. Thus, (4.50)–(4.52) yield $B_s=1$, $D_s=\frac{2}{3}$, and $B_0/B_s=3^{1/2}$ in precise agreement with (4.13).

Finally, let us consider these ideas in the context of the usual homogeneity arguments. In the one-phase region close to the critical point, Stell[16] has discussed the idea of a certain temperature change being equivalent to a certain change in the magnetization in the sense that it produces the same change in the susceptibility χ, for example. Writing $x=1-t$, we have

$$\chi\approx Cx^{-\gamma} \quad (M=0,\ x\rightarrow0+), \tag{4.55}$$

where C is a constant amplitude, and

$$\chi\approx\delta^{-1}D^{-1}M^{1-\delta} \quad (T=T_C,\ M\rightarrow0+), \tag{4.56}$$

which follows from (3.1). Thus, $Cx^{-\gamma}$ is equivalent to $\delta^{-1}D^{-1}M^{1-\delta}$, or x is equivalent to $z\equiv bM^{(\delta-1)/\gamma}$, where $b^{\gamma}=\delta CD$. Stell has shown that homogeneity of $\chi(x,z)$ yields Widom's[15] form of homogeneity, which in turn leads to the equation of state (4.5) and (4.6). By considering χ contours in the (z,x) plane and assuming homogeneity, one can show that the phase boundary is given by the straight line

$$x=-k_1z, \quad k_1=\text{const}. \tag{4.57}$$

It follows that

$$1/\beta=(\delta-1)/\gamma, \tag{4.58}$$

a well-known scaling law[4,24] which appears to hold for the Ising model (see following section).

We will now assume that the one-phase χ contours can be analytically continued into the two-phase region (lying between $x=-k_1z$ and the negative x axis), and that a limiting $\chi=\infty$ contour (or spinodal curve) exists. In general, its asymptotic equation must be the straight line

$$x=-k_2z, \quad \text{constant } k_2\neq k_1 \tag{4.59}$$

from which immediately follows

$$\beta_s=\beta, \quad B_0/B_s=(k_2/k_1)^\beta. \tag{4.60}$$

However, it is conceivable that as the critical point is approached the spinodal curve becomes asymptotically tangent to either the negative x axis or the phase boundary. Stell reports[16] that by assuming one-phase homogeneity and analyticity along T_C, Fisher has ruled out the first possibility (the only case to imply $\beta_s\neq\beta$). We have shown that the second possibility, which, as Stell points out, can lead to inequalities like $\gamma'>\gamma$, may be ruled out by assuming one-phase homogeneity and analyticity along the phase boundary. In Sec. 5, we will demonstrate the validity of this analyticity assumption. To conclude the present section, we will now report some Padé-approximant calculations based upon exact series expansions which *tend* to support the conjectured analyticity along the phase boundary.

Exact Series Expansions

Consider, first, the Padé approximants to the $\tilde{\delta}_M(v)$ series. It is found that the simple pole at $v_{\text{pb}}(M)$ is always followed by a zero, at which point the susceptibility $(\partial M/\partial\tau)_v\equiv M/[\tau\tilde{\delta}_M(v)]$ diverges to infinity. Since the location of the zero is reasonably stable (at least for the three-dimensional lattices), it should correspond to the singularity at $v_s(M)$ on the spinodal curve. Behind the zero lies a pole-zero sequence indicating a branch-point singularity at $v_s(M)$.

As implied above, the location of the leading zero is less stable for the two-dimensional lattices. A possible explanation is obtained by reinterpreting the whole structure as a pole-zero sequence beginning at $v_{\text{pb}}(M)$. This would imply a branch-point or (possibly) essential singularity at $v_{\text{pb}}(M)$. On the other hand, Δv is expected to be very small for the two-dimensional lattices, so that the uncertainty in the location of the first zero could be attributed to poor convergence. As we will now show, a study of the $\tau_M(v)$ series makes the latter explanation seem more plausible.

We saw in the last section that the Padé approximants to the $\tau_M(v)$ series have a zero at $v_{\text{pb}}(M)$. If this point were a branch point or essential singularity as discussed above, we might expect this zero to be followed by a pole, then another zero, and so on. In fact, we invariably find that the zero at $v_{\text{pb}}(M)$ is followed by a second zero, with no intervening pole.

Assuming the existence of a spinodal curve, we have estimated v_{pb} and v_s from the location of the first pole and first zero, respectively, of the pole-zero sequence for the Padé approximants to the $\hat{\delta}_M(v)$ series. For example, when $M=0.7$, we find

$$v_{\text{pb}}=0.173\pm0.001, \quad v_s=0.199\pm0.015 \quad (\text{bcc}), \tag{4.61}$$

so that

$$\Delta v=0.026\pm0.016 \quad (M=0.7, \quad \text{bcc}), \tag{4.62}$$

in reasonable agreement with (4.43). To calculate τ_s we have evaluated the approximants to the $\tau_M(v)$ series at $v=v_s$. In this way we find, for example,

$$\tau_s=-0.07_{-0.03}^{+0.01} \quad (M=0.65, \quad \text{bcc}), \tag{4.63}$$

again in reasonable agreement with (4.46). For the bcc lattice, results comparable in accuracy to (4.62) and (4.63) are found for other values of M. Unfortunately, the uncertainties in the estimates of v_s for the two-dimensional lattices are so large that the error associated with Δv and τ_s are larger than the values themselves. However, as explained earlier, such poor convergence is to be expected when the spinodal curve lies very close to the phase boundary.

We have also studied the exact high-field expansions

$$M(u,\mu)=1-\sum_{l=1}^{\infty} M_l(u)\mu^l, \tag{4.64}$$

where

$$u=\exp(-4J/k_BT)=(1-v)^2/(1+v)^2 \tag{4.65}$$

and

$$\mu=\exp(-2mH/k_BT)=(1-\tau)/(1+\tau). \tag{4.66}$$

$M_l(u)$ are polynomials in u which are available through orders $l=13$ (d,sq), $l=11$ (sc,bcc), $l=8$ (t), and $l=7$ (fcc). We have studied the Padé approximants to the $M(\mu)$ series obtained by evaluating the polynomials at fixed values of T (i.e., u) below T_c. Again the results are consistent with the existence of a spinodal curve, for although the covergence of the Padé-approximant table is not particularly good, the closest singularity appears to be in the two-phase region $\mu>1$. For example, when $T/T_C=\frac{1}{2}$, we find a singularity in the range $\mu=2$–3 for the bcc lattice, and in the range $\mu=1$–2 for the sq lattice.[25] These values of μ are in rough agreement with the values of μ_s calculated from the asymptotic formula (4.2) using (4.4), (4.31), and (4.33).

5. RELATIONS BETWEEN CRITICAL EXPONENTS PROVIDED BY RIGOROUS RESULTS AND ANALYTICITY HYPOTHESIS

In this section we examine what consequences follow from those properties which can be rigorously proved about the analytic structure of free energy. One

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important rigorous result for the ferromagnetic Ising model was proved by Yang and Lee.[8] They showed that all the singularities of the logarithm of the partition function are on the circle $|\mu|=1$. A representation of the free energy in terms of τ can be given on the basis of Yang and Lee's result as[9]

$$\frac{F}{kT}=\tfrac{1}{2}\ln[\tfrac{1}{4}(1-\tau^2)]+\int_0^\infty \ln\left(\frac{1+\omega}{1+\tau^2\omega}\right)d\varphi(\omega), \quad (5.1)$$

where $d\varphi(\omega)\geq 0$ and

$$\int_0^\infty d\varphi(\omega)=\tfrac{1}{2}. \quad (5.2)$$

The measure function φ depends on the temperature, but not on the magnetic field. Lebowitz and Penrose[10] have proved (among other things) that for the Ising ferromagnet (leaving aside the first term, which is a known function in any event), F is an analytic function of both T and τ for $\mathrm{Re}(\tau)\gtreqless 0$ and for real finite temperatures. That is to say that F is analytic in the neighborhood of all points on the positive-temperature axis ($T<\infty$) and τ in the right half-plane. In addition, Gallavotti, Miracle-Sole, and Robinson[11] have shown that we have analyticity in the neighborhood of $\tau=0$, provided the absolute value of the complex temperature is large enough. This result, together with that of Lebowitz and Penrose, has the consequence that the free energy is an analytic function of temperature and τ^2 in the cut τ^2 plane

$$-\infty\leq\tau^2\leq[R(T)]^{-1},\quad R(T)<0 \text{ for } T>T_G, \quad (5.3)$$

for some T_G.

The idea behind the result of Lebowitz and Penrose can be seen from (5.1). Penrose[26] has shown that for

$$|\mu|<\{[1+q(e^{4J/k_BT}-1)]e^{2qJ/k_BT+1}\}^{-1} \quad (5.4)$$

there is a convergent expansion of F in terms of μ.

Sykes, Essam, and Gaunt[20] have shown that all of the coefficients of μ are analytic functions (polynomials in e^{-4J/k_BT}), and hence by standard theorems from complex-variable theory, F is also an analytic function of T for the same region in τ as defined by (5.4). However, by (5.1) we can immediately extend the region, by noting that the coefficient of $d\varphi$ is bounded between 0 and τ^{-2} for all real τ, and, similarly, bounds may be gotten for τ complex. Hence, if the integral (5.1) is convergent for τ near unity ($d\varphi$ is positive real for T real and so this result will continue to hold near T real), it will also be convergent for any $\tau>0$ and more generally in the cut τ^2 plane $-\infty\leq\tau^2\leq 0$.

The first additional assumption we shall make is that T_G of (5.3) is in fact coincident with the critical temperature T_C. Fisher[27] has shown that, when considered as a function of temperature alone, the susceptibility for zero magnetic field is analytic to within 2.2% of the best estimate of the critical point for the sc lattice. In the two-dimensional case, Onsager's[28] exact zero-field result proves analyticity right up to the critical point. These results make, we feel this assumption very plausible. The same assumption was also made by Abe.[29] It is in the spirit of the analysis of the Ising model to data to assume the existence of critical exponents. We assume, in particular, that

$$R(T)\approx\mathcal{K}[(T-T_C)/T_C]^{-2\Delta}. \quad (5.5)$$

If we differentiate (5.1) with respect to the magnetic field, we get the magnetization per spin as

$$M=\tau+\int_0^\infty \frac{2\tau(1-\tau^2)\omega d\varphi(\omega)}{1+\tau^2\omega}. \quad (5.6)$$

It will be convenient to consider the related function

$$G(\tau)=\frac{M-\tau}{\tau(1-\tau^2)}=\int_0^{R(T)}\frac{d\psi(\omega)}{1+\tau^2\omega}, \quad (5.7)$$

where $d\psi(\omega)=2\omega\, d\varphi(\omega)\geq 0$. [Equation (5.7) is identical to (3.18).] For $T>T_C$, $R(T)$ is finite, and for $T\leq T_C$, $R(T)$ is infinite. The reduced magnetic susceptibility is given by

$$\chi=\left(1+\int_0^{R(T)}\frac{[1-\tau^2(3+(1+\tau^2)\omega)]d\psi(\omega)}{(1+\tau^2\omega)^2}\right)(1-\tau^2) \quad (5.8)$$

and, for $T>T_C$, the zero-field susceptibility by

$$\chi=1+\int_0^{R(T)}d\psi(\omega)$$
$$=1+G(0)\approx 1+A_0[(T-T_C)/T_C]^{-\gamma}, \quad (5.9)$$

where we here assume the existence of the critical index γ. Now

$$\frac{1}{n!}\left(-\frac{\partial}{\partial\tau^2}\right)^n G(\tau)\bigg|_{\tau=0}=\int_0^{R(T)}\omega^n d\psi(\omega)$$
$$\leq R^n(T)G(0) \quad (5.10)$$

gives an upper bound on the coefficients of $G(\tau)$, $T>T_C$. If we define

$$\frac{1}{n!}\left(-\frac{\partial}{\partial\tau^2}\right)^n G(\tau)\bigg|_{\tau=0}=A_n\left(\frac{T-T_C}{T_C}\right)^{-\gamma-2n\Delta} \quad (5.11)$$

using (5.5), (5.9), and (5.10), then using the result that

$$A_{n+1}A_{n-1}>A_n^2 \quad\text{or}\quad A_{n+1}/A_n>A_n/A_{n-1}, \quad (5.12)$$

which follows from the Cauchy-Schwartz inequality

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[28] L. Onsager, Phys. Rev. **65**, 117 (1944).
[29] R. Abe, Progr. Theoret. Phys. (Kyoto) **38**, 72 (1967).

and d'Alembert's ratio test for the radius of convergence

$$\lim_{n\to\infty} |g_{n+1}/g_n| = R(T), \tag{5.13}$$

where the g_n are the power-series coefficients in the expansion of G in powers of τ^2, we conclude that the A_n are a well-defined sequence of numbers. Consequently, if in the defining equations (5.10) and (5.11),

$$\int_0^{R(T)} \omega^n d\psi(\omega) = A_n\left(\frac{T-T_C}{T_C}\right)^{-\gamma-2n\Delta}, \tag{5.14}$$

we make the change of variables

$$w = [(T-T_C)/T_C]^{+2\Delta}\omega, \quad d\Psi(w) = [(T-T_C)/T_C]^{\gamma} d\psi(\omega), \tag{5.15}$$

then we have

$$\int_0^{\mathcal{K}} w^n d\Psi(w) = A_n. \tag{5.16}$$

Consequently,

$$\lim_{T\to T_C+}\left(\frac{T-T_C}{T_C}\right)^{\gamma} d\psi\left[\left(\frac{T-T_C}{T_C}\right)^{-2\Delta} w\right] = d\Psi(w) \tag{5.17}$$

defines a limiting measure function for the critical isotherm, at least for large ω. We now see that if $M \propto \tau^{1/\delta}$ on the critical isotherm, (5.7) implies

$$G(\tau) \sim \tau^{(1-\delta)/\delta} \tag{5.18}$$

as τ goes to zero. Rewriting (5.7) and (5.18) with (5.15), we find

$$\lim_{T\to T_C} \int_0^\infty \frac{(t)^{-\gamma} d\Psi(w)}{1+\tau^2 t^{-2\Delta} w} \sim \tau^{(1-\delta)/\delta}, \tag{5.19}$$

where now $t = (T-T_C)/T_C$. In order for (5.19) to be true for all $\tau \neq 0$ (τ small, $\tau t^{-\Delta}$ large), we must have

$$d\Psi(w) \propto w^{-(\delta+1)/2\delta} dw \tag{5.20}$$

for w small. The temperature behavior of the coefficient of $\tau^{(1-\delta)/\delta}$ is

$$t^{-\gamma+\Delta(\delta-1)/\delta} \tau^{(1-\delta)/\delta} \tag{5.21}$$

in the limit as $t \to 0+$. Hence, we conclude that

$$-\gamma + \Delta(\delta-1)/\delta \geq 0. \tag{5.22}$$

We cannot conclude strict equality because it is perfectly possible that other singularities in $G(\tau)$ besides the one which moves most quickly to $\tau = 0$ as $t \to 0$ also contribute to the behavior along the critical isotherm. We differ with Abe[29] at this point. We will give an example later to clarify it. A convenient way to rewrite inequality (5.22) is

$$\delta \geq \Delta/(\Delta-\gamma). \tag{5.23}$$

We may summarize by saying that if γ, δ, and Δ exist in the sense we have defined them for the ferromagnetic Ising model, then they must satisfy (5.23).

Let us now turn our attention to the region $T < T_C$. First we note that by (5.7) we may express $d\psi(\omega)$ in terms of $G(\tau)$,[30]

$$\psi'(\omega) = \frac{1}{\pi} \lim_{\epsilon\to 0} \operatorname{Im}\left[G\left(\frac{1}{(-\omega+i\epsilon)^{1/2}}\right)\right]\frac{1}{\omega}. \tag{5.24}$$

Thus the known analytic properties of G as detailed previously become available in the study of $\psi'(\omega)$. It follows from the series expansion available[14] that the coefficient of every power of τ may be represented in a formal expansion in $u = \exp(-4J/k_BT)$ for $T < T_C$. We shall assume—with good evidence, we feel[14]—that these formal series define finite coefficients for every order of τ for real $T < T_C$. We will further assume, as the series represent a rearrangement of *all* the terms of the (convergent) μ series which defines the function that there are no additional parts of $G(\tau)$ which have a Taylor series with all derivatives zero in the $\operatorname{Re}(\tau) \geq 0$ at $\tau = 0$. The consequence of this is that we may write

$$G(\tau) = \hat{g}_{-1}/\tau + \hat{g}_0 + \hat{g}_1\tau + \hat{g}_2\tau^2 + \cdots \tag{5.25}$$

for all $T < T_C$. By virtue of (5.24) we must then have

$$\psi'(\omega) = \frac{1}{\pi}\left[\hat{g}_{-1}\left(\frac{1}{\sqrt{\omega}}\right) - \hat{g}_1\left(\frac{1}{\sqrt{\omega}}\right)^3 + \hat{g}_3\left(\frac{1}{\sqrt{\omega}}\right)^5 - \cdots\right], \tag{5.26}$$

where the coefficients must behave as follows:

$$\hat{g}_{-1} \propto (-t)^{\beta}, \quad \hat{g}_0 \propto (-t)^{-\gamma'}, \tag{5.27}$$

by the definition of the low-temperature critical exponents.

We are now in a position to examine the combined effects of (i) the existence of the low-temperature field derivatives, (ii) the integral representation (5.7), (iii) analyticity, and (iv) the existence of various critical exponents. We focus on the behavior of $\psi'(\omega)$ near $1/\omega = 0$ for $t \to 0+$. There must be a closest branch point which approaches the origin of the $1/\sqrt{\omega}$ plane like t^{Δ} to account for the region of zero measure which, as we have seen, shrinks to zero at that rate. There could perhaps be another branch point close behind it at which the measure again becomes zero. It will suffice to consider the leading pair as $\psi' \geq 0$ and the contribution from others will add to the total result—that is, no cancellation can occur. Consequently, in this vicinity we must have

$$\psi'(\omega) \propto \lim_{\epsilon\to 0} \omega^{-1/2}\{[-\omega^{-1}+K(t+i\epsilon)^{2\Delta}]^{\delta_1} - [-\omega^{-1}+K(t-i\epsilon)^{2\Delta}]^{\delta_1}\}\{[\omega^{-1}-K(t+i\epsilon)^{2\Delta}/(1+(t+i\epsilon)^E)]^{\delta_2} - [\omega^{-1}-K(t-i\epsilon)^{2\Delta}/(1+(t-i\epsilon)^E)]^{\delta_2}\}, \tag{5.28}$$

[30] See Eq. (II.51) of Ref. 3.

where $\delta_1+\delta_2=1/2\delta$. This form is fixed by taking the limit as $t\to 0$ from (5.20), and the expression in terms of ω^{-1} comes from (5.26). To see that $\delta_1+\delta_2=1/2\delta$ we merely repeat the analysis of (5.15)–(5.20) on form (5.28) and at once obtain this restriction. We remark that Suzuki[31] worked out the asymptotic form of $\psi'(\omega)$ as $\omega\to\infty$ for mean-field theory and gets exact agreement with form (5.28), except the last factor is replaced by unity, i.e., there is no confluence of singularities. He finds $2\Delta=3$ and $\delta_1=\frac{1}{6}$, as they should be. Although the coefficient of the right-hand side of (5.28) must go to a function regular in $\omega^{-1/2}$, $0<\omega<\infty$ when t goes to zero, there can remain, for example, a fixed singularity at $\omega^{-1}=0$. The $\omega^{-1/2}$ factor in (5.28) is an example of such a singularity which produces a fixed square-root branch point (as a function of τ^2) which suddenly appears at the critical point. This branch point may be thought of as having been on a different Riemann sheet and being revealed by the motion of the critical point singularity. If the coefficient of the right-hand side of (5.28) contains an additive term like $\exp(-\omega)$, for example, there would remain an essential singularity on the line $\tau=0$, $T<T_c$. We will assume however that the index Δ' exist. More than that, we will further assume that the A_n' [analogus to (5.11) but for $T<T_c$] obey a condition similar to (5.13). That is, that the ratio A_{n+1}'/A_n' tends to a finite limit. This assumption is well supported by the numerical evidence[14] as pointed out in the previous section. It also serves to eliminate an essential singularity on the line $\tau=0$, $T<T_c$. The factor of $1+(t+i\epsilon)^E$ is to take account of the possible confluence of the singularities ($E>0$). If $E\neq 0$, then this measure leads to a value of $\gamma<\Delta(\delta-1)/\delta$ in accordance with (5.22). We know, however, that $\psi'(\omega)$ is analytic in t in a neighborhood of t real, even at $t=0$ as $G(\tau)$ is, $\mathrm{Re}\,\tau()>0$. Thus, we may analytically continue (5.28) around the apparent singularity at $t=0$ through complex values of t to $t<0$ and real. This analytic continuation must therefore extend (5.28) to $t<0$ and validates the limiting-process definition given. Hence, we find that the contribution from this singularity yields, using (5.27) and (5.28),

$$\beta=\Delta/\delta,\quad \gamma'=[(\delta-1)/\delta]\Delta. \qquad (5.29)$$

Furthermore, translating back to G from $\psi'(\omega)$ by means of (5.24), and selecting the proper square root of $-\tau^2$ to throw the singularities into the left half τ plane, we find that singularity is preceding like $|t|^{\Delta}$. However, there may be singularities in the coefficient of the right-hand side of (5.28) from another Riemann sheet which are proceeding more slowly. Hence

$$\Delta'\geq\Delta. \qquad (5.30)$$

We have now, however, established the results necessary to obtain the low-temperature analog of (5.23). Hence we conclude that

$$\delta\geq\Delta'/(\Delta'-\gamma'), \qquad (5.31)$$

since other singularities might contribute a larger value of δ, but cannot cancel the one contributed by this singularity.

From (5.1) we obtain for the zero-field free energy

$$F/kT=-\ln 2+\int_0^\infty \ln(1+\omega)d\varphi(\omega). \qquad (5.32)$$

If we use the asymptotic values (5.14)–(5.19) for the measure function, we may compute the free energy to leading order. The specific-heat critical exponent contributed by each singularity is found to be

$$\alpha=2+\gamma-2\Delta. \qquad (5.33)$$

We note that if $d\varphi$ tends smoothly to zero as ω tends to $R(T)$, the logarithmic factor in (5.32) does not carry over to the specific-heat singularity. However, in a case like (5.28), where there can be a narrow peak of measure moving to ω equals infinity and $\gamma'\neq\gamma$, then the logarithmic factor is carried over to the specific-heat singularity. The case $\alpha=0$ is special and a logarithm may or may not occur there. For the low-temperature side, asymptotic evaluation leads to the conclusion

$$\alpha'=2+\gamma'-2\Delta', \qquad (5.34)$$

for each singularity. The extra logarithmic factor does not seem to carry over to the specific-heat singularity here, except of course $\alpha'=0$ may or may not correspond to a logarithm. All of these remarks are not to say that logarithmic factors cannot occur, but that if they do occur, they will occur in the various critic a exponents in a consistent manner.

We will now give an example which shows that the room to extend our results (as distinguished from proving our hypotheses) is rather limited. Consider an Ising model made up of two noninteracting subsystems, each of which has the same critical temperature. It then follows easily that the susceptibility with the larger critical exponent will dominate and γ will be the maximum of γ_1 and γ_2. The same will be true of all the other exponents. For example, if we have relations

$$\delta_1=\Delta_1'/(\Delta_1'-\gamma_1'),\quad \delta_2=\Delta_2'/(\Delta_2'-\gamma_2'), \qquad (5.35)$$

then

$$\begin{aligned}\delta&=\max[\Delta_1'/(\Delta_1'-\gamma_1'),\Delta_2'/(\Delta_2'-\gamma_2')]\\ &\geq\max[\Delta'/(\Delta'-\gamma_1'),\Delta'/(\Delta'-\gamma_2')]\\ &=\Delta'/(\Delta'-\gamma'),\end{aligned} \qquad (5.36)$$

where

$$\Delta'=\max[\Delta_1',\Delta_2'],\quad \gamma'=\max[\gamma_1',\gamma_2'], \qquad (5.37)$$

so that even though both subsystems satisfy the Widom[32] relation, the combined system need not. Certainly one would not expect the scaling hypotheses

[31] M. Suzuki, Progr. Theoret. Phys. (Kyoto) **38**, 1225 (1967).

[32] B. Widom, J. Chem. Phys. **41**, 1633 (1964).

to be valid for such a system. Coopersmith[33] has shown that analyticity by itself does not preclude asymmetry in the critical exponents, although his example does not satisfy the conditions of the Yang-Lee theorem[8] [it violates (5.23), for example].

Let us now summarize the restriction on the possible values which the critical exponents can attain. The result can be gotten by thinking of the contribution from a set of singularities S_i. Each singularity will contribute the exponent set

$$\{S_i: \Delta_i,\delta_i,\Delta_i'\geq\Delta_i,\quad \gamma_i'=(\delta_i-1)\Delta_i'/\delta_i,\quad \gamma_i\leq\gamma_i',\\ \alpha_i'=2+\gamma_i'-2\Delta_i',\quad \alpha_i=2+\gamma_i-2\Delta_i,\\ -\beta_i=-\Delta_i'/\delta_i\}. \tag{5.38}$$

Singularities on the other sheet do not contribute to the high-temperature indices. Then any critical exponent E will be the maximum over the singularities S_i of E_i. (Note that we use $-\beta$ as the magnetization exponent, since the smallest β dominates the larger ones.) From this construction we can derive various relations. For example,

$$\Delta\leq\Delta',\quad \gamma\leq\gamma',\quad \alpha\leq\alpha',\\ \Delta'/\beta\geq\delta\geq\Delta'/(\Delta'-\gamma')\geq\Delta/(\Delta-\gamma),\\ \alpha'+2\beta+\gamma'\geq 2,\quad \alpha'+\beta(1+\delta)\geq 2. \tag{5.39}$$

We have assumed that the various exponents required exist and that the free energy is analytic for real T and H in the neighborhood of $H=0$, $T>T_C$, an extension of the proved result[11] ($T>T_G>T_C$). We also assumed the existence of all derivatives with respect to magnetic field on the phase boundary, and a condition on their magnitude.

In addition, our results imply (at least in the neighborhood of T_C) that on the magnetic phase boundary for $T<T_C$ the free energy is analytic in T and H. This property is contrary to that of the droplet model. Fisher[12,18,4] has shown that, for this model, the line $H=0$ is an essential singularity $0<T<\infty$. The droplet model is not a counterexample to our result since it fails to have the analyticity property proved by Gallavotti *et al.* for Ising models. Plainly this property is essential to our results.

Essam and Hunter[14] have made a detailed analysis of the exact series expansions for the three-dimensional Ising model and estimate

$$\Delta=1.563\pm0.003.\\ \Delta'=1.60\ \pm0.05. \tag{5.40}$$

Baker and Gaunt[7] have carefully studied the series expansions below T_C and estimate

$$\beta=0.312_{-0.005}^{+0.002}. \tag{5.41}$$

[33] M. H. Coopersmith, Phys. Rev. 172, 230 (1968).

In addition, we have the estimate[4] of

$$\gamma=1.250\pm0.003. \tag{5.42}$$

Substituting these estimates into (5.39),

$$\Delta'/\beta\geq\delta\geq\Delta/(\Delta-\gamma),$$

yields

$$5.13_{-0.19}^{+0.24}\geq\delta\geq4.99_{-0.08}^{+0.09}, \tag{5.43}$$

so that δ can differ from 5.15 by at most 0.25, which encompasses most previous estimates.

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APPENDIX: ψ POLYNOMIALS

sq Lattice

$\psi_1=-4+4M^2$,

$\psi_2=4-24M^2+20M^4$,

$\psi_3=-4+68M^2-168M^4+104M^6$,

$\psi_4=12-168M^2+760M^4-1160M^6+556M^8$,

$\psi_5=-20+436M^2-2776M^4+7192M^6-7880M^8+3048M^{10}$,

$\psi_6=44-1128M^2+9356M^4-34\,592M^6+62\,176M^8-52\,928M^{10}+17\,072M^{12}$,

$\psi_7=-84+2868M^2-30\,064M^4+145\,840M^6-371\,240M^8+508\,232M^{10}-352\,880M^{12}+97\,328M^{14}$,

$\psi_8=188-7256M^2+93\,176M^4-566\,968M^6+1\,889\,032M^8-3\,631\,064M^{10}+4\,001\,592M^{12}-2\,341\,752M^{14}+563\,052M^{16}$,

$\psi_9=-372+18\,164M^2-280\,272M^4+2\,078\,864M^6-8\,660\,120M^8+21\,699\,832M^{10}-33\,341\,968M^{12}+30\,685\,008M^{14}-15\,497\,080M^{16}+3\,297\,944M^{18}$,

$\psi_{10}=788-44\,392M^2+817\,092M^4-7\,259\,168M^6+36\,754\,592M^8-114\,841\,440M^{10}+229\,164\,816M^{12}-292\,475\,392M^{14}+230\,756\,064M^{16}-102\,397\,840M^{18}+19\,524\,880M^{20}$,

$\psi_{11}=-1604+107\,460M^2-2\,316\,072M^4+24\,277\,480M^6-146\,498\,200M^8+554\,665\,848M^{10}-1\,376\,525\,280M^{12}+2\,274\,300\,512M^{14}-2\,478\,205\,704M^{16}+1\,709\,581\,544M^{18}-676\,063\,264M^{20}+116\,677\,280M^{22}$,

$\psi_{12}=3444-258\,504M^2+6\,427\,864M^4-78\,299\,560M^6$
$+553\,952\,980M^8-2\,489\,181\,632M^{10}$
$+7\,463\,499\,392M^{12}-15\,296\,652\,096M^{14}$
$+21\,518\,331\,408M^{16}-20\,435\,567\,088M^{18}$
$+12\,516\,708\,496M^{20}-4\,461\,912\,368M^{22}$
$+702\,947\,664M^{24}$,

$\psi_{13}=-7204+620\,356M^2-17\,554\,072M^4$
$+245\,188\,312M^6-2\,004\,706\,240M^8$
$+10\,513\,555\,648M^{10}-37\,283\,928\,480M^{12}$
$+92\,073\,363\,232M^{14}-160\,287\,439\,384M^{16}$
$+196\,044\,178\,488M^{18}-164\,870\,758\,432M^{20}$
$+90\,765\,662\,624M^{22}-29\,443\,477\,952M^{24}$
$+4\,265\,303\,104M^{26}$,

$\psi_{14}=15\,660-1\,483\,368M^2+47\,311\,260M^4$
$-749\,341\,664M^6+6\,994\,337\,296M^8$
$-42\,218\,177\,936M^{10}+174\,126\,684\,064M^{12}$
$-507\,121\,822\,400M^{14}+1\,061\,173\,789\,936M^{16}$
$-1\,602\,697\,933\,600M^{18}+1\,732\,198\,074\,416M^{20}$
$-1\,306\,491\,196\,576M^{22}+652\,984\,363\,120M^{24}$
$-194\,286\,909\,008M^{26}+26\,042\,288\,800M^{28}$,

$\psi_{15}=-33\,316+3\,540\,484M^2-126\,088\,560M^4$
$+2\,243\,537\,840M^6-23\,661\,453\,648M^8$
$+162\,471\,081\,872M^{10}-768\,760\,181\,168M^{12}$
$+2\,596\,569\,460\,464M^{14}-6\,392\,150\,025\,848M^{16}$
$+11\,579\,571\,149\,976M^{18}-15\,424\,214\,072\,912M^{20}$
$+14\,922\,957\,259\,280M^{22}-10\,199\,134\,928\,144M^{24}$
$+4\,666\,432\,232\,912M^{26}-1\,282\,076\,329\,040M^{28}$
$+159\,874\,849\,808M^{30}$.

t Lattice

$\psi_1=-6+6M^2$,
$\psi_2=6-48M^2+42M^4$,
$\psi_3=6+130M^2-424M^4+288M^6$,
$\psi_4=6-144M^2+1752M^4-3552M^6+1938M^8$,
$\psi_5=6+18M^2-3888M^4+19\,464M^6$
$-28\,548M^8+12\,948M^{10}$,
$\psi_6=18+32M^2+4630M^4-62\,368M^6+194\,480M^8$
$-223\,312M^{10}+86\,520M^{12}$,
$\psi_7=66-18M^2-1728M^4+123\,840M^6-802\,788M^8$
$+1\,814\,628M^{10}-1\,713\,384M^{12}+579\,384M^{14}$,
$\psi_8=78+1488M^2-9864M^4-120\,912M^6+2\,142\,960M^8$
$-9\,070\,896M^{10}+16\,110\,408M^{12}-12\,937\,392M^{14}$
$+3\,884\,130M^{16}$,
$\psi_9=138-330M^2+36\,336M^4-158\,704M^6$
$-3\,283\,900M^8+29\,975\,580M^{10}-93\,928\,536M^{12}$
$+137\,649\,576M^{14}-96\,314\,812M^{16}+26\,024\,652M^{18}$,
$\psi_{10}=546-3168M^2-15\,642M^4+740\,640M^6$
$+279\,384M^8-62\,865\,168M^{10}+369\,200\,976M^{12}$
$-914\,667\,840M^{14}+1\,141\,580\,244M^{16}$
$-708\,376\,992M^{18}+174\,127\,020M^{20}$.

d Lattice

$\psi_1=-4+4M^2$,
$\psi_2=4-24M^2+20M^4$,
$\psi_3=-4+68M^2-168M^4+104M^6$,
$\psi_4=4-136M^2+712M^4-1128M^6+548M^8$,
$\psi_5=-4+228M^2-2104M^4+6264M^6$
$-7288M^8+2904M^{10}$,
$\psi_6=28-488M^2+5340M^4-24\,608M^6+50\,160M^8$
$-45\,888M^{10}+15\,456M^{12}$,
$\psi_7=-52+1300M^2-14\,048M^4+82\,144M^6$
$-246\,376M^8+378\,504M^{10}-284\,128M^{12}$
$+82\,656M^{14}$,
$\psi_8=100-3336M^2+39\,720M^4-263\,464M^6$
$+1\,015\,608M^8-2\,235\,560M^{10}+2\,742\,568M^{12}$
$-1\,740\,040M^{14}+444\,404M^{16}$,
$\psi_9=-148+7508M^2-110\,784M^4+840\,768M^6$
$-3\,858\,072M^8+10\,947\,960M^{10}-18\,947\,200M^{12}$
$+19\,293\,952M^{14}-10\,576\,632M^{16}+2\,402\,648M^{18}$,
$\psi_{10}=580-18\,184M^2+297\,780M^4-2\,617\,632M^6$
$+13\,984\,752M^8-48\,098\,080M^{10}+107\,318\,592M^{12}$
$-152\,676\,096M^{14}+132\,683\,872M^{16}$
$-63\,934\,256M^{18}+13\,058\,672M^{20}$,
$\psi_{11}=-1252+48\,420M^2-814\,808M^4+7\,964\,376M^6$
$-48\,733\,992M^8+196\,697\,288M^{10}$
$-535\,450\,560M^{12}+980\,841\,408M^{14}$
$-1\,183\,038\,200M^{16}+895\,925\,336M^{18}$
$-384\,748\,656M^{20}+71\,310\,640M^{22}$,
$\psi_{12}=3148-130\,920M^2+2\,323\,048M^4-24\,326\,024M^6$
$+165\,545\,772M^8-764\,053\,632M^{10}$
$+2\,448\,202\,368M^{12}-5\,480\,864\,640M^{14}$
$+8\,494\,895\,904M^{16}-8\,884\,620\,848M^{18}$
$+5\,958\,449\,264M^{20}-2\,306\,397\,616M^{22}$
$+390\,974\,176M^{24}$,

$\psi_{13}=-5860+330\,628M^2-6\,646\,920M^4+75\,256\,712M^6-558\,151\,376M^8+2\,873\,148\,112M^{10}-10\,532\,341\,184M^{12}+27\,775\,023\,552M^{14}-52\,589\,440\,600M^{16}+70\,509\,348\,472M^{18}-65\,042\,506\,832M^{20}+39\,123\,143\,824M^{22}-13\,777\,878\,896M^{24}+2\,150\,720\,368M^{26}$,

$\psi_{14}=18\,700-844\,776M^2+18\,563\,644M^4-231\,464\,096M^6+1\,873\,779\,312M^8-10\,606\,817\,072M^{10}+43\,515\,616\,352M^{12}-131\,415\,004\,736M^{14}+293\,063\,673\,264M^{16}-479\,387\,394\,016M^{18}+565\,476\,850\,352M^{20}-466\,224\,610\,656M^{22}+254\,105\,136\,752M^{24}-82\,051\,191\,664M^{26}+11\,863\,688\,640M^{28}$,

$\psi_{15}=-40\,340+2\,194\,740M^2-51\,210\,064M^4+698\,158\,992M^6-6\,200\,038\,528M^8+38\,512\,552\,000M^{10}-174\,733\,436\,432M^{12}+592\,425\,233\,744M^{14}-1\,514\,585\,190\,984M^{16}+2\,917\,028\,903\,464M^{18}-4\,191\,791\,943\,888M^{20}+4\,408\,714\,825\,744M^{22}-3\,283\,529\,402\,464M^{24}+1\,635\,230\,364\,192M^{26}-487\,317\,529\,552M^{28}+65\,596\,559\,376M^{30}$,

$\psi_{16}=113\,780-5\,886\,872M^2+142\,720\,360M^4-2\,080\,285\,816M^6+20\,115\,514\,872M^8-136\,900\,632\,792M^{10}+683\,603\,876\,712M^{12}-2\,572\,648\,458\,552M^{14}+7\,402\,922\,305\,992M^{16}-16\,362\,146\,743\,576M^{18}+27\,674\,931\,590\,984M^{20}-35\,410\,433\,388\,536M^{22}+33\,569\,953\,950\,264M^{24}-22\,783\,917\,643\,992M^{26}+10\,440\,608\,476\,808M^{28}-2\,887\,603\,419\,064M^{30}+363\,457\,909\,428M^{32}$.

sc Lattice

$\psi_1=-6+6M^2$,

$\psi_2=6-48M^2+42M^4$,

$\psi_3=-6+166M^2-460M^4+300M^6$,

$\psi_4=30-456M^2+2544M^4-4296M^6+2178M^8$,

$\psi_5=-54+1350M^2-10\,596M^4+32\,196M^6-38\,916M^8+16\,020M^{10}$,

$\psi_6=318-5248M^2+42\,946M^4-181\,216M^6+369\,428M^8-345\,328M^{10}+119\,100M^{12}$,

$\psi_7=-726+19\,782M^2-184\,584M^4+927\,528M^6-2\,616\,948M^8+3\,983\,172M^{10}-3\,021\,720M^{12}+893\,496M^{14}$,

$\psi_8=3726-80\,280M^2+818\,040M^4-4\,678\,008M^6+16\,233\,120M^8-33\,998\,232M^{10}+41\,118\,840M^{12}-26\,171\,640M^{14}+6\,754\,434M^{16}$,

$\psi_9=-9718+313\,462M^2-3\,652\,248M^4+23\,582\,584M^6-95\,235\,036M^8+248\,261\,580M^{10}-410\,841\,928M^{12}+411\,094\,696M^{14}-224\,902\,468M^{16}+51\,389\,076M^{18}$,

$\psi_{10}=49\,974-1\,297\,728M^2+16\,324\,842M^4-118\,033\,824M^6+542\,967\,612M^8-1\,669\,027\,632M^{10}+3\,455\,409\,588M^{12}-4\,709\,249\,472M^{14}+4\,010\,484\,780M^{16}-1\,920\,738\,528M^{18}+393\,110\,388M^{20}$,

$\psi_{11}=-139\,974+5\,198\,310M^2-73\,026\,276M^4+585\,585\,444M^6-3\,028\,136\,556M^8+10\,677\,478\,428M^{10}-26\,256\,889\,632M^{12}+44\,863\,474\,848M^{14}-51\,848\,181\,972M^{16}+38\,375\,893\,092M^{18}-16\,322\,543\,160M^{20}+3\,021\,287\,448M^{22}$,

$\psi_{12}=728\,022-21\,952\,200M^2+327\,269\,360M^4-2\,879\,498\,504M^6+16\,559\,709\,770M^8-65\,892\,382\,464M^{10}+186\,837\,761\,024M^{12}-380\,796\,817\,024M^{14}+552\,180\,243\,236M^{16}-553\,009\,884\,688M^{18}+361\,531\,476\,512M^{20}-138\,152\,293\,968M^{22}+23\,315\,640\,924M^{24}$.

bcc Lattice

$\psi_1=-8+8M^2$,

$\psi_2=8-80M^2+72M^4$,

$\psi_3=-8+328M^2-976M^4+656M^6$,

$\psi_4=104-1136M^2+6640M^4-11\,696M^6+6088M^8$,

$\psi_5=-200+4616M^2-34\,544M^4+108\,592M^6-135\,728M^8+57\,264M^{10}$,

$\psi_6=1880-26\,320M^2+186\,712M^4-767\,488M^6+1\,600\,768M^8-1\,539\,104M^{10}+543\,552M^{12}$,

$\psi_7=-5288+132\,392M^2-1\,106\,240M^4+5\,135\,936M^6-14\,274\,960M^8+22\,099\,472M^{10}-17\,178\,176M^{12}+5\,196\,864M^{14}$,

$$\psi_8 = 44\,072 - 771\,632M^2 + 6\,807\,856M^4 - 35\,037\,360M^6 + 114\,817\,808M^8 - 237\,744\,112M^{10} + 291\,377\,712M^{12} - 189\,484\,400M^{14} + 49\,990\,056M^{16},$$

$$\psi_9 = -143\,560 + 4\,145\,352M^2 - 42\,281\,728M^4 + 243\,122\,432M^6 - 900\,699\,312M^8 + 2\,242\,834\,736M^{10} - 3\,673\,093\,248M^{12} + 3\,713\,856\,384M^{14} - 2\,071\,075\,024M^{16} + 483\,333\,968M^{18},$$

$$\psi_{10} = 1\,165\,704 - 24\,644\,304M^2 + 264\,493\,800M^4 - 1\,684\,554\,752M^6 + 6\,997\,557\,824M^8 - 20\,002\,116\,448M^{10} + 39\,826\,568\,000M^{12} - 53\,724\,506\,368M^{14} + 46\,125\,717\,664M^{16} - 22\,473\,207\,392M^{18} + 4\,693\,526\,272M^{20},$$

$$\psi_{11} = -4\,144\,200 + 136\,480\,392M^2 - 1\,659\,001\,872M^4 + 11\,639\,673\,296M^6 - 53\,730\,081\,296M^8 + 173\,043\,357\,584M^{10} - 399\,332\,355\,136M^{12} + 658\,948\,695\,872M^{14} - 753\,636\,008\,624M^{16} + 561\,275\,110\,960M^{18} - 242\,430\,982\,208M^{20} + 45\,749\,255\,232M^{22},$$

$$\psi_{12} = 33\,266\,904 - 822\,723\,600M^2 + 10\,432\,080\,336M^4 - 79\,866\,919\,568M^6 + 406\,862\,380\,696M^8 - 1\,461\,077\,755\,840M^{10} + 3\,819\,172\,893\,504M^{12} - 7\,352\,468\,491\,584M^{14} + 10\,324\,354\,362\,976M^{16} - 10\,228\,962\,320\,512M^{18} + 6\,717\,611\,029\,696M^{20} - 2\,602\,671\,071\,808M^{22} + 447\,403\,268\,800M^{24}.$$

fcc Lattice

$$\psi_1 = -12 + 12M^2,$$

$$\psi_2 = 12 - 168M^2 + 156M^4,$$

$$\psi_3 = 36 + 764M^2 - 2792M^4 + 1992M^6,$$

$$\psi_4 = 180 - 1464M^2 + 20\,808M^4 - 44\,952M^6 + 25\,428M^8,$$

$$\psi_5 = 948 - 2484M^2 - 75\,192M^4 + 444\,696M^6 - 692\,952M^8 + 324\,984M^{10},$$

$$\psi_6 = 5556 - 13\,432M^2 + 126\,292M^4 - 2\,426\,656M^6 + 8\,510\,960M^8 - 10\,355\,296M^{10} + 4\,152\,576M^{12},$$

$$\psi_7 = 36\,132 - 75\,204M^2 - 47\,856M^4 + 7\,877\,040M^6 - 61\,407\,096M^8 + 152\,077\,272M^{10} - 151\,515\,216M^{12} + 53\,054\,928M^{14},$$

$$\psi_8 = 256\,452 - 579\,624M^2 + 288\,552M^4 - 13\,755\,144M^6 + 282\,680\,664M^8 - 1\,351\,689\,960M^{10} + 2\,586\,921\,768M^{12} - 2\,182\,086\,792M^{14} + 677\,964\,084M^{16}.$$