mine the precise properties of the polarization in the neighborhood of the boundary plane. Consistent with the approximations made in this paper we neglect the effect of the semiconducting properties on the behavior of the polarization and assume that the polarization follows closely the deformation of the lattice as determined crystallographically.

A sigificant advantage in being able to produce large single domain ferroelectric crystals, as well as sharp paraelectric-ferroelectric phase boundaries, is that one can readily study transport, optical, dielectric, and elastic properties both above and below the Curie point in unpoled crystals. We show, for example, in Figs. 3 and 4, the resistance anisotropy and infrared dichroism measured as a function of temperature on two high-quality KTN crystals. Above the Curie point where the crystals are cubic both properties are isotropic. The resistivity data of Fig. 3 obtained using a four-terminal method show that the resistance increases parallel to the polarization or c axis and decreases slightly in the perpendicular direction. The activation energy above T_c, $E_a \approx 120$ mV, corresponds to donors situated approximately 0.24 eV below the conduction band edge. The optical data of Fig. 4 were obtained at a wavelength of 1.985 μ corresponding to the peak in the near infrared donor photo-ionization absorption. These data show a discontinuous first-order change in the absorption coefficient at the Curie point. In the ferroelectric phase the absorption is greater for light polarized perpendicular to the crystal c axis ($E\perp c$). Results of a complete study of transport and optical properties of KTN in the vicinity of the Curie point will be reported in the near future.

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Ising-Model Critical Indices below the Critical Temperature*

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We review the estimates for the critical indices of the Ising model below T_C and conclude (for 3 dimensions): $\alpha'=0.066_{-0.04}^{+0.16}$, $\beta=0.312_{-0.005}^{+0.002}$, $\gamma'=1.310_{-0.05}^{+0.04}$ for the specific heat, magnetization, and magnetic susceptibility, respectively. For 2 dimensions, we estimate $\gamma'=1.75_{-0.00}^{+0.01}$. In order to explain previous estimates of $\alpha'=0$, we point out that a low power can, in practice, look deceptively like a logarithm. Finally, we discuss the behavior of the specific heat at constant magnetization.

1. INTRODUCTION AND SUMMARY

In recent years, various workers have estimated from power-series expansions the various critical indices for the two- and three-dimensional Ising model. In 1963 it was speculated[1] that a certain relation must hold between three of the critical indices below the critical point. Later that year, this conjectured equality was proved as a rigorous inequality.[2] Unfortunately, the best available estimates at that time failed, by $6\frac{1}{4}\%$, to satisfy this relation for the three-dimensional Ising model, although they satisfied it for the two-dimensional model. It is the purpose of this paper to critically re-examine the various estimates, to attempt to establish realistic error bounds on them, and to reconcile them with all available information.

We conclude from our study that C_M/C_H is probably continuous at T_c for the three-dimensional Ising model and that it is continuous for the two-dimensional model. As a consequence

$$2\leq\alpha'+2\beta+\gamma'<2+\epsilon, \tag{1.1}$$

where $\epsilon\sim0.1$ for three dimensions and 0.01 for two

* Part of this work performed under the auspices of the U. S. Atomic Energy Commission.

[1] J. W. Essam and M. E. Fisher, J. Chem. Phys. 38, 802 (1963).

[2] G. S. Rushbrooke, J. Chem. Phys. 39, 842 (1963).

dimensions. The indices α', β, and γ' refer to the specific heat, magnetization, and magnetic susceptibility, respectively. We also consider the ratio γ'/β for three-dimensional lattices and conclude

$$\gamma'/\beta=4.2\pm0.1. \tag{1.2}$$

As a third relation (for three-dimensional lattices), we use estimates of β and conclude

$$\beta=0.312_{-0.005}^{+0.002}. \tag{1.3}$$

Combining these results, we obtain the estimates

$$\gamma'=1.310_{-0.05}^{+0.04}, \tag{1.4}$$
$$\alpha'=0.066_{-0.04}^{+0.16},$$

for the critical indices. In addition we demonstrate how, to the extent for which convergence had been obtained (namely, to more than 90% of T_c), a divergence rate of $\frac{1}{16}$, say, very closely approximates a logarithm. Thus we reconcile (1.4) with previous estimates that $\alpha'=0$, which corresponds to a logarithmic divergence.

In Sec. 6 we use the results of our study of C_M/C_H to deduce the behavior of the specific heat at constant magnetization.

2. THE RUSHBROOKE-ESSAM-FISHER RELATION

Essam and Fisher[1] conjectured the following relation between the critical indices:

$$\alpha'+2\beta+\gamma'=2, \tag{2.1}$$

where for $H=0$ and $T\to T_c^-$ we have

$$\alpha'=-\lim_{T\to T_c^-}(T-T_c)\frac{d\ln C_H}{dT},$$
$$\beta=\lim_{T\to T_c^-}(T-T_c)\frac{d\ln M}{dT}, \tag{2.2}$$
$$\gamma'=-\lim_{T\to T_c^-}(T-T_c)\frac{d\ln\chi}{dT}.$$

In (2.2), C is the specific heat, M is the magnetization, χ is the magnetic susceptibility, H is the magnetic field, T is the temperature, and T_c is the critical temperature.

Rushbrooke[2] showed that the thermodynamic relation[3]

$$C_H-C_M=T(\partial M/\partial T)^2{}_H(\partial H/\partial M)_T \tag{2.3}$$

rigorously implies that

$$\alpha'+2\beta+\gamma'\geq 2. \tag{2.4}$$

In this section we investigate whether equality (2.1) or inequality (2.4) hold for the nearest-neighbor, ferromagnetic Ising model. To this end, we rearrange equation (2.3) as

$$\frac{C_M}{C_H}=1-T(\partial M/\partial T)_H{}^2/(C_H\chi). \tag{2.5}$$

Since C_M and C_H are principle specific heats,[2] their ratio is non-negative; furthermore, since the second term on the right-hand side of (2.5) is positive, C_M/C_H is less than or equal to unity. It is sufficient for equality (2.1) to hold that

$$\lim_{T\to T_c^-} C_M/C_H<1. \tag{2.6}$$

If this limit is unity, then the inequality may hold. It need not, however, because the rate of approach may be, for example, logarithmic, so that

$$\lim_{T\to T_c^-}(T-T_c)\frac{d}{dT}\ln[1-C_M/C_H]=0. \tag{2.7}$$

When $T>T_c$, $M=0$ and it follows from (2.5) that $C_M/C_H\equiv1$. The problem, then, is to decide whether C_M/C_H is continuous at T_c. We find that, in fact, the most difficult situation for interpretation, i.e., C_M/C_H apparently very close to unity, holds.

In order to investigate C_M/C_H we used the series data of Sykes, Essam, and Gaunt[4] to compute the power series expansions of

$$C_M/C_H=(2/q)u^{q/2-1}+\cdots, \tag{2.8}$$

where q is the coordination number and

$$u=\exp(-4J/kT).$$

For the simple quadratic (sq), triangular (t), diamond (d), simple cubic (sc), body-centered cubic (bcc), and face-centered cubic (fcc) lattices, we obtain series through u^n for $n=7$, 10, 10, 16, 24, and 27, respectively. Since the honeycomb lattice (h) has an odd coordination number, the expansion variable $z=u^{1/2}$ is used in (2.8) for this lattice, and the series is obtained through order z^{10}.

We now compute the $[N,N]$ and $[N,N-1]$ Padé approximants[5] to these series and form a table of values for each approximant. As can be seen from (2.8), C_M/C_H is initially zero and starts off quite small. In a favorable case, we obtain convergence up to an argument of around 96% of u_c. At this value of the argument, C_M/C_H is apparently less than $\frac{1}{2}$ for all lattices and appreciably less for some. Nevertheless, it is changing sufficiently rapidly in this region to prevent

[3] See, for example, P. S. Epstein, *Textbook of Thermodynamics* (J. Wiley & Sons, Inc., New York, 1937), Eq. (20.23).

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

[5] See G. A. Baker, Jr., in *Advances in Theoretical Physics*, edited by K. A. Brueckner (Academic Press Inc., New York, 1965), Vol. 1, p. 1, for a review article on the Padé approximant method.

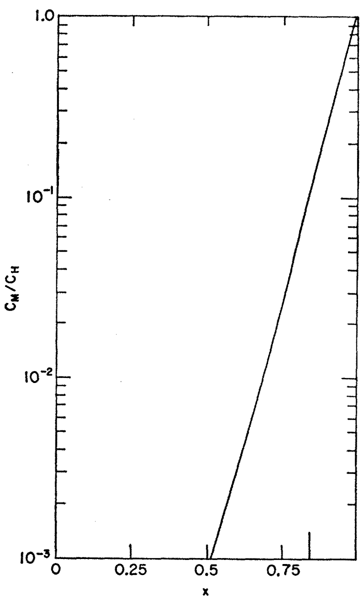

FIG. 1. C_M/C_H below T_c for the fcc lattice, based on the [13,14] Padé approximant. The horizontal scale is x of Eq. (2.9) where we have assumed $u_c = 0.66470$. The large tic mark shows the approximate limit of convergence.

one from drawing a firm conclusion about the limit (2.6) by ordinary graphical extrapolation alone.

A likely explanation for this behavior is suggested in two dimensions by the Onsager[6] solution for the specific heat at constant magnetic field. According to his result, the specific heat diverges logarithmically at T_c. Consequently, we expect, by (2.5), that the limit will be approached like $1/[\ln(1-u/u_c)]$. In order to straighten out this behavior, we introduce a new variable

$$x=\frac{\ln(1-u/u_c)/\ln(0.5)}{1+\ln(1-u/u_c)/\ln(0.5)} \tag{2.9}$$

to use as an abscissa. This change will make such trends appear linear. If we then plot C_M/C_H versus x on semilog paper to accommodate the large change in magnitude, we get very nearly straight lines aimed (with varying degrees of accuracy) at the point (1,1) for *all* lattices (and not just the two-dimensional ones), except the diamond lattice for which a lower value of about 0.3 to 0.4 is extrapolated. However, primarily because of a shorter series, convergence was obtained only to about 75% of u_c, and so this result should be less reliable than those for the other lattices. See Fig. 1 for an illustrative case.

If the inequality held instead of the equality, say,

$$\alpha'+2\beta+\gamma'=2+\epsilon, \tag{2.10}$$

then a variable based on $(1/\epsilon)[(1-u/u_c)^{-\epsilon}-1]$ instead of $-\ln(1-u/u_c)$ would be appropriate. The use of this kind of extrapolative procedure tends to lower the predicted value of C_M/C_H at $u=u_c$ and since $\epsilon>0$ requires that $C_M/C_H=1.0$ at $u=u_c'$ the possibilities are quite limited. We conclude that $\epsilon>0.1$ seems inconsistent with all the three-dimensional lattices and $\epsilon=0.0$ seems to be best in accord with the results for them all. For the two-dimensional lattices, a somewhat weaker bound on ϵ is obtained but the same general picture seems consistent with the available information.

Although the sequence of approximants has not converged very well, we mention that, in accordance with the above results, Padé analysis of $d\ln(1-C_M/C_H)/du$ indicates $\epsilon<0.3$ in two dimensions, and $\epsilon<0.09$ in three dimensions. For two dimensions, a consequence of C_M/C_H approaching unity like $1/[\ln(1-u/u_c)]$ together with the exact results on the specific heat[6,7] and on the magnetization[7] is that

$$\chi_0(T)\approx(Nm^2/kT)C^-(1-T/T_c)^{-\gamma'}, \quad (T\to T_c), \tag{2.11}$$

(where $\gamma'=1.75_{-0.00}^{+0.01}$), in accord with the previous results of Essam and Fisher.[1] The upper error estimate in (2.11) is theirs and enables us to deduce $\epsilon\leq0.01$, and the lower one follows from (2.4) and the exact results[6,7] $\alpha'=0$, $\beta=\frac{1}{8}$. Provided that the approach to the limit is logarithmic, there can be no $\ln(1-T/T_c)$ factors multiplying or dividing the right-hand side of (2.11). This has been confirmed by using the Padé-approximant method[5] to analyze the series for

$$-\chi(u_c/u)\ln(1-u/u_c) \quad\text{and}\quad -\chi/(u_c/u)\ln(1-u/u_c).$$

Estimates for the critical amplitude C^- are given by Eq. (18) of Ref. 1.

For three dimensions we obtain the relation between the critical indices,

$$2\leq\alpha'+2\beta+\gamma'<2.1. \tag{2.12}$$

We note in passing that the mean-field approximation satisfies[1] equality (2.1) with $\alpha'=0$, $\beta=\frac{1}{2}$, $\gamma'=1$, for $C_M\equiv0$ here, as can easily been seen from the structure of the energy ($E\propto M^2$). The three-dimensional spherical model,[8,9] on the other hand, is pathological in this respect, since for small H and $T<T_c$,

$$\chi\propto H^{-1/2}(1-T/T_c)^{-3/4}$$

and is thus infinite for all $T<T_c$ when H tends to zero. This result is easily obtained following the standard procedure of the theory of the spherical model.[8,9] In the limit of long-range exponential interactions[9] the mean-field results are recovered even though the above form for χ is valid at any finite range. Such behavior arises because of the nonuniform convergence to the limit.

3. THE DOMB-HUNTER RATIO

In a recent study, Domb and Hunter[10] have speculated that the ratio of critical indices γ'/β is exactly

[6] L. Onsager, Phys. Rev. **65**, 117 (1944).

[7] For a summary of the exact results, see C. Domb, Advan. Phys. **9**, Nos. 34 and 35 (1960).

[8] T. H. Berlin and M. Kac, Phys. Rev. **86**, 821 (1952).

[9] G. A. Baker, Jr., Phys. Rev. **126**, 2071 (1962).

[10] C. Domb and D. L. Hunter, Proc. Phys. Soc. (London) **86**, 1147 (1965).

an even integer. This conjecture is apparently correct for two dimensions ($\gamma'/\beta=14$) and in the mean-field approximation ($\gamma'/\beta=2$); however, as we shall see, it does not seem to be so for the three-dimensional Ising model. That there is no apparent mathematical necessity for γ'/β to be an even integer can be seen by considering the counter-example

$$\ln Z=\operatorname{Im}\{[(u/u_c-1)[(u/u_c-1)^2+H^4]^{9/8}+iH^2]^{31/52}e^{0.01i}\}+\tfrac{1}{10}H\operatorname{Im}\{(u/u_c-1+iH)^{5/16}\},\quad(3.1)$$

where $u=\exp(-4J/kT)$ and Z is the partition function per spin. This function has the critical data $\alpha'=\alpha=\frac{1}{16}$, $\beta=\frac{5}{16}$, $\gamma'=\gamma=1\frac{5}{16}$, and $\gamma'/\beta=4.2$. It also has the properties χ, C_H, C_M, and $M\operatorname{sgn}(H)$ all ≥ 0 (near the critical point). Further, for H small and T near T_c, it is of the form

$$\ln Z\approx F_0(T)+H^2F_2(T)+H^4F_4(T)+\cdots,\quad(3.2)$$

where

$$F_{2r}(T)\sim A_r(1-T/T_c)^{-\gamma-(r-1)\Delta},\; r=1,2,\cdots,\quad(3.3)$$

with $\Delta=3\frac{1}{4}$. An example with three terms instead of the two of (3.1) can be constructed with the same critical data, except $\gamma=1\frac{1}{4}$. Thus the symmetry $\gamma'=\gamma$ is not a mathematical necessity either.

Nevertheless, γ'/β is a useful quantity to estimate, because this estimation may be done in two ways which we believe are independent of each other. We may calculate easily that if $\chi\propto(1-u/u_c)^{-\gamma'}$ and $M\propto(1-u/u_c)^{\beta}$, then

$$\lim_{u\to u_c}\frac{d\ln(\chi)}{d\ln(M)}=\lim_{u\to u_c}\frac{(u-u_c)d\ln(\chi)/du}{(u-u_c)d\ln(M)/du}=-\gamma'/\beta.\quad(3.4)$$

Now we may expand $[d\ln\chi]/[d\ln M]$ as a power series in u and then use the Padé-approximant method[5] to evaluate this ratio as $u\to u_c$. The results of this evaluation are given in Table I.

We conclude from these results that

$$\gamma'/\beta=4.2\pm0.1.\quad(3.5)$$

The results on the diamond lattice are, we feel, not sufficiently converged to say more than that they are not inconsistent with the above conclusion.

A second way to obtain information on the ratio γ'/β is to study the magnetization on the critical isotherm. If we assume that

$$M\propto H^{1/\delta},\quad(T=T_c)\quad(3.6)$$

then it has been conjectured[1,11] that

$$\gamma'=\beta(\delta-1).\quad(3.7)$$

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

From the definitions (2.2), it follows that

$$\frac{\gamma'}{\beta}=-\lim_{T\to T_c^-,\,H=0^+}\frac{M(\partial^2M/\partial T\partial H)|_{H,T}}{(\partial M/\partial H)|_T(\partial M/\partial T)|_H}.\quad(3.8)$$

By the laws of partial differentiation, we may rewrite (3.8) as

$$\frac{\gamma'}{\beta}=\lim_{T\to T_c^-,\,H=0^+}\left[\frac{M(\partial^2H/\partial M^2)|_T}{(\partial H/\partial M)|_T}-\frac{M(\partial^2H/\partial T\partial M)|_{M,T}}{(\partial H/\partial T)|_M}\right].\quad(3.9)$$

If $H(T,M)$ is sufficiently well behaved, then the limit as $T\to T_c^-$ with $H=0^+$ may be replaced by the limit as $M\to 0^+$ with $T=T_c$. [The direction in the (T,M) plane is the same for these two limits provided $\beta<1$]. With this replacement for the first term, we may evaluate it from (3.6). Thus (3.9) becomes

$$\delta-1=\gamma'/\beta+\lim_{M\to 0,\,T=T_c}\frac{M(\partial^2H/\partial M\partial T)|_{M,T}}{(\partial H/\partial T)|_M}.\quad(3.10)$$

If we refer to Fig. 2, we see, as

$$\left.\frac{\partial H}{\partial T}\right|_M=-\frac{(\partial M/\partial T)|_H}{(\partial M/\partial H)|_T}\propto\frac{\beta(1-T/T_c)^{\beta-1}/T_c}{\chi},$$
$$(H=0^+,\quad T\to T_c^-),\quad(3.11)$$

that $(\partial H/\partial T)|_M$ is (a) positive on $T=T_c$, and (b) tends to zero at the critical point if $\beta+\gamma'>1$, by (3.11). Hence as the term in the limit in (3.10) is the logarithmic

TABLE I. The $[N,N]$ and $[N,N-1]$ Padé approximants to $-[d\ln(\chi)]/[d\ln(M)]$ evaluated at u_c.

	fcc	bcc	sc	d
[1,1]				2.77963
[2,1]				b
[2,2]				a
[3,2]				4.71534
[3,3]	a	a	4.24760	4.45428
[4,3]	5.16259	a	4.06029	4.48292
[4,4]	4.14936	a	4.14829	a
[5,4]	3.91190	4.44318	4.36958	a
[5,5]	4.00761	4.15742	4.31533	
[6,5]	4.02015	4.14211	a	
[6,6]	a	a	4.25561	
[7,6]	a	4.20573	a	
[7,7]	4.02906	4.18321	a	
[8,7]	4.11242	4.19061	a	
[9,9]	a	4.16062		
[10,9]	4.19171	4.13076		
[10,10]	4.30571			

[a] Approximants with close-to-each-other poles and zeros near the origin. These are omitted from the tabulation in accordance with the criterion of Sec. IIA of Ref. 5. The missing entries are not there for this same reason.
[b] Approximant does not exist. The low-order Padé approximants were not computed because of large gaps in the early part of the series.

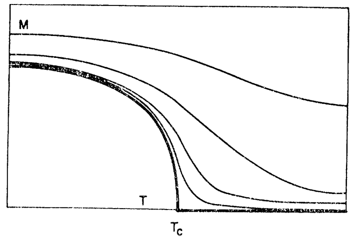

FIG. 2. Sketch of the lines of constant magnetic field in the M versus T plane near the critical point. Dark line represents $H=0^+$.

derivative of $(\partial H/\partial T)|_M$ with respect to $\ln M$ at constant T, it is necessarily positive. We remark we need only assume $(\partial H/\partial T)|_M$ is ultimately of fixed sign for this conclusion to hold.

We conclude that

$$\delta-1\geq\gamma'/\beta, \tag{3.12}$$

when

$$\beta<1, \quad \gamma'+\beta>1, \tag{3.13}$$

hold, as they do for the two- and three-dimensional Ising models, and $H(T,M)$ is sufficiently well-behaved. That (3.12) cannot in general be replaced by an equality without further assumptions can be seen from the example given by replacing in (3.1) the fractions 9/8, 31/52, and $\frac{5}{16}$ by $\frac{2}{5}$, $\frac{5}{8}$, and $\frac{1}{2}$, respectively. The critical data for that partition function are

$$\alpha'=\tfrac{7}{8}, \quad \beta=\tfrac{1}{2}, \quad \gamma'=27/40, \quad \delta=4. \tag{3.14}$$

We note that (2.4) is an inequality for this example as well. We also note that the inequality of Griffiths,[12]

$$(1+\delta)\beta\geq 2-\alpha', \tag{3.15}$$

follows from (3.12) and (2.4).

That the (T,M) plane is a sensible one in which to assume smooth behavior may be made plausible in the following way. The partition function can be written as

$$Z=\sum_{\text{all states}} e^{-\beta(E-H\mathfrak{M})}\rho(E,\mathfrak{M}), \tag{3.16}$$

where ρ gives the number of states as a function of energy E and magnetization $\mathfrak{M}$. The principal contribution will come from a single point in E, $\mathfrak{M}$ space above T_c and below T_c from two points because there is symmetry between $\pm\mathfrak{M}$. At the critical point, the maximum point bifurcates and, so to speak, turns a corner. However, in order to turn this corner, the maximum, as a function of $\mathfrak{M}$ at the critical point must be quite flat. Consequently, smooth behavior is much more plausible in terms of $\mathfrak{M}$ than H where no such argument is available. The singularities introduced in the orthogonal T direction by using T instead of E should not invalidate this assumption.

If, in addition, we assume with Griffiths[13] that $(\partial\chi/\partial H)|_T<0$ near T_c, $H=0^+$, then, as he showed, we obtain

$$\delta-1\leq\gamma'/\beta. \tag{3.17}$$

Combining (3.17) with (3.12) we have shown (3.7), Widom's conjecture. We remark that our example with critical data (3.14) does not satisfy $(\partial\chi/\partial H)|_T\lesssim 0$ because the susceptibility has a ripple in it near T_c. Nevertheless, this additional assumption is not implausible as Griffiths[13] has pointed out, although it is not required thermodynamically.

Gaunt *et al.*[14] have analyzed δ for various lattices and found

$$\delta=5.20\pm0.15, \text{ (three dimensions)}, \qquad \delta=15.00\pm0.08, \text{ (two dimensions)}. \tag{3.18}$$

These results, together with (3.5), (2.11), and the exact result $\beta=\frac{1}{8}$ (two dimensions) show that for the two- and three-dimensional Ising models, (3.7) is apparently satisfied, in accord with the plausible assumptions we have made. Alternatively, they provide additional support for the estimate (three dimensions) $\gamma'/\beta=4.2$.

4. THE CRITICAL INDICES BELOW T_c

In the previous sections, we have estimated two relations between the critical indices α', β, and γ' for three-dimensional lattices. One further relation will suffice to determine these indices. In two dimensions, α' and β are known exactly[6,7] to be

$$\alpha'=0, \quad \beta=\tfrac{1}{8}. \tag{4.1}$$

The best additional result here is Essam and Fisher's estimate[1] of $\gamma'=1.75\pm0.01$ for the triangular and simple quadratic lattices. Relation (2.4) together with (4.1) reduce this range to

$$\gamma'=1.75_{-0.00}^{+0.01}, \tag{4.2}$$

as we noted in (2.11). Although, the errors in the direct estimates on the honeycomb lattice are much larger, we may conclude (4.2) there also from the triangular lattice results on the basis of the transformation theory of Fisher.[15]

To provide a third relation for three dimensions, we have chosen to estimate β directly. We employ the method of Padé approximants applied to $(u-u_c)(d\ln M/du)$ and adopt the estimates of Baker[16] and Essam and Sykes[17] for u_c;

$$\begin{array}{ll} \text{fcc} & 0.664658, \\ \text{bcc} & 0.5326607, \\ \text{sc} & 0.411940, \\ \text{d} & 0.2278. \end{array} \tag{4.3}$$

[12] R. B. Griffiths, Phys. Rev. Letters 14, 623 (1965).
[13] R. B. Griffiths, J. Chem. Phys. 43, 1958 (1965).
[14] D. S. Gaunt, M. E. Fisher, M. F. Sykes, and J. W. Essam, Phys. Rev. Letters 13, 713 (1964).
[15] M. E. Fisher, Phys. Rev. 113, 969 (1959).
[16] G. A. Baker, Jr., Phys. Rev. 124, 768 (1961).
[17] J. W. Essam and M. F. Sykes, Physica 29, 378 (1963).

TABLE II. Estimates of β.

	fcc	bcc	sc	d
[3,2]				−0.2942
[3,3]			−0.2907	−0.2982
[4,3]			a	−0.3061
[4,4]			−0.3012	−0.3135
[5,4]		−0.2997	−0.3032	−0.3094
[5,5]		a	−0.3032	−0.3104
[7,6]		−0.3010	−0.3109	
[7,7]		−0.3051	−0.3066	
[8,7]	−0.2979	−0.3069	−0.3091	
[8,8]	−0.3046	−0.3101	−0.3132	
[9,8]	−0.3069	a	−0.3118	
[9,9]	−0.3066	−0.3389	−0.3100	
[10,9]	a	−0.3133		
[10,10]	−0.3078	−0.3156		
[11,10]	−0.3081	a		
[12,11]	a	−0.3132		
[12,12]	a	−0.3124		
[13,13]	a	−0.3133		
[14,13]	a	−0.3133		
[15,14]	−0.3077			

[a] Approximants with close-to-each-other poles and zeros near the origin. These are omitted from the tabulation in accordance with the criterion of Sec. IIA of Ref. 5.

This work parallels that of Essam and Fisher,[1] except that we have used longer series than they had available. We have given in Table II the estimates for the critical index β based on the indicated Padé approximants. We conclude for all lattices that the estimates are consistent with

$$0.307 \leq \beta \leq 0.314 \quad \text{or} \quad \beta = 0.312_{-0.005}^{+0.002}, \tag{4.4}$$

which agrees with Essam and Fisher, but with somewhat smaller errors.

To summarize the results of Secs. 2 and 3 we have, besides (4.4), the relations

$$\gamma'/\beta = 4.2 \pm 0.1, \tag{4.5}$$

$$2 \leq \alpha' + 2\beta + \gamma' < 2.1. \tag{4.6}$$

These lead to the estimates

$$\gamma' = 1.310_{-0.05}^{+0.04}, \tag{4.7}$$

$$\alpha' = 0.066_{-0.04}^{+0.16}, \tag{4.8}$$

which, together with (4.4), summarize the bounds obtained on the values of the critical indices. It is our present opinion that

$$\alpha' = \tfrac{1}{16}, \quad \beta = \tfrac{5}{16}, \quad \gamma' = 1\tfrac{5}{16}, \quad \delta = 5\tfrac{1}{5}, \tag{4.9}$$

is the set of rational indices which is most consistent with available data. Nevertheless, (4.7) and (4.8) do not convincingly rule out either $\gamma' = \gamma = 1.25$ or $\alpha' = 0$ as have been suggested,[1,17,18] although, of course, (2.4) precludes both these alternatives from holding simultaneously.

[18] G. A. Baker, Jr., Phys. Rev. **129**, 99 (1963).

Satisfactory estimates of the amplitude B in

$$M/mN \approx B(1-T/T_c)^{\beta}, \quad (T \to T_c^-), \tag{4.10}$$

have been given by Essam and Fisher[1] for the fcc, bcc, and sc lattices. We add the result for the diamond lattice:

$$B = 1.661 \pm 0.001. \tag{4.11}$$

For the susceptibility

$$\chi_0(T) \approx \frac{Nm^2}{kT} \frac{(0.193 \pm 0.002)}{[1-T/T_c]^{21/16}}, \quad (T \to T_c^-), \tag{4.12}$$

and for the three-dimensional fcc, bcc, and sc lattices summarize our best estimate near $T = T_c$. For the diamond (d) lattice, the constant is 0.191 ± 0.003. The amplitudes in (4.11) and (4.12) are determined as described in Ref. 16.

5. THE SPECIFIC HEAT AT CONSTANT MAGNETIC FIELD

In Sec. 4 we estimated that the critical index for the divergence in the specific heat was about $\frac{1}{16}$. Previously, it had been shown[18] that there is considerable evidence that the specific heat diverges very much like $\ln(1-T/T_c)$ up to 90–95% of T_c, depending upon the the lattice. For example, in Fig. 3 we have plotted $-(kT/J)^2 C_H/[4kq^2u^{q/2}(\ln(1-u/u_c))u_c/u]$ versus $-\ln(1-u/u_c)$ for the fcc lattice. The final curvature is concave downward and hence although the curve is slowly rising it shows no evidence of a singularity sharper than logarithmic, or $\alpha' = 0$. Further evidence for the diamond lattice has been given[19,20] by comparing its series (reduced to unit critical point) to that of the simple quadratic lattice (similarly reduced) which has a known logarithmic divergence.[6] There too, no evidence was found for a singularity sharper than logarithmic.

Indeed, when the ratios of corresponding coefficients were computed, they were found to change monotoni-

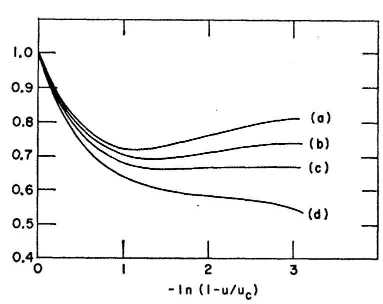

FIG. 3. C_H below T_c for the fcc lattice divided by its leading power series coefficient and divided by (a) $-\ln(1-u/u_c)/(u/u_c)$; (b) $l_{16}(u/u_c)/(u/u_c)$; (c) $l_8(u/u_c)/(u/u_c)$; (d) $l_4(u/u_c)/(u/u_c)$. The horizontal scale is $-\ln(1-u/u_c)$.

[19] D. S. Gaunt and J. W. Essam, in *Proceedings of the International Conference on Magnetism, Nottingham, 1964* (Institute of Physics and The Physical Society, London, 1965), p. 88.

[20] D. S. Gaunt, thesis, University of London (unpublished).

cally, so that the singularity in the simple quadratic lattice seemed sharper than that in the diamond lattice, if anything.

One must now inquire whether these results are strong enough to eliminate a sharper singularity. To this end we consider the functions

$$l_n(x)=n[(1-x)^{-1/n}-1]. \tag{5.1}$$

It is easy to show that

$$\lim_{n\to\infty} l_n(x)=-\ln(1-x), \tag{5.2}$$

for $x<1$, as

$$l_n(x)=x+\frac{(1+1/n)}{2}x^2+\frac{(1+1/n)(2+1/n)}{2\cdot 3}x^3+\cdots$$
$$\to x+\tfrac{1}{2}x^2+\tfrac{1}{3}x^3+\cdots. \tag{5.3}$$

Referring again to Fig. 3, we have plotted various curves using l_n as a divisor instead of ln. Curve (b), for $n=16$, corresponds to our hypothesis of $\alpha'=\frac{1}{16}$, and is similar in every way to curve (a) which uses ln, or $\alpha'=0$. Hence we conclude that $\alpha'=\frac{1}{16}$ is not excluded by these results. As a matter of fact, curve (c) corresponding to $\alpha'=\frac{1}{8}$ is practically level with only a slight downward curvature near the right end. This result suggests that $\alpha'=\frac{1}{8}$ is not inconsistent with the specific-heat results, but represents an excellent fit to the data for the fcc lattice. Values of $\alpha'>\frac{1}{8}$ both slope and curve downward, which result suggests that the assumed singularity is sharper than the correct one. The same analysis applied to the other lattices gives a best fit with $\alpha'\sim\frac{1}{16}$ for bcc lattice and $0\leq\alpha'<\frac{1}{16}$ for sc and d lattices. Values of α' greater than these lead to both slope and curvature downward.

We now consider the power of the method which compares the series for the diamond lattice and the simple quadratic lattice. We demonstrate in Table III that interpretation of this procedure is difficult, for it would seem to indicate that l_{16} diverges more slowly than the specific heat for the simple quadratic lattice which has $\alpha'=0$. While these results are not as dramatic as the sq-versus-d comparison, they are similar enough to cast doubt on the procedure.

TABLE III. Comparison of the specific heat for the simple quadratic lattice and $l_{16}(x)$.

N	{1} Coeff. (sq)	{2} Coeff. l_{16}	ratio {1}/{2}
1	0.77208	1.0	0.7721
2	0.52987	0.53125	0.9974
3	0.37880	0.36523	1.0371
4	0.29116	0.27963	1.0412
5	0.23677	0.22720	1.0421
6	0.20009	0.19170	1.0438
7	0.17359	0.16603	1.0456
8	0.15345	0.14657	1.0469
9	0.13758	0.13130	1.0478
10	0.12473	0.11899	1.0482

We mention for the sake of completeness that although they are both poorly converged, the Padé approximants to $[d\ln(M)/d\ln(C_H)]$ and $[(u-u_c)d\ln(C_H)/du]$ indicate a large value of $\alpha'\sim 0.2$.

We estimate the amplitude of $(1-T/T_c)^{-1/16}$ by considering the ratio $C_H/l_{16}(u/u_c)$, since we do not have enough power series terms (or alternatively, we lack convergence close enough to the critical point) to clearly distinguish the nature of the singularity. This lack prevents the use of the residue from a simple pole in $(C_H)^{16}$ to determine this amplitude. We obtain

$$C_H/Nk\approx A^-(1-T/T_c)^{-1/16}, \quad (T\to T_c^-), \tag{5.4}$$

with

$$\begin{aligned} A_{\rm fcc}^-&=6.47\pm0.2,\\ A_{\rm bcc}^-&=7.36\pm0.2,\\ A_{\rm sc}^-&=8.16\pm0.2,\\ A_{\rm d}^-&=9.44\pm0.2. \end{aligned} \tag{5.5}$$

6. THE SPECIFIC HEAT AT CONSTANT MAGNETIZATION

We have already remarked that in the mean-field approximation $C_M\equiv0$. Thus, $C_M/C_H=0$ if $T<T_c$ and (since $C_H=0$ above T_c) is indeterminate if $T>T_c$.

For the two-dimensional Ising model, it follows from (2.5) together with (2.11), Eq. (18) of Ref. 1, and the exact results[6,7] on the specific heat and magnetization that

$$C_M/C_H\approx 1+E/\ln(1-T/T_c), \quad (T\to T_c^-), \tag{6.1}$$

with

$$\begin{aligned} E_{\rm t}&=1.83\pm0.05,\\ E_{\rm sq}&=1.80\pm0.04,\\ E_{\rm h}&=1.86\pm0.04. \end{aligned} \tag{6.2}$$

Hence by using the exact results for C_H one derives

$$C_M\approx -A^-\ln|1-T/T_c|[1+a^-/\ln|1-T/T_c|], \quad (T\to T_c^-), \tag{6.3}$$

where

$$\begin{aligned} A_{\rm t}^-&=0.4991, & a_{\rm t}^-&=2.44\pm0.05,\\ A_{\rm sq}^-&=0.4945, & a_{\rm sq}^-&=2.42\pm0.04,\\ A_{\rm h}^-&=0.4781, & a_{\rm h}^-&=2.50\pm0.04. \end{aligned} \tag{6.4}$$

That a^- and E do not form monotonic sequences with coordination number should not be taken seriously, because the discrepancy is small compared to the errors involved.

In three dimensions, combining (5.4), (5.5), (4.10)–(4.12) and Eq. (15) of Ref. 1, we can estimate, using (2.5), that

$$\lim_{T\to T_c^-}(1-C_M/C_H)=\begin{cases}0.0018, & \text{fcc},\\ 0.0038, & \text{bcc},\\ 0.0075, & \text{sc},\\ 0.020, & \text{d}.\end{cases} \tag{6.5}$$

These small deviations are quite consistent with the estimates of Sec. 2, where we found $C_M/C_H \sim 1$ at $T=T_c$, with an error substantially larger than these deviations. We conclude that C_M/C_H is probably unity at T_c. If this is the case we cannot reject the form

$$C_H \propto [\ln(1-u/u_c)](1-u/u_c)^{-1/16}, \quad (y \to u_c^-), \quad (6.6)$$

which behaves very similarly to $l_{16}(u/u_c)$ and would yield $C_M/C_H=1$ at $T=T_c$. (However, this is not the only possibility.) The approach of C_M/C_H to the limit would then be like $1/[\ln(1-u/u_c)]$, which is consistent with our analysis in Sec. 2, and in addition [compare with (6.3) for two dimensions]

$$C_M \propto (1-T/T_c)^{-1/16} \ln(1-T/T_c) \times[1-a^-/\ln(1-T/T_c)], \quad (T \to T_c^-). \quad (6.7)$$

For the two- and three-dimensional Ising models, $C_M/C_H=1$ for $T>T_c$. Thus, we conclude in two dimensions that C_M/C_H is continuous at $T=T_c$, and that it is probably continuous in three dimensions. From the exact two-dimensional results we know that the singularity in C_H is symmetrical about T_c, and as a result (6.3) also represents the behavior of C_M above T_c. (The coefficients A^- and a^- become A^+ and a^+, respectively. We note that $A^-=A^+$ and a^+ follows from the exact results.[6,7])

$$\begin{aligned} a_t^+ &= 0.6147, \\ a_{sq}^+ &= 0.6194, \\ a_h^+ &= 0.6375. \end{aligned} \quad (6.8)$$

We note that C_M/C_H is $1-\rho^2$, where ρ is the correlation coefficient between energy fluctuations ΔE and magnetization fluctuations $\Delta\mathfrak{M}$. Its continuity fits in nicely with the arguments presented in Sec. 3, concerning the nature of $\ln Z$ near the critical point.

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We wish to acknowledge several helpful conversations with Professor M. E. Fisher and R. B. Griffiths during the course of this work.

APPENDIX

We tabulate in Table IV, for the convenience of the reader, the series for C_M/C_H which we have derived from previous results.[4]

TABLE IV. $C_M/[C_H u^{\frac{1}{2}q-1}]$.

n	fcc $q=12$	bcc $q=8$	sc $q=6$	d $q=4$	t $q=6$	sq $q=4$	H[a] $q=3$
0	0.166666667	0.25	0.333333333	0.5	0.333333333	0.5	0.66666667
1	0	0	0	−0.25	2.	3.75	−0.44444444
2	0	0	−0.111111111	−0.375	5.55555556	13.125	7.62962963
3	0	−0.0625	6.	17.4375	12.	56.9375	5.97530864
4	2.	0.5	−15.2962963	−15.84375	34.9259259	258.78125	47.9094650
5	−2.69444444	12.	38.	147.234375	66.4444444	1205.98438	−4.33470508
6	1.	−32.234375	−16.1234568	264.851563	215.320988	5731.82031	399.671696
7	2.	61.25	−36.	119.277344	397.481481		298.018595
8	16.6666667	−42.	320.781892	6603.91602	1390.27572		3471.83305
9	−42.	−86.8789063	−338.888888	4215.37402			5381.19650
10	16.0601852	771.34375	−106.174216				
11	76.	−2350.	4721.25927				
12	40.3333333	4552.70410	−14401.0449				
13	−436.222222	−3437.25	40321.2594				
14	360.777778	−9527.0625	−76477.6675				
15	858.943673	51984.5154					
16	−644.694444	−135930.646					
17	−3786.5	232618.016					
18	5790.	−166941.161					
19	6273.35185	−449586.021					
20	−14500.3533	2273561.34					
21	−21781.7685	−5950333.96					
22	64228.1574						

[a] z replaces u for the honeycomb lattice which starts with $\frac{2}{3}z+\cdots$.