PHYSICAL REVIEW B VOLUME 11, NUMBER 3 1 FEBRUARY 1975

Tests of strong scaling in the three-dimensional Ising model

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(Received 18 June 1974)

We study numerically the amplitudes $E^{\pm}(\vec{R})$ of the $|\Delta T/T_c|^{1-\alpha}$ variation in the spin-spin correlation functions $\langle s_{\vec{0}} s_{\vec{R}} \rangle$, of three-dimensional Ising models in zero field above and below T_c. By allowing for reasonable correction terms to the asymptotic behavior $E^{\pm}(\vec{R}) \approx E_0^{\pm}(R/a)^{\zeta}$, where a is the lattice spacing, we find consistency with the strong-scaling prediction $\zeta = (1-\alpha)/\nu - d + 2 - \eta \simeq 0.31$, and reasonable agreement with universality and ϵ-expansion estimates of the amplitudes $E_0^{\pm}$.

It has been shown, in various ways,[1-6] that the temperature dependence of the basic order correlation function $G(\vec{R}, T)$ and, correspondingly, of its Fourier transform $\hat{G}(\vec{k}, T)$ must mirror that of the energy or entropy. Specifically, as the temperature approaches its critical value T_c the correlation functions on the critical "isochore" (or in zero "field") at *fixed* $\vec{R}$ or fixed $\vec{k}$, should vary as $|t|^{1-\alpha}$, where $t = (T - T_c)/T_c$ (and α is the specific-heat exponent[7]). The presence and magnitude of this $|t|^{1-\alpha}$ term are important for interpreting a variety of experiments, including the temperature dependence of electrical resistivities through magnetic critical points[3] and the variation of critical light, x-ray, and neutron scattering at fixed wave number.

In this note we study the amplitudes of this singular term for three-dimensional Ising models above and below T_c. We show that they are consistent with "strong-scaling"[1,8] and universality expectations, and agree moderately well with recent renormalization-group calculations.[5,6] (A previous study[8] above T_c had suggested that strong scaling was violated.)

For an Ising system with spins $s_{\vec{R}} = \pm 1$ at lattice sites $\vec{R}$ we may write

$$G(\vec{R}, T) = \langle s_{\vec{0}} s_{\vec{R}} \rangle = G_c(\vec{R}) \mp E^{\pm}(\vec{R}) |t|^{1-\alpha} + \cdots , \quad (1)$$

as $T \to T_c \pm$, where we assume equal specific-heat exponents, $\alpha' = \alpha$.[7] {Note that no contribution of the form $|t|^{2\beta}$ should appear although at first sight one might be expected to arise from the long-range order $\langle s_{\vec{0}} s_{\vec{\infty}} \rangle = \langle s_0 \rangle^2 \sim [M_0(T)]^2$.}

The scaling hypothesis[2,7,8] for the correlation functions (in zero field) in the critical region can be expressed asymptotically as

$$G(\vec{R}, T) \approx (a/R)^{d-2+\eta} D^{\pm}(R/\xi_1) , \quad (2)$$

where a is the nearest-neighbor lattice spacing and

$$\xi_1(T) \approx f_1^{\pm} a / |t|^{\nu} \quad (3)$$

is the second-moment correlation length[2,7,8] (and we may assume $\nu = \nu'$). Alternatively one may write[2,8]

$$\hat{G}(\vec{k}, T) \approx \hat{G}(0, T) \hat{D}^{\pm}(k^2 \xi_1^2) . \quad (4)$$

According to the "strong-scaling" hypothesis[1,8,9] the asymptotic forms (2) and (3) should extend to describe the fixed $\vec{R}$ (or fixed $\vec{k}$) variation (1): if this is so one must have[1,2,9]

$$D^{\pm}(x^2) \approx D_0^{\pm\infty}/x^{2-\eta} + D_1^{\pm\infty}/x^{d+\zeta} + \cdots , \quad (5)$$

as $x \to \infty$, with

$$\zeta = (1-\alpha)/\nu - d + 2 - \eta . \quad (6)$$

Thence, for the amplitudes in (1), one obtains the prediction

$$E^{\pm}(\vec{R}) \approx E_0^{\pm}(R/a)^{\zeta} , \quad (7)$$

as $R/a \to \infty$. Adopting the values[2,7,10] $\alpha = \frac{1}{8}$, $\nu = \frac{9}{14}$, and $\eta = \frac{1}{18}$ for $d = 3$ gives $\zeta = \frac{11}{36} \simeq 0.306$. A different choice[8] of estimates for ν and η yields $\zeta \simeq 0.33$: the difference is probably indicative of the confidence level of the exponent estimates.

The predictions (6) and (7) were first investigated in detail by Ferer, Moore, and Wortis,[8] who extrapolated the high-temperature series for $\langle s_{\vec{0}} s_{\vec{R}} \rangle$ on the fcc Ising lattice to determine $E^+(\vec{R})$ for values of $(R/a)^2$ up to 11. From a plot vs $\log(R/a)$ they concluded $\zeta = 0.47 \pm 0.06$ ($T \geq T_c$), in apparant violation of the strong-scaling prediction (6).

We have recently calculated and studied[9] the correlation functions for the sc and bcc Ising lattices as a function of both magnetic field and temperature, and have, in particular, obtained low-temperature, zero-field series in powers of $u = e^{-2J/k_B T}$, to order u^{11} and u^{13}, respectively. To study the amplitudes $E^-(R)$, below T_c, we may first differentiate the series for $\langle s_{\vec{0}} s_{\vec{R}} \rangle$ with respect to T (or u) in order to sharpen the singularity and remove the leading temperature-independent term in (1). We have then formed series for the ratio

$$\mathcal{E}(\vec{R}, T) = \frac{dG(\vec{R}, T)}{dT} \Big/ \frac{dG(\vec{\delta}, T)}{dT} , \quad (8)$$

where $\vec{\delta}$ is a nearest-neighbor vector. As $T \to T_c -$ this ratio should approach $E^-(\vec{R})/E^-(\vec{\delta})$. We have found that the apparent convergence of direct Padé approximants to the series for $\mathcal{E}_c^-(\vec{R}) = \mathcal{E}(\vec{R}, T_c -)$

TABLE I. Estimates of $\mathcal{E}_c^{\pm}(\vec{R}) = E^{\pm}(\vec{R})/E^{\pm}(\vec{\delta})$. Uncertainties refer to the last decimal place quoted.

	Simple cubic		Body-centered cubic	
$(R/a)^2$	$\mathcal{E}_c^-(\vec{R})$	$\mathcal{E}_c^+(\vec{R})$	$(R/a)^2$	$\mathcal{E}_c^-(\vec{R})$
2	1.264 ± 3	1.20 ± 1	$1\frac{1}{3}$	1.1354 ± 5
3	1.375 ± 3	1.44 ± 2	$2\frac{2}{3}$	1.270 ± 5
4	1.445 ± 8	1.59 ± 3	$3\frac{2}{3}$	1.346 ± 20
5	1.52 ± 1	1.71 ± 5	4	1.373 ± 15
6	1.554 ± 5	1.78 ± 8	$5\frac{1}{3}$	1.47 ± 2
8	1.67 ± 1	1.85 ± 9	$6\frac{1}{3}$	1.51 ± 2
$9_{(300)}$	1.68 ± 1		$6\frac{2}{3}$	1.52 ± 2
$9_{(221)}$	1.72 ± 5		8	1.563 ± 10
10	1.73 ± 5		9	1.576 ± 35
11	1.77 ± 4		$10\frac{2}{3}$	1.61 ± 4
13	1.81 ± 5		12	1.63 ± 3

is surprisingly good up to $(R/a)^2 = 13$. (The usual interfering, low-T singularities seem to be suppressed in forming the ratio.) Our estimates are collected in Table I. They may be supplemented by the estimates[10,11] for $E^{\pm}(\vec{\delta})$ collected in Table II.

The function $\mathcal{E}(\vec{R})$ may also be calculated above T_c, but the resulting series converge very slowly at T_c and cannot be effectively extrapolated. This is easily seen to arise from the strong competition, for $T > T_c$, between the $|t|^{1-\alpha}$ term in (1) and the following term, namely, $E_2(\vec{R})t$. [This same competition leads to the maximum[2,3,5] in $\hat{G}(\vec{k}, T)$ at fixed $\vec{k}$ lying above but very close to T_c. Below T_c the $|t|^{1-\alpha}$ term is about 40% larger (see below) and of the same sign as the linear term; so there is no competition.]

Plots of $\ln \mathcal{E}_c^-(\vec{R})$ vs $\ln (R/a)^2$, following Ferer *et al.*, can be fitted moderately well by straight lines and suggest $\zeta = 0.39 \pm 0.04$. This is similar to the estimate of Ferer *et al.* and again disagrees with strong scaling. However, it is unreasonable in any test of strong scaling not to allow for some corrections to the expected asymptotic form. Accordingly, in Fig. 1, the estimates for $\mathcal{E}_c^{\pm}(\vec{R})$ have been plotted vs $\ln[(R/a)^2 - e_0]$, which provides for corrections to the asymptotic behavior of $E^{\pm}(\vec{R})$ of relative order $(a/R)^2$. This is most reasonable since nonuniversal corrections of just this order are known rigorously to be present in $G_c(\vec{R})$ in two dimensions [see, e.g., Ref. 2, Eq. (5.6)]. It is evident from the figure [where the dashed lines indicate the asymptotic slope predicted by (6)] that the sc data with $e_0 = 1$ and the bcc data with $e_0 = \frac{1}{4}$, are, in fact, quite *consistent* with the strong-scaling expectations.

TABLE II. Correlation amplitude estimates (see Refs. 9–11 and 13).

lattice	sc	bcc	fcc
$E^-(\vec{\delta})$	3.16 ± 18	3.23 ± 14	3.24 ± 9
$E^+(\vec{\delta})$	1.987	2.010	2.005
$D = D^{\pm}(0)$	0.3071 ± 15	0.2557 ± 9	0.2426 ± 5
f_1^+	0.4783 ± 4	0.4446 ± 4	0.4337 ± 4

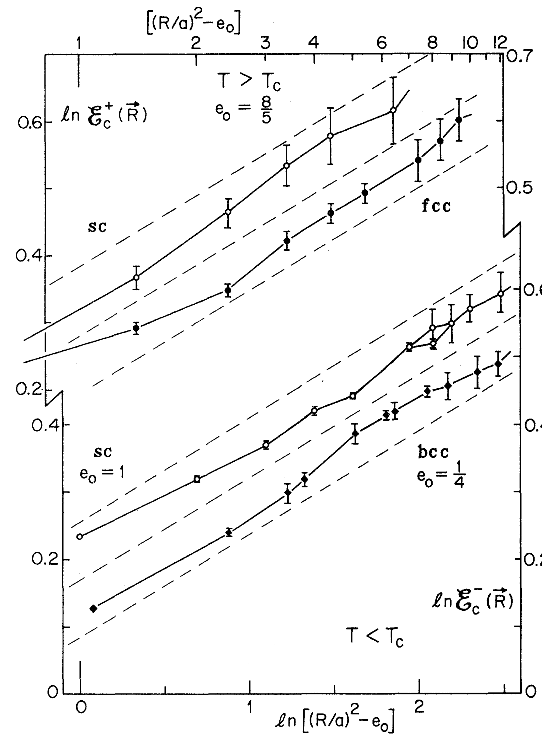

FIG. 1. Logarithmic plots of the reduced amplitudes $\mathcal{E}_c^{\pm}(\vec{R})$ of the energy singularity in the correlation functions $G(\vec{R}, T)$ vs $[(R/a)^2 - e_0]$. The dashed lines indicate the slope corresponding to the prediction $E^{\pm}(\vec{R}) \sim R^{\zeta}$, with $\zeta \simeq 0.306$.

Figure 1 also includes the data above T_c of Ferer *et al.* for the fcc lattice, together with our own new estimates for the sc lattice (see Table I and Refs. 2 and 13), both plotted with $e_0 = \frac{8}{5}$. These results now also appear consistent with $\zeta \simeq 0.306$.

Values of e_0 of order unity, such as assumed here, are certainly not to be considered surprising. Accordingly we conclude that the Ising-model data both above and below T_c are consistent with strong scaling. More pessimistically one might say that the range of R/a for which reasonably precise extrapolations may be made, is too small to yield estimates of ζ with a confidence range of better than ± 0.15.

If we accept the fits exhibited in Fig. 1 we can estimate the limiting amplitudes $E_0^{\pm}$ in (4) from the linear intercepts and the estimates (7) and (8). We find

$$E_0^- = 3.91 \pm 5 \text{ (sc)}, \qquad E_0^- = 3.64 \pm 6 \text{ (bcc)}, \qquad (9)$$

where the uncertainties arising from those in Table II have *not* been included and

$$E_0^+ = 2.76 \pm 6 \text{ (sc)}, \quad E_0^+ = 2.536 \pm 26 \text{ (fcc)}. \quad (10)$$

The dimensionless ratios $Q_4^{\pm} = E_0^{\pm}(f_1^{\pm})^{(1-\alpha)/\nu}/D$, where $D = D^{\pm}(0)$ is the critical-point decay amplitude, are expected to be universal.[12] Using (9) and the data[9,13] in Table II, together with the universal estimate[9] $f_1^+/f_1^- = 1.96 \pm 2$, leads to $Q_4^- = 1.87 \pm 10$ for the sc and bcc lattices, respectively. Above T_c we obtain $Q_4^+ = 3.29 \pm 7$ and 3.35 ± 4 for sc and fcc lattices. In view of the uncertainties, the agreement between the two pairs of values is surprisingly good.

The universal ratio $D_1^{+\infty}/D_0^{+\infty} = \hat{Q}_4^+$ of scaling function coefficients [see (5) above] can be obtained from Q_4^+ by multiplying by

$$\Gamma(2+\zeta)(\sin\tfrac{1}{2}\pi\zeta)/\Gamma(1-\eta)\cos\tfrac{1}{2}\pi\eta \simeq 0.52410 \; .$$

This gives the estimate $\hat{Q}_4^+ = 1.74 \pm 5$, which may be compared with the recent calculation of Fisher and Aharony,[5] who obtained

$$\hat{Q}_4^+ = D_1^{+\infty}/D_0^{+\infty} = 1 + \epsilon + O(\epsilon^2) = (\gamma - 1)/\alpha + O(\epsilon^2) \; , \qquad (11)$$

where $\epsilon = 4 - d$. For $d = 3$ dimensions we have $\epsilon = 1$, and predict $\hat{Q}_4^+ \simeq 2.0$. The discrepancy of about 12% must be considered quite satisfactory since the expansion is correct only to first order in ϵ. By comparison, theory predicts[14]

$$f_1^+/f_1^- = 2^{\nu}(1 + \tfrac{5}{24}\epsilon) + O(\epsilon^2) \simeq 1.89 \; , \qquad (12)$$

at $\epsilon = 1$; this is 4% lower than the series estimate[9] mentioned above. Similarly the ratio of specific-heat amplitudes is given[14] as $2^{\alpha-2}n(1+\epsilon) + O(\epsilon^2)$, with $n = 1$ for Ising systems; this predicts $A^-/A^+ \simeq 1.83$, which is 14% higher than the estimate $A^-/A^+ = E^-(\vec{\delta})/E^+(\vec{\delta}) = 1.61 \pm 6$, which follows from the data of Table I.

It is natural to expect that the universal ratio E_0^-/E_0^+ should also equal A^-/A^+. From the sc estimates we find $E_0^-/E_0^+ \simeq 1.42 \pm 13$. The bcc and fcc data can also be used if one computes $(Q_4^-/Q_4^+) \times (f_1^+/f_1^-)^{(1-\alpha)/\nu}$; this yields $E_0^-/E_0^+ \simeq 1.41 \pm 14$. As expected, universality is well confirmed but the discrepancy of 14% from the central estimate $A^-/A^+ \simeq 1.61$ seems to exceed the uncertainties. Possibly this indicates a more subtle departure from strong-scaling behavior. On the other hand it might mean that, despite the concurrence of the different estimates for Q_4^+ and Q_4^-, the values found for $E^{\pm}(\vec{R})$ at larger values of $\vec{R}$ are systematically high or low, respectively, by 10 to 15%. In view of our (unavoidable) use of Padé approximants for extrapolation below T_c, and the likelihood of significant confluent singularities in $\mathcal{E}(\vec{R}, T)$ there, this possibility is hard to exclude.

ACKNOWLEDGMENTS

We are grateful to Dr. E. Brézin for stimulating correspondance and to Professor M. Ferer for sending us details of his estimates. The support of the National Science Foundation, in part through the Materials Science Center at Cornell University, has been essential to this research.

[1]M. E. Fisher, in *Critical Phenomena*, edited by M. S. Green and J. V. Sengers, NBS Miscellaneous Publication No. 273 (U.S. GPO, Washington, D.C., 1966), p. 108.

[2]M. E. Fisher and R. J. Burford, Phys. Rev. 156, 583 (1967).

[3]M. E. Fisher and J. S. Langer, Phys. Rev. Lett. 20, 665 (1968).

[4]An argument can be based on the operator-product expansion [L. P. Kadanoff, Phys. Rev. Lett. 23, 1430 (1969); K. G. Wilson, Phys. Rev. 179, 1499 (1969), Phys. Rev. D 2, 1473 (1970)].

[5]M. E. Fisher and A. Aharony [Phys. Rev. Lett. 31, 1238 (1973); Phys. Rev. B 10, 2818 (1974)] give a renormalization-group demonstration within the $\epsilon = 4 - d$ expansion. See also Ref. 6.

[6](a) E. Brézin, D. Amit, and J. Zinn-Justin, Phys. Rev. Lett. 32, 151 (1974); (b) E. Brézin, J. C. LeGuillou, and J. Zinn-Justin, Phys. Rev. Lett. 32, 473 (1974).

[7]We use standard critical exponent notation; see e.g., M. E. Fisher Rep. Prog. Phys. 30, 615 (1967).

[8]M. Ferer, M. A. Moore, and M. Wortis, Phys. Rev. Lett. 22, 1382 (1969).

[9]H. B. Tarko and M. E. Fisher, (a) Phys. Rev. Lett. 31, 926 (1973) (note that the last entry in Table I of this paper is misprinted); (b) Phys. Rev. B 11, 1217 (1975).

[10]M. F. Sykes, D.L. Hunter, D. S. McKenzie, and B. R. Heap, J. Phys. A 5, 667 (1972).

[11]P. E. Scesney, Phys. Rev. B 1, 2274 (1970); H. Garelick and J. W. Essam, J. Phys. C 1, 1588 (1968) (note that the a^- entry of Table 4 for the fcc lattice has been replaced by the value following from D_q^{σ} (in place of D_q^{μ}) which seems more reliable in the light of universality expectations).

[12]See, e.g., Refs. 5 and 9, and references therein, in particular to P. G. Watson and to L. P. Kadanoff.

[13]D. R. Ritchie and M. E. Fisher, Phys. Rev. B 5, 2668 (1972).

[14]E. Brézin, J. C. LeGuillou, and J. Zinn-Justin, Phys. Lett. A 47, 285 (1974).