Use of Scaling Theory to Predict Amplitudes: Verification of Double-Power-Law Behavior for Crossover of Lattice Dimensionality*

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Scaling with a parameter, in contrast to ordinary scaling theory, makes predictions concerning *amplitude* functions as well as critical-point exponents. We provide the first test of these predictions, by examining the dependence of the amplitude on the anisotropy parameter $R = J_z/J_{xy}$ for the susceptibility and the second moment of the simple cubic and fcc Ising models with directional anisotropy. The "double-power-law" behavior found strongly supports the scaling predictions for thermodynamic functions and the two-spin-correlation function. Our analysis provides a measure of the ranges of R over which parameter scaling appears to hold for the simple cubic and fcc lattices. The relative domains of validity on the two lattices are interpretable in terms of the respective lattice structures.

The scaling hypothesis for thermodynamic functions and the two-spin-correlation function makes predictions about critical-point *exponents* but no predictions about the behavior of the *amplitudes* of these functions as the critical point is approached. However, an additional scaling hypothesis is possible at special symmetry points where a system changes its exponents (i.e., crosses over from one universality class[1] to another) upon variation of a parameter R in the Hamiltonian.[2] The restrictions imposed by the simultaneous validity of both hypotheses lead to the prediction that functions possess amplitudes singular in R *besides* the usual singularity along the critical line $T_c(R)$. We call the resulting product of two singular factors a "double-power" law.

Such laws have been discussed for three different systems: (i) Riedel and Wegner[2] treated magnetic systems with spin anisotropy, where the spin symmetry is subject to variation between the Ising and Heisenberg limits. (ii) Double-power laws were later proposed[3,4] for the Ising model with *lattice* anisotropy (different coupling strengths J_z, J_{xy} in different lattice directions). Here varying the anisotropy parameter $R \equiv J_z/J_{xy}$ changes the lattice dimensionality from three to two. (iii) Double-power laws are also predicted by scaling to occur for systems displaying tricritical points (e.g., metamagnets, He^3-He^4 mixtures).[5-7]

Whereas the *exponent* predictions have received considerable attention, there has to date been no confirmation of the *amplitude* predictions. In this work we test double-power laws near a symmetry point both for thermodynamic functions *and* for the two-spin-correlation function $C_2(\vec{r}) \equiv \langle s_0 s_{\vec{r}}\rangle - \langle s_0\rangle\langle s_{\vec{r}}\rangle$. Specifically, we employ high-temperature series expansions to study the amplitudes A_χ, A_μ of the susceptibility χ and the second moment of the two-spin correlation function $\mu_2 \equiv \sum_{\vec{r}} \vec{r}^{\,2} C_2(\vec{r})$ for the Ising model with directional (or "lattice") anisotropy,

$$\mathcal{H} = -J_{xy}\sum_{\langle ij\rangle}^{xy} s_i s_j - J_z \sum_{\langle ij\rangle}^{z} s_i s_j \equiv -J_{xy}\left(\sum_{\langle ij\rangle}^{xy} s_i s_j + R\sum_{\langle ij\rangle}^{z} s_i s_j\right). \tag{1}$$

Here the first sum is over nearest-neighbor (nn) spins coupled in an xy plane and the second sum is over nn spins whose relative displacement vector has a z component. For $R=0$ both the fcc and simple cubic (sc) ($d=3$) lattices reduce to uncoupled square ($d=2$) lattices.

The double-power laws for (1) that are tested in this work are[4]

$$\chi \sim R^{(\gamma-\bar{\gamma})/\varphi}[T - T_c(R)]^{-\gamma} \tag{2a}$$

and

$$\mu_2 \sim R^{[\gamma+2\nu-(\bar{\gamma}+2\bar{\nu})]/\varphi}[T - T_c(R)]^{-(\gamma+2\nu)}, \tag{2b}$$

where barred and unbarred exponents refer, respectively, to $d=2$ and $d=3$ lattices. The conceptual basis of these laws should be made clear by the following derivation of Eq. (2a).[8]

We first make the following scaling hypothesis about the point $R=0$: The Gibbs potential $\overline{G} = \overline{G}(\bar{\tau}, H, R)$ is a generalized homogeneous function (GHF) in magnetic field H, $\bar{\tau} \equiv T - T_c(R=0)$, and R, i.e., for all $\lambda > 0$, there exist three positive numbers $\bar{a}_\tau$, $\bar{a}_H$, $\bar{a}_R$ such that

$$\overline{G}(\lambda^{\bar{a}_H}H, \lambda^{\bar{a}_\tau}\bar{\tau}, \lambda^{\bar{a}_R}R) = \lambda\overline{G}(H, \bar{\tau}, R). \tag{3}$$

Since Eq. (3) holds for $R=0$, the exponents for a $d=2$ lattice are expressible in terms of the "scaling powers" $\bar{a}_H$, $\bar{a}_\tau$. Equation (3) implies[6]

$$y_0 = \overline{F}_2(y_1, y_2), \tag{4}$$

where $y_0 \equiv \overline{G}/R^{1/\bar{a}_R}$, $y_1 \equiv H/R^{\bar{a}_H/\bar{a}_R}$, and $y_2 \equiv \bar{\tau}/R^{\bar{a}_\tau/\bar{a}_R}$. The scaled variables y_0, y_1, y_2 are invariant under the transformations (parametrized by λ) $\overline{G}' = \lambda\overline{G}$, $H' = \lambda^{\bar{a}_H}H$, $\bar{\tau}' = \lambda^{\bar{a}_\tau}\bar{\tau}$, and $R' = \lambda^{\bar{a}_R}R$. Equation (4) gives the critical line $T_c(R)$ as $y_1^{(c)}=0$, $y_2^{(c)}=\text{const}$ $=\bar{\tau}^{(c)}/R^{\bar{a}_\tau/\bar{a}_R}$ or $T_c(R)-T_c(0)=\text{const}\, R^{1/\varphi}$, with $\varphi=\bar{a}_R/\bar{a}_\tau$. Independent arguments[3-4,9] yield $\varphi=\bar{\gamma}$.

The second scaling hypothesis is about points on the critical line. It is valid within the crossover region (cf. Fig. 1), and expresses invariance properties with respect to a *second* group of transformations parametrized by ρ. In order that the resulting scaling equation be consistent at small fixed R with (3), we cast it in terms of the invariants y_0, y_1, and y_2, thereby ensuring that only changes in the y_i are important. The distance from the critical line at finite R in the $H=0$ plane (of the H-T-R field space) may be measured by $\tau \equiv \bar{\tau}/(R^{\bar{a}_\tau/\bar{a}_R})-k=y_2-k$. We now define a new function $G(y_1,y_2-k)\equiv \bar{F}_2(y_1,y_2)$, and postulate that G is a GHF with scaling powers a_H and a_τ, the appropriate $d=3$ scaling powers (e.g., for the Ising model, $a_H\simeq\frac{5}{6}$, $a_\tau\simeq\frac{8}{15}$, while $\bar{a}_H=\frac{15}{16}$, $\bar{a}_\tau=\frac{1}{2}$). Thus

$$G(\rho^{a_H}y_1,\ \rho^{a_\tau}(y_2-k))=\rho G(y_1,y_2-k). \tag{5}$$

From Eq. (5) it follows that

$$G(y_1,y_2-k)=(y_2-k)^{1/a_\tau}F_1(y_1/y_2{}^{a_H/a_\tau}). \tag{6}$$

Rewriting, we obtain

$$\bar{G}(H,\bar{\tau},R)=R^{1/\bar{a}_R}(\bar{\tau}/R^{\bar{a}_\tau/\bar{a}_R}-k)^{1/a_\tau}$$

$$\times F_1\left(\frac{H/R^{\bar{a}_H/\bar{a}_R}}{(\bar{\tau}/R^{\bar{a}_\tau/\bar{a}_R}-k)^{a_H/a_\tau}}\right). \tag{7}$$

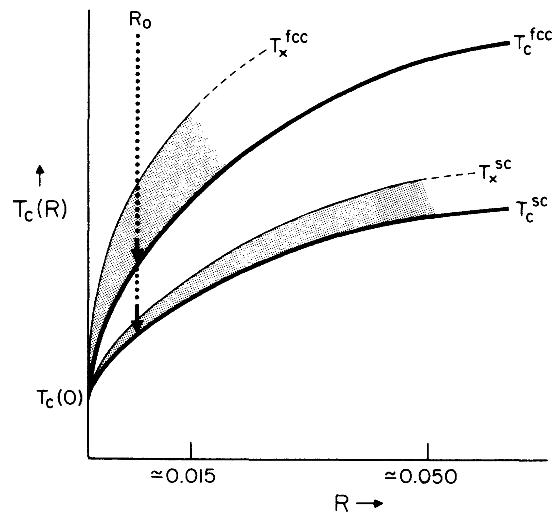

FIG. 1. Schematic diagram of the H-T-R "field" space for $H=0$. Shown are the critical lines $T_c^{sc}(R)$ and $T_c^{fcc}(R)$. [$T_c(0)$ is the square-lattice critical temperature]. The shaded regions denote the crossover regions within which two scaling hypotheses should be simultaneously valid. The "cutoffs" at $R\cong 0.015$ and $R\cong 0.050$ for the fcc and sc lattices, respectively, are based upon considerations discussed in the text (cf. Fig. 2). The vertical dotted arrow corresponds to an experiment (or series analysis) at a fixed $R=R_0$. The crossover region is appreciably broader for the fcc than the sc (cf. text).

Next, differentiation with respect to H and setting $H=0$ results in

$$\chi\sim R^{(1-2\bar{a}_H)/\bar{a}_R}\left(\frac{\bar{\tau}}{R^{\bar{a}_\tau/\bar{a}_R}}-k\right)^{(1-2a_H)/a_\tau} \tag{8}$$

Finally, upon using the relations $-\bar{\gamma}=(1-2\bar{a}_H)/\bar{a}_\tau$, $-\gamma=(1-2a_H)/a_\tau$, and $\varphi=\bar{a}_R/\bar{a}_\tau=\bar{\gamma}$, we arrive at Eq. (2a).

The analogous double-power law for μ_2, Eq. (2b), is obtained in the same fashion beginning with the two GHF hypotheses for $C_2(H,\bar{\tau},R,\vec{r})$. Upon substituting the numerical values for the $d=2$ and $d=3$ Ising models,[10] $\bar{\gamma}=\varphi=\frac{7}{4}$, $\bar{\nu}=1$, $\gamma=\frac{5}{4}$, $\nu\simeq 0.638$, we find $A_\chi(R)\sim R^{-2/7}$, $A_\mu(R)\sim R^{-0.699}$.

The amplitudes for (1) were calculated from general-R high-temperature series for a range of R from 0.001 to 0.100 on the sc and from 0.001 to 0.050 on the fcc.[11] For any given value for R, the following procedure for obtaining the $A_\chi(R)$ was used. First, the universality prediction of a constant $\frac{5}{4}$ power-law divergence is assumed, so that the series $[\chi(R)]^{4/5}$ should show a simple pole at $T_c(R)$. After forming the series $[\chi(R)]^{4/5}$, we fit it by Padé approximants (PA's). From the resulting Padé table of singularities, we determine the critical temperature $T_c(R)$ and the corresponding residue $[A_\chi(R)]^{4/5}$, predicted by (2a) to vary as $R^{-0.229}$.

An identical procedure is carried out on the $\mu_2(R)$ series, except here the PA's are to the series raised to the inverse of $(\gamma+2\nu)\simeq 2.526$. The PA's to $[\mu_2(R)]^{1/(\gamma+2\nu)}$ again should converge to the critical temperature $T_c(R)$, with a residue at the pole of $[A_\mu(R)]^{1/2.526}$. The residue is predicted by (2b) to vary as $R^{-0.277}$.

Figure 2 displays (for both the sc and fcc lattices) log-log plots for A_χ versus R and A_μ vs R. As expected, series convergence was generally better for larger R values. Our estimates of the error bars for the amplitudes are based on the extent of convergence of the Padé tables. Where no explicit error bars are indicated, the size of the points may be taken to represent an upper limit on the uncertainty. Although estimates of the $T_c(R)$ from the χ and μ_2 Padé tables are fairly consistent with each other, the convergence of the χ Padé is always superior. Therefore, the T_c determined from the χ series is used in the evaluation of the A_μ. The straight lines in the plots are the theoretical scaling predictions.

a. Susceptibility amplitudes A_χ. Examining first the A_χ plots of Fig. 2(a), we see that a line of slope 0.229 appears to provide an excellent fit on the fcc lattice in the range from $R\cong 0.004-0.015$, and on the sc from $R\cong 0.01-0.05$. Points begin to fall below the line for R outside these intervals. The deviation at higher R may be explained by the fact that the scaling hypothesis in the parameter R is assumed to hold about $R=0$ and has diminishing validity for increasing R. Indeed, *the estimates given above give some indication of how far out in R the scaling hypothesis in R holds.* Why the sc seems to scale in R further out than the fcc may be understood from consideration of the respective lattice structures. The fcc has four in-plane (xy) bonds and eight out-of-plane (z) bonds. In the sc, the ratio is exactly reversed, with four in-plane and only two out-of-plane bonds. Hence, it is quite plausible that two-dimensional behavior appears to set in sooner for the sc than the fcc as R is decreased. More precisely, the sc is more "two-dimensional" in character than the fcc in the sense that, for a fixed small value of R, one must get closer to $T_c(R)$ to find out the lattice is really three dimensional (cf. Fig. 1). We therefore expect the range of influence of R scaling to be greater for the sc than the fcc.

The deviations at small R we attribute to the failure of the finite high-temperature series to locate the correct critical temperatures. The series in this region overestimate the $T_c(R)$ and hence underestimate the amplitudes, and they become steadily worse for decreasing R. As the crossover region shrinks, an increasing number of series coefficients would be required to effectively penetrate the crossover region and locate the true critical temperature (cf. Fig. 1). For the same

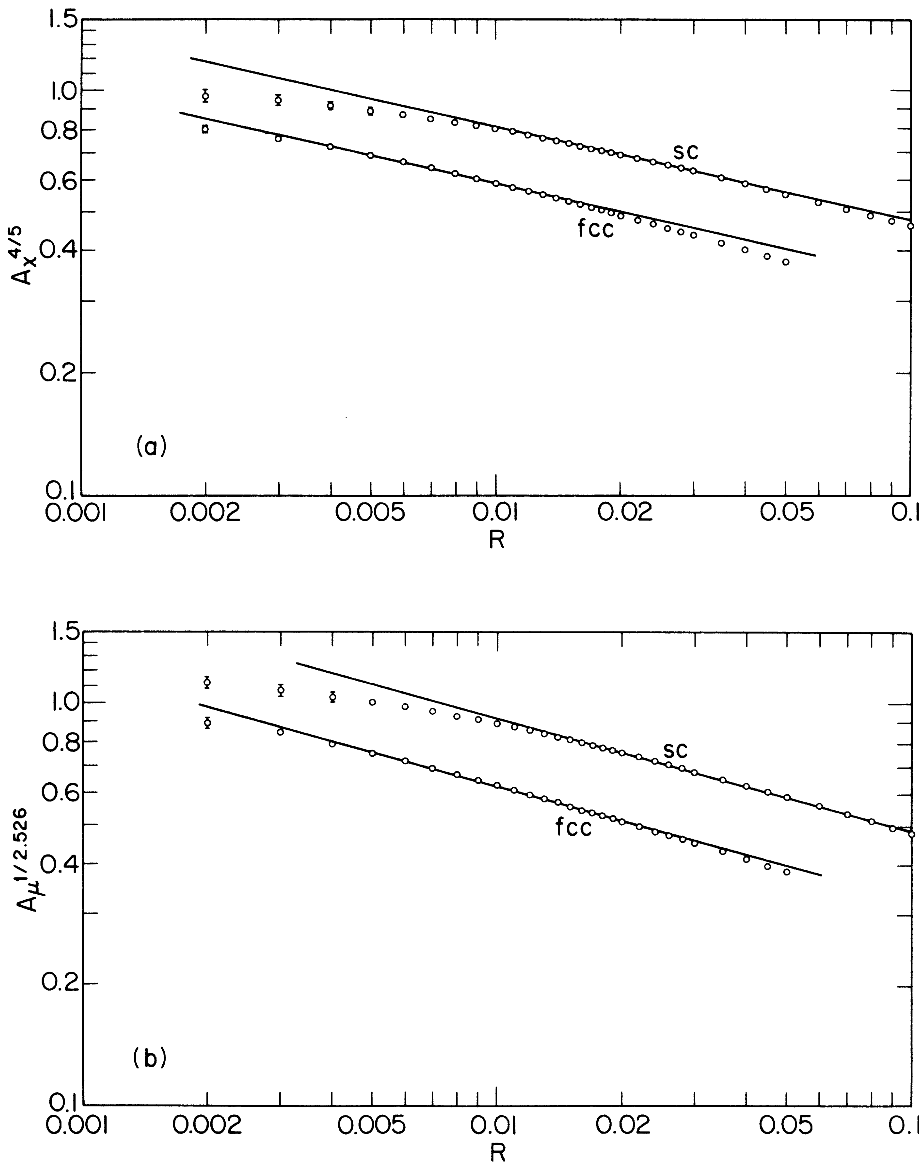

FIG. 2. (a) Log-log plot of the susceptibility amplitude $[A_x(R)]^{4/5}$ vs R. Upper points are data from sc series, lower from fcc series. Straight lines shown have slope of $\gamma^{-1}[(\gamma-\bar{\gamma})/\varphi] = -0.229$, as predicted by scaling theory. (b) Log-log plot of amplitude $[A_\mu(R)]^{1/2.526}$ vs R. Upper points are sc series data, lower are fcc data. Straight lines have slope of $(2\nu+\gamma)^{-1}[(2\nu+\gamma-2\bar{\nu}-\bar{\gamma})/\varphi] = -0.277$.

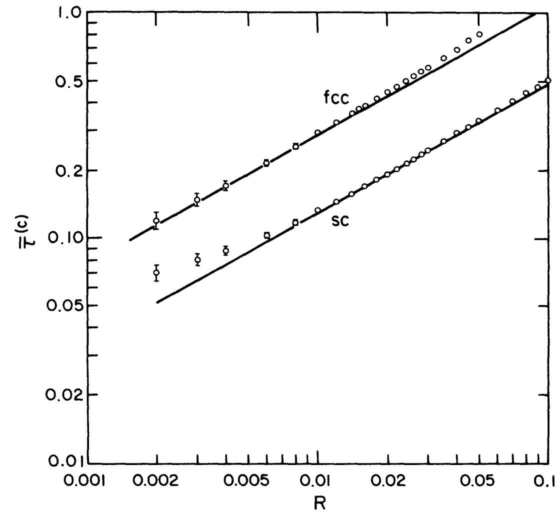

FIG. 3. Log-log plot of $\overline{\tau}^{(c)}(R) \equiv k_B[T_c(R) - T_c(0)]/J_{xy}$ vs R. Upper points are data from fcc series, lower from sc series. Straight lines have slope of $\overline{\gamma}^{-1} = \frac{4}{7}$, as predicted by parameter scaling exponent relation that $\overline{\tau}^{(c)} \sim R^{1/\varphi}$, plus the rigorous result that $\varphi = \overline{\gamma}$.

reasons stated in the last paragraph, one expects such deviations at small R to occur earlier (i.e., at larger R) for the more "two-dimensional" sc lattice than for the fcc, *and this we indeed observe*.

It is to be noted that the error bars for the points at very small R are inconsistent with the scaling prediction. This is because the Padé tables have converged to some extent, but not to the true $T_c(R)$. We emphasize that as R gets smaller, any small error in $T_c(R)$ is amplified in the corresponding amplitude $A(R)$ since both A_χ and A_μ diverge as $R \to 0$. The amplitudes should be discounted when the $T_c(R)$ from which they are calculated are no longer reliable. As an independent test on the accuracy of the $T_c(R)$, we have used the exponent parameter scaling prediction that $\overline{\tau}^{(c)} \equiv [T_c(R) - T_c(0)] \sim R^{1/\varphi} = R^{1/\overline{\gamma}}$. The *exponent* scaling predictions for this model have been strongly supported by previous numerical work.[12] On a log-log plot of $\overline{\tau}^{(c)}$ vs R, a line of slope $1/\overline{\gamma} = \frac{4}{7}$ fits the small-R data well down to $R \lesssim 0.002$ on the fcc and to $R \cong 0.010$ on the sc (cf. Fig. 3). These values therefore are estimates below which the amplitudes should be regarded as unreliable.

b. Second-moment amplitudes A_μ. The A_μ plots of Fig. 2(b) are again well described by the theoretical scaling prediction over a significant range of R values. A detailed analysis for the sc indicates that the scaling prediction fits the series data further out in R than for A_χ; for small R, the deviation sets in at $R \cong 0.015$. For the fcc A_μ data, the region where the scaling line provides an excellent fit is also shifted slightly to the right compared to the A_χ plot. The correct $T_c(R)$ for very small R should, for the reasons explained above, raise the A_μ closer to the theoretical prediction on both lattices.

In conclusion, the results from series analysis provide strong evidence supporting the double-power-law predictions, Eqs. (2a) and (2b), for the Ising model with directional anisotropy. These results constitute the first such test in the literature and include both thermodynamic scaling and correlation function scaling. Further numerical (and experimental) studies on double-power laws for models (and real materials) with crossover behavior would be very welcome.[13]

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[10]We use the value for ν given in M. A. Moore, D. Jasnow, and M. Wortis, Phys. Rev. Lett. **22**, 940 (1969). If we use $\nu = 0.643$ [as proposed in the earlier but still widely accepted work of M. E. Fisher and R. J. Burford, Phys. Rev. **156**, 583 (1967)], then one obtains the scaling prediction that $A_\mu \sim R^{-0.694}$. If the prediction $\nu = 5/8$ (which follows from $\alpha = 1/8$ and the two-exponent scaling prediction $d\nu = 2 - \alpha$) were valid, then $A_\mu \sim R^{-0.714}$. The A_μ calculation may be sufficiently refinable that it could provide evidence distinguishing possible values of ν.

[11]Tenth-order general-R series [of F. Harbus and H. E. Stanley, Phys. Rev. B **7**, 365 (1973)] were used for our analysis of both χ and μ_2 on the fcc, and for μ_2 on the sc lattice. For χ on the sc, the eleventh-order series available from J. Oitmaa and I. G. Enting [Phys. Lett. A **36**, 91 (1971)] were used.

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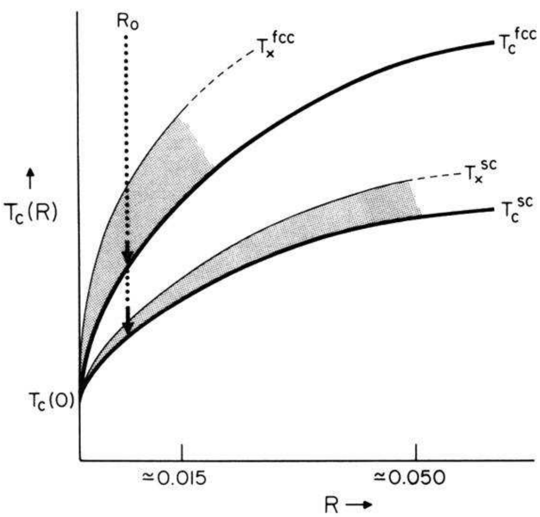
[13]Unfortunately, the numerical situation in recent studies [F.

Harbus and H. E. Stanley, Phys. Rev. Lett. **29**, 58 (1972)] of Ising-model antiferromagnets with tricritical points (TCPs) is much more difficult from the point of view of testing double-power laws. For example, completely lacking is precise knowledge of the location of the TCP and of the necessary tricritical exponents (e.g., ϕ). The Hamiltonian (1) has the distinct advantage that one knows, exactly, both the location of the "special point" in the phase diagram where the change of universality class occurs ($H = \tau\varphi = R = 0$), and the values of the appropriate exponents (e.g., $\varphi = \overline{\gamma} = 7/4$). See also F. Harbus and H. E. Stanley, Phys. Rev. B **8**, 1141 (1973); Phys. Rev. B **8**, 1156 (1973); and F. Harbus, A. Hankey, H. E. Stanley, and T. S. Chang, following paper, Phys. Rev. B **8**, 2273 (1973).



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