SCALING FORM OF THE SPIN-SPIN CORRELATION FUNCTION OF THE THREE-DIMENSIONAL ISING FERROMAGNET ABOVE THE CURIE TEMPERATURE*

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(Received 28 April 1969)

The spin-spin correlation function for the $S=\frac{1}{2}$ Ising ferromagnet is evaluated in zero magnetic field and for $T \geq T_c$ by the method of series expansions. Evidence is presented showing that the scaling of correlations is valid in the (weak) limit $r \to \infty$, κr fixed, but is not valid in the (strong) limit $\kappa a \to 0$, $r \gg a$, with κr arbitrary.

In this Letter the range of validity of the scaling form of the critical spin-spin correlation function $\Gamma(\vec{r},T)$ of the three-dimensional $S=\frac{1}{2}$ Ising ferromagnet for $T \geq T_c$ (the Curie temperature) and in zero magnetic field is discussed by means of series expansions. According to the scaling hypothesis,[1,2]

$$\Gamma(\vec{r},T)=(a/r)^{d-2+\eta}D(\kappa r) \tag{1}$$

provided that $r \gg a$ and $\kappa a \ll 1$ but for arbitrary values of the product κr. In the above, a is the nearest-neighbor lattice spacing, d is the dimensionality, and $\kappa=\kappa(T)=1/\xi(T)$ is the inverse coherence length, which, as $T \to T_c$, becomes isotropic and varies as[3] $\kappa(T)=\kappa_0\epsilon^{\nu}$, where $\epsilon=1-T_c/T$. We shall refer to (1) and the conditions which follow it as "strong scaling." Strong scaling holds for the Ising model in two dimensions.[4] As reported in an earlier publication,[5] we have obtained the first 12 coefficients in the high-temperature series expansion of $\Gamma(\vec{r},T)$ on the fcc, bcc, and simple cubic lattices. We analyzed the spherical moments of the correlation function, evaluated ν to be $0.638_{-0.001}^{+0.002}$ and η to be $0.041_{-0.003}^{+0.006}$ (in contrast to the scaling-law predictions $\nu=0.625$ and $\eta=0$), and presented evidence that (1) was at least valid in the limit κr fixed, $r \to \infty$ (we will refer to this limit as "weak scaling"[3]), i.e., that scaling holds provided distances are measured in units of the coherence length.

We shall present here the results of direct analysis of the series of Ref. 5 for the fcc lattice. Our conclusions are: (i) that there are probably deviations from strong scaling for fixed r as $\kappa a \to 0$, (ii) that these deviations are numerically small and will be difficult to detect experimentally, and (iii) that the Ornstein-Zernike (OZ) form[6]

$$\Gamma(\vec{r},T)=C(\kappa a)^{\eta}(a/r)e^{-\kappa r} \tag{2}$$

is an accurate representation of the critical correlations provided $\kappa r \gtrsim 0.1$.

Our high-temperature series expansions[5] provide all coefficients $q_n(\vec{r})$, $n \leq 12$, in the development

$$\Gamma(\vec{r},T)=\sum_{n=0} q_n(\vec{r})K^n, \tag{3}$$

where $K \equiv J/k_BT$. To evaluate $\Gamma(\vec{r},T)$ for fixed $\vec{r}$ and T we extrapolated the partial sums

$$S_N(\vec{r},T) \equiv \sum_{n=0}^{N} q_n(\vec{r})K^n.$$

It is reasonable to expect[7] that for fixed $\vec{r}$, $\Gamma(\vec{r},T)$ carries the specific heat singularity as $T \to T_c$:

$$\Gamma(\vec{r},T)=\Gamma_c(\vec{r})-E(\vec{r})\epsilon^{1-\alpha} + \text{higher powers of } \epsilon, \tag{4}$$

where $\Gamma_c(\vec{r}) \equiv \Gamma(\vec{r},T_c)$ and α, the specific-heat index, is equal to $\frac{1}{8}$ in three dimensions.[8] If this is so, then one expects

$$S_N(\vec{r},T) \sim \Gamma(\vec{r},T)+f_N(T)E(\vec{r}), \tag{5}$$

where

$$f_N(T) \equiv \epsilon^{1-\alpha} - \sum_{n=0}^{N} c_n\left(\frac{7}{8}\right)\left(\frac{K}{K_c}\right)^n;$$

$K_c \equiv J/k_BT_c$, and $c_n(\lambda)$ is the coefficient of x^n in $(1-x)^{\lambda}$. A plot of S_N vs f_N then gives $\Gamma(\vec{r},T)$ as intercept. Curvature can be taken into account by means of a Neville table.[9] Good convergence was obtained by this method for sites located five or fewer steps from the origin.[10] Values of ϵ ranging from 10^{-4} to 0.08 were used, but for the more distant sites convergence was adequate only for the larger values of ϵ.

Figure 1 shows a plot of $(r/a)^{1+\eta}\Gamma(\vec{r},T)/(\kappa r)^{\eta}$ vs[11] κr for a variety of values of r and ϵ. The fact that points for different ϵ all lie roughly on the same curve is a direct if blunt test of (1). Note that if, as is generally believed,[3,5] $D(\kappa r) \to \text{const}$ as $\kappa r \to 0$, then the curve is expected to diverge at small κr like $D(0)/(\kappa r)^{\eta}$. OZ theory

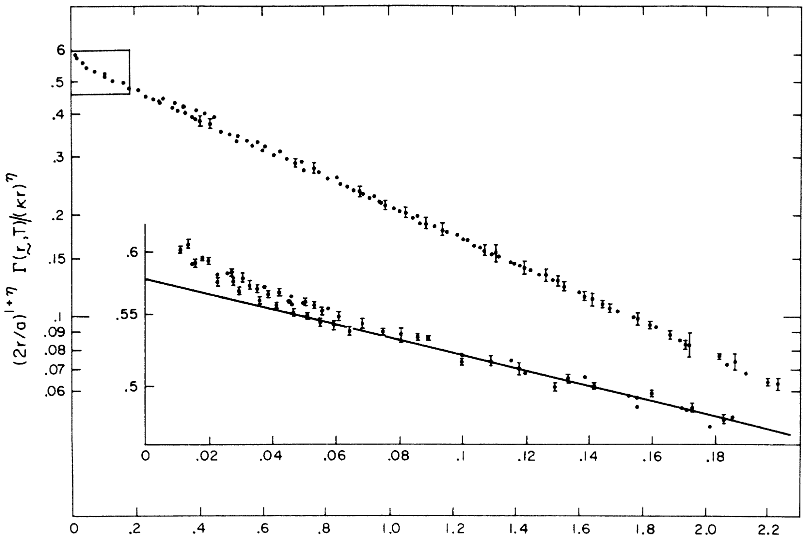

FIG. 1. The scaling of $\Gamma(\vec{r}, T)$. Figure includes points for $10^{-4} \leq \epsilon \leq 0.08$ and $1 \leq r/a \leq 5$. According to (1) vertical axis is $2^{1+\eta}D(\kappa r)/(\kappa r)^{\eta}$. OZ plots as a straight line of slope -1, the continuation of which is drawn in on the inset.

would yield a straight line in Fig. 1; so the distinct turn-up for $\kappa r \lesssim 0.1$ is evidence that $\eta > 0$. All points in Fig. 1 include generous error bars, but in many cases the errors were too small to show up on the scale of the figure. The scatter of the points can be attributed to spherical asymmetry (lattice effects) at short distances, i.e., to violations of the condition $r \gg a$. The discrepancy is largest (6% at $\epsilon = 0$) for the next-nearest-neighbor site, of the order of 1% for the seven next-nearest sites, and less than 1% for the further sites, provided that ϵ is kept less than 0.1. For larger ϵ, the coherence length becomes comparable with a lattice spacing, and big departures from spherical symmetry appear. None of the scatter can be attributed to departures from strong scaling, which, as we shall now see, are too small to be observed directly.

To make departures from strong scaling apparent, we focus on the behavior of $\Gamma(\vec{r}, T)$ for fixed r as $\epsilon \to 0$. Strong scaling requires that the coefficient of the energy-density singularity, $E(\vec{r})$ in (4), should behave for $r \gg a$ as[12]

$$E(\vec{r}) = B(r/a)^{g}, \quad g = (1-\alpha)/\nu - d + 2 - \eta$$
$$\simeq 0.33 \pm 0.01. \qquad (6)$$

Note that weak scaling, which fixes κr, makes no prediction for g. Numerical determination of g (see below) gives $g = 0.47 \pm 0.06$ in violation of strong scaling. $E(\vec{r})$ was determined by extrapolating successive estimates for $E(\vec{r})$, $nq_n(\vec{r})K_c n/|c_n(-\alpha)|(1-\alpha)$. A plot of $\ln E(\vec{r})$ vs $\ln(r/a)$ should give a straight line of slope g. Figure 2 shows such a plot for the fcc lattice for those sites for which reasonably accurate estimates of $E(\vec{r})$ were possible. Estimates of $E(\vec{r})$ are very sensitive to the value of α, but there seems little reason to doubt that α is exactly $\frac{1}{8}$. Our evaluation of g is open to the criticism that, even for the largest value of r used [the site (3, 3, 2)], the region ($r \gg a$) to which (6) applies may not have been reached. In defense, we note that $E(\vec{r})$ can be calculated exactly for the two-dimensional Ising model,[3] and it is possible to extract from its value at the nearby sites a value of $g = \frac{3}{4}$ in agreement with the exact asymptotic ($r \gg a$) calcula-

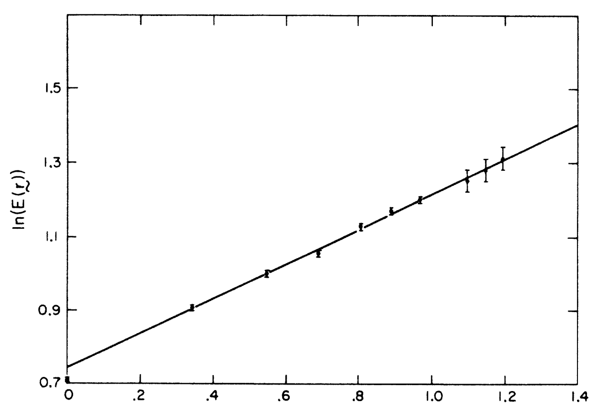

FIG. 2. Plot of $\ln E(\vec{r})$ vs $\ln(r/a)$. The slope determines $g = 0.47 \pm 0.06$.

tion.[13]

The constant B in (6) can be evaluated from the vertical intercept of Fig. 2, yielding $B = 2.1 \pm 0.1$. Recalling $D(0) = 0.246 \pm 0.003$,[3,5] it is easy to see that, in the region (small ϵ) where the expansion (4) holds, the second term is never more than a few percent of the first for the values of r for which we have reliable information. Thus, any departure from the strong-scaling prediction for the form of the second term will be difficult to see directly in Fig. 1. However, by taking the derivative of $\Gamma(\vec{r}, T)$ with respect to K, the first term in (4) is removed, and the failure of strong scaling becomes easy to detect. In Fig. 3 we have plotted the quantity

$$(\kappa r)^{\alpha/\nu}(\kappa_0 r)^{-1/\nu}\frac{\partial(r/a)^{1+\eta}\Gamma(\vec{r},T)}{\partial(K/K_c)}$$

vs κr for a variety of representative sites. $\kappa_0 a = 2.30 \pm 0.03$.[11] If strong scaling holds, then this quantity is equivalent by (1) to $-(\kappa r)^{\alpha/\nu} dD(\kappa r)/d[(\kappa r)^{1/\nu}]$ and the curves for different lattice sites must coincide, apart from small fluctuations due to departures from spherical symmetry, etc. It can be seen that there is a systematic departure from strong scaling in the region $\kappa r < 0.8$ which disappears for larger values of κr. $\partial\Gamma(\vec{r}, T)/\partial K$ was calculated in analogy to (5) by extrapolating the partial sums

$$\sum_{n=0}^{N} n q_n(\vec{r}) K^n$$

against the quantity

$$\epsilon^{-\alpha} - \sum_{n=0}^{N} c_n(-\tfrac{1}{8})(K/K_c)^n.$$

The nonscaling terms for which we have argued appear in any case to be small. They will be difficult to detect experimentally.[14] It is tempting to speculate that the breakdown of strong scaling and the failure of the scaling law $3\nu = 2-\alpha$ are related. Such deviations from "ideal" behavior may be connected with the existence of a "second length."[15] We have been unable to find an unambiguous way of extracting such a length from the series data.

We are indebted to Professor L. P. Kadanoff for discussions of these results.

*Work supported in part by the National Science Foundation under Grant No. NSF GP-7765 and the Advanced Research Projects Agency under Contract No. ARPA SD-131.

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[6]In speaking of OZ behavior we shall always mean the form Eq. (2), with the Yukawa behavior as a function of r and the factor κ^η. Note that (2) is a special case of (1). We specifically do not mean to imply the

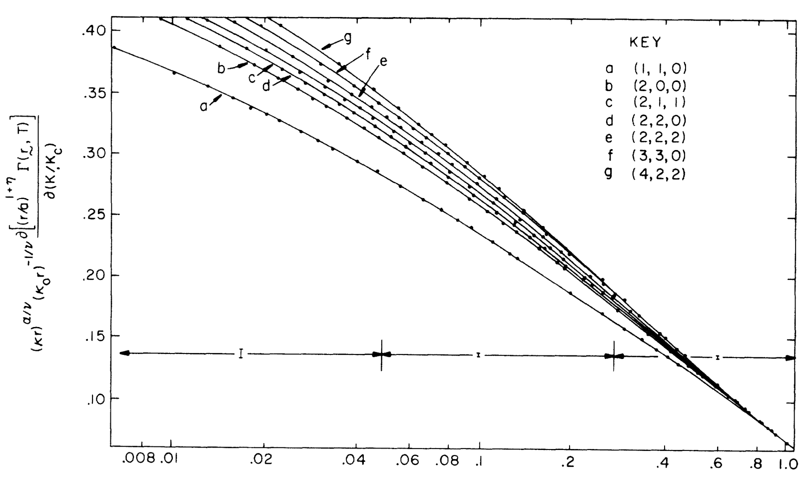

FIG. 3. Systematic deviations from scaling. According to (1) the vertical axis is $-(\kappa r)^{\alpha/\nu} dD(\kappa r)/[(\kappa r)^{1/\nu}]$, and all points should lie on a single curve. Maximum error bars for different values of κr are indicated.

"classical" critical indices $\eta = 0$ and $\nu = \frac{1}{2}$.

[7]Equation (4) is rigorous for $d=2$, and confirmed numerically, but unproven, for $d=3$. See Fisher and Burford, Ref. 3; and M. E. Fisher, in Critical Phenomena, edited by M. S. Green and J. V. Sengers (National Bureau of Standards, Washington, D. C., 1966).

[8]M. F. Sykes, J. L. Martin, and D. L. Hunter, Proc. Phys. Soc. (London) 91, 671 (1967).

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[10]For more distant sites the number of nonzero $q_n(\vec{r})$, $n \leq 12$, is insufficient for worthwhile extrapolation.

[11]Scaling depends only on the variation with temperature of $\kappa(T) = \kappa_0 \epsilon^{\nu}$. In drawing Fig. 1 we have used $\kappa_0 a = 2.30 \pm 0.03$, which consistently fits the exponential part of the large-r behavior, i.e., correctly gives the slope of $\ln[(r/a)\epsilon^{-\nu\eta}\Gamma(\vec{r},T)]$ vs $-\epsilon^{\nu}r/a$ [see Eq. (2)].

[12]Fisher, Ref. 7.

[13]V. G. Vaks, A. I. Larkin, and Yu. N. Ovchinnikov, Zh. Eksperim. i Teor. Fiz. 49, 1180 (1965) [translation: Soviet Phys.–JETP 22, 820 (1966)].

[14]Static scattering experiments measure $\chi(\vec{k},T)$, the Fourier transform of $\Gamma(\vec{r},T)$. Strong scaling predicts $\chi(\vec{k},T) = F(k/\kappa)k^{2-\eta}$ for small k and κ regardless of the ratio k/κ. Reference 3 gives scattering approximants of this type. Our prediction is that there are small nonscaling departures from this behavior, notably at fixed k as $\epsilon \to 0$. It seems likely that recent scattering experiments on lattice systems do not have sufficient resolution to detect such effects. See L. Guttmann and H. C. Schnyders, Phys. Rev. Letters 22, 520 (1969); also, J. Als-Nielsen and O. W. Dietrich, Phys. Rev. 153, 706, 711, 717 (1967).

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SPIN-POLARIZED SPLITTINGS IN THE TEMPERATURE-DEPENDENT REFLECTANCE OF EuO†

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(Received 5 May 1969)

The reflectance of EuO from above the Curie point at 69°K down to 1.5°K shows splittings in the two main peaks near 1.5 and 4.7 eV. The first peak is a polarization-dependent triplet at 1.5°K and a doublet at 70°K. The data suggest that the 1.5-eV peak is associated with the absorption edge and arises from the transition $4f^7(^8S_{7/2}) \to 4f^6(^7F_J)5d(t_{2g})$. The narrow t_{2g} sub-band is exchange split by 0.25 eV at low temperatures.

Previous optical studies of the magnetic semiconductors, EuO and other europium chalcogenides, have shown unusually large magneto-optical effects[1] and an anomalous red shift of the absorption edge upon cooling through the Curie point.[2] These effects have been ascribed to transitions from the localized europium $4f$ electron states to $5d$ energy states.[3] We have further examined the effects of magnetic ordering on the band structure by optical reflection studies of EuO beyond the absorption edge in two sets of experiments: (1) measurement of the reflectance from 0.6 to 5.2 eV at several temperatures through the Curie point, $T_C = 69$°K, down to 1.5°K and (2) examination of the first peak in the reflectance with circularly polarized light and in a magnetic field at 70 and 1.5°K. We believe the splittings of the reflectivity peak observed in these measurements indicate that the transitions are to conduction-band states which spin split at low temperatures. To our knowledge, this is the first time such structure has been seen by direct reflectance measurements through the Curie point in any ferromagnetic material.

In the first set of experiments no polarized light or magnetic field was used. The results of these measurements appear in Fig. 1. E_1 centered at 1.44 eV at 80°K is the lowest energy structure near the absorption edge at 1.2 eV.[2,4-6] E_2 is centered at 4.65 eV at 80°K.

As the temperature is lowered through T_C several striking features appear in the spectrum.

(1) E_1 appears to narrow slightly with decreasing temperature above T_C but for $T < T_C$, E_1 broadens and a second peak E_1' splits off to lower energy. As noted later in our magneto-optical measurements, there is a third peak E_1'' splitting off to higher energies, not resolved in Fig. 1 (see Fig. 2), which also contributes to the broadening.

(2) E_1 has a red shift upon cooling similar to that of the absorption edge.[6] However, the peak shift is not as great as that of the edge, the peak shifting about 0.2 eV and the edge about 0.3 eV