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Density of Zeros on the Lee-Yang Circle for Two Ising Ferromagnets*

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Extrapolations of high-field and high-temperature series expansions have been used to construct numerical approximations to the density of zeros $g(\theta)$ on the Lee-Yang circle for the Ising ferromagnets on a two-dimensional square and a three-dimensional diamond lattice. For temperatures above the critical temperature the density is zero for $|\theta| < \theta_G$ and then varies as $(\theta - \theta_G)^{\mu}$, with $\mu \simeq -0.1$ and $+0.1$ for the square and diamond lattices, respectively.

Lee and Yang[1] in 1952 pointed out that the thermodynamic properties of an Ising ferromagnet in the thermodynamic limit, in the presence (or absence) of a magnetic field H, are determined by the limiting density of zeros of the partition function, $g(\theta)$, on the unit circle $z = e^{i\theta}$ in the complex $z = \exp(-2H/T)$ plane (with H and T in suitable dimensionless units). There have been many studies of the thermodynamic properties of Ising ferromagnets, especially near the critical point,[2] but despite the fact that $g(\theta)$ (as a function of T) contains all this information, and is of fundamental significance for the theory of phase transitions,[3] very little is known about its actual form. We present below results of what we believe to be the first systematic investigation of $g(\theta)$, based on extrapolations of high-temperature and high-field series, for two Ising ferromagnets which exhibit a phase transition and a critical point: the square lattice and the diamond lattice, with nearest-neighbor interactions.

We have obtained quantitative information about some features of g previously anticipated such as the existence of a gap $|\theta| < \theta_G(T)$, centered at $\theta = 0$, in which g is zero if the temperature exceeds the critical temperature T_c. (Such a gap implies that the free energy is an analytic function of H for all real values of H including $H = 0$, and thus there is no phase transition as a function of H.[3] Such analyticity, and thereby the existence of a

gap, has been proved[4] at sufficiently high temperatures, and it is plausible to assume that it persists for all $T > T_c$.) However, some properties of g were quite unexpected. We find strong evidence that for the square lattice $g(\theta)$ diverges at $\theta = \theta_G$. That is, if we assume

$$g \sim (\theta - \theta_G)^{\mu} \tag{1}$$

near θ_G, μ is negative. For the three-dimensional diamond lattice, μ is positive, but different from a value previously suggested.[5] Also, for both the square and diamond lattices g does not appear to be a monotone function of θ for $T > T_c$ and for the square lattice, g exhibits a sharp decrease as $\theta \to \pi$, at temperatures well above T_c.

Let $M(z)$ be the magnetization of the Ising ferromagnet, equal to 1 at saturation. The high-field series[6] provides a power series expansion for $M(z)$ at $z = 0$ of which the first fourteen coefficients are known exactly for the square and diamond lattices. These coefficients are, as well, the coefficients of the Fourier cosine series for the function

$$u(\theta) = 2\pi g(\theta) = \lim_{r \to 1-} \mathrm{Re} M(re^{i\theta}), \tag{2}$$

the limit of the real part of M as z approaches the boundary of the unit circle from the inside.

For temperatures somewhat below T_c a reasonably good approximation to $u(\theta)$ is obtained by forming Padé approximants to the high-field series for $M(z)$ and using (2). The result for both square and diamond lattices is qualitatively similar to that indicated in Fig. 1(a) for the mean-field model.[7] At $\theta = 0$, u is just the spontaneous magnetization, and near this point $u(\theta)$ is approximately parabolic. With increasing θ the parabola rapidly bends over and u continues to rise at a decreasing rate as θ approaches π.

At T_c one expects[2] M to vary as $H^{1/\delta}$ for small H and hence[8] u should be proportional to $\theta^{1/\delta}$ for small θ, where δ is 15 for the square lattice and approximately 5 for the three-dimensional lattices. If $u(\theta)$ is set equal to $[\sin(\theta/2)]^{1/\delta}$ times a polynomial, the polynomial can be adjusted to give Fourier coefficients in good agreement with the high-field series. The mean-field density for $T = T_c$ is shown in Fig. 1(b) ($\delta = 3$).

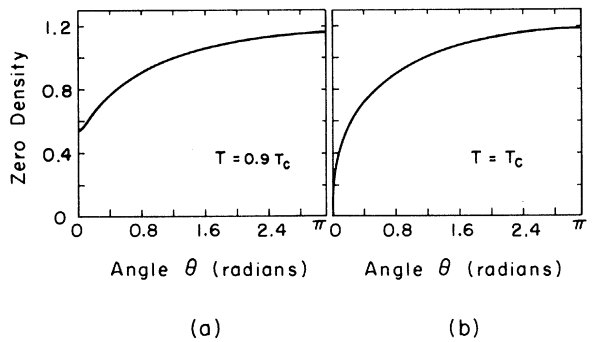

FIG. 1. The function $u(\theta)$ for the mean-field model.

For temperatures $T > T_c$, a reliable estimate for $u(\theta)$ depends on knowing the gap angle θ_G. The following technique appears to yield accurate values of θ_G for T not too close to T_c. If we define

$$\tau = \tanh(H/T) = (1 - z)/(1 + z), \tag{3}$$

then $|z| = 1$ is mapped onto the imaginary τ axis, $\tau = i\eta$, and the point $z = \exp(-i\theta_G)$ onto $\tau = i\eta_G = i\tan(\theta_G/2)$. Assuming that

$$M \sim \tau(\tau^2 + \eta_G^2)^{\mu} \tag{4}$$

for τ near $i\eta_G$, then, by (2), u or[9] g has the form (1) for $\theta > \theta_G$ while for $\eta < \eta_G$,

$$\hat{\chi} \equiv (\partial M/\partial \tau)_T \sim (\eta_G - \eta)^{\mu - 1}. \tag{5}$$

The divergence of $\hat{\chi}$ (assuming $\mu < 1$) can be used to locate η_G.

In practice it is more convenient to hold $\tau = i\eta$ fixed and search for a divergence in $\hat{\chi}$ as a function of T or, equivalently, the variable $v = \tanh(J/T)$, using high-temperature series.[10] Indeed, this procedure is essentially identical to locating an ordinary critical point in zero magnetic field by looking for a divergence of the susceptibility series. We employed a Neville table[11] to analyze the series in v (all known coefficients are positive) in order to obtain $v_G(\eta)$, the inverse function to $\eta_G(v)$. The resulting estimates for $\theta_G(T)$, whose reliability increases with increasing temperature T, are shown in Fig. 2. The curves

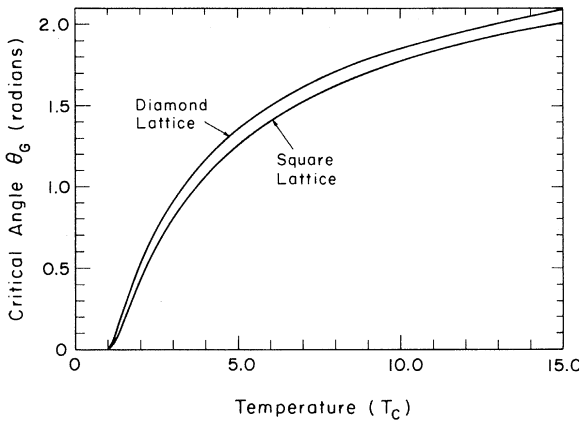

FIG. 2. The gap angle $\theta_G(T)$ for the square lattice (lower curve) and diamond lattice (upper curve).

were drawn using the formula

$$\sin(\theta_G/2) = (v_c - v)^{\Delta} f(v) \tag{6}$$

with $f(v)$ a third-order polynomial and $\Delta = \beta\delta$ the usual critical gap index. The form (6) gives excellent agreement with numerical results and has the expected variation of $\theta_G(T)$ near T_c.[12]

The high-temperature series also permits one to estimate μ, on the plausible assumption that $\hat{\chi}$ diverges as $(v_G - v)^{\mu-1}$ for fixed η. The values obtained from Padé approximants to $d(\ln\hat{\chi})/dv$ and $(v_G - v)d(\ln\hat{\chi})/dv$ showed some dependence on the temperature which is probably spurious. We know that the mean-field model[7] has $\mu = \frac{1}{2}$ at all temperatures, but our methods of analysis applied to this model gave a variation in μ similar to that obtained in the other cases, with the most rapid apparent variation occurring as T approaches T_c.

Assuming that μ is constant, we estimate a value of -0.12 ± 0.05 for the square lattice and $+0.12 \pm 0.05$ for the diamond lattice. A linear Ising chain[1] has $\mu = -0.5$ while the mean-field model, with $\mu = 0.5$, probably represents the limit of an infinite number of dimensions. Thus there seems to be a systematic increase in μ with dimensionality.

Some specific curves for $u(\theta)$ are shown in Fig. 3. Those for the square and diamond lattices were generated by computing the Fourier coefficients of u defined by[9]

$$u(\theta) = P_1(\theta - \pi)\psi^{\mu} \tag{7}$$

for $\theta_G < \theta < \pi$, with

$$\psi(\theta) = [\sin(\theta/2)]^{1/\Delta} - [\sin(\theta_G/2)]^{1/\Delta} \tag{8}$$

and P_1 a polynomial in $\theta - \pi$ containing eight terms. The rather complicated form for ψ in (8) was adopted in hopes of providing a better fit near $T = T_c$; at the temperatures illustrated in Fig. 3, $\psi = \theta - \theta_G$ would probably work equally well. The constant term in P_1 was chosen to give the value of u at $\theta = \pi$ (known exactly for the square lattice[13] and estimated by Padé approximants for the diamond lattice), and the remaining terms adjusted to minimize the mean square deviation of the Fourier coefficients from the exact values. For the square lattice, the best fit (in the sense just described) occurred if both even and odd terms were included in P_1. This seems to reflect the presence of a singularity in the form of a sharp decrease in u at $\theta = \pi$ for temperatures well above T_c. This decrease is quite evident in Fig. 3. Padé approximants to d^2M/dz^2

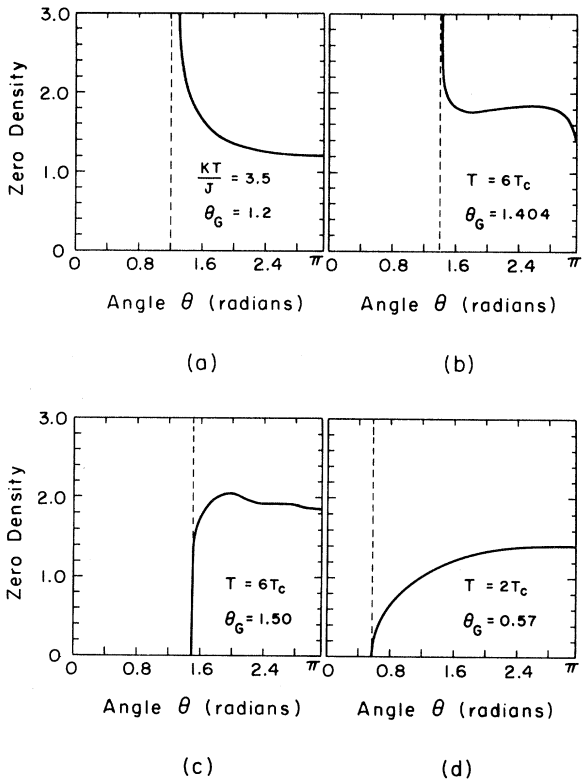

FIG. 3. The function $u(\theta)$ for (a) the linear chain, (b) the square lattice, (c) the diamond lattice, and (d) the mean-field model.

also give some evidence for a singularity at $\theta = \pi$. For the diamond lattice equally good fits were obtained if P_1 contained both even and odd powers or only even powers of $\theta - \pi$. Our calculations do not rule out the possibility of singular (nonsmooth) behavior at $\theta = \pi$, but if present it is certainly less prominent than for the square lattice. For both lattices there is a region about halfway between θ_G and π where $du/d\theta$ is positive. This seems to be a real effect, though we cannot be absolutely certain it is not an artificial result of our approximations.

At temperatures less than twice the critical temperature, we added to (7) a term

$$P_2(\theta - \pi)\psi^{\beta} \tag{9}$$

with P_2 another polynomial, and β the usual spontaneous magnetization critical index ($\frac{1}{8}$ for the square lattice and approximately $\frac{5}{16}$ for the diamond lattice). The form (9) was suggested by some work of Suzuki[5] and seemed to give good agreement with the high-field series for temperatures near the critical temperature, where the "leading" singularity (7) has a much smaller amplitude than at high temperatures. Of course, if

our hypothesis about the constancy of μ is correct, there must be at least a small contribution from a term of the form (7) at any temperature above T_c, showing that the actual density has a more complicated structure than Suzuki proposed.

In summary, numerical investigations of the density of zeros on the Lee-Yang circle for a two-dimensional and a three-dimensional Ising model indicate few surprises for $T \leq T_c$, but suggest that above T_c the behavior near θ_G is dominated by a singularity with an exponent μ whose connection with other "critical" exponents is at present not clear. Also, $g(\theta)$ is not a monotone function of θ for T substantially greater than T_c, unlike the situation in the one-dimensional Ising and mean-field models. Finally, for the two-dimensional lattice there is strong evidence of some sort of singular behavior at $\theta = \pi$ for $T > T_c$.

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[9]Note that $g(\theta)$ is a symmetric function, $g(\theta) = g(-\theta)$.

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Character of Excitations in Substitutionally Disordered Antiferromagnets

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Magnetic excitations in several single crystals of the systems K(Co, Mn)F_3 and (Co, Mn)F_2 have been studied by neutron inelastic scattering. It is found that two branches of well-defined magnetic excitations, both of which exhibit propagating character, occur at certain compositions. The dispersion relation for two branches of propagating excitations cannot be adequately described by current theories, but an extension of Anderson's criterion for localization in disordered alloys gives approximate agreement with the observed character.

The excitations in randomly disordered systems may have either localized or nonlocalized character. Although Anderson[1] first investigated the conditions for localization in 1958, there is still considerable disagreement[2] about the detailed behavior. The theoretical work has dealt mainly with electron states; but, in principle, the problem is the same for a wide class of excitations and in particular for spin waves, which have the advantage that they can be studied directly by neutron inelastic scattering. We report here measurements on disordered antiferromagnets that for the first time show the existence of two branches of propagating excitations in a disordered quasibinary system. Current Green-function theories for antiferromagnets cannot describe the results, but the character of the excitations is reasonably well described by a localization criterion of the Anderson form.

The measurements were carried out by means of neutron inelastic scattering using a triple-axis crystal spectrometer controlled so that the wave-