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Magnetic Tricritical Points in Ising Antiferromagnets

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(Received 20 December 1971)

The thermodynamic properties of the antiferromagnetic Ising simple cubic and square lattices with nearest-neighbor and next-nearest-neighbor interactions have been studied using a Monte Carlo technique. Although both systems were found to possess magnetic tricritical points, their behavior in the "tricritical region" differed from that found in He^3-He^4 mixtures.

Over the past decade tremendous interest has been generated regarding the thermodynamic properties of both magnetic and gas-liquid systems near their critical points. New stimulus has been added recently by Griffiths[1] who examined the region of the two-fluid critical mixing point in He^3-He^4 mixtures and pointed out that the critical temperature corresponded to a thermodynamic "tricritical point," T_t. In addition, his examination of the experimental results showed that "classical theory"[2] clearly failed near T_t. Since there is no reason to expect any relation to the ordinary critical region, the "tricritical region" represents a totally new thermodynamic puzzle. Analogous tricritical behavior is also to be expected in magnetic systems (with suitable transformation of variables), and indeed magnetic tricritical points have been observed in $FeCl_2$,[3] $Ni(NO_3)\cdot 2H_2O$,[4] and dysprosium aluminum garnet (DyAlG).[5] Unfortunately, the experiments on these systems were not intended to probe the tricritical region and only in the case of DyAlG was the experimental resolution sufficient to map out the thermodynamic behavior near T_t. In DyAlG, however, the situation is complicated by the dominance of long-range dipolar interactions. Griffiths[1] used general arguments to propose a "scaling" form for the free energy. This expression appears quite successful for He^3-He^4, and an analogous form should apply to magnetic systems. Beyond this, theoretical support is very sparse.[6] Molecular field theory [7-9] does predict the existence of tricritical points in magnetic systems with competing interactions; however, this model fails completely in the ordinary critical region and should not be expected to be reliable near T_t. Because of the difficulty of including both competing interactions and a magnetic field in the Hamiltonian, series expansions have not been derived for any lattice. (The nearest neighbor only case has been considered.[10]) Thus, the only information available regarding magnetic systems comes from a small number of experimental reports of tricritical points in anisotropic systems.

It was our desire to investigate simple two- and three-dimensional magnetic systems in order to further our understanding of magnetic tricritical points. The disadvantage of working with finite systems must not be taken too lightly; however, there are obvious advantages to performing experiments at constant volume on a pure sample possessing no strains or imperfections. (Theoretical models generally have these features "built in.") Monte Carlo studies were made of the 50×50 square lattice, and the $12\times 12\times 12$ simple cubic (sc) lattice. In both cases periodic boundary conditions were applied, and the interaction Hamiltonian included both nearest-neighbor (nn) and next-nearest-neighbor (nnn) interactions:

$$\mathcal{H}=\sum_{\text{nn pairs }(ij)} K_{\text{nn}}\sigma_{iz}\sigma_{jz} + \sum_{\text{nnn pairs }(ik)} K_{\text{nnn}}\sigma_{iz}\sigma_{kz}+\sum_i g\mu_B H\sigma_{iz}, \quad (1)$$

where $\sigma_{iz}, \sigma_{jz}, \sigma_{kz}=\pm 1$. The relative magnitudes of the competing interactions ($\alpha=K_{\text{nnn}}/K_{\text{nn}}$) were allowed to vary, but K_{nn} was constrained to be positive in order to ensure the basic stability of the low-temperature antiferromagnetic state. The method used was an important sampling technique described by Fosdick.[11] (A brief discussion of our procedure was presented earlier,[12] and full details will be explained in a forthcoming publication.) Data were generally taken isothermally with the field both increasing and decreasing in order to test for reversibility. Additional experiments were performed with the field fixed and the temperature varying. Averages of the magnetization and internal energy were determined for each temperature and field. In an effort to ascertain the general reliability of our data we made a number of runs under conditions for which the results were already known quite accurately. Zero-field transition temperatures, for various α, were in excellent agreement with the series expansion results of Dalton and Wood[13]; in addition, for $\alpha=0$ the critical field H^c and critical magnetization M^c, i.e., $M(H=H^c)$, agreed closely with series-expansion results.[10]

The results of our experiments showed that in both the sq and sc lattices tricritical points did occur for antiferromagnetic nn interactions and ferromagnetic nnn coupling, i.e., $K_{\text{nn}}>0$ and $\alpha<0$. In all cases the critical-field curve was smooth and continuous as a function of temperature showing no "kinks" at T_t. Examination of the M-vs-H plots showed that between T_N and T_t the transition from the antiferromagnetic to paramagnetic state was at least second order with no discontinuity in the magnetization and no irreversibilities. (In comparison with He^3-He^4 mixtures, this part of the critical-field curve could be termed the "line of magnetic λ transitions.") Below T_t the transitions were clearly first order with discontinuities in the magnetization and pronounced hysteresis. In these cases a modified rule of equal areas was used to find the actual transition field. The resultant critical phase lines in the M-T plane are plotted in Fig. 1 for one value of α for each lattice; the data points are expressed in terms of the reduced magnetization $m=M/M_{\text{sat}}$, where M_{sat} is the saturation magnetization. The values of α were chosen so that the ratio of the total *inter*-sublattice and *intra*-sublattice interaction strength was the same for both lattices. It is obvious from these results that, as in the case of He^3-He^4 mixtures, the upper arm of the two-state coexistence curve does *not* join smoothly into the curve of critical magnetization on the line of magnetic λ transitions. Several runs were also made on smaller lattices in order to determine the effect of finite lattice size. As a general rule, the smaller the lattice the more "smeared out" the antiferromagnetic-paramagnetic transition was and the more T_t was depressed. Also, as the system moved away from T_t the magnetic properties very quickly became less dependent on sam-

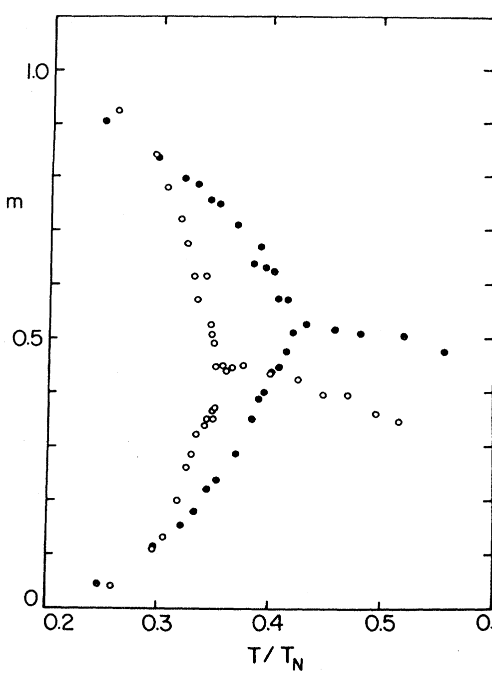

FIG. 1. Reduced magnetization at the critical field as a function of temperature. Open circles, results for the sq lattice, $\alpha=-0.5$; filled circles, results for the sc lattic, $\alpha=-0.25$.

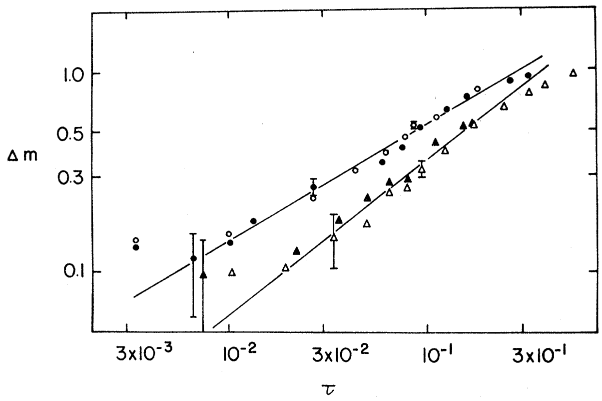

FIG. 2. Discontinuity in the reduced magnetization at the critical field as $T \to T_t$ from below. Results for the sq lattice: filled circles, $\alpha = -0.5$; open circles, $\alpha = -1.0$. Results for the sq lattice: filled triangles, $\alpha = -0.25$; open triangles, $\alpha = -0.50$.

ple size. These data indicated that the results reported here for larger lattices should be quite reliable for $|(T - T_t)/T_t| \simeq 10^{-2}$.

As is usual in the analysis of critical phenomena, we shall assume that the discontinuity in the magnetization disappears as a simple power law as the two-state coexistence curve merges into magnetic λ line:

$$\Delta m = R\tau^{\rho}, \tag{2}$$

where R is a constant, $\tau = |T - T_t|/T_t$, and ρ is a tricritical exponent. In order to test for this type of behavior, we have made plots of Δm vs τ on a log-log scale (see Fig. 2). The slopes of the best straight lines which fit the data appear to depend on the lattice but *not* on the choice of α. For the sq lattice we find $\rho = 0.58 \pm 0.11$ and for the sc lattice $\rho = 0.78 \pm 0.20$. Thus, the value $\rho = 1$ obtained from molecular field theory[9] appears to be an artifact of the theory. It appears then that ρ depends on lattice structure, or at least dimensionality, but not on the relative magnitudes of the competing interactions. An interesting comparison can be made with He^3-He^4 for which the experimental results[14] strongly suggest that ρ is very near to 1.

Outside the mixed phase region the magnetic susceptibility describes the nature of the phase transition. In analogy with ordinary critical points, we shall assume that the susceptibility for m equal to its tricritical value m_t diverges, for T greater than T_t, as a simple power:

$$\chi_T(m = m_t) \propto \tau^{-\epsilon}. \tag{3}$$

The differential isothermal susceptibility was de-

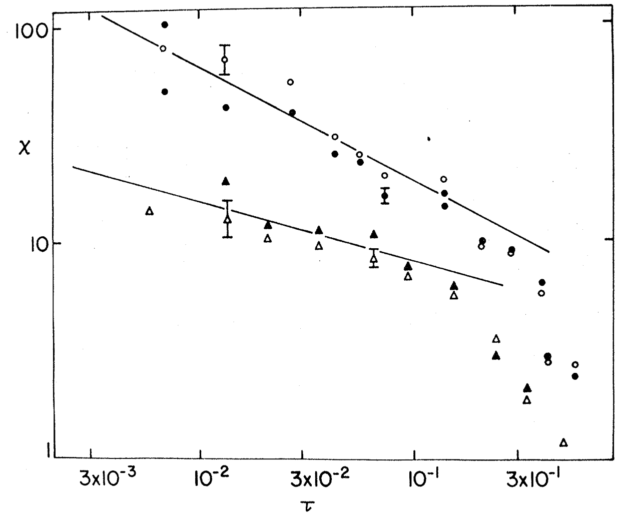

FIG. 3. Divergence of the reduced differential magnetic susceptibility at $m = m_t$ as $T \to T_t$ from above. Results for the sq lattice, $\alpha = -0.5$: open circles, $(dm/dH)_{m=m_t}$; filled circles $\chi_{\text{fluct.}}$. Results for the sc lattice, $\alpha = -0.25$: open triangles, $(dm/dH)_{m=m_t}$; filled triangles, $\chi_{\text{fluct.}}$.

termined graphically from the m-vs-H curves, and in Fig. 3 we have plotted the differential susceptibility

$$(dm/dH)_{m_t} = \chi_T(m = m_t)$$

versus τ on a log-log scale, $\alpha = -0.5$ for the sq lattice and $\alpha = -0.25$ for the sc lattice. We have also determined the susceptibility from the fluctuation theorem:

$$\chi_{\text{fluct}} = (\lambda/T)(\langle m^2\rangle - \langle m\rangle^2) \tag{4}$$

where $\langle m^2\rangle$ is the mean square magnetization, $\langle m\rangle$ is the mean magnetization, λ is a normalization constant, and T is temperature. These results are also shown in Fig. 3. For the sq lattice we find $\epsilon = 0.53 \pm 0.14$ and for the sc lattice $\epsilon = 0.29 \pm 0.18$. The data for other α values yielded the same ϵ's for the respective lattices. Although the large experimental errors preclude any definite conclusions, our values certainly appear to be different from the experimental result $\epsilon = 1.0 \pm 0.1$ determined for He^3-He^4 mixtures.[15]

These results must, of course, be regarded rather cautiously since the size of the tricritical region is not yet known. It does nonetheless appear that magnetic tricritical points should be common since the conditions for their existence do not appear stringent. In the systems studied here the tricritical behavior is in clear disagreement with molecular field theory. At the moment it is not clear why He^3-He^4 mixtures differ in their tricritical behavior from these simple magnetic systems, although recent series expansion results[16] on the Blume-Emery-Griffiths[17] model suggest that the differences in the Hamiltonian may be responsible. Thus, we feel that there is a whole new range of thermodynamic phase diagram to be studied theoretically. In particular, we feel it would be most interesting to see the results of more careful experiments on real systems, and of series expansions studies for a variety of lattices.

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Transcendence of the Law of Baryon-Number Conservation in Black-Hole Physics*

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(Received 1 November 1971)

The following result is stated: A black hole in its final state can be endowed with no exterior scalar, vector, or spin-2 meson fields. We conclude that such a black hole is not subject to the strong interactions which are mediated by meson fields such as the π, ρ, and f, and that consequently a useful definition of baryon number cannot be given for such an object.

It is the present belief that, from the point of view of an exterior observer, the final state of the total gravitational collapse of a massive star is a stationary black hole.[1] It has been conjectured that mass, charge, and angular momentum are the *only* independent properties of such black holes. More precisely, this Israel-Carter conjecture states that the exterior of an isolated stationary black hole is *completely* described by a Kerr-Newman (charged Kerr) solution of the Einstein-Maxwell equations. Such a solution has only three parameters: the mass, charge, and angular momentum of the black hole.[1] This conjecture is supported by much evidence, but principally by theorems of Israel,[2] Carter,[3] Hawking,[4] and Wald.[5]

The above theorems do not explicitly allow for the effects of the weak and strong interactions of the stellar material out of which the black hole was formed. Hartle[6] and Teitelboim[7] have considered the possible effects of the weak interactions on the problem. Hartle concludes that a Kerr black hole cannot interact with the exterior world by means of the weak interactions which are mediated by neutrino fields. By a different method, Teitelboim obtains a similar result for the spherically symmetric case, and concludes that the black-hole's lepton number cannot be measured from its exterior by means of the weak interactions (which are characteristic of all leptons). This conclusion supports Wheeler's argument that the law of conservation of lepton number is transcended in black-hole physics.[8] Both Hartle's and Teitelboim's results support the Israel-Carter conjecture in the realm of the weak interactions.