Integer Optimization and Zero-Temperature Fixed Point in Ising Random-Field Systems

Andrew T. Ogielski
AT&T Bell Laboratories, Murray Hill, New Jersey 07974
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Phase transition in $d=3$ ferromagnetic Ising models with random fields is analyzed directly at the zero-temperature critical point. Critical behavior is extracted from correlation functions averaged over an ensemble of exact ground states obtained with a new integer optimization algorithm. For Gaussian distribution of random fields finite-size scaling demonstrates a continuous phase transition with effective disconnected susceptibility exponent $\tilde{\eta} \approx -0.9$, correlation-length exponent $\nu \approx 1.0$, and magnetization exponent $\beta \approx 0.05$.

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New scaling hypotheses were proposed in several recent articles to explain the critical behavior[1-4] and nonequilibrium phenomena[1,2] in Ising systems with random fields (RF) coupling to the order parameter. The scenario is restricted to an unspecified class of RF distributions such that the transition is *continuous* along the entire phase boundary, and as a result of the dominance of spatial RF fluctuations over thermal fluctuations the critical behavior is controlled by a zero-temperature fixed point with temperature dangerously irrelevant.[5] The hyperscaling is modified to $(d-\theta)\nu = 2-\alpha$, where θ is a third independent exponent, and extremely slow relaxation is explained by activated dynamics with relaxation time scaling in a Vogel-Fulcher–type manner, $\ln\tau \sim \xi^z$, with z assumed equal to θ.

These conjectures provided a plausible explanation of experiments on the most studied RF systems, dilute antiferromagnets in a field,[6] and were supported by large Monte Carlo simulations.[7] However, because of slow relaxation it is exceedingly difficult to test the scaling in the crucial regime close to the transition, especially at low T (strong fields) where crossover effects do not distort the asymptotic RF critical behavior. In this report I discuss the scaling analysis of numerical solutions of RF Ising models obtained with a new *nonrelaxational* algorithm, thus completely avoiding the equilibration problem.

Static critical behavior in strong random fields can be obtained from a zero-temperature theory alone. In statistical mechanics of random systems at $T=0$ one has to compute correlation functions of interest in the exact ground state for each particular configuration of the disorder variables (here, random fields), and subsequently average over the ensemble of disorder configurations. Such a task can be performed by a computer for a range of lattice sizes and a range of parameters characterizing the distribution of disorder. The algorithm used to generate exact ground states is described further in the text.

I consider the ferromagnetic RF Ising models defined by a nearest-neighbor Hamiltonian

$$H = -J\sum_{xy} S_x S_y - \sum_x h_x S_x, \tag{1}$$

with uncorrelated random fields h_x on sites of a cubic L^3 lattice with periodic boundary conditions. I computed the *disconnected* correlation functions

$$\chi_L(q) = (1/L^3)\langle |S_q|^2\rangle_c, \tag{2}$$

average ground-state energy $E_0(h) = \langle H\rangle_c$, and magnetization $M(h) = (1/L^3)\langle |S_{q=0}|\rangle_c$. The brackets $\langle \cdots \rangle_c$ denote configurational averaging, and S_q is the Fourier-transformed spin variable. The correlation function (2) at $q=0$ defines the disconnected susceptibility χ_L. I used several finite-size scaling techniques to investigate the nature of the transition and to locate the critical value of RF variance h_c^2 and, when applicable, to obtain the estimates of critical exponents.

For the Gaussian distribution of RF with variance h^2 and zero mean I find a *continuous* transition to a ferromagnetic state. There is no evidence for any "domain phase"[8] above the transition. The estimates of the disconnected susceptibility exponent $\tilde{\eta}$ (defined by $\chi \sim \xi^{2-\tilde{\eta}}$) and of the correlation length exponent ν are

$$\tilde{\eta} = -0.9, \quad \nu = 1.0. \tag{3}$$

The uncertainty in these values (estimated to be about 10%) is due mainly to corrections to scaling, whose form is not known, rather than to statistical errors. The critical field h_c and $\tilde{\eta}$ were determined from the plot of the ratios[9] $\zeta_{L,L'} = \ln(\chi_L/\chi_{L'})/\ln(L/L')$ vs h for distinct pairs of lattice sizes in the range from 4^3 to 32^3. In the scaling limit (large L and L') a simple power law $\chi_L = \chi_0 L^{2-\tilde{\eta}}$ expected at h_c should make all curves intersect at a single point with coordinates h_c, $2-\tilde{\eta}$. Figure 1 shows a magnified intersection region near h_c for some values of L and L'. One can clearly see the effects of corrections to scaling which, although numerically small, are not completely negligible. The proximity of $2-\tilde{\eta}$ to its upper bound of 3 re-

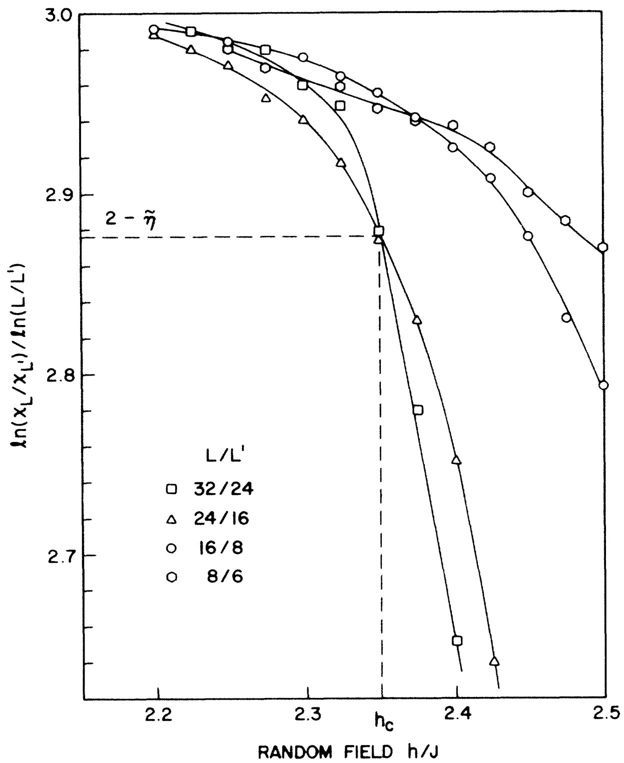

FIG. 1. Plot of the ratios $\ln(\chi_L/\chi_{L'})/\ln(L/L')$ vs the standard deviation h of the Gaussian-distributed random fields. Corrections to scaling are seen in the shift of the intersection point corresponding to small ($L=6,8,16$) and to larger lattices ($L=16,24,32$).

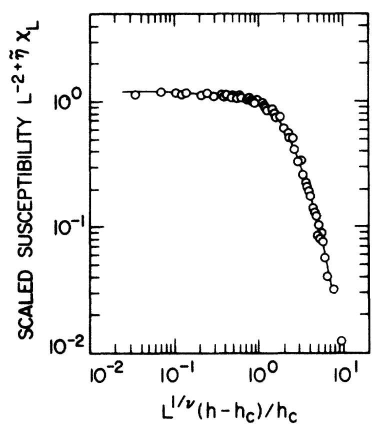

FIG. 2. The scaling function $L^{-2+\tilde{\eta}}\chi_L=f((h/h_c-1)L^{1/\nu})$ plotted with use of the values $\nu=1.0$ and $\tilde{\eta}=-0.9$, $h_c=2.35$. Lattice sizes $L=8$, 16, 24, and 32.

quired very high-precision in computation of χ_L, and the error was kept in the range from 0.1% to 1%, often even less.

Exponents $\tilde{\eta}$ and ν together were found from matching of the data to obtain the scaling function f, $\chi_L \approx L^{2-\tilde{\eta}} f((h-h_c)L^{1/\nu})$ (Fig. 2), and ν itself was also found from the size dependence of the "apparent" critical field $h_c(L)$. The latter is defined by the inflection point of the magnetization curves (Fig. 3), and is expected to scale as $h_c(L) \approx h_c + aL^{-1/\nu}$. I also computed the correlation length ξ for $L=32$ above h_c [$\chi_L(q)$ was fitted by a squared Lorentzian at small momenta], and for a rather narrow range of fields where finite-size effects can be ignored I find again that $\xi \sim (h-h_c)^{-\nu}$ with $\nu \approx 1$ describes the data well. In addition, a somewhat more noisy plot of the ratios $\chi_L(q=0)/\chi_L(q=1)$ vs h for different lattice sizes (Fig. 4) unmistakably showed an intersection of all curves in the vicinity of h_c, which provided further evidence that transition is continuous and that the expected scaling formula $\chi_L(q=0)/\chi_L(q=1) \sim f(\xi/L)$ holds.

The sensitivity of these methods varies, but estimates of exponents were consistently in good agreement from one case to another.

From the scaling law $\beta=\nu(1+\tilde{\eta})/2$ (Ref. 2) I obtain a very small value for the magnetization exponent: $\beta \approx 0.05$. A steep magnetization curve appears as one of characteristic features of the transition, but should not be confused with a discontinuity. The estimates (3) for $\tilde{\eta}$ and ν agree with the less accurate numbers -1.0 ± 0.3 and 1.3 ± 0.3, respectively, found in Monte Carlo simulations of dilute antiferromagnets[7]

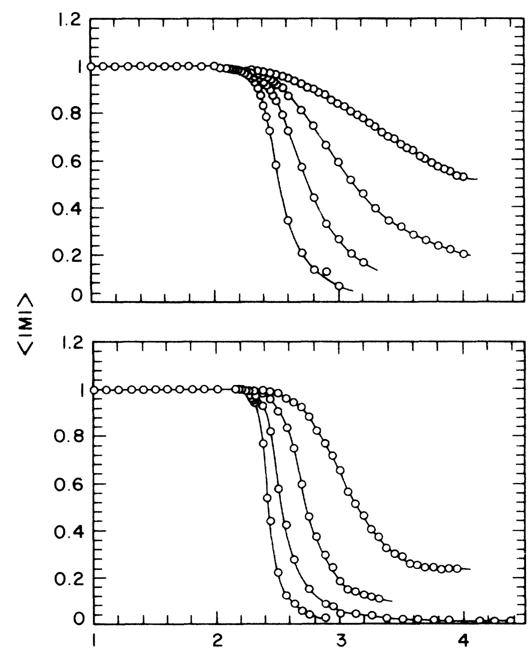

FIG. 3. Average absolute value of the magnetization $\langle|M(h)|\rangle_c$ for the binary $\pm h$ (bottom) and for the Gaussian (top) distribution of random fields. Continuous lines are guides to the eye. Lattice sizes $L=4$, 8, 16, and 32.

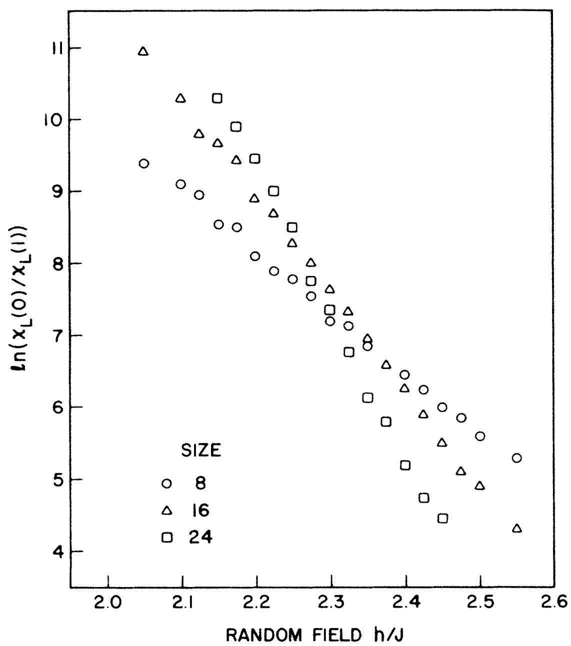

FIG. 4. The ratios $\chi_L(q=0)/\chi_L(q=1)$ of disconnected correlation function for several lattice sizes.

away from the crossover region, and also agree with the expansion[3] to first order in $\epsilon=d-2$ which yields $\tilde{\eta}=-1, \nu=1$.

Results for another RF distribution studied, the discrete $\pm h$ field with probability $\frac{1}{2}$ for each value, proved more difficult to interpret. In contrast to the Gaussian case the mean-field theory predicts here a first-order transition in the low-temperature limit.[10] Finite-size scaling analysis was performed on the $\pm h$ model in the same way as described above for the Gaussian case. My numerical solutions unambiguously show a transition to a ferromagnetic state (cf. Fig. 3), but while the correlation length grows rapidly as $h \rightarrow h_c$, one does *not* see the crossing of lines in scaling plots analogous to Figs. 1 and 4. Instead, the ratios $\zeta_{L,L'}$ all converge together only in the ferromagnetic phase towards the limiting value of 3, and merely fan out in stronger fields without intersecting. Magnetization curves which are steeper than in Gaussian case, and the absence of clear-cut signals for a continuous transition in the finite-size scaling plots, suggest the possibility that the transition is weakly first order in strong discrete $\pm h$ random fields. The technique used in this work does not allow extensions to nonzero temperatures, so we cannot say anything about the possible existence of a tricritical point, nor about the order of the transition in weak random fields. Young and Nauenberg[11] interpreted their Monte Carlo data in weak random fields in favor of a first-order transition; however, then one expects large crossover effects[7] which obscure the asymptotic critical behavior. More work is needed to resolve the puzzles of the discrete $\pm h$ RF model.

Let me turn now to the method used to generate the ground states. The details will be presented elsewhere.

Construction of exact lowest energy states is a quadratic integer optimization problem. In contrast to $d>2$ frustrated systems, where the problem is *NP* complete,[12] it was recently brought to the attention of physicists[13] that earlier mathematical work allows one to find ground states for models with arbitrary (even random) but *not frustrated* exchange interactions and arbitrary random fields in polynomially bounded computing time. The problem can be reformulated[14] as a minimum-weighted-cut problem on a certain associated graph, which in turn is related to a highly developed theory of network flows.[15] Although for short-range Ising models the corresponding graph is extremely sparse, until recently the available algorithms were nonlocal and too slow to generate large numbers of ground states for big lattices necessary in systematic scaling analysis. I implemented a new minimum-cut algorithm,[16] which is local and after some careful programming proved to be considerably faster. Interestingly enough, the execution time grows visibly in the neighborhood of the critical point, which indicates larger fluctuations in positions of bigger ordered domains of comparable energy.

The number of ground states with independent RF configurations used in the averaging was determined by the acceptable error of χ_L, and ranged from 20 000 for the smallest size (4^3) through intermediate values for 6^3, 8^3, 12^3, 16^3, and 24^3 lattices to several hundred configurations for size 32^3. I also found some ground states for up to $50^3=125\,000$ spin variables (which is a rather large optimization problem!), but longer computing time did not allow reduction of statistical errors enough. For each value of the RF variance h^2 a completely different set of RF configurations was generated.

The results of this work lead to following conclusion:

(1) At least for continuous RF distributions such as the Gaussian, there indeed is a continuous phase transition in the strong-field regime, and one expects that the transition remains continuous along the entire phase boundary. This contrasts with extrapolations of high-temperature series which in $d=3$ were previously interpreted in favor of a first-order transition.[17] Much longer series are evidently required for the correct interpretation. The results also do not support the picture of an equilibrium "domain phase" above the ferromagnetic phase boundary.

(2) Mean-field theory appears to predict correctly the existence of distinct RF universality classes characterized by the shape of RF distribution.

(3) When the proposed relation $\theta=\eta-\tilde{\eta}$ and the

exact bound $\eta > 0.5$ are used together with (3) in the hyperscaling law $(d-\theta)\nu = 2-\alpha$ we find that the specific-heat exponent α is positive and may be as large as 0.5!

(4) Slow dynamics[7,18] and crossovers make it unlikely that asymptotic critical exponents could be easily estimated in experiments on dilute antiferromagnets. In experimentally realizable weak random fields one can maintain equilibrium only not too close to the phase boundary, and effective exponents may significantly differ from asymptotic ones. Birefringence experiments[19] showed a sharpening of the specific-heat peak in stronger random fields, which was described by a logarithmic singularity ($\alpha = 0$). A larger positive value of α is indicated in the present work. This discrepancy can be resolved if one observes that on experimental time scales large localized ordered domains are completely frozen, as seen in neutron-scattering experiments,[20] and only the fluctuations on short length scales can occur: Fluctuations of large domains would give large contributions to the magnetic specific heat, thus enhancing the divergence even more. An experiment on time-dependent specific heat would be very interesting.

(5) It is worth noting that there is no simple relation between exponentially growing relaxation times and computational complexity of obtaining exact optimal solutions (ground states). In the random-field systems simulated annealing[21] is unable to produce correct ground states in any reasonable amount of time; but the optimization problem can be easily solved in a polynomial time with a deterministic algorithm.

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