Structure factor of the three-dimensional random-field *XY* model: Monte Carlo calculations

Ronald Fisch[*]

382 Willowbrook Drive, North Brunswick, New Jersey 08902, USA

We have performed Monte Carlo studies of the three-dimensional random-field *XY* model on $L \times L \times L$ simple cubic lattices, with random-field strengths of $h_r = 1$ and 2. We present results for the angle-averaged magnetic structure factor $S(k)$ at $L = 64$. Our results appear to indicate a phase transition into a ferromagnetic state. This is made possible by the existence of a Griffiths singularity. It appears that at the phase transition, M^2 jumps to zero discontinuously, with a latent heat which is probably subextensive.

I. INTRODUCTION

Some time ago, Monte Carlo calculations[1,2] indicated that there appeared to be a region of quasi-long-range order (QLRO) in the phase diagram of the three-dimensional (3D) random-field *XY* model (RFXYM), at weak random field and low temperature. Some recent functional renormalization group calculations[3,4] have questioned this. Therefore, since there have been substantial improvements in computing power over the last ten years, the author felt it worthwhile to conduct another Monte Carlo study of this model.

For fixed-length classical spins, the Hamiltonian of the RFXYM is

$$H = -J \sum_{\langle ij \rangle} \cos(\phi_i - \phi_j) - h_r \sum_i \cos(\phi_i - \theta_i). \quad (1)$$

Each ϕ_i is a dynamical variable which takes on values between 0 and 2π. The $\langle ij \rangle$ indicates here a sum over nearest neighbors on a simple cubic lattice of size $L \times L \times L$. We choose each θ_i to be an independent identically distributed quenched random variable, with the probability distribution

$$P(\theta_i) = 1/2\pi \quad (2)$$

for θ_i between 0 and 2π. This Hamiltonian is closely related to models of vortex lattices and charge density waves.

Larkin[5] studied a model for a vortex lattice in a superconductor. His model replaces the spin-exchange term of the Hamiltonian with a harmonic potential, so that each ϕ_i is no longer restricted to lie in a compact interval. He argued that for any nonzero value of h_r, this model has no ferromagnetic phase on a lattice whose dimension d is less than or equal to 4. A more intuitive derivation of this result was given by Imry and Ma,[6] who assumed that the increase in the energy of an L^d lattice when the order parameter is twisted at a boundary scales as L^{d-2}.

As argued by Imry and Ma,[6] and later justified more carefully,[7,8] within a perturbative ϵ expansion, one finds the phenomenon of "dimensional reduction." The critical exponents of any d-dimensional $O(N)$ random-field model (where N is the number of components of the spin on each site) appear to be identical to those of an ordinary $O(N)$ model of dimension $d-2$. For the Ising ($N=1$) case, this was shown rigorously to be incorrect.[9,10]

Because translation invariance is broken for any nonzero h_r, it seems quite implausible that the twist energy for Eq. (1)

scales as L^{d-2}, even though this is correct to all orders in perturbation theory. An alternative derivation by Aizenman and Wehr,[11,12] which claims to be mathematically rigorous, also makes an assumption equivalent to translation invariance. Although the average over the probability distribution of random fields restores translation invariance, one must take the infinite volume limit first. It is not correct to interchange the infinite volume limit with the average over random fields.

The basic point is that the Imry-Ma argument for continuous spins [$O(N)$ with $N \geq 2$] is not self-consistent. One begins by assuming that the random field is weak so that the twist energy scales as L^{d-2}, as in the absence of the random field. Then, one shows that if $d \leq 4$, this cannot be true for large enough L. The only conclusion which should be drawn from this is that a deeper analysis of what is going on is needed in that case.

II. GRIFFITHS PHASE

A mechanism which causes the breakdown of perturbation theory in the presence of quenched randomness at the critical temperature T_c of the pure ferromagnet was discovered by Griffiths[13] in the special case of a bond-diluted Ising model. It was later shown explicitly[14] that the magnetization per unit volume $\vec{M}(\vec{H})$ has an essential singularity at $\vec{H}=0$ (where $\vec{H}$ is a uniform field) at and below T_c. The result was then extended to the case of binary ferromagnetic alloys.[15] It was later argued that this result could be extended beyond the Ising model to $O(N)$ models[16] and that the Griffiths singularity will exist whenever the specific heat is divergent at T_c for the pure model, so that the bond randomness is a relevant perturbation.[17]

This argument appears to imply that it is never correct to use a perturbation theory of the standard type (e.g., an ϵ expansion) when the randomness is a relevant perturbation. On the other hand, an ϵ expansion is only an asymptotic series even in the nonrandom case. Thus, one may hope that it might continue to be useful even in the presence of the Griffiths singularity.

The original concept of Griffiths[13] was a singularity caused by the contributions of large, isolated clusters of spins. Hertz *et al.*[18] developed a more intuitive picture of the Griffiths singularity in random bond models, which was de-

veloped further by Bray and Moore.[19,20] These authors showed that the same type of singular behavior would be a consequence of a Lifshits tail of localized eigenvectors of the inverse magnetic susceptibility matrix χ^{-1} near the band edge at eigenvalue zero.

If one generalizes the idea of the Griffiths singularity from these random bond models to random-field models, one finds similarities but also important differences. The magnetic structure factor, $S(\vec{\mathbf{k}}) = \langle |\vec{\mathbf{M}}(\vec{\mathbf{k}})|^2 \rangle$, for XY spins is

$$S(\vec{\mathbf{k}}) = L^{-3} \sum_{i,j} \cos(\vec{\mathbf{k}} \cdot \vec{\mathbf{r}}_{ij}) \langle \cos(\phi_i - \phi_j) \rangle, \tag{3}$$

where $\vec{\mathbf{r}}_{ij}$ is the vector on the lattice which starts at site i and ends at site j and here the angle brackets denote a thermal average. For a random-field model, unlike a random bond model, the longitudinal part of the magnetic susceptibility χ, which is given by

$$T\chi(\vec{\mathbf{k}}) = 1 - M^2 + L^{-3} \sum_{i \neq j} \cos(\vec{\mathbf{k}} \cdot \vec{\mathbf{r}}_{ij})(\langle \cos(\phi_i - \phi_j) \rangle - Q_{ij}), \tag{4}$$

is not the same as S even above T_c. For XY spins,

$$Q_{ij} = \langle \cos(\phi_i) \rangle \langle \cos(\phi_j) \rangle + \langle \sin(\phi_i) \rangle \langle \sin(\phi_j) \rangle \tag{5}$$

and

$$M^2 = L^{-3} \sum_i Q_{ii} = L^{-3} \sum_i \langle \cos(\phi_i) \rangle^2 + \langle \sin(\phi_i) \rangle^2. \tag{6}$$

When there is a ferromagnetic phase transition, $S(\vec{\mathbf{k}} = 0)$ has a stronger divergence than $\chi(\vec{\mathbf{k}} = 0)$. Thus, it is S, and not χ, which is the best place to look for an essential singularity in the random-field model. There may also be an effect[19] in χ, but we should look in the place where the effect is expected to be largest.

The author is not aware of any explicit studies on the question of the occurrence of Lifshits tails in a matrix which has the form of $S(\vec{\mathbf{k}})$. The natural generalization of the Harris criterion is that the Griffiths singularity should be found in $S(\vec{\mathbf{k}} = 0)$ at the T_c of the pure $O(N)$ ferromagnet for any finite N and any $d > 2$. This is because the response of the pure system to a weak uniform $\vec{H}$ field is always divergent at T_c, i.e., the susceptibility exponent γ is always positive.[21]

A detailed numerical study of the 3D Ising model in a random field (RFIM) at $T = 0$ has been performed by Middleton and Fisher.[22] These authors find that the 3D RFIM has a ferromagnetic critical point and that the order parameter exponent β has a small but positive value. For weak random fields, the 3D RFIM still has two low-temperature (ferromagnetic) Gibbs states, even though the random fields have destroyed the Kramers degeneracy. The current author believes that the existence of multiple ferromagnetic Gibbs states is required for the existence of a critical point with a positive β.

Middleton and Fisher found no explicit evidence for the existence of a Griffiths phase in the RFIM, although they agree that such a phase should exist. Middleton[23] has also studied the four-dimensional (4D) RFIM at $T = 0$.

The scalar quantity $\langle M^2 \rangle$ is a well-defined function of the lattice size L for finite lattices, which, with high probability, approaches its large L limit smoothly as L increases. The vector $\vec{\mathbf{M}}$, on the other hand, is not really a well-behaved function of L for an XY model in a random field. Knowing the local direction in which $\vec{\mathbf{M}}$ is pointing, averaged over some small part of the lattice, may not give us a strong constraint on what $\langle \vec{\mathbf{M}} \rangle$ for the entire lattice will be.

III. NUMERICAL RESULTS FOR $S(k)$

In this work, we will present results for the average over angles of $S(\vec{\mathbf{k}})$, which we write as $S(k)$. The data were obtained from $L \times L \times L$ simple cubic lattices with $L = 64$ using periodic boundary conditions. Some preliminary studies for smaller values of L were also done. The calculations were done using a 12-state clock model, i.e., a $\mathbf{Z}_{12}$ approximation[2] to the XY model of Eq. (1). The strengths of the random field for which data were obtained are $h_r = 1$ and 2. These sets of parameters allow the use of a lookup table for the Boltzmann factors because all the energies in the problem are expressible as sums of integers and integer multiples of $\sqrt{3}$.[24]

This discretization of the phase space of the model has significant effects at very low T, but the effects at the temperatures we study here are expected to be negligible compared to our statistical errors. The probability distributions for the local magnetization of equilibrium states which are calculated for the $\mathbf{Z}_{12}$ model are found to have very small contributions from the third and higher harmonics of $\cos(\phi)$ and $\sin(\phi)$. This is a strong evidence that the 12-state clock model is an accurate approximation to the XY model within our range of parameters.

The program uses two linear congruential pseudorandom number generators, one for choosing the values of the θ_i and a different one for the Monte Carlo spin flips, which are performed by a single-spin-flip heat-bath algorithm. The code was checked by setting $h_r = 0$ and seeing that the expected behavior of the pure ferromagnetic system was produced correctly.

Four different $L = 64$ realizations of the random fields θ_i were used. The same four samples of random fields were used for all values of T and both values of h_r. Each lattice was started off in a random spin state at $T/J = 2.3125$, significantly above the T_c for the pure model, and cooled slowly. Thermal averages for $S(\vec{\mathbf{k}})$ were obtained at a set of temperatures. At each T, a sequence of 12 spin states obtained at intervals of 20 480 Monte Carlo steps (MCS) per spin was Fourier transformed and averaged. The data were then binned according to the value of k^2 to give the angle-averaged $S(k)$. Finally, a logarithmically weighted average over the four samples was performed.

The data for $h_r = 1$ at T/J between 1.3125 and 2.0 are shown in Fig. 1. At $T/J = 2.0$, S is clearly flattening out for $k < 0.1$. As T is lowered, weight is shifted from large values of k toward $k = 0$. For all the smaller values of T/J shown in the figure, the correlation length ξ is clearly larger than the size of the samples, $L = 64$. All of these large ξ samples show an Ak^{-3} behavior at small k and the coefficient A is, within
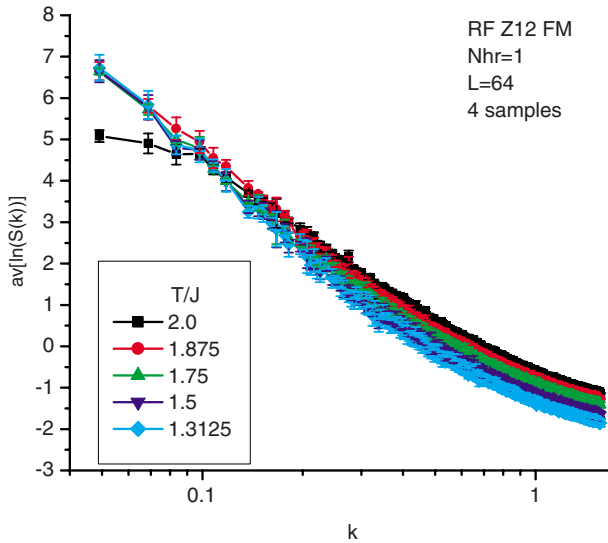
FIG. 1. (Color online) Angle-averaged structure factor for $64 \times 64 \times 64$ lattices with $h_r = 1$ at various temperatures. The error bars indicate one standard deviation statistical error and the x axis is scaled logarithmically.
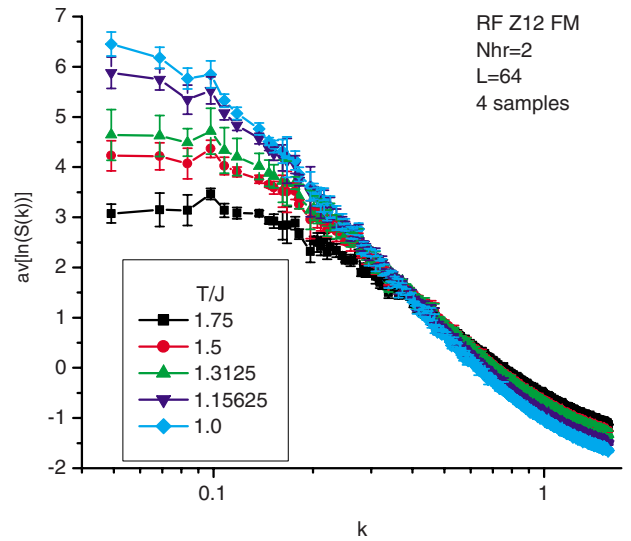

FIG. 2. (Color online) Angle-averaged structure factor for $64 \times 64 \times 64$ lattices with $h_r = 2$ at various temperatures. The error bars indicate one standard deviation statistical error and the x axis is scaled logarithmically.

our statistical errors, independent of T. This apparently universal behavior is consistent with the prediction of Giamarchi and Le Doussal[25] for the 3D elastic glass model. For the elastic glass model, this Ak^{-3} behavior has been verified numerically by McNamara *et al.*[26] For the RFXYM, however, we know that this behavior cannot hold down to $k=0$ because the fixed length of the XY spins yields a sum rule for S,

$$\sum_{\vec{k}} S(\vec{k}) = L^3. \qquad (7)$$

There is also some interesting information to be learned from the dynamical behavior. Below $T/J = 1.875$, one of the four samples shows a strong hysteresis and a second one shows a mild hysteresis. This may indicate the existence of a first-order phase transition for $h_r = 1$ at $T/J \approx 1.80$. The hysteresis goes away as we continue to still lower T. The value of ξ under these conditions is clearly bigger than $L = 64$, however. Therefore, we cannot say exactly what is going on here from these data.

Due to the sum rule, Eq. (7), we know that the Ak^{-3} behavior which is seen in Fig. 1 *cannot* be the correct behavior at small k for very large lattices. Increasing the size of our lattice by a significant amount is rather impractical. However, it is impossible to distinguish between a ferromagnetic state and the QLRO state claimed in the earlier Monte Carlo studies[1,2] without studying the true small k limit.

Another way to learn more about the behavior is to decrease ξ by increasing h_r. In Fig. 2, we display $S(k)$ data from four $h_r = 2$ samples obtained using the same procedures as before. In this case, the peak at $\vec{k} = 0$ continues to grow as we lower T, but there does not appear to be any simple scaling behavior. The peaks are very flat near $\vec{k} = 0$. An attempt to fit the data by a Lorentzian shape, or even a Lorentzian raised to some power, is not satisfactory.

At $T/J = 0.875$, a system which is started in an initially ordered state shows no sign of relaxing into the low M^2 state which is found by slow cooling, even on time scales of 10^6 MCS per spin. In Fig. 3, we show $\langle \ln[S(k)] \rangle$, with $h_r = 2$, at this temperature averaged over the same four samples for both types of initial conditions. From this figure, we see that although the two initial conditions give significantly different values of $\langle M^2 \rangle$, the rest of $\langle \ln[S(k)] \rangle$ is almost the same. The peak in $\langle \ln[S(k)] \rangle$ has continued to sharpen slowly with the reduction in T. The values of $\langle \ln[S(0)] \rangle$, not shown in Fig. 3, are 11.54 ± 0.11 for the initially ordered state and 8.26 ± 0.28 for the slow-cooled state.

The ordered initial conditions give slightly lower values of the energy per spin, as we will discuss in more detail in
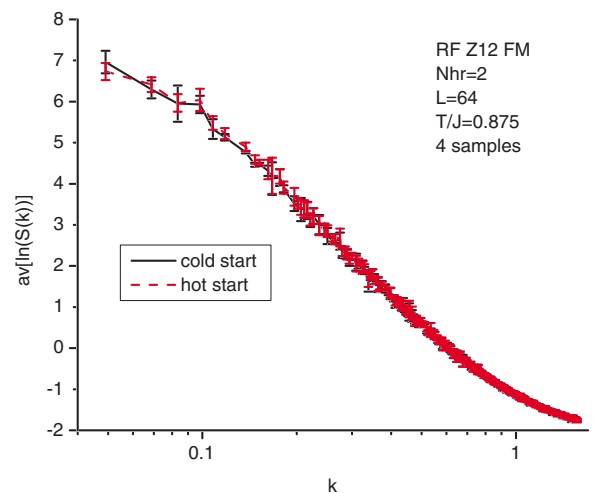

FIG. 3. (Color online) Angle-averaged structure factor for $64 \times 64 \times 64$ lattices with $h_r = 2$ at $T/J = 0.875$, using both hot start and ordered start initial conditions. The error bars indicate one standard deviation statistical error and the x axis is scaled logarithmically.

the next section. A careful study to find the highest value of T for which the metastability exists was not performed. For $h_r=2$, unlike $h_r=1$, the relaxation time gets increasingly longer as we continue to lower T beyond the point where metastability first appears.

IV. DISCUSSION

If, as argued by Imry and Ma, the random-field energy dominates the spin-exchange energy for the 3D RFXYM, how could it be possible to have a ferromagnetic phase? To understand this, we need to think carefully about finite-size scaling.

Consider a very large system at $T=0$, with $h_r=1$ (for example). Since there is no degeneracy due to symmetry, and the energy is not quantized, we expect that the ground state for any particular sample of random fields should be unique, with probability 1. If $d>4$, then we expect that $S(\vec{k})$ has a δ-function peak at $\vec{k}=0$ of strength $M^2(T=0)>0$. If we consider some low but finite T, we expect that, in thermodynamic equilibrium, many states will contribute to $S(\vec{k})$. These states should have similar values of $M^2>0$, but the direction of $\vec{M}$ ought to be randomly distributed on the unit circle, so that $\langle\vec{M}\rangle\approx0$.

In $d=3$, the Monte Carlo results presented here do not indicate that there are many states with similar values of $M^2>0$, but very different values of the direction of $\vec{M}$, contributing substantially to the equilibrium Gibbs state. This may happen as a rare event in a few samples, but it is unlikely to be observed. There is, however, an alternative road to ferromagnetism.

Let us consider some very large but finite 3D sample. As Bray has argued,[20] χ^{-1} has a Lifshits tail of localized states near eigenvalue 0. These localized states occur in regions of the sample in which the average local random field has a large magnitude but a random direction. At any temperature, each such localized state corresponds to a compact cluster of spins which is pinned to point in a direction which is approximately parallel to the local field in that neighborhood.

When we lower T, the eigenvalue spectrum of χ^{-1} will be modified, as discussed by Hertz *et al.*[18] For $d>4$, the mobility edge will move down to zero, and the sample polarizes into the renormalized band-edge state. In three dimensions, this type of continuous process cannot occur. However, it may become possible, at a low enough T, for the state of minimum eigenvalue to polarize most of the sample, without completely destroying the other stable clusters.

A condition which makes it favorable for this process to occur is that the density of localized states should be low and that the size of a typical localized state should be small compared to the average nearest neighbor distance between the localized states. Whether this is possible may thus depend on the details of the distribution of random fields. An earlier calculation[2] using a different type of random-field distribution provided evidence for a continuous phase transition.

A small difference in energy per spin,

$$\langle\Delta E\rangle=(-1.24\pm0.25)\times10^{-3} \text{ J/spin}, \qquad (8)$$

was found in our $L=64$ results for $h_r=2$ at $T/J=0.875$ between the slowly cooled states and the states relaxed from ordered initial conditions. In order to reach this low energy state, the direction of the initial $\vec{M}$ must be close to the direction of $\langle\vec{M}\rangle$ for the slow-cooled state. Using an initial $\vec{M}$ which is not close to this direction results in a state which has a higher energy than the slow-cooled state.

The author believes that this energy is subextensive. This means that, as $L\to\infty$, $\langle\Delta E\rangle\to0$, but $L^3\langle\Delta E\rangle\to\infty$. In these terms, the energy difference quoted above is -325 ± 66 J. Thus, the Boltzmann factor, $\exp(-325/0.875)$, for the weighting of the two separate free energy minima is extremely small. Since, of course, the free energies of the two Gibbs states must be equal at the phase transition, this Boltzmann factor must be compensated by the entropy difference between them.

It has been known for a long time that something similar occurs[27,28] in the one-dimensional Ising model with inverse-square law long-range interactions. For this model, it is known that the correlation length diverges at T_c,[29] so that T_c is a critical point with $\beta=0$. A phase transition of this type is also believed to occur in the k-core percolation model,[30] which has been suggested as the model for the ordinary glass transition.

A rather similar subextensive singularity was recently seen in a type of two-dimensional Ising spin glass.[31] If this effect also occurs in the Ising spin glass in higher dimensions, where $T_c>0$, it provides an explanation for the puzzling behavior of the high-temperature series for the Ising spin glass[32] since we know that for random bond Ising models, the Griffiths singularity appears in four dimensions. This is consistent with the ideas of Bray and Moore.[19,20]

A phase transition at about $T/J\approx1.80$ for $h_r=1$ and $T/J\approx0.90$ for $h_r=2$ is in good agreement with the work of Gingras and Huse,[1] who worked at $T/J=1.5$ and estimated the transition to be at $h_r\approx1.35$.

V. SUMMARY

In this work, we have performed Monte Carlo studies of the 3D RFXYM on $L=64$ simple cubic lattices, with random-field strengths of $h_r=1$ and 2. We present results for the structure factor $S(k)$ at a sequence of temperatures. We argue that our results appear to indicate a phase transition into a ferromagnetic state. This is made possible by the existence of a Griffiths singularity, which invalidates the Imry-Ma analysis. At the phase transition, M^2 seems to jump to zero discontinuously, but with a latent heat per spin which probably goes to zero as $L\to\infty$.

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*ron@princeton.edu

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