Low-temperature behavior of random-anisotropy magnets

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An improved computer annealing algorithm has been used to study the low-energy states of magnets with strong random anisotropy on simple-cubic lattices. For classical Heisenberg spins with isotropically random uniaxial anisotropy, the ferromagnetic correlations at $T=0$ can be described by a scaling exponent η of about 0.2 and a correlation length of about 10 lattice units. The ground-state energy E_0 is $(-1.118\pm0.003)J$. For XY spins with random p-fold anisotropy, the ground states are ferromagnetic, with magnetizations of 0.45 ± 0.02, 0.715 ± 0.015, and 0.843 ± 0.006, for $p=2$, 3, and 4, respectively, and the values of E_0/J are -1.5075 ± 0.0015, -2.229 ± 0.003, and -2.543 ± 0.002.

I. INTRODUCTION

The behavior of magnets with random local anisotropy has attracted a great deal of attention for nearly twenty years. Despite the large volume of work that has been done, and the real progress that has been made, some of the simplest questions about the nature of the ground state of a strongly disordered three-dimensional magnet have remained unanswered. The reason for this is that actually finding the ground state of such a system is an extremely difficult computational problem. In this work, we will use a simulated-annealing technique to study several such systems. We will see how the behavior of the magnetic order in the ground state depends on the type of random anisotropy which is used.

The canonical model for random-anisotropy magnets was proposed by Harris, Plischke, and Zuckermann[1] (HPZ):

$$H_{\rm HPZ}=-J\sum_{\langle ij\rangle}\sum_{\alpha=1}^{m}S_i^\alpha S_j^\alpha-D\sum_i\left[\sum_{\alpha=1}^{m}(\hat{\mathbf{n}}_i^\alpha S_i^\alpha)^2-1\right], \quad (1)$$

where S_i is an m-component spin and the $\hat{\mathbf{n}}_i$ are uncorrelated random m-component unit vectors. HPZ showed that a mean-field approximation gives a ferromagnetic phase for this Hamiltonian at low temperatures. Equation (1) can also give rise to spin-glass behavior under certain conditions, as was made clear by later work.[2,3]

When we go to the strong-anisotropy limit, $D/J\to\infty$, each spin is constrained to be parallel to its local anisotropy axis. Equation (1) then reduces to

$$H_\infty=-J\sum_{\langle ij\rangle}(\hat{\mathbf{n}}_i\cdot\hat{\mathbf{n}}_j)S_iS_j \quad (2)$$

in the absence of an external magnetic field. Each S_i is now an Ising variable, which takes on only the values ±1. This Hamiltonian was solved in the infinite range case by Derrida and Vannimenus,[4] and it is convenient for both computer modeling[5,6] and high-temperature series expansion.[7-9]

The random-anisotropy term in Eq. (1) can easily be generalized to higher-order types of anisotropy. It is particularly interesting to do this for the $m=2$ case. For $m>2$, higher-order random anisotropies will generate random uniaxial anisotropy terms under a renormalization-group transformation,[10] so that no qualitatively new behavior is expected. For XY spins we can transform each spin variable, $\mathbf{S}_i$, into an angular variable, θ_i. Equation (1) is then generalized to the case of p-fold random anisotropy by writing

$$H_p=-J\sum_{\langle ij\rangle}\cos(\theta_i-\theta_j)-D\sum_i\{\cos[p(\theta_i-\phi_i)]-1\}, \quad (3)$$

where ϕ_i is the angular coordinate of $\hat{\mathbf{n}}_i$. Equation (3) has been studied[11] in two spatial dimensions ($d=2$) and also[12] in $d=2+\epsilon$. It was shown that, at least for small D, the Kosterlitz-Thouless phase survives the addition of the random anisotropy term if $p\geq3$. What makes this particularly noteworthy is the argument by Pelcovits, Pytte, and Rudnick,[13] who claim that there can be no ferromagnetism at finite temperature in the presence of a random anisotropy term when $d<4$. (The analysis given by Pelcovits[13] is for the $p=2$ case, but it easily generalizes to arbitrary p.) If we were to accept that the lower critical dimension for ferromagnetism in the presence of random anisotropy is $d=4$, then it becomes extremely difficult to explain how the ferromagnetic correlations can decay slowly at large distances in $d=2$, so as to allow the survival of the Kosterlitz-Thouless phase.

Part of the resolution of this apparent paradox seems to be that the lower critical dimension for ferromagnetism when $m=2$ is $d=3$, rather than 4. This result is indicated by the analysis of high-temperature series expansions[9] for Eq. (2). The question is not completely answered, however, since neither the series expansions nor other techniques[14] suggest that the magnetic correlations decay slowly at large distances for $d=2$. What is claimed in the work by Houghton, Kenway, and Ying,[11] and Cardy and Ostland[11] is that, if D is small, there is an intermediate range of temperatures where the range of the ferromagnetic correlations is determined by the distance between vortex pairs. The Kosterlitz-Thouless mechanism would then operate in this range of temperatures.

Taking the $D/J\to\infty$ limit of Eq. (3), we obtain

$$H_{p,\infty}=-J\sum_{\langle ij\rangle}\cos\left[\frac{2\pi}{p}(q_i-q_j)-\phi_{ij}\right], \quad (4)$$

where $\phi_{ij}=\phi_i-\phi_j$, and each q_i is now a $\mathbf{Z}_p$ variable, which takes on all integer values between 0 and $p-1$. If we remove the randomness from Eq. (4) by setting all of the $\phi_{ij}=0$, we are left with the standard p-state vector Potts (clock) model.[15] For $p\geq 3$, the vector Potts model has a first-order transition to the ferromagnetic state when $d=3$. At the mean-field level,[4] the inclusion of the random ϕ_{ij} terms changes the nature of the model in a dramatic fashion. The ground state now has a macroscopic rotational invariance, rather than the discrete p-fold invariance of the vector Potts model. This might appear to change the behavior of the domain-wall energy from that characteristic of a system with discrete symmetry to that of a system with continuous symmetry. But the actual symmetry group of the ground state is still only the p-fold discrete rotation invariance, so it may not be correct to use an Imry-Ma type argument[13] to claim that the lower critical dimension must be $d=4$.

This issue has arisen before, in the context of the Ising spin glass.[16,17] In order that the domain-wall energy behave as in a system of continuous symmetry, it would be necessary that there exist distinct ground states which are not related by the p-fold invariance. The existence of such states would allow domain walls to spread out in space at a very low cost in energy, by mixing two nonequivalent ground states. One of the results of the calculations described here is that such states do not exist for $m=2$ random-anisotropy models in three dimensions. This confirms the conclusion of the high-temperature series work,[9] that the lower critical dimension for ferromagnetism in these models is $d=3$, not 4.

II. CALCULATIONAL PROCEDURE

Taking the $D/J\to\infty$ limit gives an enormous simplification in the nature of the problem of finding the ground state, since it is then only necessary to deal with a discrete phase space, rather than a continuous one. There is no reason, however, to believe that the behavior is singular in this limit. Our results will be qualitatively valid for all large values of D/J. The first large-scale attempt to study the structure of the ground state of a random anisotropy model was performed by Jayaprakash and Kirkpatrick,[5] (JK), who studied the $m=2$ case of Eq. (2) on square lattices, and the $m=3$ case on simple cubic lattices. These authors were primarily interested in studying finite temperature properties, so they used a Monte Carlo spin-flip algorithm. This limited their ability to locate the ground states of large lattices. JK introduced two techniques to the study of this problem which were used in the current work: a multiple-spin-flip algorithm, and repeated low-temperature annealing.

If one wishes to concentrate solely on the ground-state properties,[6] a Monte Carlo algorithm is very inefficient, because a substantial fraction of the computing time is used by calculating Boltzmann factors. This results from the fact that the spin-spin interaction energies are different for each spin. It is much better to use an energy criterion: a spin is flipped if and only if the energy cost is less than $\epsilon(t)$, which may be either positive or negative. After each two or three passes through the entire lattice, ϵ is changed. At the end, one sets $\epsilon=0$, and then iterates until a metastable state is reached. The annealing schedule, $\epsilon(t)$ should be adapted to the problem. It would not be optimal to use the same $\epsilon(t)$ for all values of m and p.

Since each finite lattice with its own set of random axes has different individual properties, it is necessary to study a number of lattices of each size, in order to obtain the properties of the distribution of lattices of that size. Naturally, this substantially increases the amount of computer time which is needed, relative to what one would need to study a nonrandom problem. It is particularly true that the magnetization of the ground state can vary greatly from one lattice to the next of a given size.

Starting from an arbitrary initial configuration, we are unlikely to reach a very low energy state in one annealing cycle. Therefore, a number of initial configurations were used for each lattice, and this number was increased as the lattice size was made larger. For small lattices one can then pick out the lowest-energy state which is found by this procedure, and assume with a reasonable degree of confidence that it is the ground state. For lattices of 1000 spins or more, however, it is not practical to use enough initial configurations to find the ground state in this way. For these larger lattices, one picks out a small number of the lowest-energy states found by starting from arbitrary initial configurations, and subjects them to further annealing. This process eventually converges: given sufficient annealing, the different states begin to have a high degree of overlap. The fact that this occurs tells us we have almost surely found a good approximation to the true ground state. It also tells us that the ground state is essentially unique, and that the domain-wall energy is not very small. The convergence of the different states occurs fairly rapidly for XY spins, and with some difficulty for $m=3$ spins. It was found that lattices up to $20\times20\times20$ could be studied for $m=2$, but for $m=3$ it was only practical to go up to $16\times16\times16$.

The sets of random axes were chosen in the same way as in the previous study.[6] This made it possible to restudy the same lattices which were used before. For most of the larger lattices, the annealing algorithm was able to find states of lower energy than found previously. This was due partly to improvements in the program, and partly to the availability of greater computing resources than before. These improvements have also made it possible to work with larger lattices. The reader should understand that in some cases the program has not succeeded in finding the exact ground states of these large lattices. We must be satisfied with the more modest goal of finding a metastable state which has a high degree of overlap (typically about 95%) with the true ground state.

This is sufficient for our estimates of the properties of the ground state to be reasonably accurate.

III. NUMERICAL RESULTS

$L \times L \times L$ simple cubic lattices with periodic boundary conditions were studied, with L up to 16 for the $m=3$ case of Eq. (2), and L up to 20 for the $m=2$ cases, Eq. (4), with $p=2$, 3, and 4. It turns out that, for a given L, the $m=3$ case requires much more computer time. This is because the domain-wall energy is much lower for $m=3$, which allows a much larger number of low-lying metastable states to exist. The results for the ground-state energy E_0 and the square of the ground-state magnetization, M^2, for $m=3$ lattices in the range $3 \le L \le 16$ are given in Table I. The improved algorithm for finding the ground state has resulted in a lowering of the estimates[6] of E_0 for the larger lattices, and small changes in the estimates of M^2. A simple extrapolation of $E_0(L)$ to large L gives

$$E_0=(-1.118\pm0.003)J \quad \text{for } m=3 .$$

A log-log plot of M^2 vs L is shown in Fig. 1. It is clear that the slope of $M^2(L)$ is becoming more negative as L increases. It appears that the slope will eventually go to -3 for large L, which is the result for correlations of finite range in $d=3$. The spin-spin correlations are described by the usual form,

$$[\mathbf{S}_i\cdot\mathbf{S}_j]_c \sim \frac{A}{|\mathbf{r}_i-\mathbf{r}_j|^{d-2+\eta}}\exp(-|\mathbf{r}_i-\mathbf{r}_j|/\xi_0) , \tag{5}$$

where η is the spin scaling exponent, and ξ_0 is the zero-temperature correlation length. The brackets, $[\ ]_c$, indicate a configuration average over the random axes. Since ξ_0 is not infinite, η cannot be precisely defined, but we can estimate that $\eta\approx0.2$ and $\xi_0\approx10$. There is no true ferromagnetism for $m=3$ on the simple cubic lattice. This is probably true for all three-dimensional lattices.[9] These conclusions agree well with prior work,[5,6] but are more precise.

It is worth remarking, however, that the short-range order is so strong that it will have large effects. Large ferromagnetic correlation lengths have been observed in small-angle neutron-scattering experiments[18] on amorphous RFe_2 samples (where R stands for rare earth). We

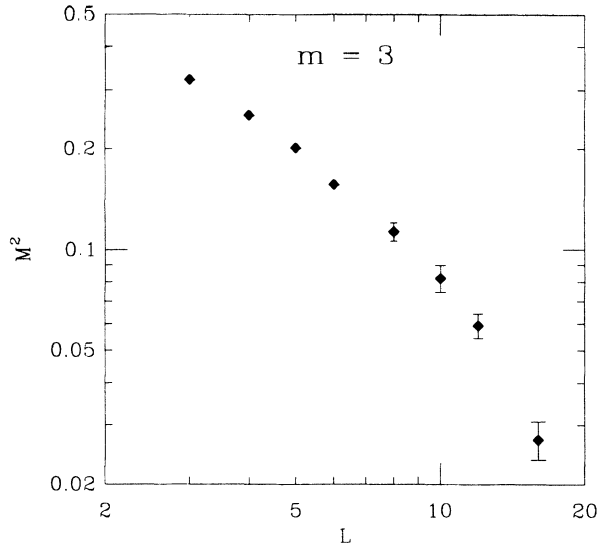

FIG. 1. Configuration average of the square of the magnetization, $[M^2]_c$, vs lattice size, L, for $L\times L\times L$ simple cubic lattices, for the random uniaxial anisotropy model with $m=3$ and $D/J=\infty$. Both axes have logarithmic scales. The error bars show one standard deviation.

can see that the existence of a substantial correlation length does *not* prove that D/J is small, as has sometimes been assumed.

The results for the XY model with strong random uniaxial anisotropy [Eq. (2) with $m=2$, or, equivalently, Eq. (4) with $p=2$] are given in Table II. In Fig. 2 we see a semi-log plot of $1/M^2$ vs L. Going out to $L=20$ does not rigorously prove anything about the limit $L\to\infty$, but the finite lattice data rule out a decrease of M^2 to zero which is faster than $1/\log(L)$. The data are well fit by

$$M_0=0.45\pm0.02 \quad \text{and} \quad E_0=(-1.5075\pm0.0015)J$$

for $L\to\infty$ with $m=2$ and $p=2$. This value of M_0, the magnetization of the ground state, is only about 70% of the mean-field theory value, $2/\pi$. It is not clear that ferromagnetism will be stable at even very low nonzero temperatures, and it seems unlikely that M will remain finite up to $T_c=1.78J$, the temperature at which the magnetic susceptibility diverges.[9] So there is probably a range of

TABLE I. Ground-state data for $L\times L\times L$ simple cubic lattices with $m=3$. M^2 and ΔM^2 are the average and standard deviation of the distribution of ground-state magnetization squared. E_0 and ΔE_0 are the average and standard deviation of the ground-state energy distribution (in units of J).

L	Samples	M^2	ΔM^2	E_0	ΔE_0
3	192	0.3224	0.0687	−1.1680	0.1129
4	128	0.2521	0.0547	−1.1335	0.0740
5	96	0.2015	0.0412	−1.1311	0.0504
6	64	0.1558	0.0436	−1.1245	0.0356
8	48	0.1128	0.0470	−1.1209	0.0208
10	32	0.0821	0.0426	−1.1196	0.0170
12	24	0.0593	0.0238	−1.1198	0.0132
16	16	0.0272	0.0135	−1.1185	0.0088

TABLE II. Ground-state data for $L\times L\times L$ simple cubic lattices with $m=2$ and $p=2$. Column labels are the same as in Table I.

L	Samples	M^2	ΔM^2	E_0	ΔE_0
3	192	0.4779	0.0678	−1.5845	0.1496
4	128	0.4244	0.0562	−1.5458	0.1001
5	96	0.3837	0.0413	−1.5345	0.0517
6	64	0.3596	0.0416	−1.5238	0.0465
8	40	0.3193	0.0375	−1.5101	0.0312
10	32	0.2884	0.0290	−1.5086	0.0239
12	32	0.2665	0.0247	−1.5082	0.0137
16	32	0.2425	0.0307	−1.5083	0.0118
20	24	0.2290	0.0280	−1.5077	0.0057

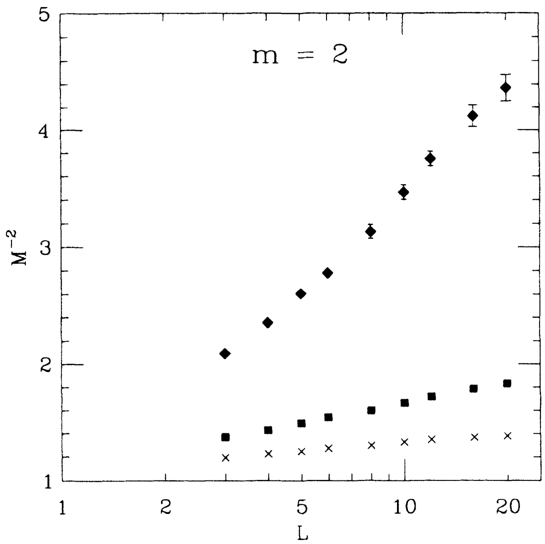

FIG. 2. Inverse of the square of the magnetization, $1/[M^2]_c$, vs lattice size, L, for $L\times L\times L$ simple cubic lattices, for the random uniaxial anisotropy model with $m=2$ and $D/J=\infty$. The L axis is scaled logarithmically. The error bars show one standard deviation. Diamonds: $p=2$; squares: $p=3$; crosses: $p=4$.

T, which may extend down to 0, where $M=0$ and $\chi=\infty$. A phase of this type was originally predicted by Aharony and Pytte,[19] although their prediction was not specific to the $m=2$ case.

The distribution of effective fields for this system is shown in Fig. 3. The shape of the distribution is qualitatively similar to what was found by JK (Ref. 5) for the $m=3$ case. The density of states at low fields is somewhat smaller, and the peak is moved out, as one would expect. This is simply a reflection of the fact that the distribution of effective fields is not sensitive to the existence of long-range order in these random anisotropy magnets. Even the infinite range model[4] has a finite density of states at zero field. Since the dominant low-energy excitations are localized single spin flips, it is hard to accept the validity of a spin-wave analysis[13] of the low-temperature behavior.

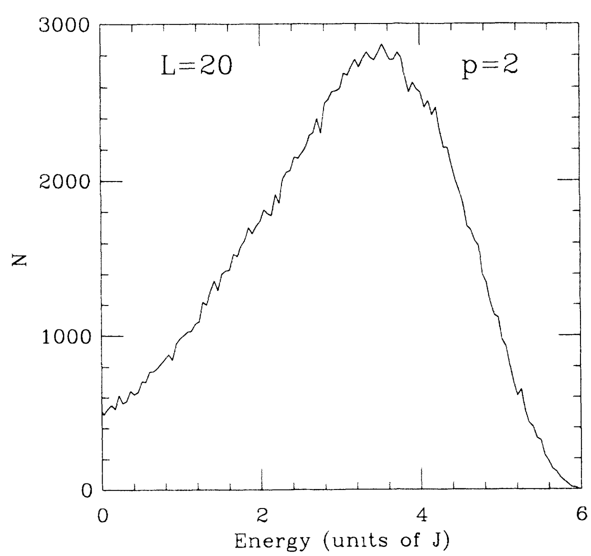

FIG. 3. Density of states for the distribution of effective fields for the $L=20$ lattices with XY spins and $p=2$.

TABLE III. Ground-state data for $L\times L\times L$ simple cubic lattices with $m=2$ and $p=3$. Column labels are the same as in Table I.

L	Samples	M^2	ΔM^2	E_0	ΔE_0
3	192	0.7298	0.0410	−2.2886	0.0848
4	128	0.6996	0.0319	−2.2711	0.0514
5	96	0.6698	0.0286	−2.2465	0.0349
6	64	0.6483	0.0290	−2.2409	0.0306
8	48	0.6253	0.0227	−2.2396	0.0178
10	40	0.6008	0.0185	−2.2359	0.0118
12	32	0.5818	0.0264	−2.2353	0.0088
16	32	0.5596	0.0194	−2.2321	0.0060
20	24	0.5460	0.0207	−2.2299	0.0044

The data for Eq. (4) with $p=3$ and $p=4$ are shown in Tables III and IV, respectively. These systems are strongly ferromagnetic, and they have rather large domain-wall energies. Therefore the ferromagnetism should be stable up to temperatures of about $2J$ in these cases. The extrapolations to $L\to\infty$ are estimated to be

$$M_0=0.715\pm0.015 \text{ and } E_0=-2.229\pm0.003J$$

for $p=3$, and

$$M_0=0.843\pm0.006 \text{ and } E_0=-2.543\pm0.002J$$

for $p=4$. The widths of the distributions for M_0 and E_0 become progressively smaller as we move from $p=2$, to 3, to 4. Clearly, the effects of the randomness become weaker as p increases.

TABLE IV. Ground-state data for $L\times L\times L$ simple cubic lattices with $m=2$ and $p=4$. Column labels are the same as in Table I.

L	Samples	M^2	ΔM^2	E_0	ΔE_0
3	192	0.8358	0.0281	−2.5749	0.0578
4	128	0.8144	0.0226	−2.5604	0.0301
5	96	0.8000	0.0193	−2.5554	0.0200
6	64	0.7840	0.0181	−2.5523	0.0147
8	48	0.7698	0.0149	−2.5497	0.0103
10	40	0.7521	0.0157	−2.5466	0.0081
12	32	0.7411	0.0146	−2.5448	0.0052
16	32	0.7307	0.0144	−2.5441	0.0042
20	24	0.7241	0.0129	−2.5437	0.0028

IV. DISCUSSION

The systems studied in this work display a fairly wide range of behavior. For the $m=2$ model with $p=4$, the randomness does not seem to matter that much, since the behavior is not that different from the nonrandom $p=4$ vector Potts model. Domain walls are very well defined, and metastable states do not seem to be very important. It may be, however, that more dramatic effects do occur near the ferromagnetic transition temperature, T_c. The nonrandom vector Potts models have first-order transitions in $d=3$. The effects of randomness on first-order phase transitions are not, in general, well understood. It is often stated that a "smearing" of the transition will occur, but the meaning of this term is rather vague. It would not be surprising if an Aharony-Pytte phase existed in a narrow band of temperature, between the ferromagnetic phase and the paramagnetic phase. This question must be left to future work.

On the other hand, the behavior of the $m=3$ model is dominated by the metastable states. In this case, the analysis of Pelcovits, Pytte, and Rudnick, which assumes that the domain walls can spread out as in a system of continuous symmetry, seem to work rather well, despite the discreteness induced by the strong anisotropy. The short-range order is highly ferromagnetic, even in this strong anisotropy limit. This indicates that there will be a giant peak in the magnetic susceptibility at low temperatures, which may be difficult to distinguish experimently from true ferromagnetism.

Chakrabarti[20] has claimed that there is a spin-glass freezing transition at a temperature $T_f=1.0J$ for the $m=3$ case on the simple cubic lattice. It is clear, however, that there is a large variation of the ferromagnetic correlation length, ξ, in this temperature range, which was missed by his calculation. It may be that there is a spin-glass freezing at a somewhat lower temperature, e.g., $0.5J$, and that this is what prevents ξ from diverging as $T\rightarrow 0$. Chakrabarti's results are a nonequilibrium effect, which arise from his use of a single-spin-flip Monte Carlo algorithm.

The case of $m=2$ with $p=2$ is intermediate between these two extremes. It probably has ferromagnetic order at $T=0$, but this order is rather weak, and will be easily destroyed by thermal excitations. It should display an Aharony-Pytte phase over a fairly wide range of temperature. It was predicted by Pelcovits,[13] based on a spin-wave analysis for the small D limit, that this behavior would occur in $d=4$ for XY spins. It would be very useful to have a simple explanation of why the effect actually occurs in $d=3$.

V. SUMMARY

In this work, a computer annealing algorithm has been used to study the ground-state properties of random anisotropy magnets of several types, on simple cubic lattices. We see that the nature of the ground state depends on the number of spin components. Random axes uniformly distributed over the sphere give rise to a ferromagnetic correlation length of about ten lattice units, but no true long-range order. Ferromagnetism occurs for random anisotropy distributed in a plane, for any value of p. As p increases, the behavior becomes increasingly similar to that of a vector Potts model.

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