Phase transitions in cubic models with random anisotropic exchange

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A Monte Carlo algorithm has been used to study a three-component cubic spin model with a type of random diagonal anisotropic exchange on simple cubic lattices, in the strong anisotropy limit. There is a narrow region of "domain ferromagnet" phase between the ordinary ferromagnet and the spin-glass phase, which also has a domain structure in this model. Even with the presence of the domain structures, the spin-glass freezing appears to take place via a mobility edge transition that is similar to the process which occurs in the Ising spin glass.

I. INTRODUCTION

It was demonstrated over ten years $ago¹$ that, if one wishes to reproduce the spin-freezing transition seen in many real experimental systems,² it is essential to add anisotropic interactions to the three-dimensional Heisenberg spin-glass model. Within a mean-field theory or even an ε expansion about six dimensions, $3⁻⁵$ this addition of anisotropic interactions causes the model to cross over to the Ising spin-glass universality class. Some of the most carefully studied experimental systems, such as CuMn and AuFe, are crystalline alloys with an average cubic symmetry. Until recently,⁶ the possible effects of this average cubic symmetry on the spin-glass freezing transition have been largely ignored. A renormalizationgroup calculation by Aharony⁷ gave the result that a weak cubic anisotropy should not affect the freezing transition. However, we now know that the lower critical dimension of the isotropic Heisenberg spin glass is four.⁵ This invalidates the assumptions of Aharony's calculation. Reasoning by analogy with the situation for cubic ferromagnets in two dimensions,^{8,9} it might be anticipat ed that an average cubic symmetry would cause the spinglass transition in a three-dimensional system to become $\text{discontinuous}^{10}$ when the number of spin components is three or more.

In this work we will present evidence that a transition with a new type of domain spin glass, bearing some resemblance to the one seen in $CuMn₀$ ⁶ occurs in a particular three-dimensional model which includes threecomponent spins, random anisotropic spin exchange, and a strong cubic anisotropy which favors the cube axis directions. No clear evidence is seen for discontinuous behavior, however. If the appropriate compensation is made for the increase in the number of spin components, the freezing transition is rather similar to the one seen in the usual Ising spin glass.

There has been some recent numerical work 11,12 on models which add a random off-diagonal spin exchange to the Heisenberg spin glass. Because the probability distribution of the random spin exchange in these models is not invariant under rotations, these models have an effective average cubic symmetry. It has been found, as expected, that these models have spin-freezing transitions at some $T_g > 0$ in three dimensions. It is fair to say that the nature of the freezing transition remains somewhat unclear. In the author's opinion, the crucial difficulty is the lack of a fundamental understanding of the behavior of the Hertz, Fleishman, and Anderson model¹³ in a three-dimensional system.

II. RANDOM ANISOTROPIC EXCHANGE MODEL

We consider the simplest model which will suffice for the questions we wish to study. The Hamiltonian for a three-component spin model with a random nearestneighbor anisotropic exchange and a cubic crystalline anisotropy is

$$
H = -\sum_{\langle ij \rangle} \sum_{\alpha,\beta=1}^{3} S_i^{\alpha} J_{ij}^{\alpha\beta} S_j^{\beta} - K \sum_{i} \left[\sum_{\alpha=1}^{3} (S_i^{\alpha})^4 - 1 \right]. \tag{1}
$$

In order to make the calculation tractable, we will work in the limit $K \rightarrow \infty$, so that each spin has only six possible states, parallel and antiparallel to the cube axes. We choose the spins to be classical and of unit length, and to lie on the sites of a simple cubic lattice. The notation $\langle ij \rangle$ denotes that i and j are nearest neighbors. In order to specify the model completely, we must choose a probability distribution, $P(J)$, for the exchange matrices. In this work we assume that each J_{ii} is independent, and selected from the one-parameter probability distribution

$$
P(J) = x \delta(J - J_0)
$$

+ $\frac{1-x}{3} [\delta(J - J_1) + \delta(J - J_2) + \delta(J - J_3)]$, (2)

where the J_{μ} are a set of diagonal 3X3 matrices. Their diagonal elements are

$$
J_0^{\alpha\alpha} = (1, 1, 1) ,
$$

\n
$$
J_1^{\alpha\alpha} = (1, -1, -1) ,
$$

\n
$$
J_2^{\alpha\alpha} = (-1, 1, -1) ,
$$

\n
$$
J_3^{\alpha\alpha} = (-1, -1, 1) .
$$

\n(3)

Thus for $x = 1$ we recover the nonrandom cubic ferromagnet, and for $x = 0.25$ the expectation value of each

component $\langle J^{\alpha\beta} \rangle$ is zero. For any value of x, Eq. (2) treats all three of the spin components equivalently, on the average. With the restriction that each spin can only point in one of the six axis directions, Eq. (1) then reduces to

$$
H = -\sum_{\langle ij \rangle} \sum_{\alpha=1}^{3} S_i^{\alpha} J_{ij}^{\alpha \alpha} S_j^{\alpha} . \tag{4}
$$

The reader should note that for a simple cubic lattice where all of the J matrices were, for instance, J_2 , there would be no frustration and the model could be turned into a ferromagnet by a gauge transformation. The effects which we wish to study arise from the random mixing of the different J matrices on the lattice. This model may be thought of as consisting of three Ising spin-glass models coupled together by the fixed-lengthspin constraint. [Note that if we were to choose a probability distribution in which each diagonal element $J_{ii}^{\alpha\alpha}$ was independent, we would require eight different J_{μ} matrices, with the additional four generated by multiplying each of the diagonal elements of the four J_{μ} in Eq. (3) by each of the diagonal elements of the four J_{μ} in Eq. (3) by -1 .] Thus, within a mean-field theory or an ε expansion about six dimensions, $3⁻⁵$ the critical behavior should indeed be that of an Ising spin glass. Our numerical results indicate that new phenomena, not present in a mean-field theory, can occur in three dimensions. The spin-glass phase in this model is then of a new type, but it is not clear that the critical behavior is qualitatively different.

The four J matrices of Eq. (3) form a group under matrix multiplication. They all have the property that the product of their diagonal elements (and thus their determinant) is 1. As a result of this, if we consider the product of the J_{ii} around a plaquette on the lattice, we will find that either none or else two of the spin components are frustrated. If two of the spin components are frustrated around a plaquette, then it is favorable for the spins around that plaquette to point along the third, unfrustrated axis, in order to achieve a low energy. Thus the choice of J matrices of Eq. (3) is very efficient in generating a random anisotropy energy. This is precisely what we wish to achieve.

The effective random anisotropy energy induces a local quadrupolar order at each site. This effective random quadrupolar field tends to destroy the long-range magnetic or spin-glass order by encouraging the system to break up into domains of short-range quadrupolar order. It is not possible, however, to deduce what the favored axis will be at a particular site merely by examining the J matrices which connect that site to its nearest neighbors. The anisotropy comes from going around a plaquette, just as the frustration in the Ising spin glass does.

Other choices using the full set of eight diagonal J_i which treat all axes equivalently (on the average) would be expected to display the same qualitative behavior. Our objective is to choose the set of Γ s which will show us the asymptotic long-distance behavior on the shortest possible length scale. This is necessary in order that our numerical calculations with limited computing resources will give us the answers to the questions under study. A

less advantageous choice of the \mathcal{S} s might have led to incorrect conclusions about the nature of the true longrange behavior of these systems. We do not claim that this Hamiltonian provides a good microscopic description of any real physical system. We hope that the behavior which we find in this model is a useful representation of the complex behavior seen in the physical systems that we are trying to understand.

It would not be surprising if there were ways of parametrizing a probability distribution for the eight J_{μ} matrices which maintained the average cubic symmetry but did not have domain phases. In any event, one could certainly create a model with such a phase diagram by adding an attractive biquadratic term

$$
H_b = -K_b \sum_{\langle ij \rangle} \sum_{\alpha=1}^{3} (S_i^{\alpha} S_j^{\alpha})^2
$$
 (5)

to the Hamiltonian, with a large K_b . With the inclusion of this term, it should be possible to find trajectories in "Hamiltonian space" for which there is a (presumably first-order) phase transition from the Ising spin-glass phase to the domain spin-glass phase. Thus we do not claim that an Ising spin-glass phase transition cannot occur in a Hamiltonian of this type, but only that it need not occur, and that other interesting possibilities exist. It is also likely that the behavior for negative K , where the spins prefer to point along the body diagonals, is different in some respects from the $K > 0$ model studied in this work. This would be similar to the situation in nonrandom cubic ferromagnets, 10 where the transition never becomes first order when $K < 0$.

III. MONTE CARLO SIMULATION

The Hamiltonian of Eq. (4), with the probability distribution of Eq. (2), was studied using Monte Carlo simulations on simple cubic lattices with periodic boundary conditions. The computer program used a standard heat-bath algorithm, and was similar to the one used earlier to study the cubic model with random single-site uniaxial anisotropy.¹⁴ For each Monte Carlo step, the value of a spin was reassigned to one of the six allowed values, weighted according to the Boltzmann factors, and without reference to the prior value of that spin. In order to avoid unwanted correlations, the random number generator which was used to Rip the spins according to the Boltzmann factors was completely different from the one which was used to choose the J matrices. The model was studied for values of x ranging between 0.25 and 1, on $L \times L \times L$ lattices with L between 16 and 48. In many ways the results for the diagonal random anisotropic exchange cubic model are similar to the results for the random single-site uniaxial anisotropy cubic model. This is not surprising, since a coarse graining of the anisotropic exchange model gives single-site anisotropy terms in the Hamiltonian. The major difference here is that the anisotropic exchange model has a spin-glass phase at low temperatures for x less than about 0.65. There was no spinglass phase in the model studied in Ref. 14 because a purely ferromagnetic exchange was used. If a random, but isotropic, exchange is added to the model of Ref. 14, this would be expected to have a spin-glass phase also.

The results for the phase diagram of the diagonal random anisotropic exchange cubic model on a simple cubic lattice are shown in Fig. 1. Based on symmetry considerations (i.e., cubic terms in a Landau free-energy functional), we would expect all of the transitions to be discontinuous. However, we should expect that strong enough randomness will smear out the latent heat in this model. Indeed, for x close to 1 the randomness is only a weak perturbation of the simple ferromagnet, and the behavior is not changed qualitatively, except that the latent heat at the freezing transition is smeared out. There is a narrow region of x, lying approximately between 0.65 and 0.73, in which a "domain ferromagnet" phase, similar to the one found in Ref. 14, appears to be the stable phase. For smaller values of x , there is no evidence of ferromagnetism at low temperatures, and there appears to be a transition into a spin-glass phase. The domain structure, with independent ordering¹⁴ along the three cube axes, persists into the spin-glass region.

In the spin-glass phase, the characteristic length for a "blob" of spins predominantly oriented along one of the axes is about eight lattice constants. A result of this is that an $L = 16$ system is too small to give useful results. At low T it tends to become dominated by a single domain, which wraps around the periodic boundary conditions. This means that large lattices must be used to understand the long-range behavior. Because of the domain structure, the spin correlations cannot be described by a single characteristic length scale. The spinglass phase may appear to be Ising-like at short distances, but at longer distances the domain structure will become dominant. The domain structure observed in a layer of the lattice just above the observed freezing temperature for $x = 0.25$ is shown in Fig. 2. The amount of local qua-

FIG. 1. Phase diagram of the diagonal random anisotropic exchange cubic model on simple cubic lattices. The plotting symbols show actual data points, and the dot-dashed lines indicate phase transitions. The FM-dFM and dFM-dSG phase boundaries were not observed directly.

$x = 0.250$ 32 1 1	$temp = 0.675$	
quadrupolar domains	$layer = 1$	
33033333333333300301111111002033		
03303000333033300330111110000003		
11011100000333330030111103330001		
11011000033300303330100330030001		
11111030333310330001101330330301		
22011333330300000001111110300300		
33311333330333000001111001100220		
33300303011333010000011000110022		
33300000011111111000000030112222		
33333300011122011100002000002220		
33333322222222011111220002022220		
03333322222222221111220022202200		
03333322202222220111110002222220		
33333302202222221111103002222022		
00022202020002221101102222222222		
02222222220000001111002222222022		
22222222003330000033332220200200		
02220222203333333330000220222222		
02200222233333003311002222222033		
22022220033333333011022200220332		
20022222003333333001122220022002		
20300222000033330000022222220002		
03302222222200330111022222220222		
00300202022200301112022222000223		
30222200000201111200000222003330		
30322000020221111022022222000333		
03302000020222111022222220333333		
30300003333222110002222203033333		
33333033333020000220000333330333		
33333033030020022200110333333333		
33333330033300000031111311030303		

FIG. 2. Spatial distribution of the local quadrupolar order for a layer of an $L = 32$ simple cubic lattice of the diagonal random anisotropic exchange cubic model with $x = 0.25$. The symbols 1, 2, and 3 indicate that the spin was observed to spend more than half of its time oriented along the x , y , and z axes, respectively. The remainder of the spins are denoted with the symbol 0. The data were obtained from a sequence of 192 states of a single $L = 32$ simple cubic lattice with $T/J = 0.675$, using an interval of 2560 Monte Carlo steps per spin between states.

drupolar ordering changes smoothly, but significantly, in this range of T . This, by itself, is a major factor in the slowing down of the kinetics, but it need not be related to any long-range ordering.

With only three types of domains, as in our simple model, it appears that true long-range order persists in the domain spin glass, just as it does in the threecomponent domain ferromagnet. At $x = 0.25$ there seems to be a true thermodynamic phase transition into a spin-glass phase at a temperature of $T_g / J = 0.67 \pm 0.03$. This conclusion is, however, based largely on the study of a single $L = 32$ system, out to times of 5×10^5 Monte Carlo steps per spin. It would be highly desirable to study an $L = 64$ lattice for somewhat longer times.

It should be noticed that, within the statistical errors, the T_g for this model is equal to the T_g of the $\pm J$ Ising spin glass¹⁵ divided by $\sqrt{3}$. This relationship is precisely what is predicted by a tree-level high-temperature perturbation theory, which finds that T_g scales like the inverse square root of the number of spin components.¹⁶ Despite the obvious difference in the natures of the lowtemperature phases of these models, this simple relation between the T_g values suggests that the same mechanism is driving the transition in both cases. In this context, it

is noteworthy that the freezing transition in the Ising spin glass can be analyzed in terms of domain walls.¹⁷

IV. MOBILITY EDGE TRANSITION

Based on a Landau-Ginsburg theory for the Edwards-Anderson¹⁸ spin-glass order parameter, q , one would predict that in this model q jumps discontinuously at T_g . The simulations do not support such a picture of the spin-glass freezing transition. The freezing occurs in a highly inhomogeneous fashion, and does not appear to be well-characterized by the configuration-averaged value of q.

Qualitatively, the kinetics of this model at $T/J = 0.675$ are similar to those of the random chiral model¹⁹ just above its freezing transition. The spectrum of local relaxation times at this temperature, shown in Fig. 3, is even broader here than in the latter model. This is probably due to the fact that the relaxation times of most of the spins which sit in a boundary layer between two differently oriented quadrupolar domains remain very short even at this temperature. The spatial distribution of the relaxation times of the spins, for the same layer of the lattice as in Fig. 2, is displayed in Fig. 4. There are "nuggets" of slowly relaxing spins, examples of which are visible in Fig. 4, embedded in some of the blobs. These nuggets correspond to the localized eigenvectors of the susceptibility matrix.^{13,19} Note that nuggets do not extend across domain boundaries. (This is much easier to see when the domain structure is displayed in color.)

Due to the broad tail of the distribution of relaxation times, and the fact that the fraction of the spins which are in this tail (i.e., the nuggets) is small, the long-time kinetics are not well-described by the average relaxation time. The typical distance between nuggets appears to be about 10–12 lattice constants. Therefore, for $L = 32$, the

FIG. 3. Histogram of the spin-Hip frequency for individual spins of the diagonal random anisotropic exchange cubic model with $x = 0.25$, and $T/J = 0.675$. The y axis is scaled logarithmically. The data set is the same one used for Fig. 2.

FIG. 4. Spatial distribution of the spin-flip frequency for the same layer of the same lattice used in Fig. 2. The data set is the same one used for Figs. 2 and 3. The scale of relaxation times is logarithmic, with larger numbers denoting longer relaxation times, and $T/J = 0.675$.

number of spins in the nuggets which dominate the slow relaxation behavior near the freezing temperature is comparable to $L^{3/2}$. This means that a description in terms of the configuration-average value of q is not even qualitatively valid near T_g . It may be that a description in terms of the configuration-average value of q becomes useful on larger length scales, but a naive extrapolation of the results on accessible scales leads one to believe that the glassy structure is fractal on all length scales.

As originally pointed out by Anderson²⁰ in 1970, the freezing of a single nugget cannot give true long-range order. However, the nuggets will interact with each other through the effective medium of the rapidly relaxing spins, and this can lead to long-range order. This mobili- $\frac{1}{x}$ edge transition^{13,21-23} has no natural counterpart in an infinite-range model.

Let us define

$$
q_{ij}(t) = \sum_{\alpha=1}^{3} \left\langle S_i^{\alpha}(0) S_j^{\alpha}(t) \right\rangle , \qquad (6)
$$

where the bracket, $\langle \rangle$, denotes a thermal expectation value. Now set $T=T_g$, and choose t_0 to be some large inite time, such as $10⁵$ Monte Carlo steps per spin. Then, in a large system, for most choices of the sites i and j , $q_{ij}(t_0)$ will be essentially zero, even if i and j are the same. If i and j both belong to the same nugget, however, then $|q_{ij}(t_0)|$ will be close to 1; this follows from the definition of a nugget. Only one of the spin components makes a significant contribution: the one which lies along the local axis of quadrupolar order.

Now consider sites i and j belonging to different nuggets. If they belong to different domains, then $q_{ii}(t_0)$ will be zero, because the local quadrupolar axes of i and j are orthogonal. If i and j belong to the different nuggets in the same domain, however, then $\left| \sum_{\alpha=1}^{3} S_i(0)S_j(t_0) \right|$ will again be close to 1, since t_0 is not a long enough time to allow relaxation of nuggets. In order to obtain the thermal expectation value for this case by the Monte Carlo simulation we must allow the system to evolve for a longer time, t_1 , of perhaps 10⁶ Monte Carlo steps per spin, so that the nuggets can equilibrate with each other. This is similar in spirit to Sompolinsky's analysis²⁴ of the infinite range Ising spin glass, in which there is an infinite hierarchy of time scales for $T \leq T_g$.

When the temperature is reduced to 0.65, it is obvious that a significant fraction of the system has become rather rigid, and it then becomes very difficult to run an $L = 32$ lattice long enough to observe the equilibrium behavior. It is not completely clear whether this is due to a true spin-glass freezing transition or is merely a finitetime effect.²⁵ In the case of the random chiral model, the author considers the evidence¹⁹ for a true phase transition to be convincing. It is likely that the result for the model considered here is the same.

V. DISCUSSION

This domain spin glass with three types of domains resembles, but is simpler than, the 12 Q-domain state which Werner⁶ has suggested for the spin-glass phase in CuMn. (The allowed Q vectors in CuMn do not lie along the high-symmetry cube axes.) Werner's 12 O-domain state should not have this kind of "simple" long-range spin-glass order, because the domains associated with a particular Q vector will apparently consist of disconnected finite clusters. Domain structures also exist in Cr antiferromagnet phases, 26 and a conceptually similar domain

structure has been proposed to explain β critobalite.^{27,28}

A domain spin-glass phase with only two types of domains was studied in the diluted Ising antiferromagnet in a magnetic field by Nowak and Usadel.²⁹ These authors were able to study very large systems for their model, and they found evidence that their domain state had a fractal structure. Chamberlin and Haines³⁰ have argued for the existence of a similar fractal structure in AuFe, based on their magnetic relaxation measurements.

The relevance of percolation effects of this sort for the existence of spin-glass phases has been emphasized recently by Celik, Hansmann, and Katoot, 31 who studied the van Hemmen model. It may be, however, that the presence of all 12 types of Q domains in a lowtemperature sample of CuMn is a nonequilibrium effect, analogous to polycrystallinity.

Another possibility which must be considered is that there may be energetic constraints on the ways in which the different Q domains are arranged, which could force the existence of some kind of topological long-range order. $32,33$ The experiment of Monod and Prejean 34 indicates that there is long-range rigidity of the domain structure in CuMn. One might expect the behavior of Werner's model to be more similar to that of the $K < 0$ model, which has eight favored directions for the spins. The $K > 0$ model has the unique property that the favored axes are a11 mutually orthogonal. This simplifies the energetics of the domain walls, and makes it difficult for the internal state of a domain to affect the internal states of its neighbors. This allows the ordering along different axes to proceed almost independently.

In this work we have used Monte Carlo simulations to investigate the behavior of a cubic magnet with threecomponent spins and a random diagonal nearestneighbor anisotropic exchange on a simple cubic lattice. In addition to the previously known phases, there is a new type of domain spin-glass phase, which apparently can exist at finite temperature in three dimensions. This domain spin-glass appears to be similar to structures which have been seen in various experimental systems.

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