Infinite Susceptibility Phase in Planar Random-Anisotropy Magnets

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A Monte Carlo algorithm has been used to study the random-anisotropy model with two-component spins on simple cubic lattices, in the strong anisotropy limit. The magnetic susceptibility diverges at a temperature of $T_c/J=1.91\pm0.03$, but no singular behavior is observable in the specific heat near T_c. The two-spin correlation function at T_c is described by a critical exponent $\eta=0.04\pm0.04$. The magnetization of the ground state of a lattice of size L is approximately $1/[0.37\ln(L)+1]$ per spin. At $T=0$ the value of η_1 is -0.34 ± 0.06, which agrees with small-angle neutron-scattering experiments on certain amorphous magnetic alloys.

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The magnetic properties of amorphous rare-earth–transition-metal alloys have been studied for about twenty years,[1] and a significant amount of work has been done. Perhaps most striking was the discovery that at low temperatures the small-angle elastic-scattering intensity for neutrons, which is proportional to the equal-time two-spin correlation function, behaves as $k^{-2.4}$, where k is the magnitude of the momentum transfer. This phenomenon was seen in amorphous alloys of TbFe,[2] HoFe,[3] and ErCo.[4] The effect does not occur in YFe or GdFe alloys, so it appears to be caused by the random single-site anisotropy which acts on the non-S-state rare-earth atoms in these amorphous alloys. An explanation of the $k^{-2.4}$ law has remained as a major challenge to our understanding of these materials.

The Hamiltonian which is used to model these random-anisotropy magnets was introduced by Harris, Plischke, and Zuckermann[5] (HPZ). In its general form, it may be written as

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

where each S_i is an m-component spin and the $\hat{\mathbf{n}}_i$ are uncorrelated random m-component unit vectors. The constants J and D are assumed to be positive. HPZ showed that a mean-field approximation for this Hamiltonian gives a ferromagnetic phase at low temperatures. Equation (1) can also give rise to spin-glass behavior under certain conditions, as was made clear by later work.[6,7]

When we go to the strong anisotropy limit, $D/J\rightarrow\infty$, 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.[8] It is convenient for both computer modeling[9,10] and high-temperature series expansions,[11–13] and it can also be used as a starting point for real-space renormalization-group calculations.[7,12,14] In this work we present the results of large-scale Monte Carlo simulations of Eq. (2), for the case of planar random anisotropy ($m=2$) on simple cubic lattices ($d=3$). This case was predicted[7,13,15] to be especially interesting, and we will see that the results fully justify our expectations.

Monte Carlo calculations of Eq. (2) for the cases $m=2$ in $d=2$ and $m=3$ in $d=3$ were performed by Jayaprakash and Kirkpatrick,[9] who found that the standard single-spin-flip heat-bath method was not an effective technique for this problem. They found it necessary to use a combination of single-spin, pair-spin, and four-spin flips in order to achieve a workable algorithm. The case we study in this work, $m=2$ in $d=3$, is not as frustrated as those studied by Jayaprakash and Kirkpatrick, so four-spin flips were not used. A Monte Carlo cycle consisted of four single-spin-flip passes through the lattice alternating with three pair-flip passes (one for each direction). A program using a version[16] of the Swendsen-Wang[17] cluster method was also tried. Even near T_c, the heat-bath method using a combination of single-spin and pair-spin flips was about 6 times as efficient as the cluster method, for $32\times32\times32$ lattices ($L=32$).

The algorithm was tested on several lattices of size $L=20$ which had been studied previously[10] by a nonequilibrium simulated-annealing method. It was found that the Monte Carlo program worked quite well down to the lowest temperatures. The low-temperature states found by the Monte Carlo method for these $L=20$ lattices had a high degree of overlap with the lowest-energy states of the same lattices found by the simulated-annealing method. This is significant, as it indicates that the ground states of these lattices are essentially unique. Therefore, the scaling concepts which have been developed by Fisher and Huse[18] to describe the low-temperature behavior of the three-dimensional Ising spin glass should also be applicable to the $m=2$ random-anisotropy

magnet in $d=3$. The numerical values of the scaling exponents should be different, since for this model the domain walls are much stiffer than for the Ising spin glass.

The program was then used to study larger lattices. It was not difficult to work with $L=32$ lattices, and even $L=48$ lattices could be successfully cooled down to low temperatures if some care was exercised. Sharp freezing transitions were exhibited by these lattices. This means that correlation times increased rapidly as T was lowered. T_c was taken to be the highest temperature for which the lattice remained substantially correlated over a time of 2000 Monte Carlo cycles. Correlation times at $T=T_c+0.05J$ were typically an order of magnitude less than this. (The reader should remember that each of these cycles is equivalent to a large number of single-spin-flip passes through the lattice.) For the $L=32$ lattices, the freezing occurred in the temperature range $1.95 \leq T_c/J \leq 2.00$, and for the $L=48$ lattices it occurred at $1.92 \leq T_c/J \leq 1.95$. The ranges indicate the variation in T_c among lattices of the same size. These variations were highly correlated with variations in the ground-state energy, as one would expect. The variations in T_c were about a factor of 4 larger than the variations in the ground-state energy, however. No significant correlation was observed between these quantities and variations in the ground-state magnetization. Each lattice was cooled down through T_c several times, in order to insure that the system did not get stuck in a large-scale metastable state. Data obtained from the lowest-energy state found for each of these lattices are displayed in Table I, along with data previously obtained by the simulated-annealing method[10] for smaller lattices.

The program was also used to study two $L=64$ lattices. Both of these lattices froze at about $1.93J$. For these very large lattices, an attempt to find the ground states was judged to be impractical. Considering all of the data, and allowing for the shift of the freezing temperature as a function of size, we can estimate that

$$T_c/J=1.91\pm0.03 \tag{3}$$

in the limit $L\rightarrow\infty$. Although there is a broad maximum in the specific heat, centered at about $1.95J$, this peak does not appear to "sharpen up" as L becomes larger. Therefore, within the accuracy of the calculation, there is no evidence for any singular behavior of the specific heat at the freezing transition. "Cold start" initial conditions (using a fully magnetized initial state) were also used, to test for a possible first-order transition. No evidence for any discontinuous behavior at T_c was found. The value of T_c found here is slightly higher than the one which was quoted on the basis of extrapolation of the high-temperature susceptibility series.[13] This difference is not very meaningful, as the high-temperature series were deliberately analyzed using assumptions which would give the lowest reasonable value of T_c.

An inspection of Table I reveals that the (normalized) magnetization of the ground state exhibits a slow decay as a function of L. We define the average magnetization $M(L)$ to be the square root of $M^2(L)$, as given in Table I. (Since the width of the distribution is not large, and scales approximately as the average value, the precise definition we use is not crucial.) By plotting the data as shown in Fig. 1, we see that they are fit remarkably well by the simple equation

$$M(L)=[0.37\ln(L)+1]^{-1}. \tag{4}$$

TABLE I. Ground-state data for the $m=2$ random-anisotropy magnet on $L\times L\times L$ simple cubic lattices. M^2 and ΔM^2 are the average and standard deviation of the ground-state distribution of 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	0.4779	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
32	16	0.1965	0.0166	−1.5052	0.0033
48	4	0.1695	0.0140	−1.5063	0.0014

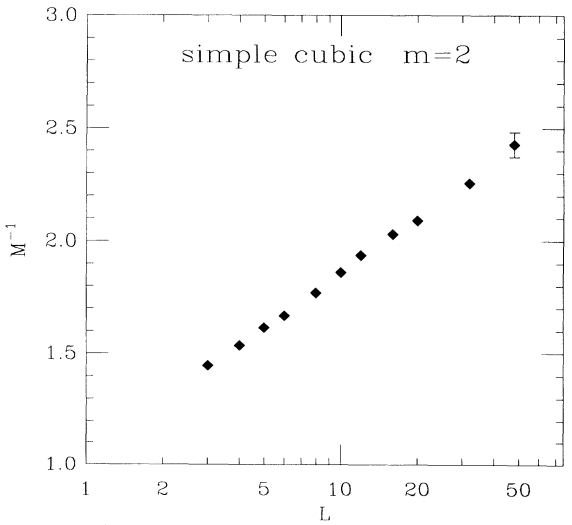

FIG. 1. Inverse of the average magnetization (as defined in the text), $1/M$, vs lattice size, L, for $L\times L\times L$ simple cubic lattices, for the random-anisotropy model with $m=2$ and $D/J=\infty$. The L axis is scaled logarithmically. The error bars for $L=48$ show 1 standard deviation. The error bars for smaller L would be about the same size as the plotting symbols.

The form of Eq. (4) is likely to be universal, although the constant which multiplies $\ln(L)$ should be a function of D/J, etc. An analytical derivation of Eq. (4) would presumably involve the free energy of vortex lines. This general scenario was proposed by Fisher,[15] building upon some ideas of Halperin[19] regarding the role of vortex lines in three-dimensional XY models. Random-anisotropy models possess a long-wavelength instability[20] for $d=3$, but when $m=2$ this is not sufficient[19,21] to destroy the long-range spin correlations. A phase with an infinite magnetic susceptibility, but no true magnetization, was first proposed for three-dimensional random-anisotropy models by Aharony and Pytte,[22] for somewhat different reasons.

One can also consider the effect of higher-order random anisotropies.[23,24] Renormalization-group expansions about both four dimensions[23] and two dimensions[24] give the result that a threefold random anisotropy should be irrelevant for $m=2$ in $d=3$. This has been confirmed by numerical work.[10,25] Therefore, the infinite susceptibility phase appears to be unique to the case of twofold random anisotropy. The threefold random-anisotropy system also shows[25] a well-defined XY-like specific-heat peak at T_c, in contrast to the twofold case.

To compare our computer simulations with the small-angle neutron-scattering (SANS) experiments,[2-4,26] we calculate the angle-averaged two-spin correlation function $C_2(k)$ by Fourier transforming the spin states, and then squaring. The results for $T=0$ are shown in Fig. 2, with the octagons giving the average over the $L=32$ lattice ground states, and the plusses for $L=48$. The data for the two lattice sizes fall right on top of each other, within the statistical accuracy, as they should. On this log-log plot, the data at small k can be fit by a straight line with a slope of -2.34 ± 0.06, in excellent agreement with the $k^{-2.4}$ law found at low temperatures by the experiments. This exponent is conventionally[22] called $2-\eta_1$, so the result may be written

$$\eta_1=-0.34\pm0.06. \tag{5}$$

The experimental papers claim that this exponent should be corrected for systematic errors. This will not affect the agreement between the simulations and the experiments, as similar correction factors are applicable to both sets of data. It might be objected that the experiments should correspond to an $m=3$ model, rather than $m=2$. The experimental samples were made by sputtering, however, and such samples usually have a significant amount of growth-induced anisotropy. Amorphous Dy-Cu, which is a good $m=3$ system, does not exhibit these effects.[27,28] Since the structure of the experimental systems is quite complex, the ability of the relatively simple Hamiltonian, Eq. (2), to reproduce the primary features of their behavior is a very significant result.

Results for $C_2(k)$ at $T=1.95J$ are shown in Fig. 3. These data are the angle-averaged Fourier transforms of twelve statistically independent equilibrium spin states, six each from two different $L=64$ lattices. A temperature slightly greater than T_c was used in order to insure that these states were truly independent equilibrium states. By fitting the small-k data with a straight line, as before, we obtain the critical exponent

$$\eta=0.04\pm0.04. \tag{6}$$

This is indistinguishable from the value of η for an isotropic $m=2$ magnet (or, for that matter, an $m=1$ or iso-

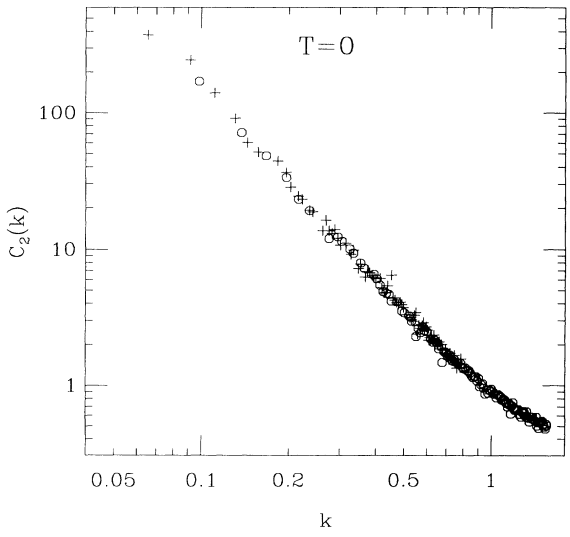

FIG. 2. Angle-averaged two-spin correlation at $T=0$, for the $m=2$ random-anisotropy model. Octagons show data from $32\times32\times32$ simple cubic lattices, and the plusses from $48\times48\times48$ lattices.

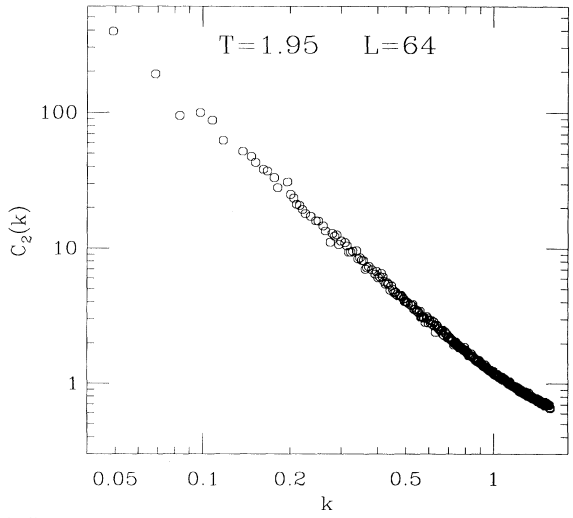

FIG. 3. Angle-averaged two-spin correlation at $T=1.95J$, for the $m=2$ random-anisotropy model. Data from $64\times64\times64$ simple cubic lattices.

tropic $m=3$ magnet). It is clear from these data that the entire $L=64$ lattice is correlated at $T=1.95J$. In contrast, the data for $T=2.00J$ (not displayed) show clear evidence of rounding of the small-k peak. This indicates that we are looking at a sharp phase transition, rather than some kinetic effect.

The random-anisotropy model has also been used to describe certain crystalline metallic alloys.[29-32] Therefore, the results presented here are likely to find a broad range of applicability. In the presence of an underlying crystalline lattice, care must be exercised in the determination of which universality class a particular experimental system should correspond to $m=1$, 2, or 3, or perhaps something more complicated.

In summary, large-scale Monte Carlo simulations of the $m=2$ random-anisotropy magnet have been performed. The results indicate the presence of a sharp, continuous phase transition, but no singularity is found in the specific heat at T_c. The low-temperature phase is characterized by infinite-range ferromagnetic correlations, but no true magnetization. The long-wavelength behavior of the two-spin correlation function matches the form which has been found by small-angle neutron-scattering in certain amorphous rare-earth–transition-metal alloys.

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[1]Progress in this field may be followed through the Proceedings of the Annual Conference on Magnetism and Magnetic Materials, which, for the past several years, has appeared in the Journal of Applied Physics.

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