Ferromagnetism in the XY model with random threefold anisotropy

Ronald Fisch
Department of Physics, Washington University, St. Louis, Missouri 63130
(Received 6 January 1992)

A Monte Carlo algorithm has been used to study the XY model with random threefold single-site anisotropy on simple cubic lattices, in the strong-anisotropy limit. The model has a pure XY-like ferromagnetic critical point at $T_c/J=2.190\pm0.005$. The zero-field thermodynamic functions remain close to those of the simple XY model down to $T\approx2.00J$. The ground state has an energy per spin of $E_0/J=-2.2305\pm0.0010$ and a magnetization per spin of $M_0=0.720\pm0.003$.

I. INTRODUCTION

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

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

where each S_i is an m-component unit-length spin, and the $\hat{\mathbf{n}}_i$ are uncorrelated random m-component unit vectors that are distributed uniformly over the m sphere. HPZ showed that a mean-field approximation gives a ferromagnetic phase for this Hamiltonian at low temperatures. There has been a large amount of subsequent work, whose object has been to go beyond the mean-field theory and to understand the behavior of two- and three-dimensional systems.

The random anisotropy term in Eq. (1) can easily be generalized[2–4] to higher-order types of anisotropy. It is particularly interesting to do this for XY spins, the $m=2$ case of Eq. (1). For $m>2$, higher-order random anisotropies will generate random uniaxial anisotropy terms under a renormalization-group transformation,[3,4] 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

$$H_p=-J\sum_{\langle ij\rangle}\cos(\theta_i-\theta_j)-D\sum_i\{\cos[p(\theta_i-\phi_i)]-1\}, \quad (2)$$

where ϕ_i is the angular coordinate of $\hat{\mathbf{n}}_i$.

Much progress has been made in analyzing Eq. (2) for the case of two spatial dimensions ($d=2$). It was shown[5,6] that the Kosterlitz-Thouless phase survives in the presence of the random anisotropy term when $p\geq3$, at least for small D. This result made it seem reasonable that these $p\geq3$ models should be ferromagnetic for $d=3$. Based on a spin-wave argument, however, Pelcovits, and co-workers[7,8] had claimed that in the presence of a random anisotropy there could be no ferromagnetism at $T>0$ when $d\leq4$, so this was discounted. (The analysis given by Pelcovits[8] is for the $p=2$ case, but it easily generalizes to arbitrary p.) Doubts about the validity of this spin-wave argument for an XY model had been raised earlier, by Halperin,[9] who pointed out that a spin-wave instability cannot destroy the magnetization in this case.[10] Sourlas,[11] and Villain and Semeria[12] also discussed some weaknesses in the spin-wave perturbation theory treatment of Pelcovits, and co-workers.

Subsequent work[13–16] has shown that for XY spins the lower critical dimension for ferromagnetism when $p=2$ is $d=3$, rather than 4. Renormalization-group arguments,[2,17] treating the random anisotropy in the small D/J limit, gave the result that for $p\geq3$ the randomness is irrelevant. This means that the disorder induced by the quenched random anisotropy is qualitatively indistinguishable from thermal disorder, at least near the critical temperature T_c. Thus, near T_c, the system is expected to behave like a simple XY ferromagnet, even in the presence of the $p=3$ random anisotropy.

The calculations of Sourlas,[11] and Villain and Semeria,[12] however, have shown that we must regard these perturbative arguments with some suspicion. Therefore, it is important to check the results by doing Monte Carlo simulations. Reed[18] has presented the results of such simulations for both the $p=2$ and 3 random anisotropy models with $D/J=1$ on simple cubic lattices. He found that for lattice sizes that could be studied by computer, the behavior near T_c was quite similar to that of a pure XY ferromagnet without anisotropy. Reed expressed the opinion that this was a finite-size effect, and that if it were possible to study much larger lattices the magnetic order would be seen to vanish at large distances.

An alternative to using larger lattices is to use larger values of D/J. This should cause any such qualitatively new behavior, if it exists, to occur at smaller, and perhaps accessible, length scales. For the $p=2$ case, such behavior was indeed found.[16] In this work, we present results for $p=3$, where no such deviations from pure XY-type critical behavior have been encountered. The author believes that the lattice sizes used were sufficiently large that they indicate the lack of such deviations from pure XY behavior even for infinite systems. This, of course, should not be considered a proof, but it does agree with the renormalization-group results.[17]

II. CALCULATIONS

Taking the $D/J \to \infty$ limit of Eq. (2) enormously simplifies the nature of the problem of performing Monte Carlo simulations. It is then only necessary to deal with a discrete phase space, rather than a continuous one. There is no reason,[11] however, to believe that the behavior is singular in this limit. Our results will be qualitatively valid for all large values of D/J. Upon taking this limit, we obtain

$$H_{p,\infty} = -J \sum_{\langle ij \rangle} \cos\left[\frac{2\pi}{p}(q_i - q_j) - (\phi_i - \phi_j)\right], \quad (3)$$

where each q_i is now a $\mathbb{Z}_p$ variable, which takes on all integer values between 0 and $p-1$. If we remove the randomness from Eq. (3) by setting all of the $\phi_i = 0$, we are left with the standard p-state vector Potts (clock) model.[19] For $p=3$, the vector Potts model has a first-order transition into the ferromagnetic state when $d=3$. Alternatively, we could (for example) set all of the ϕ_i on the A sublattice equal to 0, and all of the ϕ_i on the B sublattice equal to π, which yields the antiferromagnetic p-state clock model. For even p the ferromagnetic and antiferromagnetic models can be mapped into each other by a gauge transformation. This cannot be done for odd p, and the $p=3$ antiferromagnetic clock model is believed to be in the XY universality class.[20,21]

At the mean-field level,[22] the inclusion of the random ϕ_i terms changes the nature of the model in a dramatic fashion. The probability distribution for the random anisotropy terms has a continuous rotational invariance, rather than the discrete p-fold invariance of the vector Potts model. Although 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, that is an artifact of the mean-field theory. The actual symmetry group of the ground state is only the p-fold discrete rotation invariance. The energy barriers to rotation of the magnetization that are produced by the random anisotropy may only grow like the square root of the volume. However, when the volume becomes large, they still become much larger than thermal activation energies, and they diverge in the thermodynamic limit.

On a Cayley tree, one can replace Eq. (3) by the random chiral model,[23,24]

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

where the ϕ_{ij} are independent random variables. This, however, does not work for a lattice that contains closed loops. To illustrate this, we observe that Eq. (3) is the same if the probability distribution for the ϕ_i is chosen to be uniform on $[-\pi/p, \pi/p]$ or $[-\pi, \pi]$. In contrast, if the probability distribution of the ϕ_{ij} is uniform on $[-\pi/p, \pi/p]$, then the ground state of Eq. (4) is a simple ferromagnet, while a distribution of the ϕ_{ij}, which is uniform on $[-\pi, \pi]$, gives a ground state for Eq. (4) that is highly frustrated, and has no ferromagnetic long-range order in the ground state. Analyses of the Chen-Lubensky[25] type, which assume that Eq. (3) can be approximated by Eq. (4), are of dubious validity.

The reader should note that in the $p=2$ case Eq. (4) reduces to a form of the Ising spin glass. It is not true that Eq. (3) can be reduced to an Ising spin glass for $p=2$, except on a tree graph. Despite this, for $p \geq 3$ it may be that the critical point of Eq. (3) corresponds to some critical point of Eq. (4), within a range of probability distributions of the ϕ_{ij}. Preliminary results[26] from Monte Carlo simulations of Eq. (4) with $p=3$ on simple cubic lattices do appear to display a continuous transition from paramagnet to ferromagnet for some distributions of the ϕ_{ij}. It is difficult, however, to determine the precise nature of this critical point from the numerical data.

In this paper, we report the results of studying Eq. (3) with $p=3$. The Monte Carlo program that was used in this work was a straightforward modification of the one used[16] for the $p=2$ case. Calculations were performed on $L \times L \times L$ simple cubic lattices of sizes $L=32$ and 48. A Monte Carlo cycle consisted of six single-spin-flip passes through the lattice interleaved with three pair-flip passes (one for each type of pair). No metastability problems were encountered near T_c for the $p=3$ case, in contrast to the earlier $p=2$ work. This is because T_c is higher for $p=3$, while the activation barriers are lower. For $p=3$, the kinetic freezing occurs below T_c, with the freezing temperature increasing to T_c as L is increased. Twelve $L=32$ lattices were successfully cooled to $T=0$, and two $L=48$ lattices were studied near the critical temperature. Despite the absence of metastability problems, the Monte Carlo algorithm is intrinsically slower for $p=3$ than for $p=2$, as one must consider three possible states for each spin, rather than two.

Figure 1 shows the zero-field specific heat c_H as a function of temperature, in the range $1.3 < T/J < 2.3$, for Eq.

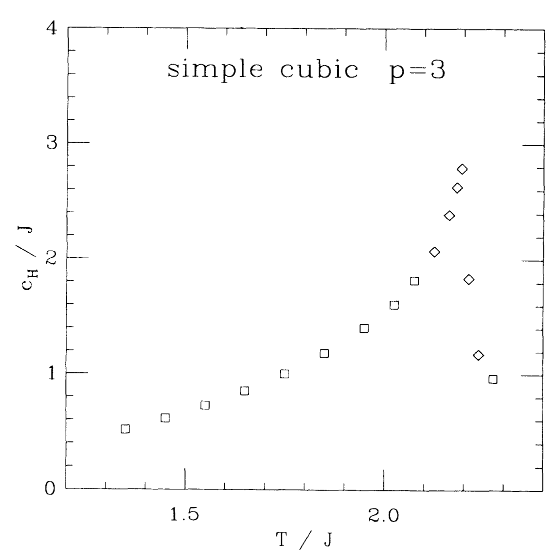

FIG. 1. Zero-field specific heat vs temperature for the random $p=3$ anisotropy model with $D/J=\infty$. Squares show data from $32 \times 32 \times 32$ simple cubic lattices, and diamonds are data from $48 \times 48 \times 48$ lattices. The error bars (not shown) would be smaller than the plotting symbols.

(3) with $p=3$. The data points were obtained by numerically differentiating the energy per spin E with respect to the temperature. They represent the average over all of the $L=32$ lattices, except in the critical region, where the $L=48$ lattices were used. Measuring c_H by using energy fluctuations gave similar results, but with larger statistical errors. The critical point occurs at

$$T_c/J=2.190\pm0.005 , \quad (5)$$

which is only about 0.5% lower than the T_c for the simple XY model on this lattice.[27–29] For the $L=48$ lattices, the value of E at $T/J=2.20$ is -0.991 ± 0.002, where the "error" reflects the difference in energy between different lattices, rather than the uncertainty for a particular lattice. This is also extremely close to the value of E at the same temperature for the simple XY model. By comparing with the results of Li and Teitel,[27] we see that the entire c_H vs T curve remains close to that of the pure XY model down to a temperature of about $T/J=2.00$, 10% below T_c. If c_H is a monotonic function of D/J, which seems likely, then it follows that the dependence on D/J is remarkably small at these temperatures. This is consistent with Reed's results[18] for $D/J=1$.

For $p\geq 4$, the results would be even closer to those of the pure XY model, since in the limit $p\rightarrow\infty$ we recover the XY model. This is in marked contrast to the situation for $p=2$. In that case c_H is much lower for $2.0<T/J<2.4$, and an E of -0.99 is not achieved until $T/J\approx 1.95$, which happens to be just above the T_c of the $p=2$ model.[16] Since the entropy S is the integral of c_H/T, this means that $S(T_c)$, measured relative to $S(T=\infty)$, is significantly lower for $p=2$ than it is for larger p. Therefore, it is not so surprising that the nature of the phase transition that occurs in the $p=2$ model on this lattice[14–16] is different from what we see here.

For $p\geq 3$, there is a spontaneous magnetization M in the low-temperature phase. Figure 2 shows the average value of M^2 as a function of T for $p=3$. Again, by comparing with the results of Li and Teitel,[27] we see that the behavior of the $p=3$ model remains close to that of the pure XY model down to about $T/J\approx 2.00$, and then deviates noticeably. The finite-size effects visible near T_c are comparable in magnitude to those of the XY model, although the sample-to-sample fluctuations cause the statistical errors to be somewhat larger. Thus, we verify that the $p=3$ model shows no observable deviations from pure XY behavior near T_c, as predicted by the small D/J renormalization group arguments.

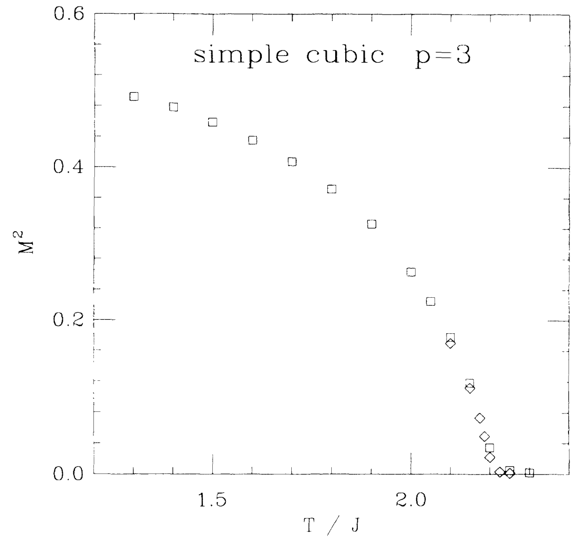

FIG. 2. Magnetization squared vs temperature for the random $p=3$ anisotropy model with $D/J=\infty$. Squares show data from $32\times32\times32$ simple cubic lattices, and diamonds are from $48\times48\times48$ lattices. The error bars (not shown) would be smaller than the plotting symbols.

The computer simulations also make clear why the instability found by Pelcovits and co-workers[7,8] does not destroy the magnetization. While it is true that below T_c the transverse fluctuations of the magnetization are much larger than the longitudinal ones, they are not purely diffusive. The phase space is divided into three well-defined equivalent minima. There are restoring forces in the transverse direction, and there is no Goldstone mode. The barriers between the phase-space minima (and thus the surface tension) disappear continuously as we approach T_c, so the model becomes XY-like near T_c. It is true that the $T=0$, XY fixed point is unstable to the introduction of random anisotropy, but the $T=0$, random anisotropy fixed point is also ferromagnetic.[22]

Ground-state properties are displayed in Table I, as a

TABLE I. Ground-state data for $L\times L\times L$ simple cubic lattices for XY spins with $p=3$. M_0 and ΔM_0 are the average and standard deviation of the magnetization distribution for ground states. E_0 and ΔE_0 are the average and standard deviation of the ground-state energy distribution (in units of J).

L	Samples	M_0	ΔM_0	E_0	ΔE_0
3	192	0.8539	0.0241	−2.2886	0.0848
4	128	0.8362	0.0191	−2.2711	0.0514
5	96	0.8182	0.0175	−2.2465	0.0349
6	64	0.8050	0.0182	−2.2409	0.0306
8	48	0.7906	0.0143	−2.2396	0.0178
10	40	0.7750	0.0120	−2.2359	0.0118
12	32	0.7626	0.0173	−2.2353	0.0088
16	32	0.7479	0.0130	−2.2321	0.0060
20	24	0.7388	0.0140	−2.2299	0.0044
32	12	0.7300	0.0093	−2.2307	0.0021

function of L. The data for $L \leq 20$ were obtained previously,[30] by a simulated annealing method. If we extrapolate values of the ground-state energy and the ground-state magnetization to $L = \infty$ we find

$$E_0 = -2.2305 \pm 0.0010 \text{ and } M_0 = 0.720 \pm 0.003 \ . \quad (6)$$

These values are significantly more precise than the earlier estimates.[30] The approximate ground states, which are found by the computer for the $L = 32$ lattices, are estimated to be about 95% correct, and the errors consist of isolated clusters of a few hundred spins or less each. Therefore, systematic errors should be smaller than the statistical errors. Figure 3 shows the extrapolation of M_0. We see that

$$M_0(L) - M_0(\infty) = 1.75 L^{-3/2} \ , \quad (7)$$

provides a remarkably accurate fit to the data, for all $L \geq 10$. Considering the statistical error bars, some of this apparent precision must be fortuitous, but it is evident that the transverse magnetic correlation length of the ground state is rather short. If we assume that the sample-to-sample fluctuations of M induced by the random anisotropy are functionally equivalent to thermal fluctuations, then the value of $-\frac{3}{2}$ for the exponent on the right-hand side of Eq. (7) can be predicted by finite-size-scaling theory.[31]

This point deserves further emphasis. The excellent fit of Eq. (7), the $L^{-3/2}$ finite-size effect, to the magnetization data of Fig. 3 is strong evidence for the essential uniqueness of the ordered state (up to the trivial threefold degeneracy). If there was a Goldstone mode, then the magnetization ought to display an L^{-1} finite-size scaling. Since Pelcovits, Pytte, and Rudnick[7,8] have shown that a magnetization with a Goldstone mode is not possible for this model when $d < 4$, we have a consistent picture. If one did not know that the destruction of the magnetization in this model was impossible without the creation of vortex lines,[9,10] this would all seem rather implausible. It must be that these vortex lines provide a long-range force that stabilizes the magnetization and causes the evasion of Goldstone's theorem.

III. DISCUSSION

The general reader may have gotten the impression, up to this point, that it should have been obvious *a priori* that our Monte Carlo results would turn out as they have. While it follows from renormalization-group universality arguments that Eq. (2) should have the same behavior for essentially all three-dimensional lattices when D is small enough, this is not true in the large D/J limit. It may be true, for instance, that for $p = 3$, Eq. (3) does not have a ferromagnetic phase on the diamond lattice, which has a coordination of only four neighbors per site.

Perhaps the most remarkable aspect of the work de-

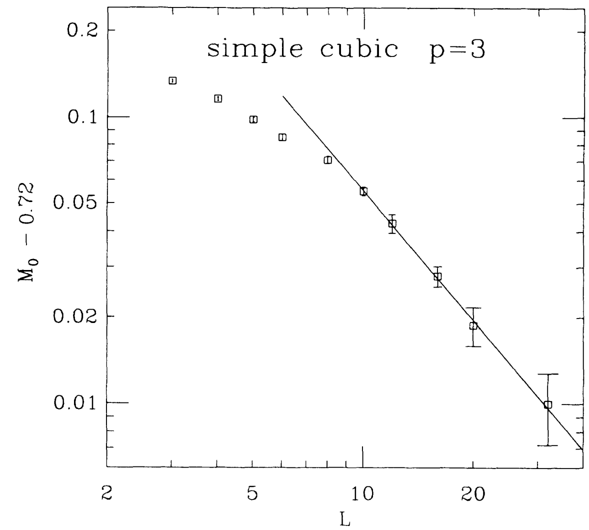

FIG. 3. Average ground-state magnetization minus 0.72 vs lattice size L for $L \times L \times L$ simple cubic lattices, for the random $p = 3$ anisotropy model with $D/J = \infty$. Both axes are scaled logarithmically. The error bars show one σ, and the straight line has a slope of $-\frac{3}{2}$.

scribed here is that the strong random threefold anisotropy changes the ground-state energy of this model by 25.7%, while the critical temperature changes by only 0.5%. The author's prior expectation, based on the previous results for the $p = 2$ random anisotropy model, was that the critical point would be depressed by about 5%. Further, within the accuracy of the simulations, the energy at the critical point is unchanged by the $p = 3$ random anisotropy. These results appear to indicate that the $p = 3$ random anisotropy does not couple directly to the operators that are relevant at the critical point. This is a much stronger result than merely saying that the model remains in the XY universality class. It seems difficult to understand this effect in terms of a spin-wave type of analysis. Therefore, it is probably another manifestation of the importance of vortex lines to the critical behavior of the three-dimensional XY model.

In this work we have presented a Monte Carlo calculation of the XY model with random $p = 3$ anisotropy on simple cubic lattices, in the strong-anisotropy limit. The model turns out to be in the universality class of the pure $d = 3$ XY model. More surprisingly, the behavior for $T \geq 2.00J$ is very insensitive to the presence of the random anisotropy, which appears to act merely as a weak additional source of pseudo-thermal fluctuations.

ACKNOWLEDGMENTS

The author thanks N. Sourlas for telling him of Ref. 11 and A. N. Berker for pointing out that the results of Ref. 31 could be used in this context.

[1]R. Harris, M. Plischke, and M. J. Zuckermann, Phys. Rev. Lett. **31**, 160 (1973).
[2]A. Aharony, J. Phys. C **14**, L841 (1981).
[3]Y. Y. Goldschmidt, Nucl. Phys. **B220**, 351 (1983).
[4]D. S. Fisher, Phys. Rev. B **31**, 7233 (1985).
[5]A. Houghton, R. D. Kenway, and S. C. Ying, Phys. Rev. B **23**, 298 (1981).
[6]J. Cardy and S. Ostlund, Phys. Rev. B **25**, 6899 (1982).
[7]R. A. Pelcovits, E. Pytte, and J. Rudnick, Phys. Rev. Lett. **40**, 476 (1978).
[8]R. A. Pelcovits, Phys. Rev. B **19**, 465 (1979).
[9]B. I. Halperin, in *Physics of Defects, Les Houches 1980,* edited by R. Balian, M. Kleman, and J.-P. Poirier (North-Holland, Amsterdam, 1981), p. 813.
[10]G. Kohring, R. E. Shrock, and P. Wills, Phys. Rev. Lett. **57**, 1358 (1986).
[11]N. Sourlas, J. Phys. (Paris) Lett. **42**, L233 (1981).
[12]J. Villain and B. Semeria, J. Phys. (Paris) Lett. **44**, L889 (1983).
[13]A. J. Bray and M. A. Moore, J. Phys. C **18**, L139 (1985).
[14]R. Fisch and A. B. Harris, Phys. Rev. B **41**, 11 305 (1990).
[15]R. Fisch, Phys. Rev. B **41**, 11 705 (1990).
[16]R. Fisch, Phys. Rev. Lett. **66**, 2041 (1991).
[17]Y. Y. Goldschmidt and B. Schaub, Phys. Rev. B **30**, 2977 (1984); Nucl. Phys. **B251**, 77 (1985).
[18]P. Reed, J. Phys. A **24**, L117 (1991).
[19]R. Savit, Rev. Mod. Phys. **52**, 453 (1980); F. Y. Wu, *ibid.* **54**, 235 (1982).
[20]J. R. Banavar, G. S. Grest, and D. Jasnow, Phys. Rev. Lett. **45**, 1424 (1980); Phys. Rev. B **25**, 4639 (1982).
[21]J. S. Wang, R. H. Swendsen, and R. Kotecky, Phys. Rev. Lett. **63**, 109 (1989); Phys. Rev. B **42**, 2465 (1990).
[22]B. Derrida and J. Vannimenus, J. Phys. C **13**, 3261 (1980).
[23]H. Nishimori and M. J. Stephen, Phys. Rev. B **27**, 5644 (1983).
[24]D. J. Gross, I. Kanter, and H. Sompolinsky, Phys. Rev. Lett. **55**, 304 (1985).
[25]J. H. Chen and T. C. Lubensky, Phys. Rev. B **16**, 2106 (1977).
[26]R. Fisch, Bull. Am. Phys. Soc. **37**, 236 (1992); and (unpublished).
[27]Y.-H. Li and S. Teitel, Phys. Rev. B **40**, 9122 (1989).
[28]M. Hasenbusch and S. Meyer, Phys. Lett. B **241**, 238 (1990).
[29]W. Janke, Phys. Lett. A **148**, 306 (1990).
[30]R. Fisch, Phys. Rev. B **42**, 540 (1990).
[31]M. E. Fisher and A. N. Berker, Phys. Rev. B **26**, 2507 (1982).