PHYSICAL REVIEW B VOLUME 36, NUMBER 13 1 NOVEMBER 1987

Chiral order in a two-dimensional XY spin glass

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(Received 13 April 1987)

Ordering phenomena in the two-dimensional XY (plane-rotator) spin glass are studied by Monte Carlo simulations, with particular attention to the behavior of the chirality, which is an Ising-like multispin variable associated with a broken reflection symmetry. The chiral degrees of freedom are found to order in a markedly different manner from the XY spins: Indeed, the chiral susceptibility can be accurately mapped onto the spin-glass susceptibility of a pure *Ising* spin glass.

I. INTRODUCTION

It was pointed out by Villain that the ground state of certain frustrated vector spin systems could display a twofold, Ising-like degeneracy,[1] in addition to a continuous degeneracy associated with the original spin symmetries. This twofold degree of freedom is called "chirality," and is closely related to a reflection symmetry of the system. Villain analyzed the properties of an XY spin-glass model in two dimensions, and suggested the importance of this "chiral" degree of freedom for the spin-glass behavior.[1] The detailed nature of a possible chiral ordering and its relation to the usual spin ordering are still intriguing issues. In this article, we report on the results of extensive Monte Carlo simulations for the $\pm J$ XY model on the square lattice,[2] the simplest spin-glass model which can sustain a chiral degree of freedom. We introduce a chirality variable, define the corresponding "chiral susceptibility," and calculate it together with the conventional spin-glass susceptibility. It is concluded that the conventional spin-glass susceptibility diverges at zero temperature as a power law, characterized by an exponent consistent with the estimates of other authors.[3] By contrast, the chiral susceptibility turns out to exhibit a significantly different behavior: Indeed, it diverges in essentially the same way as the spin-glass susceptibility of a pure *Ising* spin glass.

II. CHIRALITY

Our model is the two-dimensional $\pm J$ plane-rotator or XY model on the square lattice with two-component, fixed-length spins ($\mathbf{s}_i$) with orientations θ_i. The Hamiltonian is

$$\mathcal{H} = \sum_{\langle ij \rangle} J_{ij} \mathbf{s}_i \cdot \mathbf{s}_j = \sum_{\langle ij \rangle} J_{ij} \cos(\theta_i - \theta_j) \ , \tag{1}$$

where the sum runs over nearest-neighbor pairs $\langle ij \rangle$, while the J_{ij} are independent random variables taking the values $+J$ and $-J$ with equal probability.

Consider, first, the global symmetry of the model. If all spins in a ground state are rotated equally, one obtains another ground state. In unfrustrated systems, such as regular ferromagnets or collinear antiferromagnets, this operation generates all possible ground states. In a frustrated system like our model this is no longer so. In fact, if one makes a global spin *reflection* in a ground state with respect to an arbitrary axis in the spin space, one can obtain a distinct ground state which cannot be reached by any rotation from the original state. Thus the full set of ground states consists of at least two disconnected manifolds, which are characterized by opposite *chiralities*. This is illustrated for a single isolated frustrated plaquette in Fig. 1: A global spin reflection of the state (a) with respect to the x or y axis, yields the states (b) or (c), respectively, which cannot be generated by a global rotation from the state (a); on the other hand, the states (b) and (c) can be connected by a global rotation (of 180°).

Evidently, chiral order can be regarded as a manifestation of the breaking of a reflection symmetry, namely of the Z_2 symmetry relating the two equivalent but disconnected sets of ordered states with opposite chiralities. Recent studies on *regularly* frustrated XY systems have indeed revealed that the existence of chiral degrees of freedom deeply influences the nature of the phase transition.[4] Therefore, even in spin glasses, it is likely that the

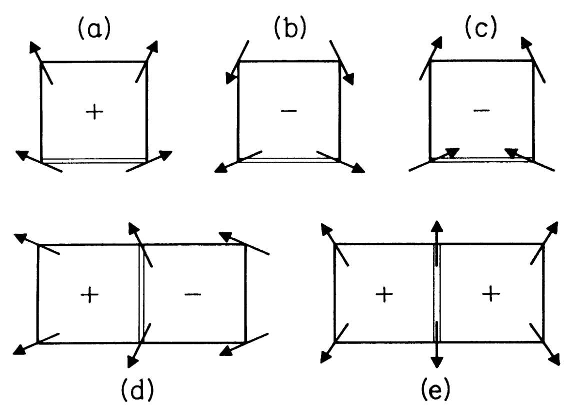

FIG. 1. Various spin configurations on frustrated plaquettes. A bold line represents a ferromagnetic bond while a double line represents an antiferromagnetic bond. The signs inside the plaquettes denote the sign of the local chirality.

chirality plays a crucial role in the ordering phenomenon.

In order to provide a concrete definition of chirality, consider an elementary plaquette α in the lattice consisting of four spins. The local chirality, κ_α, at a plaquette α, will be defined by the scalar

$$\kappa_\alpha = 2^{-3/2} \sum_{\langle ij \rangle^\alpha} \mathrm{sgn}(J_{ij}) \sin(\theta_i - \theta_j) , \tag{2}$$

where the summation runs over a directed contour of, say, clockwise orientation, along the sides of the plaquette. Note that κ_α is invariant under any global rotation of the spins whereas it changes sign under any global reflection $\theta_i \to 2\theta_0 - \theta_i$, where θ_0 specifies the axis of reflection. In any ground state of an unfrustrated plaquette one has $\kappa_\alpha = 0$, but in a ground state of an isolated frustrated plaquette, one has $\kappa_\alpha = +1$ or $\kappa_\alpha = -1$. In the examples in Fig. 1, the state (a) has a $+1$ chirality whereas the states (b) and (c) have $\kappa = -1$. In the ground state of two adjacent frustrated plaquettes, the local chiralities have opposite signs, as shown in Fig. 1(d). A lowest metastable excited state having both chiralities of the same sign is illustrated in Fig. 1(e); its energy lies $[(7/\sqrt{2}) - 4]J$ above the ground state (d). Roughly speaking this implies that the κ_α can be regarded, in this case, as Ising-like variables coupled with an effective antiferromagnetic interaction $J_I = [(7/2\sqrt{2}) - 2]J \simeq 0.47J$.

The chiral susceptibility for a spin glass is naturally defined by

$$\chi_\kappa = N^{-1} \sum_\alpha \sum_\beta [\langle \kappa_\alpha \kappa_\beta \rangle^2]_J , \tag{3}$$

where N is the total number of spins, $\langle \cdots \rangle$ denotes a thermal average while $[\cdots]_J$ indicates a configurational average over the bond distribution. This susceptibility should diverge when chiral ordering takes place. The spin-glass susceptibility may be defined in the usual way as

$$\chi_{\mathrm{SG}} = N^{-1} \sum_i \sum_j [\langle \mathbf{s}_i \cdot \mathbf{s}_j \rangle^2]_J . \tag{4}$$

In principle, there are several ways in which the spin and chiral components might order: They could both order at the same temperature or they might order separately. In the present model, there are strong indications from both Monte Carlo simulations[3] and a numerical domain-wall renormalization-group calculation[5] that the standard spin-glass ordering occurs only at zero temperature. In particular, Jain and Young[3] concluded from their simulation that the spin-glass susceptibility diverged at zero temperature as $\chi_{\mathrm{SG}} \propto T^{-\gamma}$ with exponent $\gamma = 1.80 \pm 0.05$. An interesting question, therefore, is whether chiral ordering occurs only at zero temperature, simultaneously with the spin-glass ordering, or, instead, at a finite temperature. In either case, the nature of the associated critical behavior is also of interest.

III. MONTE CARLO SIMULATIONS

In order to answer these questions, we have performed Monte Carlo simulations using the standard Metropolis method. Systems with periodic boundary conditions of sizes $N = L \times L$ with $L = 10$, 14, and 20 were studied. A total of t ($> 10^4$) Monte Carlo steps per spin (MCS/S) were generated in each run. The first t_0 MCS/S were discarded to ensure equilibration and the subsequent $t - t_0$ MCS/S were used to evaluate the chiral and the spin-glass susceptibilities via (3) and (4). At each temperature a total of from $t = 4 \times 10^4$ up to 3×10^5 MCS/S were generated with $10^4 \le t_0 \le 10^5$. The configurational average was taken over 20 samples for each temperature and lattice size. We could equilibrate the system for temperatures $T/J \geqq 0.25$ (in units with $k_B = 1$). The lowest temperature we could reach matches that attained by Jain and Young[3] but our overall sampling times were considerably longer than theirs.

Figure 2 exhibits the temperature and size dependences of the spin glass and the chiral susceptibilities, χ_{SG} and χ_κ, on a log-log plot. The data for χ_{SG} lie close to a straight line, which suggests a simple power-law divergence at zero temperature. The associated exponent is estimated as $\gamma = 1.9 \pm 0.1$, which is consistent with the estimate $\gamma = 1.80 \pm 0.05$ of Jain and Young.[3] On the other hand, χ_κ is much smaller and the data display a strong upward curvature which cannot reasonably be fitted by a straight line. Thus, even if the transition occurs at zero temperature, the effective exponent, $\gamma_\kappa^{\mathrm{eff}} = d(\ln \chi_\kappa)/d[(\ln T/J)]$, increases with decreasing temperature, at least in the investigated temperature range, $T \geqq 0.25J$.

In contrast to a standard Ising spin, the magnitude of the local chirality variable κ_α, defined in (2), varies with temperature to some extent: See Fig. 3(a). In order to allow for this short-range order effect in χ_κ and to make the correspondence with Ising spins closer, we define a reduced chiral susceptibility $\tilde{\chi}_\kappa$ by dividing χ_κ by the appropriate power of the magnitude of the local chirality:

$$\tilde{\chi}_\kappa = \chi_\kappa / \langle \kappa^2 \rangle^2, \ \langle \kappa^2 \rangle \equiv N^{-1} \sum_\alpha [\langle \kappa_\alpha^2 \rangle]_J . \tag{5}$$

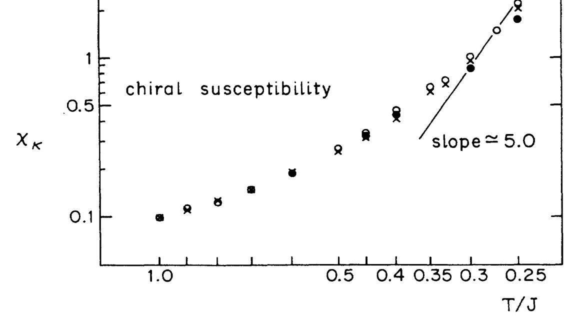

FIG. 2. Temperature dependence of the spin-glass susceptibility, χ_{SG}, and the chiral susceptibility, χ_κ, on a log-log plot for periodic $L \times L$ square lattices with $L = 10$, 14, and 20.

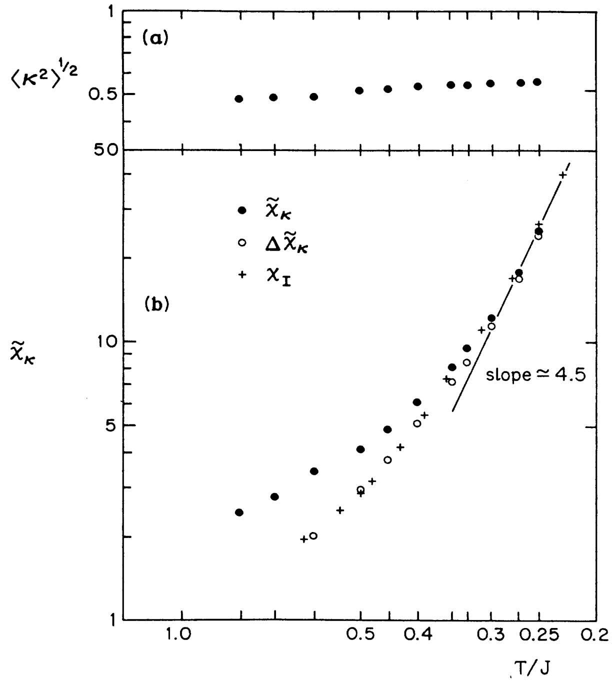

FIG. 3. (a) Variation of the rms single-plaquette chirality, $\langle\kappa^2\rangle^{1/2}$, defined in Eq. (5). (b) Behavior of the reduced chiral susceptibility $\tilde{\chi}_\kappa$, defined in Eq (5), for a 20×20 lattice (solid dots) and of the difference susceptibility $\Delta\tilde{\chi}_\kappa=\tilde{\chi}_\kappa(T)-\tilde{\chi}_\kappa(\infty)$ (open circles), compared with the spin-glass susceptibility χ_I obtained by Swendsen and Wang (Ref. 6) for a pure Ising spin glass with rescaled coupling $J_I=\frac{1}{4}J$ (crosses).

The results for the largest lattice size ($L=20$) are shown in Fig. 3(b). The data still cannot be fitted with a straight line: The effective exponent $\gamma_\kappa^{\mathrm{eff}}$ still increases markedly as T decreases. In the high-temperature limit, $\tilde{\chi}_\kappa$ approaches the value $\tilde{\chi}_\kappa(\infty)=\frac{5}{4}$. When $T\to\infty$, however, the system loses even short-range order and the physical meaning of chirality becomes obscure. Thus, it is reasonable to regard $\tilde{\chi}_\kappa(\infty)$ as a background and to examine $\Delta\tilde{\chi}_\kappa=\tilde{\chi}_\kappa(T)-\tilde{\chi}_\kappa(\infty)$ which is represented by the open circles in Fig. 3(b). It is interesting that both $\tilde{\chi}_\kappa$ and $\Delta\tilde{\chi}_\kappa$ yield almost the same effective exponent, namely $\gamma_\kappa^{\mathrm{eff}}\simeq4.5$, at the lowest temperatures studied. This value, and the overall behavior of $\Delta\tilde{\chi}_\kappa$ is, in fact, fairly insensitive to the $\langle\kappa^2\rangle^2$ factor; without this factor we would estimate $\gamma_\kappa^{\mathrm{eff}}\simeq5.0$. Of course, it is possible that $\gamma_\kappa^{\mathrm{eff}}$ increases further at temperatures $T<0.25J$ where we could not equilibrate the system because of the extremely slow relaxation processes.

It should be noticed, however, that the behavior of the chiral susceptibility found in Fig. 3 is quite similar to the behavior of the spin-glass susceptibility observed in the two-dimensional *Ising* spin glass. Thus, Swendsen and Wang[6] calculated the spin-glass susceptibility χ_I of the $\pm J$ Ising model on the square lattice, and also found that the effective exponent γ^{eff} increased as T fell. Furthermore, they estimated a limiting value $\gamma\simeq5.3$; this is reasonably close to our own low-temperature estimate $\gamma_\kappa^{\mathrm{eff}}\simeq4.5$, although this might well increase further at lower temperatures. To test the correspondence more closely we have plotted χ_I as obtained by Swendsen and Wang for the Ising spin glass, after a rescaling of the units of energy and temperature. The best fit to $\Delta\tilde{\chi}_\kappa$ is obtained by choosing J_I, the bond energy of the $\pm J$ Ising spin glass, as $J_I=\frac{1}{4}J$: See the crosses in Fig. 3(b).

The close similarity between χ_I and $\Delta\tilde{\chi}_\kappa$ is not entirely unexpected, because chirality is essentially an Ising-like variable. Indeed, Villain[1] showed that the chiral component in the present model is equivalent to a site-diluted Ising system with long-range, antiferromagnetic logarithmic Coulomb interactions, *provided* that the contribution of spin waves and thermally excited vortices can be neglected. When the effects of vortices are taken into account, the Coulombic interactions might be screened at large distances. This suggests that, although the two models are not completely equivalent, they share several basic ingredients, in particular the same symmetry and local frustration: This similarity seems to explain the observed resemblance of the chiral susceptibility of our *XY* spin-glass model to the spin-glass susceptibility of the pure Ising spin glass. Indeed, in some regularly frustrated *XY* models, a similar correspondence has also been observed. For example, for the *XY* model on the so-called odd lattice (in which bonds on every other row of a square lattice are antiferromagnetic while all other bonds are ferromagnetic), Monte Carlo simulations indicate that the chiral components have two-dimensional Ising-like critical properties.[4] The transition temperature for the odd lattice was estimated as $T_c\simeq0.45J$.[4] On comparison with the standard square-lattice Ising model this indicates an energy rescaling $J_I\simeq0.40J$. This is not so far from $J_I\simeq0.47J$ which we obtained by direct study of the twinned frustrated plaquettes in Fig. 1. In the full *XY* spin-glass model, the corresponding relation deduced from the fit in Fig. 3(b), is $J_I\simeq0.25J$. From a theoretical perspective this relation now seems very reasonable if one notes that the density of frustrated plaquettes in the fully random model is precisely one-half that in the fully frustrated odd lattice.

Although the preponderance of theory[7] now suggest that the pure Ising spin glass in two dimensions orders only at $T=0$, the Monte Carlo data alone cannot rule out a transition with $T_c>0$. Thus Swendsen and Wang reported[6] that their data were consistent with $T_c\simeq0.28J_I$. Likewise, our data for $\tilde{\chi}_\kappa$ in the *XY* spin glass can be fitted in the range $0.25J\leq T\leq0.50J$ to $C/[(T/T_c)-1]^\gamma$ with $T_c\simeq0.20J$, $\gamma\simeq1.0$, and $C\simeq6.2$. However, an exponential divergence at $T=0$ of the form $\tilde{\chi}_\kappa\approx C_0\exp[c_1(J/T)^\sigma]$ with $\sigma\simeq1.4$, $C_0\simeq1.4$, and $c_1\simeq0.42$ also provides a good fit in the range $0.25J<T<0.8J$. Thus while we cannot rule out chiral ordering in the *XY* spin glass at $T_c>0$ the similarity to the pure Ising spin glass certainly favors a transition only at $T_c=0$.

IV. DISCUSSIONS

Even if chiral ordering occurs only at $T=0$ in two dimensions, as we conclude from our study, chiral ordering at nonzero temperature might well occur *in three dimensions*. Thus it is now well established that the three-dimensional Ising spin glass with short-range interactions does have a nonzero transition temperature.[8] Although the close analogy which we have demonstrated in two dimensions between chiral and Ising spin variables is less precise, in three dimensions, because of additional geometrical constraints on the chirality distribution,[9] the basic analogy as regards symmetry and frustration should still hold. This suggests that chiral ordering should occur at nonzero temperature. On the other hand, several calculations suggest that normal spin-glass ordering occurs only at $T=0$ in three-dimensional XY spin glasses.[3,5] If so, the occurrence of chiral ordering at $T>0$ would mean that the ordered state was characterized by a broken reflection symmetry but with rotational symmetry preserved. The question of whether such an unusual phase really arises in three dimensions remains most interesting.

Finally, consider the possibility of chiral ordering in a Heisenberg spin glass.[10] In this case, at least three spins are necessary to define chirality in contrast to the XY case. One possible definition of local chirality is

$$\kappa = \det[\mathbf{s}_1,\mathbf{s}_2,\mathbf{s}_3] = \mathbf{s}_1\times\mathbf{s}_2\cdot\mathbf{s}_3 \ .$$

A Heisenberg spin glass can sustain chirality provided the spin directions in the ordered state are not confined to a common two-dimensional plane in the three-dimensional spin space. On the other hand, if the ordered-state spin configuration is contained in a two-dimensional subspace, there is no nontrivial, Ising-like chirality variable. A numerical study by Henley[10] suggested that the Heisenberg spin glass could sustain chirality. If this is so, essentially similar chiral ordering phenomena should be expected also in Heisenberg spin glasses, which might shed new light on the nature of the experimentally observed spin-glass transition.

ACKNOWLEDGMENTS

The authors are grateful to M. E. Fisher for discussions and for reading the manuscript; to D. A. Huse for his useful comments on techniques of data analysis; and to R. H. Swendsen and J. Wang for sending us their numerical data. Thanks are also due to M. A. Moore, C. L. Henley, and R. R. P. Singh for discussions. The numerical calculations were performed on the M280H computer at the Institute of Statistical Mathematics. This study was carried out under the Institute of Statistical Mathematics Cooperative Research Program (Contract No. 86-ISM CRP-24). One of the authors (H.K.) thanks the Nishina Memorial Foundation for financial support and the U.S. National Science Foundation for incidental support through the Condensed Matter Theory Program (under Grant No. DMR-87-01223).

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[1]J. Villain, J. Phys. C **10**, 4793 (1977).

[2]A preliminary account of the simulations was presented in H. Kawamura and M. Tanemura, J. Phys. Soc. Jpn. **54**, 4479 (1985).

[3]S. Jain and A. P. Young, J. Phys. C **19**, 3913 (1986).

[4]S. Teitel and C. Jayaprakash, Phys. Rev B **27**, 598 (1983).

[5]B. W. Morris, S. G. Colborne, M. A. Moore, A. J. Bray, and J. Canisius, J. Phys. C **19**, 1157 (1986).

[6]R. H. Swendsen and J. Wang, Phys. Rev. Lett. **57**, 2607 (1986).

[7]See, for example, D. A. Huse and I. Morgenstern, Phys. Rev. B **32**, 3032 (1985).

[8]A. J. Bray and M. A. Moore, J. Phys. C **17**, L463 (1984); Phys. Rev. B **31**, 631 (1985); W. L. McMillan, *ibid.* **30**, 476 (1984); **31**, 340 (1985); R. N. Bhatt and A. P. Young, Phys. Rev. Lett. **54**, 924 (1985); A. T. Ogielsky and I. Morgenstern *ibid.* **54**, 928 (1985); A. T. Ogielsky, Phys. Rev. B **32**, 7384 (1985); R. R. P. Singh and S. Chakravarty, Phys. Rev. Lett. **57**, 245 (1986).

[9]J. Villain, J. Phys. C **11**, 745 (1978).

[10]C. L. Henley, Ann. Phys. (N.Y.) **156**, 324 (1984); **156**, 368 (1984).