Chiral Ordering in Heisenberg Spin Glasses in Two and Three Dimensions

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The nearest-neighbor Heisenberg spin glass in two and three dimensions is studied by means of a $T=0$ domain-wall renormalization-group method with a focus on the chiral ordering. In $d=2$ dimensions, both the spin and chiral components order at zero temperature with different correlation-length exponents, while $d=3$ appears to be just above the lower critical dimension of the chiral component $d_l^{(c)}$, though the possibility that $d_l^{(c)}=3$ cannot be ruled out. A *chirality driven mechanism* is proposed as a new possible mechanism of experimentally observed spin-glass transitions.

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Frustration in vector spin systems often gives rise to the noncollinear or canted spin ordering. Such frustration-induced noncollinear spin structure is known to bear a discrete degeneracy, called *chirality* [1], where the noncollinear spin structure is either right or left handed. In *regularly* frustrated vector spin systems in three spatial dimensions such as stacked-triangular antiferromagnets and helimagnets, it has recently been recognized that a new type of symmetry associated with this chiral degeneracy leads to novel critical behavior which most probably lies in a new universality class, sometimes called *chiral universality class* [2]. Novel critical properties were also reported recently in the corresponding two-dimensional chiral spin systems [3].

In *randomly* frustrated vector spin systems such as XY and Heisenberg spin glasses, chirality is also expected to play an important role as was first suggested by Villain [1]. Although the study of chirality in vector spin glasses has been rather scarce so far, its potential importance in elucidating the nature of the spin-glass transition should be born in mind in view of its crucial importance in understanding the phase transition of regularly frustrated vector spin systems. Furthermore, one may also notice an interesting but hitherto unsuspected possibility that such an Ising-like chiral degree of freedom "hidden" in vector spin glasses might offer an entirely new perspective [4(a)] in understanding the yet incompletely solved issue concerning the nature of experimentally observed spin-glass transitions: Namely, although most of the real spin-glass materials are well approximated by an isotropic Heisenberg model, experimentally observed spin-glass transitions appear to be well described by an anisotropic *Ising* spin glass [5]. A puzzling point here is that no detectable sign of Heisenberg-to-Ising crossover has been observed in experiments which is usually expected to occur if the observed Ising-like critical behavior is caused by the weak magnetic anisotropy inherent to real spin glasses [5–7].

Recent numerical studies on the chirality ordering in an $(n=2)$-component XY spin glass have revealed interesting new features [4,8–10]. In two dimensions, Kawamura and Tanemura observed through a Monte Carlo simulation [4] and a domain-wall renormalization-group (DWRG) analysis [8] that the ordering tendency of chirality was much enhanced as compared with the original XY spin, although both the chirality and XY spin ordered at zero temperature. In fact, these authors claimed the existence of two distinct diverging length scales in this zero-temperature transition, the associated spin and chiral correlation-length exponents being $\nu=1.2\pm0.15$ and $\nu_\kappa=2.6\pm0.3$, respectively [8]. This rather unusual property was also observed by the recent Monte Carlo calculation by Ray and Moore, who found $\nu\simeq1.0$ and $\nu_\kappa\simeq2.0$ [9]. For a *three-dimensional XY* spin glass, Kawamura and Tanemura reported the evidence of a finite-temperature chiral-glass ordering without the conventional spin-glass order parameter [8]. The low-temperature phase is then an unusual "chiral phase" where a reflection symmetry is broken with a rotation symmetry being preserved.

By constrast, few calculations have been made on the chirality ordering of an $(n=3)$-component *Heisenberg* spin glass, a good zeroth-order approximation to real spin glasses. Numerical studies based on Monte Carlo (MC) simulations and DWRG methods were made by several authors for three-dimensional short-range Heisenberg spin glasses, with no particular attention to the chirality [6,11–13]. These authors agreed that the conventional spin-glass ordering occurred only at zero temperature, but very little is known about its chiral ordering [14].

In the present Letter, I investigate the random $\pm J$ and Gaussian Heisenberg models at zero temperature in both two and three dimensions based on a numerical DWRG method, with a focus on its *chiral ordering*. The model is the nearest-neighbor classical Heisenberg model on a $(d=2)$-dimensional square and a $(d=3)$-dimensional simple cubic lattice defined by

$$\mathcal{H}=-\sum_{\langle ij\rangle}J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j\,, \tag{1}$$

where $\mathbf{S}_i$ is a three-component unit vector and the sum runs over all nearest-neighbor pairs. The J_{ij} are independent random variables either with the binary distribution taking the values $+J$ and $-J$ with equal probability, or with the Gaussian distribution with zero mean and the variance J.

The local chirality κ_i may be defined by the scalar

[4(a),6]

$$\kappa_i = \mathbf{S}_{i+\delta_1} \cdot (\mathbf{S}_i \times \mathbf{S}_{i+\delta_2}) , \tag{2}$$

where $i+\delta_1$ and $i+\delta_2$ denote two distinct nearest-neighbor sites of the site i. Note that the scalar chirality defined by Eq. (2) is *cubic* in the original spin variables, in contrast to the chirality for the XY spins which is *quadratic* in the spins. Note also that the chirality is a pseudoscalar in the sense that it is invariant under global spin rotation but changes its sign under global spin reflection (or inversion which can be viewed as a combination of reflection and rotation). Evidently, chiral order can be regarded as a manifestation of the breaking of the reflection symmetry.

In the standard DWRG method [7(a),11,12], the domain-wall energy for a given sample of linear dimension L is defined as a difference between the two ground-state energies for periodic and antiperiodic boundary conditions. Usually, the variance of the distribution of this energy difference over samples, $W(L) = [\epsilon^2]_J^{1/2}$ with $\epsilon \equiv E_{\mathrm{P}} - E_{\mathrm{AP}}$, is taken as a measure of the averaged domain-wall energy, where E_{P} and E_{AP} are the total ground-state energies for periodic and antiperiodic boundary conditions, respectively, and $[\cdots]_J$ denotes a bond average. When $W(L)$ behaves as $W(L) \propto L^{-y}$ for $L \gg 1$, either positive or negative y is associated with a zero-temperature or a finite-temperature phase transition, respectively. If the transition occurs at zero temperature ($y > 0$), in particular, the associated correlation-length exponent ν is expected to be determined via the relation $\nu = 1/y$.

In the case of an XY spin glass, the application of antiperiodic boundary conditions does not cause the flipping of chirality [8]. In the Heisenberg case, by contrast, the application of antiperiodic boundary conditions causes the flipping of chirality and introduces a *chiral domain wall* into the sample, in addition to the conventional *spin domain wall* which accompanies a continuous rotation of spins. Thus, in the Heisenberg case, even the standard domain-wall energy should include the contributions of both the chiral and the spin domain wall. If so, the observation of a zero-temperature transition in Refs. [11] and [12] seems to exclude the possibility of a finite-temperature chiral ordering either in two or three dimensions. However, since the investigated lattice sizes were rather small, there remains a possibility that the contribution of the chiral domain wall was masked by that of the spin domain wall in Refs. [11] and [12].

In order to detect the contribution of the chiral domain wall in a Heisenberg spin glass more directly, I introduce two new types of boundary conditions: One is "reflection boundary conditions" in which boundary spins are reflected with respect to a fixed plane in the spin space, say the x-y plane, as $\mathbf{S}_i \rightarrow (S_i^x, S_i^y, -S_i^z)$; the other is "rotation boundary conditions" in which boundary spins are rotated by 180° around a fixed axis in the spin space, say the z axis, as $\mathbf{S}_i \rightarrow (-S_i^x, -S_i^y, S_i^z)$. In practice, I impose reflection (or rotation) boundary conditions in one direction and periodic boundary conditions in the remaining $d-1$ directions. Evidently, reflection boundary conditions accompany the flipping of chirality and introduce a chiral domain wall into the sample, whereas rotation boundary conditions do not. Thus, the difference between the ground-state energies for reflection and rotation boundary conditions, $\epsilon_c = E_{\mathrm{ref}} - E_{\mathrm{rot}}$, should contain the contribution of the chiral domain wall.

The advantage of using ϵ_c instead of ϵ defined above as a measure of the chiral domain wall is that the contribution of the spin domain wall is more or less canceled in ϵ_c. The reason is the following: It is found that the ground-state energy for reflection (or rotation) boundary conditions is somewhat lower than that for periodic (or antiperiodic) boundary conditions, namely, one has $[E_{\mathrm{ref}}]_J = [E_{\mathrm{rot}}]_J < [E_{\mathrm{P}}]_J = [E_{\mathrm{AP}}]_J$. This energy difference should be attributed to the contribution of the spin domain wall, since no chirality flipping occurs between reflection and antiperiodic boundary conditions (or between rotation and periodic boundary conditions). This means that the application of reflection or rotation boundary conditions releases the spin domain wall. Roughly speaking, both reflection and rotation boundary conditions tend to bring on the spin-domain-wall off states, while periodic (antiperiodic) boundary conditions tend to bring on the spin-domain-wall on/off (off/on) state with equal probability. Consequently by considering $[E_{\mathrm{rot}}]_J$ and $[E_{\mathrm{ref}}]_J$ instead of $[E_{\mathrm{P}}]_J$ and $[E_{\mathrm{AP}}]_J$ the contribution of the spin domain wall is canceled in ϵ_c.

As a measure of the spin domain wall, I adopt the energy difference between the periodic and rotation boundary conditions, $\epsilon_s = E_{\mathrm{P}} - E_{\mathrm{rot}}$, since by this definition the contribution of the chiral domain wall is expected to be canceled. Finally, the chiral- and spin-domain-wall energies averaged over samples, W_c and W_s, are defined by the variance

$$W_{c,s}(L) = [(\epsilon_{c,s} - [\epsilon_{c,s}]_J)^2]_J^{1/2} . \tag{3}$$

Concerning the corresponding odd quantities, one expects from the above discussion that $[\epsilon_c]_J$ should vanish while $[\epsilon_s]_J$ should exhibit the scaling behavior of the spin domain wall. These requirements may be used as a check of consistency.

The lattice sizes studied are $L = 4$–14 at $d = 2$, and $L = 3$–6 at $d = 3$. Sample averages are taken over 50000 ($L = 4$), 10000 ($L = 6$), 5000 ($L = 8, 10, 12$), and 3000 ($L = 14$) independent bond realizations at $d = 2$, and 50000 ($L = 3$), 30000 ($L = 4$), 4000 ($L = 5$), and 3000 ($L = 6$) at $d = 3$. The ground-state energy is estimated by repeating a spin-quench algorithm many times [7(a),8]. In fact, I have made 5 ($L = 4, 6$), 10 ($L = 8$), 20 ($L = 10$), 30 ($L = 12$), and 100 ($L = 14$) trials for each sample at $d = 2$, and 5 ($L = 3, 4$), 40 ($L = 5$), and 100 ($L = 6$) trials at $d = 3$.

The L dependence of the calculated W_s and W_c is displayed in Figs. 1(a) and 1(b) in each case of $d=2$ and $d=3$. In $d=2$ dimensions, both W_s and W_c are found to be iterated toward weak coupling for both kinds of bond distributions, indicating that both the spin and chirality exhibit a zero-temperature transition. Indeed, the data for W_s lie on a straight line reasonably well at $10 \leq L \leq 14$ with a slope $y \simeq 0.83$ ($\pm J$) or $y \simeq 1.05$ (Gaussian), while the data for W_c lie on a straight line reasonably well at $8 \leq L \leq 14$ with a slope $y \simeq 0.48$ ($\pm J$) or $y \simeq 0.47$ (Gaussian). The result clearly indicates that the Heisenberg spin and chirality bear mutually different correlation-length exponents at the zero-temperature transition; namely, one has $\nu = 1/y = 1.2 \pm 0.15$, $\nu_\kappa = 1/y_\kappa = 2.1 \pm 0.2$ for the $\pm J$ distribution, and $\nu = 1.0 \pm 0.15$, $\nu_\kappa = 2.1 \pm 0.2$ for the Gaussian distribution. Concerning the corresponding odd quantities, $[\epsilon_c]_J$ is found to vanish within the error bar, while the scaling plot for $[\epsilon_s]_J$ (not shown here) yields $y \simeq 0.99$ for both bond distributions, consistent with the values obtained above from the variance. The present estimates for the standard spin-glass correlation-length exponent ν are considerably larger than the previous DWRG estimate for the Gaussian distribution, $\nu = 0.714 \pm 0.015$ [12], but close to the Migdal-Kadanoff RG estimate, $\nu \simeq 1.08$ [7(a)], and to the estimates for the two-dimensional XY spin glass, $\nu = 1.09 \pm 0.05$ (DWRG, Gaussian) [7(a)], $\nu = 1.2 \pm 0.2$ (DWRG, $\pm J$) [8], and $\nu = 1.0 \pm 0.06$ (MC, $\pm J$ and Gaussian) [9]. On the other hand, the estimate for ν_κ is new and is rather close to the corresponding value for the XY spin glass [8,9].

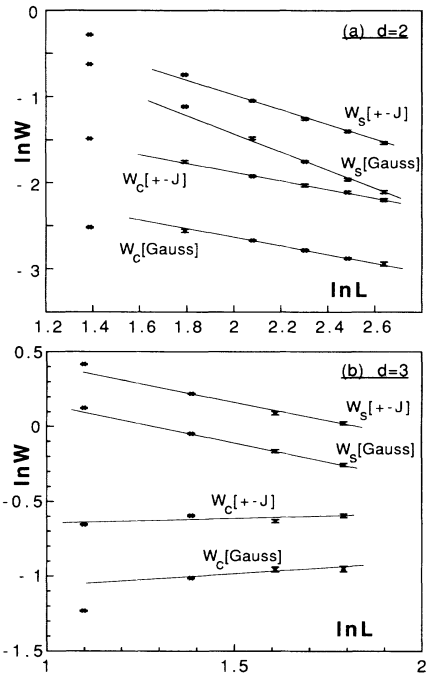

FIG. 1. L dependence of the spin-domain-wall energy W_s and of the chiral-domain-wall energy W_c on a log-log plot for the nearest-neighbor Heisenberg spin glass (a) on a $L \times L$ square lattice and (b) on a $L \times L \times L$ simple cubic lattice, for both the $\pm J$ and Gaussian bond distributions. The error bar on each point is one σ associated with sample average.

In the $d=3$ case, W_s is iterated toward weak coupling for both kinds of bond distributions, which indicates that an ordinary spin-glass ordering occurs only at zero temperature consistent with a common belief. Indeed, the data for W_s lie on a straight line reasonably well at $4 \leq L \leq 6$ with a slope $y \simeq 0.49$ ($\pm J$) or $y \simeq 0.51$ (Gaussian), yielding the correlation-length exponent $\nu = 2.0 \pm 0.2$ for both bond distributions. Concerning the odd quantities, $[\epsilon_c]_J$ is found to vanish within the error bar as expected, while the scaling plot for $[\epsilon_s]_J$ yields $y \simeq 0.46$ ($\pm J$) or $y \simeq 0.36$ (Gaussian) though the data are rather noisy in this case. The present estimate for ν is again somewhat larger than the previous numerical estimates by other authors; $\nu = 1.54 \pm 0.19$ (DWRG, Gaussian) [12], $\nu \simeq 1.14$ (MC, Gaussian) [6], and $\nu = 1.35 \pm 0.05$ (MC, $\pm J$) [13], but come rather close to the Migdal-Kadanoff RG value, $\nu \simeq 2.3$ [7(a)], and the DWRG estimates for the three-dimensional XY spin glass, $\nu = 2.2 \pm 0.05$ (Gaussian) [7(a)] and $\nu = 2.4 \pm 0.3$ ($\pm J$) [8].

By contrast, one finds nearly marginal behavior for the chiral-domain-wall energy. In the $\pm J$ case, the calculated W_c shows only weak size dependence except for a small even-odd effect. The straight-line fit to the data yields a slope $y_\kappa \simeq -0.07$ which is slightly negative but is fairly close to zero. In the Gaussian case, W_c appears to be iterated toward strong coupling for very small lattices, although nearly marginal behavior reminiscent of the one observed in the $\pm J$ case is found for larger lattices. The straight-line fit to the data at $4 \leq L \leq 6$ yields $y_\kappa \simeq 0.15$, and the one at $5 \leq L \leq 6$ yields $y_\kappa \simeq -0.03$. Thus, I conclude that $d=3$ is close to the lower critical dimension (LCD) of the chiral component. The occurrence of a chiral-glass transition at a low but finite temperature seems to be favored from the data, although in view of the smallness of the obtained $|y_\kappa|$ values the possibility of a zero-temperature transition with the exponentially diverging chiral correlation length, $\xi_\kappa \sim \exp(A/T^\theta)$, cannot be ruled out. It should also be noticed here that, even if a short-range Heisenberg spin glass might not exhibit a finite-temperature chiral ordering, the corresponding long-range RKKY spin glass may well exhibit one.

In view of the observations that the chirality in various chiral spin systems often behaves like an Ising variable [3,4,8,10], it seems not so unreasonable to expect that the exponents associated with a possible finite-temperature chiral-glass transition are close to, if not completely identical with, the 3D Ising spin-glass exponents. Then, it would not be so premature to give the following conjecture on the nature of experimentally observed spin-glass transitions: *Spin-glass transition in canonical spin*

glasses might essentially be chirality driven. Of course, if the experimental system were completely isotropic without any magnetic anisotropy, a finite-temperature chiral ordering, if any, would not be detectable by measuring the conventional nonlinear susceptibility since the chiral ordering in an isotropic system does not accompany the divergence of the standard spin-glass susceptibility. However, in the presence of weak magnetic anisotropy, the situation could be different since such anisotropy could "mix" the spin and chirality degrees of freedom which were separated by symmetry in a fully isotropic case. Then, the chiral-glass transition, which is hidden in the chirality in the absence of magnetic anisotropy, might manifest itself in the divergence of the conventional spin-glass susceptibility through the coupling between the spin and chirality generated by the weak magnetic anisotropy.

Note that such a picture can immediately explain the reason why Heisenberg-to-Ising crossover is not observed in experiments, because even in a fully isotropic case an "Ising-like" behavior already exists over a wide temperature range but only hidden in the chirality. As one switches on the magnetic anisotropy D, the amplitude of the Ising-like singularity in the nonlinear susceptibility would increase from zero. If the chiral ordering in an isotropic system takes place at a finite temperature, the transition temperature T_{SG} in the presence of weak magnetic anisotropy would behave as $T_{SG}(D) \to T_{SG}(0) > 0$ as $D \to 0$, while if $d=3$ is just at the LCD of the chiral component, it would behave as $T_{SG}(D) \propto J/[\ln(J/D)]^{1/\theta}$. The predicted anisotropy dependence of T_{SG} is distinct from the ones given in Ref. [7], and may be testable by careful experiments or numerical simulations.

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