Nature of the Ordering in the Three-Dimensional *XY* Spin Glass

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Spin and chirality orderings of a three-dimensional *XY* spin glass are studied by extensive Monte Carlo simulations. By calculating an appropriately defined spin-overlap distribution function, we show that the finite-temperature chiral-glass transition does not accompany the standard spin-glass order, giving support to the spin-chirality decoupling picture. Critical behavior of the chiral-glass transition turns out to be different from that of the Ising spin glass. The chiral-glass ordered state exhibits a one-step-like peculiar replica-symmetry breaking.

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Considerable attention has recently been paid to the ordering of the *XY* spin-glass (SG) model with two-component vector spins. The reason for such interest is probably twofold. First, the *XY* SG has found experimental realizations, not only in SG magnets with an easy-plane-type anisotropy, but also in ceramic high-T_c superconductors with the d-wave pairing symmetry which can be regarded as a random Josephson network [1]. Recently, the latter system has been studied extensively [2–5], and the *XY* SG is expected to serve as a reference model in interpreting the experimental data.

The second reason for interest in this model is more conceptual. Namely, this model is the simplest realization of the random and frustrated models with *vector* internal (or spin) degrees of freedom. Ever since the pioneering work of Villain [6], this type of model has been known to sustain nontrivial "chiral" degrees of freedom corresponding to the sense of the noncollinear ordered-state structure stabilized by frustration. The ongoing controversy is mainly concerned with how the spin and the chirality order in such chiral systems.

Earlier numerical studies suggested that the *XY* SG in less than four dimensions did not exhibit any finite-temperature transition [7,8]. In a series of papers on the *XY* SG in two and three dimensions, however, Kawamura and Tanemura observed a novel possibility arguing that the chirality associated with Z_2 spin reflection was "decoupled" from the spin associated with SO(2) spin rotation on sufficient long length and time scales (spin-chirality decoupling) [9–11]. More specifically, they claimed that, in two dimensions (2D), while both the spin and the chirality order simultaneously at zero temperature, the associated spin and chirality correlation-length exponents are mutually different, i.e., $\nu_s \simeq 1$ for the spin and $\nu_\kappa \simeq 2$ for the chirality [9,10]. In 3D, they suggested the occurrence of a novel chiral-glass transition at a finite temperature, where only the chirality exhibited a glassy long-range order (LRO) without the conventional SG order [10,11].

For the 2D *XY* SG, the general concept of such a spin-chirality decoupling was recently challenged. Kosterlitz and Akino claimed on the basis of their numerical domain-wall renormalization-group (DWRG) calculation that the spin- and chiral-correlation-length exponents at the $T = 0$ transition are common, i.e., $\nu_s = \nu_\kappa \simeq 2.7$ [12], while Ney-Nifle and Hilhorst made an analytical argument for a certain 2D *XY* model that the equality $\nu_s = \nu_\kappa$ should hold [13]. By contrast, direct Monte Carlo simulations on the 2D *XY* SG have invariably suggested $\nu_\kappa \simeq 2 > \nu_s \simeq 1$, apparently supporting the spin-chirality decoupling picture [14–17].

In 3D, Granato recently suggested on the basis of a dynamical simulation of the $\pm J$ *XY* model that the spin and the chirality order simultaneously at $T \simeq 0.4J$ with $\nu_s = 1.2(4)$ [18]. This observation might indicate the absence of the spin-chirality decoupling in 3D. Meanwhile, on the basis of a numerical DWRG calculation, Maucourt and Grempel suggested that the SG order might occur at a nonzero temperature *below* the chiral-glass transition temperature, i.e., $0 < T_{\mathrm{SG}} < T_{\mathrm{CG}}$ [19].

The purpose of the present Letter is to make further extensive Monte Carlo (MC) simulations on the 3D *XY* SG to clarify some of the issues concerning this model. Our main goal here is twofold. First, we wish to study the controversial issue mentioned above, i.e., whether the chiral-glass order accompanies the standard SG order or not. Second, we study whether the ordered state of the 3D *XY* SG, either the chiral-glass or the spin-glass, accompanies the replica-symmetry breaking (RSB), and if so, reveals its nature. We have found strong numerical evidence that the chiral-glass transition does not accompany the standard SG order, and that the chiral-glass state exhibits a one-step-like peculiar RSB.

The model we consider is the 3D *XY* (plane rotator) model, defined by the Hamiltonian

$$\mathcal{H} = -\sum_{\langle ij \rangle} J_{ij} \vec{S}_i \cdot \vec{S}_j = -\sum_{\langle ij \rangle} J_{ij} \cos(\theta_i - \theta_j), \quad (1)$$

where $\vec{S}_i$ is the two-component unit vector at the ith site on a 3D simple cubic lattice, while the nearest-neighbor random coupling J_{ij} is assumed to take either the value J or $-J$ with equal probability ($\pm J$ distribution). The local chirality may be defined at each elementary plaquette α of the lattice by

$$\kappa_\alpha = (1/2\sqrt{2}) \sum_{\langle ij \rangle} \mathrm{sgn}(J_{ij}) \sin(\theta_i - \theta_j), \qquad (2)$$

where the summation is taken over four bonds surrounding the plaquette α in a clockwise direction. The chirality is a pseudoscalar invariant under the SO(2) spin rotation, but changes its sign under Z_2 spin reflection.

Using the temperature-exchange MC method [20], we have performed a large-scale MC simulation superseding the previous simulations [8,11]. Equilibration is checked by monitoring the convergence of physical quantities as in Ref. [21], while, for a subset of samples, the stability of the result is checked by making longer runs and by adding more temperature points in the higher temperature regime. By running two independent sequences of systems (replicas 1 and 2) in parallel, we compute a scalar chiral overlap q_κ between the chiralities of the two replicas by $q_\kappa = \frac{1}{3N} \sum_\alpha \kappa_\alpha^{(1)} \kappa_\alpha^{(2)}$, as well as a spin-overlap tensor $q_{\mu\nu}$ between the μ and ν ($\mu, \nu = x, y$) components of the spin by $q_{\mu\nu} = \frac{1}{N} \sum_i S_{i\mu}^{(1)} S_{i\nu}^{(2)}$. Then, in terms of these overlaps, we calculate the Binder ratios of the chirality g_κ, and of the XY spin g_s, defined in the standard manner: See Refs. [11,22] for a detailed definition. The lattice sizes studied are $L = 6, 8, 10, 12$, and 16 with periodic boundary conditions. Sample average is taken over 1500 ($L = 6$), 1200 ($L = 8$), 640 ($L = 10$), 296 ($L = 12$), and 136 ($L = 16$) independent bond realizations.

As can be seen from Fig. 1(a), the Binder ratio of the chirality g_κ exhibits a negative dip which, with increasing L, tends to deepen and shift toward lower temperature. Furthermore, g_κ of various L cross at a temperature slightly above the dip temperature T_{dip} *on the negative side of* g_κ, eventually merging at temperatures lower than T_{dip}. We note that the observed behavior of g_κ is similar to the one recently observed in the 3D Heisenberg SG [22]. As argued in Ref. [22], the persistence of a negative dip and the crossing occurring at $g_\kappa < 0$ is strongly suggestive of a finite-temperature chiral-glass transition at which $g_\kappa(T_{\mathrm{CG}}^-)$ and $g_\kappa(T_{\mathrm{CG}})$ take a *negative* value in the $L \to \infty$ limit. In the inset of Fig. 1(a), we plot the negative-dip temperature $T_{\mathrm{dip}}(L)$ versus $1/L$. The data lie on a straight line fairly well, and its extrapolation to $1/L = 0$ gives an estimate of the bulk chiral-glass transition temperature $T_{\mathrm{CG}}/J \sim 0.41$. [More precisely, $T_{\mathrm{CG}}(L)$ should scale with L^{1/ν_κ} where ν_κ is the chiral-glass correlation-length exponent. As shown below, our estimate of $\nu_\kappa \simeq 1.2$ comes close to unity, more or less justifying the linear extrapolation employed here. Extrapolation with respect to $L^{1/1.2}$ yields $T_{\mathrm{CG}}/J \sim 0.38$.] Our present estimate of T_{CG} is somewhat higher than the previous estimate of Ref. [11], but is in agreement with the estimate of Ref. [18]. In Ref. [11], T_{CG} was determined as a point where g_κ appeared to merge on the positive side of g_κ, yielding an estimate $T_{\mathrm{CG}} = 0.32(3)$. However, since

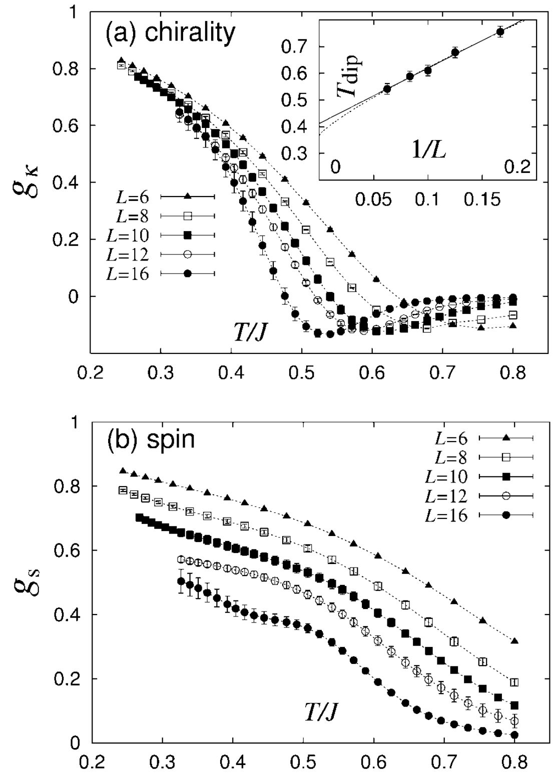

FIG. 1. The temperature and size dependence of the Binder ratios of the chirality (a), and of the spin (b). Inset of (a) displays the negative-dip temperature versus $1/L$. The solid and broken lines are the best fits assuming the $1/L$ and $1/L^{1/1.2}$ dependence, respectively.

the merging of $g_\kappa(L)$ develops very slowly with L, it is not easy to precisely locate the merging point and we believe our present estimate of T_{CG} is more reliable than that of Ref. [11].

In sharp contrast to g_κ, the Binder ratio of the XY spin g_s decreases monotonically toward zero with increasing L, without a negative dip or a crossing, suggesting that XY spin remains disordered even below T_{CG}.

We also calculate the chirality autocorrelation function defined by

$$C_\kappa(t) = \frac{1}{3N} \sum_\alpha [\langle \kappa_\alpha(t_0) \kappa_\alpha(t + t_0) \rangle], \qquad (3)$$

where $\langle \cdots \rangle$ and $[\cdots]$ represent the thermal average and the sample average, respectively. MC simulation is performed here according to the standard Metropolis updating. The starting spin configuration at $t = t_0$ is taken from the equilibrium spin configurations generated in our exchange MC runs. The result, shown in Fig. 2 on a log-log plot, suggests that the chiral-glass transition occurs at $T/J = 0.39(3)$, in agreement with the above estimate. Below $T = T_{\mathrm{CG}}$, $C_\kappa(t)$ shows an upward curvature indicating that the chiral-glass state has a rigid LRO characterized by a finite chiral Edward-Anderson order parameter $q_{\mathrm{CG}}^{\mathrm{EA}} > 0$. In order to see the possible finite-size effect in

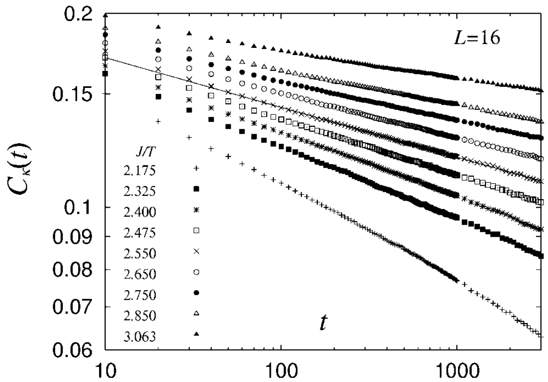

FIG. 2. Log-log plot of the time dependence of the equilibrium chirality autocorrelation function for $L = 16$ at several temperatures. The best straight-line fit of the data, represented by the solid line, is obtained at $T/J \sim 0.39$ with a slope ~ 0.077.

our estimate of $T_{\rm CG}$, we also take a limited amount of data for $L = 20$ (30 samples only) for comparison, and have checked that the present estimate of $T_{\rm CG}$ is indeed stable.

With setting $T_{\rm CG}/J = 0.39$ as determined above, we perform the standard finite-size scaling of the chiral-glass order parameter $[\langle q_\kappa^2 \rangle]$ and of the chiral autocorrelation function, to estimate various chiral-glass exponents. We then get $\nu_\kappa = 1.2(2)$, $\eta_\kappa = 0.15(20)$, $z_\kappa = 7.4(10)$. As compared with the estimates of Ref. [11], $\nu_\kappa \sim 1.5$ and $\eta_\kappa \sim -0.4$, η_κ is considerably larger, mostly due to the difference in the estimated $T_{\rm CG}$ values. We note that the present ν_κ and η_κ values are clearly different from those of the standard 3D Ising SG, suggesting that the chiral-glass transition lies in a universality class different from the Ising class.

The observed deviation from the Ising behaviors, not only in the critical properties but also in g_κ, is likely to arise from the long-range nature of the chirality-chirality interaction [6]. Indeed, in case of the 3D *XY* SG *coupled to fluctuating gauge fields* where the chirality-chirality interaction becomes *short ranged* due to screening, the exponents turn out to be close to the standard 3D Ising SG values and the negative dip in g_κ is absent, in sharp contrast to the present results [23].

In order to probe the possible RSB in the chiral-glass ordered state, we display in Fig. 3(a) the distribution function of the chiral-overlap defined by $P(q'_\kappa) = [\langle \delta(q_\kappa - q'_\kappa) \rangle]$ at $J/T = 2.95$ well below $T_{\rm CG}$. The existence of a growing "central peak" at $q_\kappa = 0$ for larger L, in addition to the standard "side peaks" corresponding to $\pm q_{\rm CG}^{\rm EA}$, suggests the occurrence of a one-step-like peculiar RSB in the chiral-glass ordered state. Similar behavior was recently observed in the chiral-glass state of the 3D Heisenberg SG [22]. The existence of a negative dip in the Binder ratio g_κ is fully consistent with the occurrence of such a one-step-like RSB [24].

We next turn to the spin-overlap distribution. While the spin-overlap distribution is originally defined in the four-component tensor space, we introduce here the

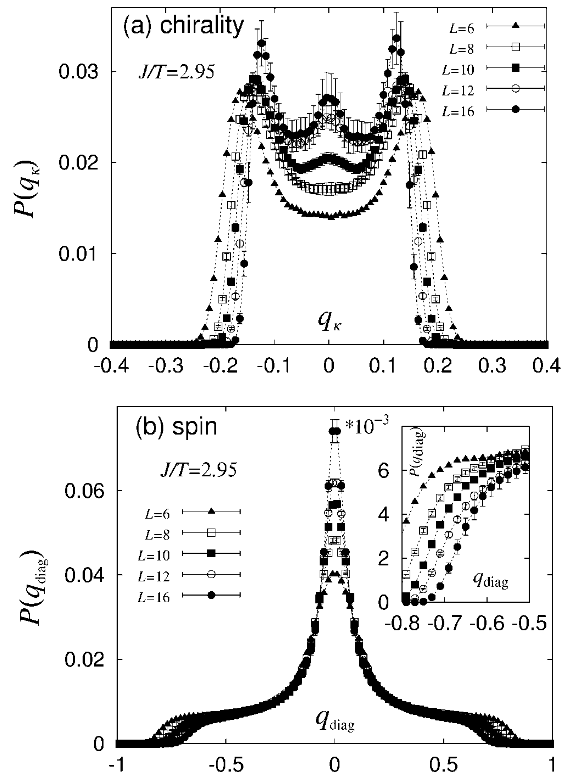

FIG. 3. Chiral-overlap distribution function (a), and diagonal spin-overlap distribution function (b), at $J/T = 2.95$ well below $T_{\rm CG}$. Inset of (b) is a magnified view of the shoulder part of $P(q_{\rm diag})$.

projected distribution function defined in terms of the "diagonal" overlap which is the trace (diagonal sum) of $q_{\mu\nu}$'s, $q_{\rm diag} = \sum_\mu q_{\mu\mu} = \frac{1}{N}\sum_i \vec{S}_i^{(1)} \cdot \vec{S}_i^{(2)}$. The distribution function $P(q_{\rm diag})$ is symmetric with respect to $q_{\rm diag} = 0$. In the high-temperature phase, each $q_{\mu\nu}$ is expected in the $L \to \infty$ limit to be Gaussian distributed around $q_{\mu\nu} = 0$, and so is $q_{\rm diag}$. Now, let us hypothesize that there exists a *spin*-glass ordered state with a nonzero Edwards-Anderson SG order parameter $q_{\rm SG}^{\rm EA} > 0$. Reflecting the fact that $q_{\rm diag}$ transforms nontrivially under independent O(2) rotations on the two replicas, even a self-overlap has nontrivial weights in $P(q_{\rm diag})$ other than at $\pm q_{\rm SG}^{\rm EA}$. In the $L \to \infty$ limit, the self-overlap part of $P(q_{\rm diag})$ should be given by

$$P(q_{\rm diag}) = \frac{1}{2}\,\delta(q_{\rm diag}) + \frac{1}{2\pi}\,\frac{1}{(q_{\rm SG}^{\rm EA})^2 - q_{\rm diag}^2}. \qquad (4)$$

The derivation is straightforward: When the two (essentially identical) ordered states in the two replicas are connected via a *proper* global rotation of the rotation-angle Θ, the diagonal overlap is given by $q_{\rm diag} = q_{\rm SG}^{\rm EA}\cos\Theta$. Uniformly distributed Θ then gives the second term of Eq. (4). When the two ordered states are connected via an *improper* global rotation, the diagonal overlap can be given by $q_{\rm diag} = q_{\rm SG}^{\rm EA}\sum_i \cos(2\alpha - 2\theta_i^{(1)})/N$, where α is an angle of the reflection axis with respect to the x axis in spin space, and $\theta_i^{(1)}$ denotes the direction of the ith spin in replica 1. Since spins should be oriented randomly on long length scale in the SG ordered state, $q_{\rm diag}$ given above should vanish in the $L \to \infty$ limit for arbitrary α, contributing a delta function at $q_{\rm diag} = 0$, the first term of Eq. (4). If the SG ordered state hypothesized here accompanies RSB, the associated nontrivial contribution would be added to the one given by Eq. (4). In any case, an important observation here is that, as long as the ordered state possesses a finite SG LRO, the diverging peak should arise in $P(q_{\rm diag})$ at $q_{\rm diag} = \pm q_{\rm SG}^{\rm EA}$, irrespective of the occurrence of the RSB.

We show in Fig. 3(b) the calculated $P(q_{\rm diag})$ at $J/T = 2.95$, well below $T_{\rm CG}$. The calculated $P(q_{\rm diag})$ exhibits symmetric shoulders at nonzero values of $q_{\rm diag}$, but as shown in the inset, these shoulders get suppressed with increasing L, *not showing a divergent behavior.* We also calculate $P(q_{\rm diag})$ up to a still lower temperature $J/T = 7$, though only for smaller lattices $L = 4, 6, 8$, to observe an essentially similar behavior. Hence, we conclude that the chiral-glass ordered state does not accompany the standard SG order with nonzero $q_{\rm SG}^{\rm EA}$, at least up to temperatures $\approx T_{\rm CG}/3$. No evidence of the successive chiral and spin transitions suggested in Ref. [19] was found. Strictly speaking, the observed suppression of the shoulder is still not inconsistent with the Kosterlitz-Thouless(KT)-like critical ordered state. However, such a critical SG ordered state is not supported by our data of g_s in Fig. 1(b). Furthermore, the *spin*-glass exponent reported in Ref. [18] assuming the simultaneous spin and chiral transition, $\nu_s = 1.2(4)$, is far from the lower-critical-dimension value, $\nu = \infty$, generically expected in such a KT transition.

Finally, we refer to the possible cause why simultaneous spin and chiral orderings were apparently observed in certain numerical simulations. We believe this to be related to the length and time scale of measurements. We stress that the spin-chirality decoupling is a long-scale phenomenon: At short scale, the chirality is never independent of the spin by its definition, roughly being its squared. Hence, the behavior of the spin-correlation related quantities, including the SG order parameter which is a summed correlation, might reflect the critical singularity associated with the chirality up to a certain length and time scale. If so, apparent, *not true*, "spin-glass exponents" at $T = T_{\rm CG}$ would be $\nu_s' \sim \nu_\kappa \sim 1.2$ and $\eta_s' \sim -0.4$, the latter being derived from the short-scale relation, $1 + \eta_\kappa \sim 2(1 + \eta_s')$. However, such a disguised criticality in the spin sector is only a short-scale phenomenon, not a true critical phenomenon. The length and time scales above which the spin-chirality separation becomes evident in correlations should roughly be given by the (finite) SG correlation length and correlation time at $T = T_{\rm CG}$. We estimate these scales roughly of order 10 lattice spacings and some 10^5 MC time steps (in the standard Metropolis dynamics). Meanwhile, the reason why the spin-chirality decoupling looks evident already for smaller lattices in other types of quantities such as $P(q_{\rm diag})$ and g_s remains to be understood.

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