Dynamical Simulation of Spin-Glass and Chiral-Glass Orderings in Three-Dimensional Heisenberg Spin Glasses

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Spin-glass and chiral-glass orderings in three-dimensional Heisenberg spin glasses are studied with and without random magnetic anisotropy by dynamical Monte Carlo simulations. In the isotropic case, clear evidence of a finite-temperature chiral-glass transition is presented. While the spin autocorrelation exhibits only an interrupted aging, the chirality autocorrelation persists to exhibit a pronounced aging effect reminiscent of the one observed in the mean-field model. In the anisotropic case, asymptotic mixing of the spin and the chirality is observed in the off-equilibrium dynamics. [S0031-9007(98)06365-0]

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Recently, there arose a growing interest both theoretically and experimentally in the off-equilibrium dynamical properties of glassy systems. In particular, aging phenomena observed in spin glasses [1] have attracted the attention of researchers [2]. Unlike systems in thermal equilibrium, relaxation of physical quantities depends not only on the observation time t but also on the waiting time t_w, i.e., how long one waits at a given state before the measurements. Recent studies have revealed that the off-equilibrium dynamics in the spin-glass state generally has two characteristic time regimes [2,3]. One is a short-time regime, $t_0 \ll t \ll t_w$ (t_0 is a microscopic time scale), called "quasiequilibrium regime," and the other is a long-time regime, $t \gg t_w$, called "aging regime" or "out-of-equilibrium regime." In the quasiequilibrium regime, the relaxation is stationary and the fluctuation-dissipation theorem (FDT) holds. The autocorrelation function at times t_w and $t + t_w$ is expected to behave as

$$C(t_w, t + t_w) \approx q^{\mathrm{EA}} + \frac{C}{t^{\lambda}} \to q^{\mathrm{EA}}, \tag{1}$$

where q^{EA} is the equilibrium Edwards-Anderson (EA) order parameter. In the aging regime, the relaxation becomes nonstationary, FDT is broken, and the autocorrelation function decays to zero as $t \to \infty$ for fixed t_w.

On the theoretical side, both analytical and numerical studies of off-equilibrium dynamics of spin glasses have so far been limited to *Ising-like* models, including the Edwards-Anderson model with short-range interaction [4–6] or the mean-field models with long-range interaction [3,7,8]. Although these analyses on Ising-like models succeeded in reproducing some of the features of experimental results, many of the real spin-glass magnets are Heisenberg-like in the sense that the magnetic anisotropy is much weaker than the isotropic exchange interaction. Thus, in order to make a direct link between theory and experiment, it is clearly desirable to study the dynamical properties of *Heisenberg-like* spin-glass models.

Even at the static level, the nature of the experimentally observed spin-glass transition and the spin-glass states is not fully understood. Although experiments have provided strong evidence that spin-glass magnets exhibit an equilibrium phase transition at a finite temperature, numerical studies indicated that the standard spin-glass order occurred only at zero temperature in a three-dimensional (3D) Heisenberg spin glass [9–12]. While weak magnetic anisotropy inherent to real materials is often invoked to explain this apparent discrepancy, it remains puzzling that no detectable sign of Heisenberg-to-Ising crossover has been observed in experiments, which is usually expected to occur if the observed spin-glass transition is caused by the weak magnetic anisotropy [9,10].

In order to solve this apparent puzzle, a chirality mechanism of experimentally observed spin-glass transitions was recently proposed by the author [11], on the assumption that an isotropic 3D Heisenberg spin glass exhibited a finite-temperature *chiral-glass* transition without the conventional spin-glass order, in which only spin-reflection symmetry was broken while preserving spin-rotation symmetry. "Chirality" is an Ising-like multispin variable representing the sense or the handedness of the noncollinear spin structures. It was argued that, in real spin-glass magnets, the spin and the chirality were "mixed" due to the weak magnetic anisotropy, and the chiral-glass transition was then "revealed" via anomaly in experimentally accessible quantities. Meanwhile, the theoretical question as to whether there really occurs such a finite-temperature chiral-glass transition in an isotropic 3D Heisenberg spin glass remains somewhat inconclusive [11,12].

In view of the absence of an off-equilibrium simulation of Heisenberg spin glasses, and also of the possible important role played by the chirality, I report in this Letter the results of extensive dynamical Monte Carlo simulations on isotropic and anisotropic 3D Heisenberg spin glasses, in which the properties of the spin and the chirality are studied.

The model is the classical Heisenberg model on a simple cubic lattice with the nearest-neighbor random Gaussian couplings, J_{ij} and $D_{ij}^{\mu\nu}$, defined by the Hamiltonian

$$\mathcal{H} = -\sum_{\langle ij\rangle}(J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j + D_{ij}^{\mu\nu} S_i^{\mu} S_i^{\nu}), \qquad (2)$$

where $\mathbf{S}_i = (S_i^x, S_i^y, S_i^z)$ is a three-component unit vector, and the sum runs over all nearest-neighbor pairs with $N = L \times L \times L$ spins. J_{ij} is the isotropic exchange coupling with zero mean and variance J, while $D_{ij}^{\mu\nu}$ $(\mu, \nu = x, y, z)$ is the random magnetic anisotropy with zero mean and variance D which is assumed to be symmetric and traceless, $D_{ij}^{\mu\nu} = D_{ij}^{\nu\mu}$ and $\sum_{\mu} D_{ij}^{\mu\mu} = 0$.

The local chirality at the ith site and in the μth direction, $\chi_{i\mu}$, may be defined for three neighboring spins by the scalar [9,12],

$$\chi_{i\mu} = \mathbf{S}_{i+\hat{\mathbf{e}}_\mu} \cdot (\mathbf{S}_i \times \mathbf{S}_{i-\hat{\mathbf{e}}_\mu}), \qquad (3)$$

where $\hat{\mathbf{e}}_\mu$ $(\mu = x, y, z)$ denotes a unit lattice vector along the μ axis. Note that the chirality defined by Eq. (3) is a pseudoscalar in the sense that it is invariant under global spin rotation but changes sign under global spin reflection or inversion.

The spin and chirality autocorrelation functions are defined by

$$C_s(t_w, t + t_w) = \frac{1}{N}\sum_i [\langle \boldsymbol{S}_i(t_w) \cdot \boldsymbol{S}_i(t + t_w)\rangle], \qquad (4)$$

$$C_\chi(t_w, t + t_w) = \frac{1}{3N}\sum_{i,\mu} [\langle \chi_{i\mu}(t_w)\chi_{i\mu}(t + t_w)\rangle], \qquad (5)$$

where $\langle\cdots\rangle$ represents the thermal average and $[\cdots]$ represents the average over bond disorder.

Monte Carlo simulation is performed based on the standard single spin-flip heat-bath method. Starting from completely random initial configurations, the system is quenched to a working temperature. A total of about 3×10^5 Monte Carlo steps per spin (MCS) are generated in each run. A sample average is taken over 30–120 independent bond realizations. The lattice size mainly studied is $L = 16$ with periodic boundary conditions, while in some cases lattices with $L = 12$ and 24 are also studied.

Let us begin with the fully isotropic case, $D = 0$. The spin and chirality autocorrelation functions at a low temperature $T/J = 0.05$ are shown in Fig. 1 as a function of t. For larger t_w, the curves of the spin autocorrelation function C_s come on top of each other in the long-time regime, indicating that the stationary relaxation is recovered and aging is interrupted. This behavior has been expected because the 3D Heisenberg spin glass is believed to have no standard spin-glass order [9–12]. Similar interrupted aging was observed in the 2D Ising spin glass which did not have an equilibrium spin-glass order [5]. By contrast, the chiral autocorrelation function C_χ shows an entirely different behavior: Following the initial decay, it exhibits a clear plateau at about $t \sim t_w$ and then drops sharply for $t > t_w$. It also shows an eminent aging effect, namely, as one waits longer, the relaxation becomes slower and the plateaulike behavior at $t \sim t_w$ becomes more pronounced.

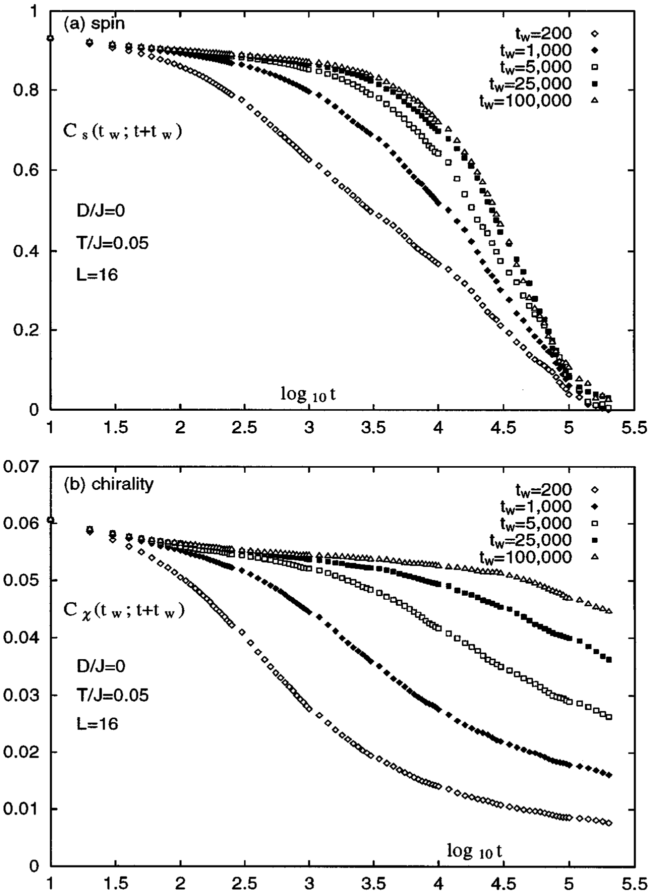

FIG. 1. Spin (a) and chirality (b) autocorrelation functions of a 3D isotropic Heisenberg spin glass at a temperature $T/J = 0.05$ plotted versus $\log_{10} t$ for various waiting times t_w. The lattice size is $L = 16$ averaged over 66 samples.

In Fig. 2, C_s and C_χ are replotted as a function of the scaled time t/t_w. Reflecting its interrupted aging, the curves of C_s for larger t_w now lie below the ones for smaller t_w (*subaging*). By contrast, the curves of C_χ for various t_w cross at about $t/t_w \sim 1$, and at $t > t_w$, the data for larger t_w lie *above* the ones for smaller t_w (*superaging*). Such superaging behavior of C_χ means that the aging in chirality is more enhanced than the one expected from the naive t/t_w scaling. Note that, although the chirality is an Ising-like variable from symmetry, the observed superaging behavior is in contrast to the aging behavior of the 3D EA model which was found to satisfy a good t/t_w scaling in the aging regime [5]. It should also be noticed that the plateaulike behavior observed here has been hardly noticeable in simulations of the 3D EA model. Rather, the behavior of C_χ observed here is reminiscent of the one observed in the mean-field model such as the Sherrington-Kirkpatrick (SK) model [7,8]. This correspondence might suggest that an effective interaction between the chiralities is long ranged.

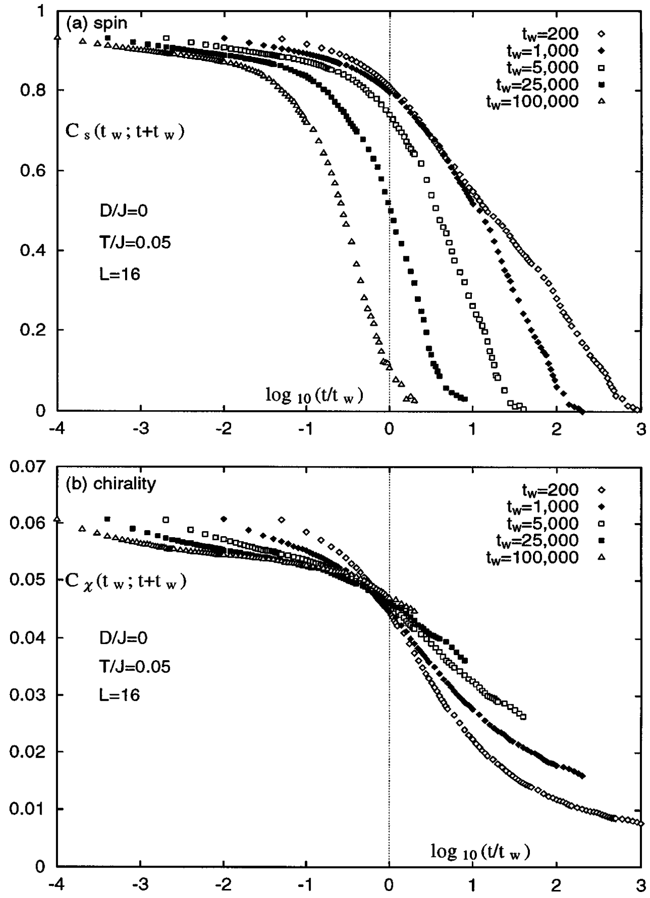

FIG. 2. The same data as in Fig. 1, but plotted versus $\log_{10}(t/t_w)$.

While the plateaulike behavior observed in C_χ is already suggestive of a nonzero *chiral* Edwards-Anderson order parameter $q_{\rm CG}^{\rm EA} > 0$, more quantitative analysis similar to the one recently done by Parisi *et al.* for the 4D Ising spin glass [6] is performed to extract $q_{\rm CG}^{\rm EA}$ from the data of C_χ in the quasiequilibrium regime. Finiteness of $q_{\rm CG}^{\rm EA}$ is also visible in a log-log plot of C_χ versus t as shown in the inset of Fig. 3, where the data show a clear upward curvature. I extract $q_{\rm CG}^{\rm EA}$ by fitting the data of C_χ for $t_w = 3 \times 10^5$ to the power-law form of Eq. (1) in the time range $40 \leq t \leq 3\,000$. The obtained $q_{\rm CG}^{\rm EA}$, plotted as a function of temperature in Fig. 3, clearly indicates the occurrence of a finite-temperature chiral-glass transition at $T_{\rm CG}/J = 0.157 \pm 0.01$ with the associated order-parameter exponent $\beta_{\rm CG} = 1.1 \pm 0.1$. The size dependence turns out to be rather small, although the mean values of $q_{\rm CG}^{\rm EA}$ tend to slightly increase around $T_{\rm CG}$ with increasing L. Since both finite-size and finite-t_w effects tend to underestimate $q_{\rm CG}^{\rm EA}$, one may regard the present result as rather strong evidence of the occurrence of a finite-temperature chiral-glass transition.

The associated exponent $\beta_{\rm CG} \sim 1.1$ is considerably larger than the value of the 3D EA model $\beta \sim 0.5$ [10], but is close to the value of the mean-field model $\beta = 1$. This suggests that the universality class of the chiral-glass transition of the 3D Heisenberg spin glass might be different from that of the standard 3D Ising spin glass. According to the chirality mechanism, the criticality of real spin-glass transitions should be the same as that of the chiral-glass transition of an isotropic Heisenberg spin glass, so long as the magnitude of random anisotropy is not too strong. If one tentatively accepts this scenario, the present result opens up a new interesting possibility that the universality class of many of real spin-glass transitions might differ from that of the standard Ising spin glass, contrary to common belief.

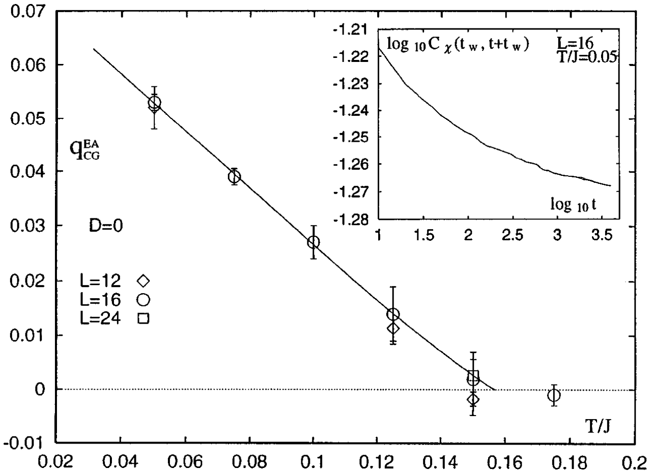

FIG. 3. Temperature dependence of the Edwards-Anderson order parameter of the chirality of a 3D isotropic Heisenberg spin glass. The data are averaged over 30–120 samples. Inset exhibits the log-log plot of the t dependence of the chiral autocorrelation function in the quasiequilibrium regime for $L = 16$, $T/J = 0.05$, and $t_w = 3 \times 10^5$.

In the presence of weak anisotropy $D > 0$, the chirality scenario predicts at the static level that the transition behavior of chirality remains essentially the same as in the isotropic case, whereas the spin is mixed into the chirality, asymptotically showing the same transition behavior as the chirality [11]. In order to see whether such "spin-chirality mixing" occurs in the off-equilibrium dynamics, further dynamical simulations are performed for the models with random anisotropies $D/J = 0.01 \sim 1$. While chirality exhibits essentially the same dynamical behavior as in the isotropic case (not shown here), the behavior of spin at $t > t_w$ changed significantly in the presence of anisotropy. As an example, the spin autocorrelation in the case of weak anisotropy $D/J = 0.01$ is shown in Fig. 4. Even for such small anisotropy, spin is found to show *superaging* behavior asymptotically at $t \gg t_w$ similar to that of the chirality in the fully isotropic case, demonstrating the chirality-spin mixing.

Experimentally, thermoremanent magnetization (TRM) or zero-field-cooled (ZFC) magnetization is found to show an approximate t/t_w scaling in the aging regime, with

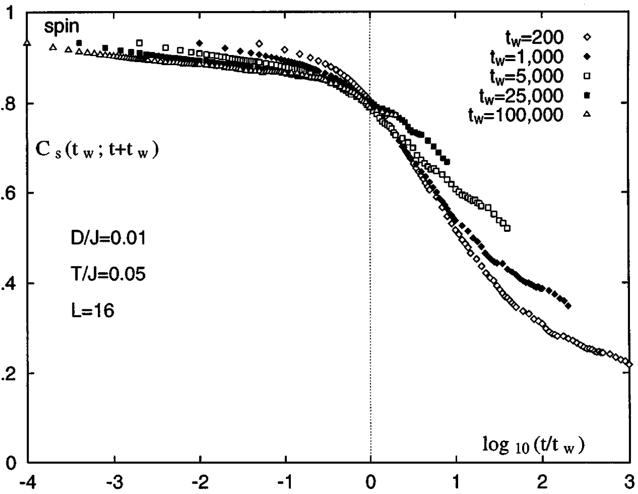

FIG. 4. Spin autocorrelation function of the weakly anisotropic 3D Heisenberg spin glass with $D/J = 0.01$ plotted versus $\log_{10}(t/t_w)$. The lattice size is $L = 16$ averaged over 60 samples and the temperature is $T/J = 0.05$.

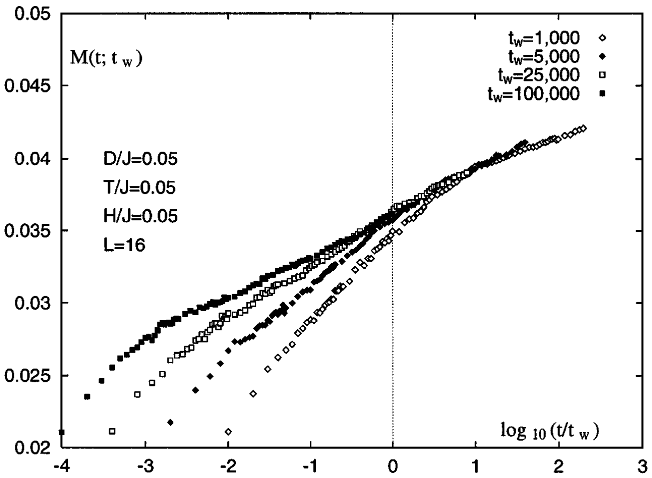

FIG. 5. Zero-field-cooled magnetization of an anisotropic 3D Heisenberg spin glass with $D/J = 0.05$ plotted versus $\log_{10} t$. The field is $H/J = 0.05$ and the temperature is $T/J = 0.05$. The lattice size is $L = 16$ averaged over 80 samples.

small deviation from the perfect scaling in the direction of subaging [2]. Although this seems in apparent contrast to the present result, it should be noticed that standard aging experiments have been made by measuring the magnetic response, not the autocorrelation. Recent numerical simulation by Yoshino *et al.* revealed that, at least in the case of the SK model, TRM showed the subaging even when the spin correlation showed the superaging [13]. Thus, I also calculate the ZFC magnetization for an anisotropic model with $D/J = 0.05$: After the initial quench, the system is evolved in zero field during t_w MCS. Then, an external field of intensity $H/J = 0.05$ is turned on and the subsequent growth of the magnetization $M(t; t_w)$ is recorded. As can be seen from Fig. 5, the data show the near t/t_w scaling in the aging regime $t > t_w$, where the spin autocorrelation shows the superaging. Thus, the observed tendency is roughly consistent with experiments. It might be interesting to experimentally investigate the aging properties of *spin correlation* of Heisenberg-like magnets in the search for possible superaging behavior.

In summary, equilibrium and off-equilibrium properties of the spin and chirality order in 3D Heisenberg spin glasses are studied with and without random anisotropy by dynamical Monte Carlo simulations. The results are basically consistent with the chirality mechanism: In the isotropic case, spin and chirality show very different dynamical behaviors consistent with the "spin-chirality separation," whereas in the anisotropic case, spin shows the same asymptotic behavior as chirality, consistent with the "spin-chirality mixing" due to the magnetic anisotropy. Furthermore, clear evidence for the occurrence of a finite-temperature chiral-glass transition in an isotropic 3D Heisenberg spin glass is presented.

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