Spin-Glass and Chiral-Glass Transitions in a $\pm J$ Heisenberg Spin-Glass Model in Three Dimensions

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The three-dimensional $\pm J$ Heisenberg spin-glass model is investigated by the non-equilibrium relaxation method from the paramagnetic state. Finite-size effects in the non-equilibrium relaxation are analyzed, and the relaxation functions of the spin-glass susceptibility and the chiral-glass susceptibility in the infinite-size system are obtained. The finite-time scaling analysis gives the spin-glass transition at $T_{\text{sg}}/J = 0.21^{+0.01}_{-0.02}$ and the chiral-glass transition at $T_{\text{cg}}/J = 0.22^{+0.01}_{-0.02}$. The results suggest that both transitions occur simultaneously. The critical exponent of the spin-glass susceptibility is estimated as $\gamma_{\text{sg}} = 1.7 \pm 0.3$, which makes an agreement with the experiments of the insulating and the canonical spin-glass materials.

75.10.Nr, 75.40.Mg, 64.60.Cn, 64.60.Fr

It has been an unsettled issue whether a short-ranged spin-glass model can explain the spin-glass transition observed in real materials. The existence of the spin-glass transition in the Ising model has been widely recognized: various types of investigations gave consistent values of the transition temperature. The recent large-scale simulation study evaluated the critical exponents which quantitatively agree with the measurements of the Ising model. The spins and the magnetic interactions of many spin-glass materials are mostly isotropic, and the anisotropy effect can be regarded as a secondary effect. Therefore, the Heisenberg model with random interactions is considered to be the simplest theoretical model. The problem is whether this model exhibits the spin-glass transition or not. Previous numerical investigations suggest that the finite-temperature transition does not occur.

In order to solve this contradiction, Kawamura introduced the chirality mechanism. The chirality is a variable whose absolute value corresponds to a volume of a parallelepiped spanned by three spins, and whose sign represents the handedness of the spin structure. In the chirality mechanism, the chirality is considered to freeze randomly at a finite temperature without the conventional spin-glass order. The experimentally-observed spin-glass anomaly is considered as an outcome of a mixture of the chirality with the spin by the weak magnetic anisotropies. The existence of the chiral-glass transition has been confirmed by several numerical analyses. However, it was pointed out recently by one of the present authors (S. E.) that the finite-temperature spin-glass transition may exist by examining the stiffness of the system when all the spins on a surface are rotated and reversed, respectively. The same evidence was also reported by a dynamical Monte Carlo simulation which removes the global spin rotation.

In this Letter, we focus on the existence or the nonexistence of the spin-glass and the chiral-glass transitions. By employing the non-equilibrium relaxation method, we have revealed that both transitions may occur simultaneously at a finite temperature $T/J \approx 0.21$. This result possibly settles the discrepancies between the experiments and the theories in the Heisenberg spin glass in three dimensions.

In the simulational studies of the phase transitions, one obtains equilibrium quantities in finite-size systems, and the finite-size scaling is utilized to extract the thermodynamic properties from them. However, the dynamics of the simulations become very slow due to the randomness and frustration in the spin-glass models, which makes it hard to realize the equilibrium state in large systems. The system size accessible by the equilibrium simulations is restricted to linear sizes $L \sim 30$ up to now. In this situation, reliability of the finite-size scaling might become doubtful, which causes controversial conclusions of the existence or the nonexistence of the spin-glass transition depending on the sizes and the temperatures of the data used. In this Letter, we follow a completely alternative approach to the thermodynamic limit, i.e., we observe the relaxation of the infinite-size system to the equilibrium state. In order to extract the equilibrium properties, the finite-time scaling analysis is utilized instead of the conventional finite-size scaling. This approach is known as the non-equilibrium relaxation (NER) method. Actually, we prepare a very large lattice with the paramagnetic state (perfectly random spin configuration), and observe the relaxation of the susceptibility. The simulations are stopped before the finite-size effect appears. Time dependences of the susceptibility diverge algebraically as $\chi(t) \sim t^{\gamma/z\nu}$ in the critical region, while it converges to a finite value in the paramagnetic region. We detect the phase transition by this difference. Another advantage of this strategy is an absence of a trivial exponential decay due to the global spin rotation. Since the spin autocorrelation function is essentially a one-body function about the spin, one may en-
counter this exponential decay even in the ordered phase after a time scale of the global spin rotation. [3]

We consider the \( \pm J \) Heisenberg spin-glass model on a simple cubic lattice of \( N = L \times L \times (L+1) \) under the skew periodic boundary conditions, \( \mathcal{H} = - \sum_{(i,j)} J_{ij} S_i \cdot S_j \). The exchange interactions \( J_{ij} \) take a value of \( +J \) or \( -J \) with the same probability, and \( S_i \) is a three-component vector spin with \( |S_i| = 1 \). The summation runs over all the nearest-neighbor spin pairs. We evaluate the spin-glass susceptibility, \( \chi_{sg} \), and the chiral-glass susceptibility, \( \chi_{cg} \), through the following relations.

\[
\chi_{sg} = \frac{1}{N} \sum_{i,j} \left[ \langle S_i \cdot S_j \rangle^2 \right]_c = N \sum_{\mu,\nu} \left[ \langle q_{\mu,\nu}^2 \rangle \right]_c, \quad (1)
\]

\[
\chi_{cg} = \frac{1}{3N} \left[ \left( \sum_{i,\mu} C^{(a)}_{i,\mu} C^{(b)}_{i,\mu} \right)^2 \right]_c, \quad (2)
\]

where \( q_{\mu,\nu} = (1/N) \sum_i S^{(a)}_{i,\mu} S^{(b)}_{i,\nu} \) is a replica overlap between the \( \mu \) component of a spin \( i \) on a replica (a), \( S^{(a)}_{i,\mu} \), and the \( \nu \) component of the spin on a replica (b), \( S^{(b)}_{i,\nu} \). The bracket \([ \cdot \cdot \cdot ]_c \) denotes the configurational average, while \( \langle \cdot \cdot \cdot \rangle \) denotes the thermal average. The indices, \( \mu \) and \( \nu \), stand for three components of spins: \( x, y, \) and \( z \).

The local chirality \( C^{(a)}_{i,\mu} \) is defined by three neighboring spins as \( C^{(a)}_{i,\mu} = S^{(a)}_{i+\hat{e}_x} \cdot (S^{(a)}_{i+\hat{e}_y} \times S^{(a)}_{i+\hat{e}_z}) \), and \( \hat{e}_\mu \) denotes a unit lattice vector along the \( \mu \) axis.

We use the single-spin-flip algorithm with the bath probability. [3] For a given random bond configuration, eight replicas are prepared with different random initial spin configurations. Each replica is updated in parallel by a different random number sequence, and twenty eight replica-overlaps are calculated and averaged. Note that these data are correlated with each other, and only seven among them are independent. Then, we take averages of \( \chi_{sg}(t) \) and \( \chi_{cg}(t) \) over the bond distributions. Typical numbers of the bond configurations are tens to thousands depending on the sizes, the temperatures, and the time ranges.

From the non-equilibrium relaxation functions of \( \chi_{sg} \) and \( \chi_{cg} \), we extract the equilibrium properties and estimate the transition temperature by the finite-time scaling analysis, [2][4], which is a direct interpretation of the conventional finite-size scaling through the relation,

\[
\tau \sim \xi^z. \]

We determine the correlation time \( \tau(T) \) at each temperature and a combined exponent \( \lambda(\equiv \gamma/z\nu) \) so that the scaled functions, \( \chi(t) t^{-\lambda} \), for various temperatures fall onto a single curve when plotted against \( t/\tau(T) \). Then, we extrapolate \( \tau(T) \) with an assumption that they diverge algebraically when the temperature approaches the transition temperature \( T_c \) as \( \tau(T) \propto (T - T_c)^{-z\nu} \).

We obtain the most probable estimate for \( T_c \) by the least-square fitting of this form.

In the finite-time scaling, it is crucial to use the data free from the finite-size effect. We estimate a characteris-
ered to correspond to the chiral correlation length. If one tries to detect \( T_{cg} \) solely by finding the algebraic relaxation behavior, he may be misled to a wrong temperature where \( \xi = L \) instead of \( \xi = \infty \). Therefore, the chiral-glass transition temperature tends to be overestimated, and the spin-glass transition temperature is to be underestimated, if the system size is insufficient.

As shown in Fig. 1, the initial relaxation of the spin-glass susceptibility continues until \( t \sim 10^3 \) steps, then it exhibits the critical relaxation. In the finite-time scaling analysis, we must discard this initial relaxation data. It is also noticed that the finite-size effects of the small sizes \( (L \leq 19) \) appear before the initial relaxation ends. The critical phenomena may not be extracted from the equilibrium states of such small systems.

\[
0.24 \leq T/J \leq 0.32. \quad \text{The data in the initial relaxation are discarded. The scaling function converges to a } t^{-\lambda} \text{ line in the equilibrium region } (t/\tau(T) \rightarrow \infty), \text{ where the susceptibility converges to an equilibrium value in the infinite system. On the other hand, it becomes a flat line in the non-equilibrium limit, } t/\tau(T) \rightarrow 0, \text{ since the susceptibility behaves as } \chi(t) \sim t^\lambda \text{ in the critical region. Therefore, this curve interpolates the non-equilibrium and the equilibrium limits.}
\]

The correlation time is extrapolated by \((T - T_c)^{-z\nu}\), and we obtain the transition temperature that gives the best least-square fitting. The exponent is estimated to be \( z\nu = 4.7 \pm 0.8 \). Combining this value with \( \lambda = \gamma/z\nu = 0.36 \pm 0.02 \), the exponent for the spin-glass susceptibility is estimated.

\[
T_{sg}/J = 0.21^{+0.01}_{-0.02}, \quad \gamma_{sg} = 1.7 \pm 0.3.
\]

This transition temperature agrees well with that obtained by the defect free-energy method, \cite{13} and that obtained by the dynamical simulations. \cite{24} The exponent is consistent to that of the non-linear susceptibility in real spin-glass compounds: \( \gamma = 2.2 \pm 0.1 \) (CuMn & AgMn) \cite{29} and \( \gamma = 2.3 \pm 0.4 \) (Cd Cr\(_{2}\times0.85\)In\(_{2}\times0.85\)S\(_4\)). \cite{30} This may suggest that the present theoretical model is relevant to the spin-glass materials. Estimates and the comparison of other exponents are left for a future investigation. It requires more detailed and accurate calculations of the Binder ratio, which diverges in the critical region as \( t^{-d/\nu} \). Preliminary calculations of the Binder ratio, however, suggest that the size effects and the sample dependences are much severer than those of the susceptibility. The algebraic divergence is only observed in lattices larger than \( L = 19 \), below which the finite-size effects appear in the initial relaxation. The details will be reported elsewhere.

Analyses of the chiral-glass transition are done in the same procedure. Note that the amplitude of \( \chi_{cg} \) is smaller than that of \( \chi_{sg} \) about two digits, which causes rather large numerical errors. A possible value of \( \lambda \) ranges as \( \lambda = 0.23 \pm 0.04 \). The transition temperature and its exponent are obtained as

\[
T_{cg}/J = 0.22^{+0.01}_{-0.04}, \quad \gamma_{cg} = 1.0 \pm 0.5.
\]

Note that this value is consistent with the estimate obtained by the equilibrium simulations which gives \( T_{cg} \sim 0.21 \). \cite{24} The value of \( \gamma_{cg} \) does not contradict with that of the model with the Gaussian bond distributions. \cite{14} The exponents \( \lambda \) for \( \chi_{sg} \) and \( \chi_{cg} \) estimated in the scaling also coincide with the slope of the relaxation functions at the transition temperature in Fig. 1. This evidence supports the validity of the present analysis. By the results presented in this Letter, it is conjectured that the spin-glass transition and the chiral-glass transition occur at the same temperature. Since the chirality must freeze.

FIG. 2. (a) The finite-time scaling of \( \chi_{sg}(t) \) with \( \lambda = \gamma/z\nu = 0.36 \) and \( \chi_{cg}(t) \) (multiplied by 300) with \( \lambda = 0.24 \). The \( t^{-\lambda} \) are depicted by straight lines. The data of \( L = 59 \) at \( T/J = 0.32, 0.29, 0.28, 0.27, 0.26, 0.25, \) and \( 0.24 \) are plotted. (b) Extrapolations of the correlation time \( \tau(T) \) of \( \chi_{sg} \) and \( \chi_{cg} \) obtained by the scaling. The transition temperatures are estimated so as to minimize the least-square errors. Six temperatures ranging \( 0.24 \leq T/J \leq 0.29 \) are used.

Results of the finite-time scaling of the spin-glass susceptibility and the chiral-glass susceptibility are shown in Fig. 2. The combined exponent \( \lambda \) and the correlation time \( \tau(T) \) are estimated by using the data of \( L = 59 \) until \( t = 70000 \) steps at seven temperatures ranging \( \sqrt{T/J} \leq 10^3 \) steps, then it exhibits the critical relaxation. In the finite-time scaling analysis, we must discard this initial relaxation data. It is also noticed that the finite-size effects of the small sizes \( (L \leq 19) \) appear before the initial relaxation ends. The critical phenomena may not be extracted from the equilibrium states of such small systems.
if the spin freezes, the transition is possibly driven by the spin degrees of freedom.

We have observed the simultaneous finite-temperature spin-glass transition and the chiral-glass transition in the $\pm J$ Heisenberg model in three dimensions. This was made possible by observing the non-equilibrium relaxation of the infinite-size system started from the paramagnetic state. We consider the inconsistency of the present results with those of the previous investigations \[5–11\] can be explained by the differences of the lattice size and the temperature range investigated. Generally, if one mixes the data above and below this crossover temperature, the finite-size scaling analysis may lead to a wrong conclusion. Generally, frustration causes a longer correlation length, and the size of the system is sometimes essential to detect the phase transition particularly in frustrated systems. \[2\] In the present non-equilibrium relaxation analysis, we have used only data of the temperatures and the time ranges where they can be considered as the infinite system. The time range is limited within $10^3$ steps, however, it is enough to equilibrate the system at higher temperatures, $T/J \sim 0.3$, where we start the scaling analysis. We gradually lower the temperature so that the scaled relaxation functions overlap with each other to ride on a single curve. At lower temperatures, $T/J \sim 0.24$, $10^5$ steps correspond to a time scale that the finiteness of the correlation length begins to appear, i.e., the relaxation function begins to bend. In order to see a longer relaxation, we need to enlarge the system size to eliminate the size effect. This must become much more time-consuming and we leave it for the future study. However, it should be noticed that the finite-size effect appears quite early in the relaxation process as shown in Fig. 4 and what is slow is the relaxation to the equilibrium state after this “finite-size” characteristic time scale. The relaxation of the infinite system might be simple: after an initial relaxation of $10^3$ steps, the critical relaxation continues to infinity. As for the relation between the model and real spin-glass materials, the critical exponent obtained by the scaling, $\gamma_{sg} \sim 1.7$, agrees with the experiments.

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