Spin and chirality autocorrelation functions of a Heisenberg spin-glass model

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We study the spin and the chirality autocorrelation functions $C_S(t)$ and $C_\chi(t)$ of the $\pm J$ Heisenberg model in three dimensions to examine the chirality mechanism of the spin-glass (SG) phase transition proposed by Kawamura, which says that it is not the spins but the chiralities of the spins that are ordered in Heisenberg SG systems. Using a dynamical simulation method that removes the drift of the system, we show that an apparent difference in the dynamics between the spin and chirality comes from the drift and suggest that the spins and the chiralities are ordered simultaneously.

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It has been believed that the spin-glass (SG) phase is realized in three dimensions (3D) for the Ising model[1,2] but not for the XY and Heisenberg models.[3–6] Thus, the SG phases observed in experiments were suggested to be realized due to magnetic anisotropies.[7,8] However, it remains puzzling that no sign of Heisenberg-Ising crossover has been detected experimentally,[5,9,10] which is expected if the observed finite temperature phase transition is due to a weak magnetic anisotropy. Recently, Hukushima and Kawamura have proposed a chirality mechanism to solve the puzzle.[11–14] They considered the chirality described by neighboring three spins. It has either positive or negative value, just like the Ising spin. Kawamura[11–13] claimed that, in the 3D XY and Heisenberg SG models, a chiral-glass (CG) phase transition occurs at a finite temperature $T_{\mathrm{CG}}\neq 0$, but the SG phase is absent. He argued that, in real SG magnets, the spin and the chirality are mixed due to a weak magnetic anisotropy, and the CG transition is revealed as anomalies in experimentally accessible quantities. According to this interpretation, the SG phase transition never occurs in Heisenberg-like systems, and what was observed in experiments is nothing but the CG phase transition. This mechanism is quite interesting, because it calls for reconsideration of the SG phase transition from both theoretical and experimental points of view.

However, there are some basic problems in the basis of the chirality mechanism. One is the $T=0$ stiffness exponent of the chiralities θ_{C} and that of the spins θ_{S}. Kawamura[11] estimated $\theta_{\mathrm{C}}>0$ and $\theta_{\mathrm{S}}<0$ in the 3D XY and Heisenberg SG models, having used a conventional defect energy method.[3,15,16] However, recent studies threw some doubt on that method itself.[17–20] Another problem is the dynamics of the system. Kawamura[13] and Hukushima and Kawamura[14] calculated the chirality autocorrelation function $C_\chi(t)$ and the spin autocorrelation function $C_S(t)$ of 3D Heisenberg SG models with and without a weak anisotropy D. They found that, even for $D=0$, $C_\chi(t)$ exhibits a pronounced aging effect reminiscent of the one observed in the mean-field model,[21] while $C_S(t)$ exhibits a similar aging effect only when $D\neq 0$. However, when one considers dynamical properties of the Heisenberg model with $D=0$, one should pay special attention to the thermal drift of the system, i.e., the global rotation of the system.[22] Although this drift does not affect the static spin correlations and becomes negligible in large systems, some of the dynamical simulation data inevitably suffer from this effect. The spin autocorrelation function $C_S(t)$ diminishes by this drift, whereas the chirality autocorrelation $C_\chi(t)$ does not, because the chiralities are invariant under global rotation of the system. Thus, the difference in the behavior between $C_S(t)$ and $C_\chi(t)$ might come from this drift.

In this paper, we show that, in the $\pm J$ Heisenberg model, the apparent difference between $C_S(t)$ and $C_\chi(t)$ comes from the drift of the system. We propose a dynamical simulation method that removes the drift of the system. Using the method, we first show that $C_S(t)$ exhibits properties quite similar to those of $C_\chi(t)$. Then, applying the same off-equilibrium Monte Carlo simulation method that was used by Kawamura,[13] we estimate values of the Edward-Anderson order parameters of the spin and the chirality and find that both have finite values at low temperatures and vanish at almost the same temperature of $T\sim 0.18J$. Thus, we suggest that the spins and the chiralities are ordered simultaneously.

We start with the $\pm J$ Heisenberg model on a simple cubic lattice of $L\times L\times(L+1)$ $(\equiv N)$ with skew boundary conditions along two L directions and a periodic boundary condition along the $(L+1)$ direction. The Hamiltonian is described by

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

where $\boldsymbol{S}_i$ is the Heisenberg spin of $|\boldsymbol{S}_i|=1$ and $\langle ij\rangle$ runs over all nearest-neighbor pairs. The exchange interaction (bond) J_{ij} takes either $+J$ or $-J$ with the same probability of 1/2.

We consider the dynamical properties of the system calculating the spin autocorrelation function. In order to consider these properties of an infinitely large system, we remove the effect of the drift applying the uniform rotation to the system so that

$$S=\sum_i |R(t)\boldsymbol{S}_i(t+t_w)-\boldsymbol{S}_i(t_w)|^2 \tag{2}$$

becomes minimum, where $R(t)$ is the rotation matrix, and $\{\boldsymbol{S}_i(t_w)\}$ and $\{\boldsymbol{S}_i(t+t_w)\}$ are the spin configurations at times t_w and $t+t_w$, respectively. We can successively determine

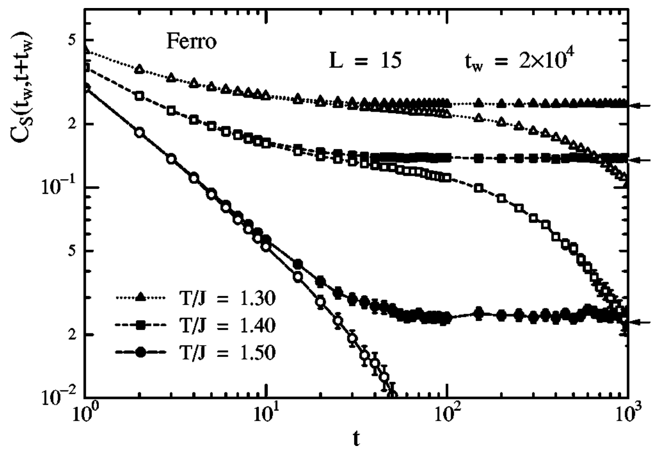

FIG. 1. The spin autocorrelation functions of the ferromagnetic Heisenberg model in 3D plotted vs t for a waiting time $t_w=2\times10^4$ at temperatures around the Curie temperature of $T_C/J\sim1.45$. The solid and open symbols are data from the fixed and the drifting systems, respectively. The arrows indicate the equilibrium values of the square of the magnetization $\langle(\boldsymbol{M}/N)^2\rangle$.

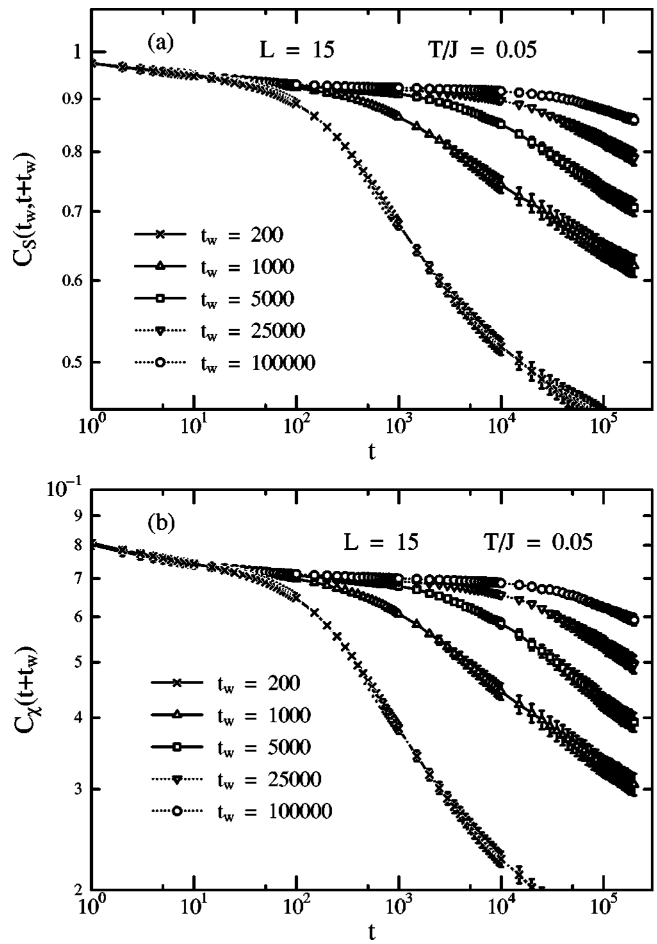

FIG. 2. The autocorrelation functions of (a) the spin C_S and (b) the chirality C_χ of the $\pm J$ Heisenberg model plotted vs t for different waiting time t_w. The data are averaged over 32 samples of the lattice size $L=15$.

$R(t)$, because $R(t)=E$ at $t=0$ and it changes step by step as t goes by, where E is the unit matrix.[23] Hereafter, we call the system described by $\{\boldsymbol{S}_i(t)\}$ the drifting system and that by $\{\tilde{\boldsymbol{S}}_i(t+t_w)\equiv R(t)\boldsymbol{S}_i(t+t_w)\}$ the fixed system. The spin autocorrelation function $C_S(t_w,t+t_w)$ of the fixed system is defined as

$$C_S(t_w,t+t_w)=\frac{1}{N}\sum_i\,[\langle\tilde{\boldsymbol{S}}_i(t+t_w)\tilde{\boldsymbol{S}}_i(t_w)\rangle], \tag{3}$$

where $\langle\cdots\rangle$ and $[\cdots]$ mean the thermal average and the bond distribution average, respectively. The chirality autocorrelation function is also defined as

$$C_\chi(t_w,t+t_w)=\frac{1}{3N}\sum_{i\mu}\,[\langle\chi_{i\mu}(t+t_w)\chi_{i\mu}(t_w)\rangle], \tag{4}$$

where $\chi_{i\mu}$ is the chirality at the ith site and in the μth direction defined by $\chi_{i\mu}=\boldsymbol{S}_{i+\hat{e}_\mu}\cdot(\boldsymbol{S}_i\times\boldsymbol{S}_{i-\hat{e}_\mu})$ with $\hat{e}_\mu(\mu=x,y,z)$ being a unit lattice vector along the μ axis. Note again that the chirality $\chi_{i\mu}$ is invariant under the global spin rotation, and then the chirality autocorrelation functions of both the drifting and fixed systems are completely the same and described by Eq. (4). Before applying this method to the present model, we test it in the 3D ferromagnetic Heisenberg model. The results are shown in Fig. 1. It is found that the spin autocorrelation function of the fixed system with a large t_w approaches the equilibrium value of the square of the order parameter, $\langle(\boldsymbol{M}/N)^2\rangle$, with $\boldsymbol{M}$ being the total magnetization, whereas that of the drifting system rapidly decays with increasing t. This result indicates that the effect of the drift can be removed properly by the present method.

We perform the same simulation that was done by Kawamura[13] using the standard single-spin-flip heat-bath Monte Carlo (MC) method. That is, starting with a random initial spin configuration, the system is quenched to a working temperature, and after waiting t_w MC steps per spin (MCS) the autocorrelation functions are measured up to about 2×10^5 MCS. A sample average is taken over about 32 independent bond distributions. The results of $C_S(t_w,t+t_w)$ and $C_\chi(t_w,t+t_w)$ for different t_w are presented in Fig. 2 as functions of t. It is seen that $C_S(t_w,t+t_w)$ exhibits an aging effect quite similar to that of $C_\chi(t_w,t+t_w)$, implying that the spin and the chirality possess similar dynamical properties. To examine this point in more detail, we plot in Fig. 3 the ratio $T(t_w,t+t_w)\equiv C_\chi/C_S$ for a fixed $t_w=10^5$ at different temperatures. At all the temperatures, $T(t_w,t+t_w)$ slowly decreases as t goes by, revealing that C_S decays more slowly than C_χ. This result suggests that, if the ordering of the chiralities is realized, the same is true for the spins.

Next, we estimate values of the Edward-Anderson order parameters of the spin and the chirality, q_{SG} and q_{CG}, applying the method proposed by Parisi *et al.*[24] and used by Kawamura.[13] That is, these values are extracted by fitting the data of C_S and C_χ for $t_w=3\times10^5$ to the power-law form of

$$C_S(t_w,t+t_w)\sim q_{\mathrm{SG}}+\frac{A_S}{t^{\lambda_S}}, \tag{5}$$

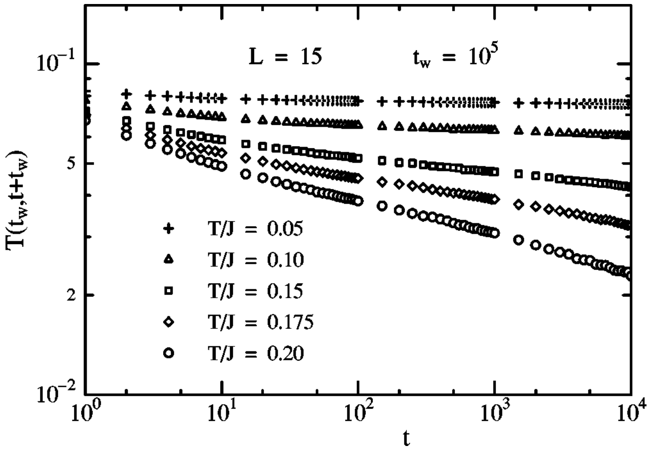

FIG. 3. The ratio of the chirality to the spin autocorrelation functions $T(t_w,t+t_w)\equiv C_\chi/C_S$ of the $\pm J$ Heisenberg model plotted vs t. The data are averaged over 32 samples of the lattice size $L=15$.

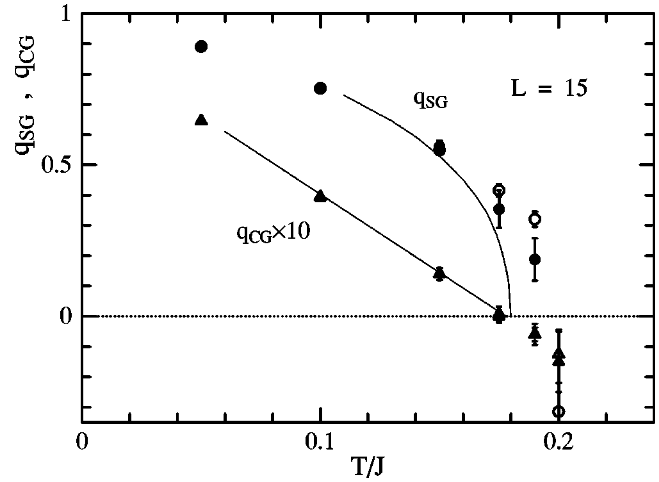

FIG. 4. Temperature dependences of the Edwards-Anderson order parameters of the spin and the chirality, q_{SG} and q_{CG}, of the $\pm J$ Heisenberg model. Open and solid symbols indicate those extracted in the time ranges of $30\leqslant t\leqslant 3000$ and $50\leqslant t\leqslant 5000$, respectively. The data are averaged over 32–200 samples. Lines are guides to the eye.

$$C_\chi(t_w,t+t_w)\sim q_{\mathrm{CG}}+\frac{A_\chi}{t^{\lambda_\chi}}, \tag{6}$$

in the two time ranges of $30\leqslant t\leqslant 3000$ and $50\leqslant t\leqslant 5000$, where A_S, A_χ, λ_S, and λ_χ are constants. The obtained q_{SG} and q_{CG} are plotted as functions of temperature in Fig. 4. Both quantities have positive, nonvanishing values at low temperatures and seem to vanish at almost the same temperature of $T\sim 0.18J$.[25] This result also suggests that the phase transitions of the spin and the chirality exist at $T\neq 0$ and they occur at the same temperature.

In summary, we have revealed that the apparent difference in the dynamical property between the spin and the chirality comes from the drift of the system. The off-equilibrium Monte Carlo simulation suggests the occurrence of the SG phase transition at $T_{\mathrm{SG}}\sim 0.18J$. This view is compatible with our recent studies of the stiffness of the system, which suggest that, contrary to previous studies,[3,4,11] the stiffness exponent θ_{S} of the spin has the positive value of $\theta_{\mathrm{S}}\sim 0.8$ at $T=0$ (Ref. 20) and changes its sign at $T\sim 0.19J$.[26] Thus we think that the SG phase will be realized at finite temperatures even when the anisotropy is absent. However, further studies are necessary to establish the finite-temperature SG transition.[27]

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[23] It is well known that any rotation matrix R is described by $R=\exp(D)$ with D being an antisymmetric matrix. If $R(t)$ is given as $R(t)=\exp[D(t)]$, then $R(t+1)$ can be readily obtained by putting $R(t+1)=\exp(\delta D)\exp[D(t)]$ and using Newton-Raphson method.
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[25] Since q_{SG} and q_{CG} should be positive or 0, the extrapolation function of Eq. (5) becomes meaningless for $T \geqslant 0.19J$ for q_{CG} and $T \geqslant 0.20J$ for q_{SG}. This fact implys that $T_{\mathrm{CG}} < 0.19J$ and $T_{\mathrm{SG}} < 0.20J$.

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[27] We have also studied properties in the equilibrium state and found that the SG susceptibility χ_{SG} exhibits a divergent singularity at $T \sim 0.18J$. However, it was reported that the spin Binder parameter g_{SG} (and also the chirality Binder parameter g_{CG}) exhibits strange temperature dependences (Ref. 14). Further studies are necessary to make clear the relationship between the phase transition and the behaviors of these Binder parameters.