Effect of Anisotropy on a Short-Range $\pm J$ Heisenberg Spin Glass in Three Dimensions

F. Matsubara, T. Iyota, and S. Inawashiro
Department of Applied Physics, Tohoku University, Sendai 980, Japan
(Received 30 January 1991)

A short-range $\pm J$ Heisenberg spin glass with and without anisotropy on a simple cubic lattice is studied by using a hybrid Monte Carlo spin-dynamics method. The anisotropy leads to a cusplike peak of the susceptibility χ and a very slow relaxation of the spin configuration at low temperatures. From a finite-size-scaling analysis of the spin-glass susceptibility χ_{sg}, we find, for the first time, that the anisotropy induces a phase transition.

PACS numbers: 75.10.Jm, 75.10.Nr, 75.40.Mg

The experimental evidence for a phase transition in spin glasses is now convincing [1]. The computer simulations [2–4] and other numerical studies [5,6] of Ising spin glasses also strongly suggest that a phase transition takes place in three-dimensional systems. However, similar computer simulations of XY [7,8] and Heisenberg [8–10] systems suggest that there is no phase transition in three-dimensional systems, even when the spin interactions are of long-range Ruderman-Kittel-Kasuya-Yoshida (RKKY) character [11,12]. This is quite mysterious, because the best-studied spin glasses (e.g., *Cu*Mn, *Ag*Mn, $Eu_xSr_{1-x}S$) are Heisenberg-like systems. In an attempt to resolve this problem, the effect of anisotropy which comes from Dzyaloshinsky-Moriya (DM) or dipolar coupling which is always present has been discussed. Walstedt and Walker [13] first investigated the effect of a weak pseudodipolar coupling in a RKKY system using a microcanonical Monte Carlo method and found that the coupling leads to a cusplike peak of the susceptibility. However, they did not discuss whether the peak reveals the phase transition or not. Bray and Moore [14] speculated that the anisotropy induces Ising critical behavior. Using a scaling argument, Morris *et al.* [8] estimated that, in the short-range spin glass, the transition temperature $T_c \propto J(D/J)^{1/4}$, where J is the average of absolute values of isotropic couplings and D is that of anisotropic couplings. Bray, Moore, and Young [15] argued that the transition temperature of the RKKY system has a much weaker dependence on the anisotropy of $T_c \propto J/[\ln(J/D)]^{1/2}$. Hence, even if a very weak anisotropy exists, the phase transition is expected to occur at a finite temperature. Detailed computer simulations of the Heisenberg spin glass with the anisotropy are necessary to examine whether the anisotropy really induces the spin-glass phase transition or not, and, if it does, how the transition temperature depends on the anisotropy.

In this Letter, we study the effect of the anisotropy in a short-range Heisenberg spin glass on the simple cubic lattice using a hybrid Monte Carlo spin-dynamics (HMCSD) method proposed by us [16]. Since the method takes into account the intrinsic spin dynamics of the classical Heisenberg model, it simulates the system more realistically than the conventional Monte Carlo (MC) method. Moreover, the method drastically reduces computer CPU time. In particular, within a reasonable computer time, we could clearly reveal the absence of the phase transition in the isotropic short-range Heisenberg spin glass.

We start with the classical Heisenberg model on the simple cubic lattice described by the Hamiltonian

$$H=\sum_{\langle ij\rangle}\left[J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j+\sum_{\alpha\neq\beta}D_{ij}^{\alpha\beta}S_i^{\alpha}S_j^{\beta}\right], \tag{1}$$

where $|\mathbf{S}_i|=1$, $J_{ij}=J$ or $-J$ with probabilities of $\frac{1}{2}$, and $\langle ij\rangle$ runs over all nearest-neighbor pairs on a lattice. Here we assume that the anisotropy comes from pseudodipolar couplings and impose the following restriction:

$$D_{ij}^{\alpha\beta}=D_{ji}^{\alpha\beta}=D_{ij}^{\beta\alpha}. \tag{2}$$

Since the essence of the anisotropy is in the tensorial structure of the couplings, we assume for simplicity that $D_{ij}^{\alpha\beta}$ are uniform random values between $-D$ and D.

We briefly mention the method [16]. The spin dynamics of the model is described by the following equation of motion:

$$\hbar\frac{d}{dt}\mathbf{S}_i=[\mathbf{S}_i\times\mathbf{H}_i], \tag{3}$$

where $\mathbf{H}_i=-\partial H/\partial\mathbf{S}_i$. In this case, the energy and total magnetization $\mathbf{M}=\sum\mathbf{S}_i$ are conserved. Then, we combine a standard MC method (Metropolis method) to realize a thermal equilibrium. The procedure of the simulation is as follows. After spins of a given ratio are refreshed by the MC method (here half the spins are refreshed), all the spins are moved simultaneously by Eq. (3) in the time interval t_0. These steps are repeated throughout the simulation. Hereafter we measure the time and temperature in the units of $\hbar/J=1$ and $k_B=1$. When $t_0\ll 1$, the system is governed by the stochastic kinetics, whereas, when spins are not refreshed at all, the system is governed by the spin dynamics. We make the simulation with $t_0=0.2$, because this value is economical to obtain physical quantities [16]. To avoid compounding errors in the integration of Eq. (3), we use the Runge-Kutta method with the time mesh of $\Delta t=0.1$.

We treat the model on the simple cubic lattices of

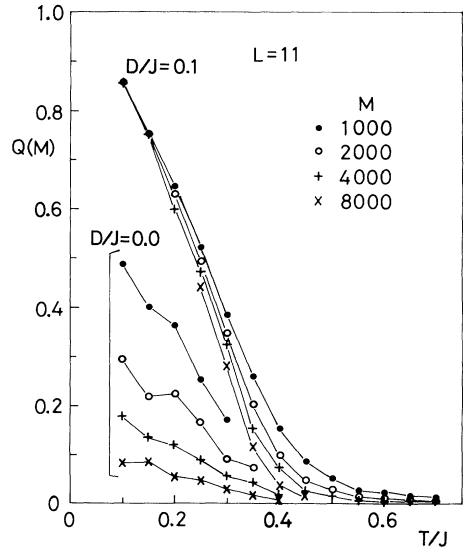

FIG. 1. The spin-glass order parameter $Q(M)$'s for different MCS's of M.

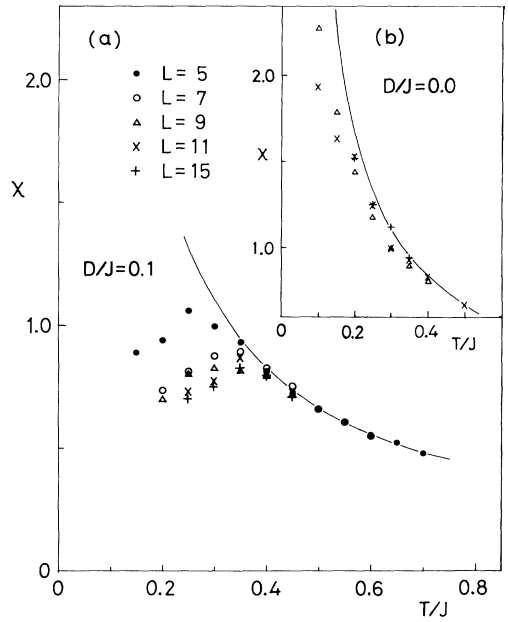

FIG. 2. Susceptibilities for different lattices. The results are those for $M=8000$ ($L=9$, 11, and 15) and those for $M=4000$ ($L=5$ and 7). Solid lines indicate the Curie law of $\chi=J/3T$.

$N=L\times L\times(L+1)$ sites with a periodic boundary condition. We use a gradual-cooling method. After the first 2000 (or 4000) MC steps per spin (MCS) are discarded, data of the next M MCS ($M=4000$ for $L=5$ and 7, $M=8000$ for $L=9$ and 11, and $M=16000$ for $L=15$) are used to calculate physical quantities. Numbers of samples prepared in this simulation are 20–30 for $L\leq 9$, 10–20 for $L=11$, and 6 for $L=15$. We calculate the susceptibility χ, spin-glass order parameter $Q(M)$, and spin-glass susceptibility $\chi_{\rm sg}$. The latter two are conventionally defined by

$$Q(M)=\frac{1}{N}\sum_{i}^{N}\left\langle\left[\frac{1}{M}\sum_{m}^{M}\mathbf{S}_i(m)\right]^2\right\rangle_J \tag{4}$$

and

$$\chi_{\rm sg}=\frac{1}{N}\left\langle\sum_{ij}\langle\mathbf{S}_i\cdot\mathbf{S}_j\rangle_T^2\right\rangle_J , \tag{5}$$

where $\langle\cdots\rangle_J$ means the sample average. Using a technique similar to that of Bhatt and Young [2], we estimate both the lower and upper bounds of $\chi_{\rm sg}$. Only when the two bounds agree are results accepted for a scaling analysis described below.

In Fig. 1, $Q(M)$'s for $D/J=0.1$ are presented for different values of M together with those for $D=0$. As the temperature is decreased, $Q(M)$ increases abruptly below a temperature ($T/J=0.35$). At low temperatures, $Q(M)$ reduces little as M increases revealing a very slow relaxation characteristic to the spin-glass phase. These properties are in striking contrast with those of the isotropic case ($D=0$), where no spin-glass phase occurs at finite temperatures [8–10,16]. These results indicate that the anisotropy induces the spin-glass phase at low temperatures.

In Fig. 2(a), the susceptibility χ for the same anisotropy $D/J=0.1$ is presented. It exhibits a cusplike peak at the same temperature of $T/J=0.35$ *even for smaller lattices.* Below this temperature, χ exhibits a small M dependence, revealing slow relaxation of the spin configuration. On the other hand, χ for $D=0$ shown in Fig. 2(b) increases monotonically according to the Curie law *even for larger lattices.* These also indicate the occurrence of the spin-glass phase for $D\neq 0$.

In Fig. 3(a), $\chi_{\rm sg}$'s for $D/J=0.1$ are plotted at different temperatures as functions of the lattice size N. For $T/J\geq 0.35$, the results reveal a power-law decay of the correlation, $\langle\langle\mathbf{S}_i\cdot\mathbf{S}_j\rangle_T^2\rangle_J$, with increasing $|i-j|$, whereas those at $T/J=0.3$ and 0.25 suggest it has an algebraic decay. We expect that the phase transition takes place between $T/J=0.3$ and 0.35. On the other hand, for $D=0$, the results of the plots shown in Fig. 3(b) reveal the power-law decay of the correlation at least down to $T/J=0.20$. For $T/J<0.2$, we could not obtain reliable values of $\chi_{\rm sg}$ for larger lattices, because the difference between the two bounds of $\chi_{\rm sg}$ becomes significant.

To estimate the transition temperature T_c, we make a finite-size scaling [17]. If the transition occurs, $\chi_{\rm sg}$ will behave as

$$\chi_{\rm sg}=L^{2-\eta}\chi[L^{1/\nu}(T-T_c)/J] , \tag{6}$$

where ν is the exponent of the correlation length and η is the exponent which describes the decay of the correlation at T_c. The scaling plots of the data of $D/J=0.1$ for lattices of $L\geq 7$ are shown in Fig. 4 [18]. When $T_c/J=0.30^{+0.02}_{-0.05}$, all the points for $T/J\geq 0.30$ can be scaled

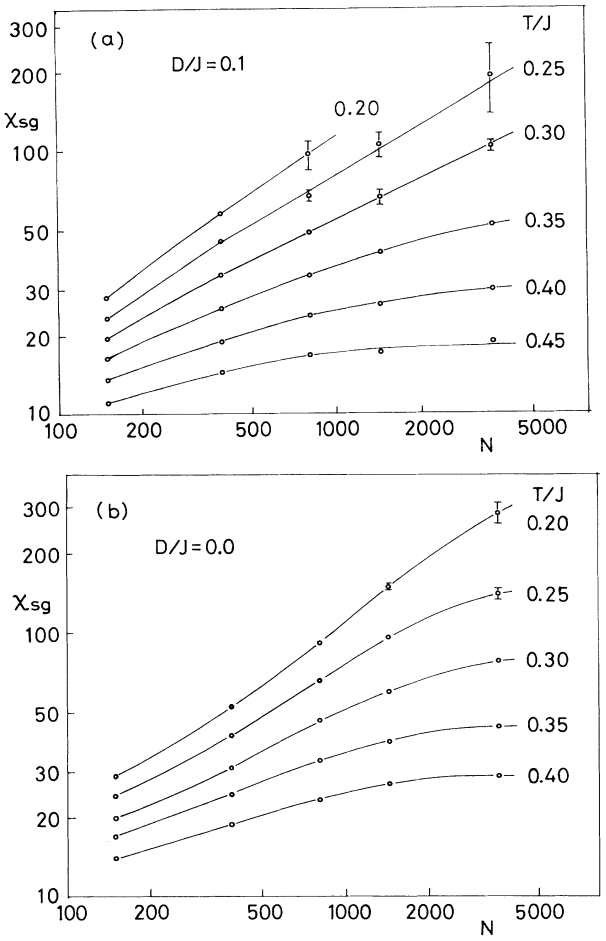

FIG. 3. χ_{sg} vs N on a log-log plot. The top and bottom of the error bar indicate the upper and lower bounds of χ_{sg} estimated by using a technique similar to Bhatt and Young [2]. Only when the two bounds agree are data accepted for the scaling analysis in Fig. 4. Note that the slope of the line at $T/J=0.30$ is $(2-\eta)/3\sim 0.5$, leading to $\eta\sim 0.5$.

well. Values of the exponents determined in this analysis are $\eta=0.7^{+0.2}_{-0.4}$ and $\nu=1.15\pm 0.10$. T_c obtained here is in agreement with that suggested from the temperature dependences of $Q(M)$ and χ, and the value of $\eta\sim 0.7$ is also compatible with $\eta\sim 0.5$ estimated from the slope of the plots in Fig. 3(a). On the other hand, for $D/J=0$, all the points can be scaled well if we choose $T_c/J<0.1$. When we take $T_c=0$, which is predicted by previous studies [8–10], and confirmed by the present studies of $Q(M)$ and χ, we obtain $\eta=-(0.9\text{–}1.0)$ and $\nu=1.35\pm 0.05$. Our value of $\nu\sim 1.35$ is compatible with those estimated previously, i.e., $\nu=1.54\pm 0.19$ by McMillan [9] and $\nu\sim 1.4$ by Olive, Young, and Sherrington [10]. This also proves the validity of the HMCSD method.

Quite similar results are obtained in another case of $D/J=0.05$. From the finite-size scaling, we get $T_c/J=0.25^{+0.02}_{-0.10}$ and similar values of the exponents η

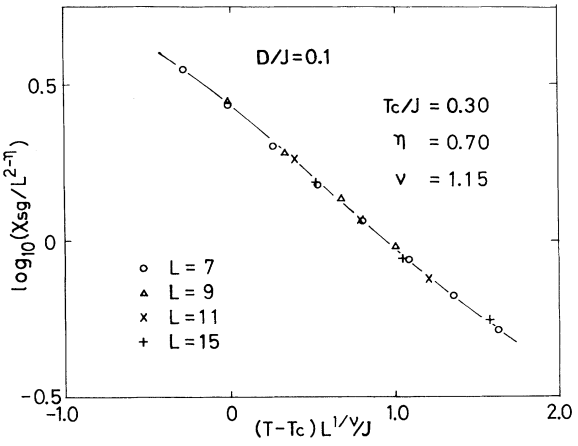

FIG. 4. A finite-size scaling for $L\geq 7$. The solid line is a guide to the eye.

$=0.6^{+0.2}_{-0.5}$ and $\nu=1.20\pm 0.10$.

From these results, we may conclude that the anisotropy induces the phase transition at a finite temperature. In this sense, the Heisenberg spin glass with anisotropy resembles the Ising spin glass. However, the spin structure of the Heisenberg spin glass is quite different from that of the Ising spin glass. We have also calculated the distribution of the spin directions and found that, even for $T<T_c$, the distribution is almost uniform in the three-dimensional space. The critical exponent $\nu\sim 1.2$ is almost the same as those predicted in the Ising spin glass, i.e., $\nu=1.4$ by Bhatt and Young [2], and $\nu=1.2$ by Ogielski [3]. However, the exponent $\eta\sim 0.6$ in our model is much larger than $\eta=-(0.3\text{–}0.2)$ predicted in the Ising spin glass [2,3,5,6]. This will be due to the difference in the spin structure between the two spin glasses. In fact, the spin correlation will decay more rapidly in the Heisenberg model than in the Ising model because of the uniform distribution of the spin directions. The difference of η together with the different spin structure strongly suggests that the Heisenberg spin glass with the random anisotropy belongs to another universality class.

The other point to be studied is how T_c depends on D. At present, it is difficult to give a conclusive answer to this question because we estimate T_c only for two values of D. We should mention, however, that our results suggest a weak dependence of T_c on D. Here, we examine the prediction of $T_c/J\propto(D/J)^x$ with $x\sim\frac{1}{4}$ which is given by Morris *et al.* [8] based on a scaling argument. A plausible fit is shown in Fig. 5, where $x=\frac{1}{4}$ is used. Our result is not incompatible with the theoretical prediction. Of course, our values of T_c are not accurate enough and we cannot exclude the possibility of another value of x. Further computer simulations are necessary to give the dependence of T_c on D.

In this Letter, we have studied the short-range $\pm J$ Heisenberg spin glass with anisotropy using the HMCSD method, and found for the first time that the anisotropy

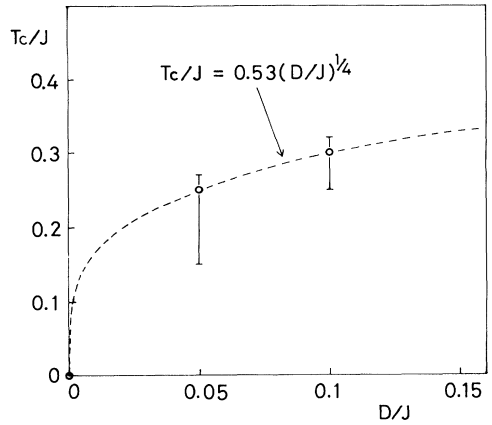

FIG. 5. Dependence of the transition temperature T_c on D.

induces the phase transition at a finite temperature. We believe that this answers the primary question of why the spin-glass phase occurs in the real world, although our model is a simplified one and the magnitude of the anisotropy used here is much stronger than those of real substances. Similar studies for realistic systems such as the RKKY system with the dipolar interaction are also desired to obtain more detailed knowledge of real spin glasses. Finally, we should emphasize that all the things presented in this Letter were obtained by the HMCSD method *within Monte Carlo steps much smaller than those of the conventional MC method.*

The authors wish to thank Dr. T. Shirakura for valuable discussions.

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[17] See, e.g., M. N. Barber, in *Phase Transitions and Critical Phenomena,* edited by C. Domb and J. Lebowitz (Academic, New York, 1983), Vol. 8, p. 146.
[18] Note that the data of the smallest lattice ($L=5$) cannot be scaled well. In this case, the total anisotropy energy of the system, the order of which is given by DN, will be too small to pin the spin configuration. In fact, almost the same values of χ_{sg} are obtained for the cases of both $D/J=0$ and 0.1.