Journal of Magnetism and Magnetic Materials 177–181 (1998) 69–70

Equilibrium simulation of chiral-glass order in a three-dimensional Heisenberg spin glass

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Abstract

Spin-glass and chiral-glass ordering of the three-dimensional Heisenberg spin glass with random Gaussian couplings are investigated by means of a Monte Carlo simulation based on an extended ensemble method.

Keywords: Spin glass; Heisenberg spin glass; Monte Carlo simulation; Phase transitions – spin glass; Chirality

Experiments have provided strong evidence that spin-glass magnets exhibit an equilibrium phase transition at a finite temperature. Although an isotropic Heisenberg model is expected to be a good reference system for many real spin glasses, numerical studies indicated that the standard spin-glass transition in vector spin glasses, including XY and Heisenberg models, occurred only at zero temperature in three dimensions (3D). While magnetic anisotropy inherent to real materials is often invoked to explain this apparent discrepancy, the true nature of the experimental spin-glass transition remains unclear. Especially puzzling point is that no detectable sign of Heisenberg-to-Ising crossover has been observed in experiments which is usually expected to occur if the observed Ising-like transition behavior is caused by the weak magnetic anisotropy [1–3].

In order to solve this apparent puzzle, a 'chirality' mechanism of experimentally observed spin-glass transitions was recently proposed [4, 5], on the assumption that isotropic vector spin glasses in 3D exhibit a finite-temperature *chiral-glass* transition without a conventional spin-glass order parameter, in which only spin-reflection symmetry is broken with preserving spin-rotation symmetry. 'Chirality' is an Ising-like quantity representing the sense or the handedness of the noncollinear spin structures induced by spin frustration. Strong support for the occurrence of such a finite-temperature chiral-glass transition was reported in the XY case in previous numerical simulations [6], but the situation remains far from clear in the Heisenberg case [4, 7]. In this paper, we wish to report on our recent Monte Carlo simulation of a three-dimensional Heisenberg spin glass, trying to shed further light on the nature of the chiral-glass order in spin-glass magnets.

Our model is the classical Heisenberg model on a $d = 3$-dimensional simple cubic lattice with the nearest-neighbor random Gaussian couplings J_{ij} with zero mean and variance J, defined by the Hamiltonian,

$$\mathscr{H} = -\sum_{<ij>} J_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j, \tag{1}$$

where $\boldsymbol{S}_i = (S_i^x, S_i^y, S_i^z)$ is a three-component unit vector, and the sum runs over all nearest-neighbor pairs with $N = L \times L \times L$ spins. 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 [8, 9],

$$\chi_{i\mu} = \boldsymbol{S}_{i+\hat{e}_\mu} \cdot (\boldsymbol{S}_i \times \boldsymbol{S}_{i-\hat{e}_\mu}), \tag{2}$$

where $\hat{e}_\mu (\mu = x, y, z)$ denotes a unit lattice vector along the μ-axis. The chirality defined by Eq. (2) is invariant under global spin rotation but changing sign under global spin reflection or inversion. Note that the chirality takes a nonzero value for any noncoplanar spin configuration but vanishes for any planar spin configuration.

By utilizing an 'extended ensemble' algorithm recently developed by Hukushima and Nemoto [10], we simulated the model (1) and succeeded in equilibrating

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PII S0304-8853(97)00436-8

the system down to the temperature considerably lower than those attained in the previous simulations. We run in parallel two independent replicas with the same bond realization and compute an overlap between the chiral variables in the two replicas,

$$q_\chi = \frac{1}{3N}\sum_{i,\mu} \chi_{i\mu}^{(1)}\chi_{i\mu}^{(2)}. \tag{3}$$

In terms of this chiral overlap, q_χ, the Binder cumulant of the chirality, g_{CG}, is calculated by

$$g_{CG} = \frac{1}{2}\left(3 - \frac{[\langle q_\chi^4\rangle]}{[\langle q_\chi^2\rangle]^2}\right). \tag{4}$$

where $\langle\cdots\rangle$ represents thermal average and $[\cdots]$ represents the average over bond disorder. At the possible chiral-glass transition point, curves of g_{CG} against T for different L should merge or intersect asymptotically.

For the case of the Heisenberg spin, one can introduce an appropriate Binder cumulant in terms of a tensor overlap $q_{\mu\nu}$ ($\mu,\nu = x, y, z$) with $3^2 = 9$ independent components

$$q_{\mu\nu} \equiv \frac{1}{3N}\sum_i S_{i\mu}^{(1)}S_{i\nu}^{(2)} \quad (\mu,\nu = x, y, z), \tag{5}$$

via the relation

$$g_{SG} = \frac{1}{2}\left(11 - 9\frac{\sum_{\mu,\nu,\delta,\rho}[\langle q_{\mu\nu}^2\, q_{\delta\rho}^2\rangle]}{(\sum_{\mu,\nu}[\langle q_{\mu\nu}^2\rangle])^2}\right). \tag{6}$$

The lattice sizes studied are $L = 6$, 8, 10, 12 with periodic boundary conditions. In our simulation, whole configurations at two neighboring temperatures of the same sample are occasionally exchanged [10] with the system remaining at equilibrium. In the case of $L = 12$, for example, we prepare 50 temperature points distributed in the range $0.08J$–$0.25J$ for a given sample, and perform 4.7×10^5 exchanges per temperature of the whole lattices combined with the same number of standard single-spin-flip heat-bath sweeps. For $L = 12$, we equilibrate the system down to the temperature $T = 0.08J$, which is lower than the minimum attained previously, e.g., $T = 0.12J$ of Ref. [7]. Sample average is taken over 1000 ($L = 4$), 800 ($L = 8$), 400 ($L = 10$) and 144 ($L = 12$) independent bond realizations.

The size and temperature dependence of the Binder cumulants of the spin and of the chirality, g_{SG} and g_{CG}, are shown in Figs. 1 and 2, respectively. As can be seen from Fig. 1, g_{SG} constantly decreases with increasing L at all temperatures studied, indicating that the conventional spin-glass order occurs only at zero temperature, consistent with the previous results [7, 8]. A closer inspection of Fig. 1, however, reveals that g_{SG} for larger lattices ($L = 10$, 12) exhibits an anomalous 'upturn' around $T \sim 0.1J$, suggesting a change in the ordering behavior. As can be seen from Fig. 2, the curves of g_{CG} for different L merge around $T \sim 0.1J$, which is suggestive of the occurrence of a finite-temperature chiral-glass transition without the conventional spin-glass order at a low but finite temperature, $T_{CG} > 0$. Indeed, we have performed a more detailed finite-size scaling analysis of the data to find that $T_{CG} > 0$ is favored over $T_{CG} = 0$, although the possibility of $T_{CG} = 0$ cannot still be ruled out completely. Further studies are now in progress with the hope to settle this issue.

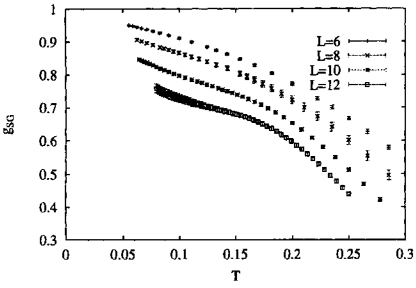

Fig. 1. The temperature and size dependence of the Binder cumulant of the Heisenberg spin, g_{SG}.

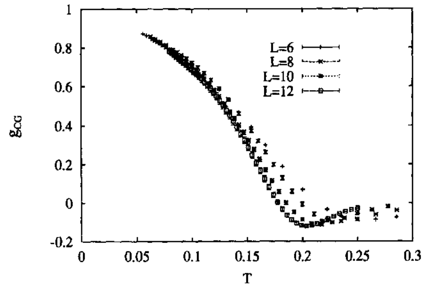

Fig. 2. The temperature and size dependence of the Binder cumulant of the chirality, g_{CG}.

The numerical calculation was performed on the FACOM VPP500 at the supercomputer center, Institute of Solid State Physics, University of Tokyo.

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