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Gabay–Toulouse phase transition in Heisenberg spin glasses in three dimensions

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Abstract

We examine three-dimensional $\pm J$ Heisenberg models with and without random anisotropies in a magnetic field. We calculate both the stiffness exponent θ_s at zero temperature and spin-glass correlation lengths for the longitudinal and transverse spin components at finite temperatures. We suggest that, contrary to a chirality scenario predicted by Kawamura and his co-workers (Kawamura 1992 *Phys. Rev. Lett.* **68** 3785, 1998 *Phys. Rev. Lett.* **80** 5421, Hukushima and Kawamura 2000 *Phys. Rev. E* **61** R1008), a Gabay–Toulouse phase transition might occur when the anisotropies are absent, although the results, except for the correlation length of the chirality for larger sizes, suggest no phase transition when they are present.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

Phase transitions of three-dimensional (3D) Heisenberg spin glass (SG) models have attracted much interest in recent years. Two phase-transition scenarios are involved in controversy. One is the *SG scenario*, in which a usual SG phase transition takes place at a finite temperature. However, this scenario has been believed to hold only when anisotropies are present [1]. The other is a *chirality glass (CG) scenario*, proposed by Kawamura and his co-workers [2–4]. In the CG scenario, not the spins, but also the local chiralities freeze at a finite temperature. In this scenario, the SG phase transition never occurs in isotropic SG models. The freezing of the spins was suggested to occur through coupling of the spins and the local chiralities by random anisotropies.

Kawamura and his co-workers gave three pieces of evidence of the CG scenario in the isotropic case: the stiffness exponent for the chiralities is positive $\theta_\chi > 0$, whereas that for the spins is negative $\theta_s < 0$ [2]; only the chirality autocorrelation exhibits a pronounced aging effect at low temperatures [3]; and the chirality overlap distribution $P(q_\chi)$ exhibits a one-step-like replica symmetry breaking (RSB) behavior [4]. However, re-examinations of those

properties revealed different aspects: the stiffness exponent for the spins in a lattice with open boundaries is positive $\theta_s > 0$ [5, 6]; the spin autocorrelation of a system, in which a uniform rotation is removed, exhibits an aging effect similar to that of the chirality autocorrelation [7, 8]; and the SG overlap distribution also exhibits the one-step-like RSB behavior, if we select the SG order parameter appropriately [9]. Recently, the SG phase transition temperature T_{SG} and the CG phase transition temperature T_{CG} were estimated using a non-equilibrium relaxation method [10] and the scaling method of the SG correlation length [11]. Results suggested that $T_{SG} = T_{CG}$ in both methods. Based on those results, the SG scenario has also come back into the isotropic models.

The controversy surrounding those two scenarios has reached a new stage. It has been speculated that true SG properties are visible only in large lattices, e.g., the $L \times L \times L$ lattice with $L \geq 20$, because the coupling of the spins and the local chiralities, which exists even for the isotropic model in small lattices, might loosen for $L \rightarrow \infty$ [12]. Campos *et al* recently studied the model for big lattices ($L = 24$ and 32) [13] to resolve this issue. Their results suggest that the lower critical dimension d_l of this model is equal to or slightly smaller than 3 ($d_l \leq 3$) and that a large finite size correction exists in the scaling property of the model with $d = 3$. Having taken into account this correction, they also suggested that $T_{SG} = T_{CG}$. However, objections exist in relation to their interpretation [14]. Unfortunately, it is too difficult to resolve this issue herein.

Two scenarios predict different aspects for a finite magnetic field $H \neq 0$. In the SG scenario, a usual phase transition will take place, which is characterized by a freezing of the transverse component of the spin, i.e., a Gabay–Toulouse (GT) phase transition [15]. In the CG scenario, the CG phase transition will occur, but the SG phase transition is absent [17]. More interesting is a case in which anisotropies D are present. Imagawa and Kawamura predicted that the CG transition still occurs even at $D \neq 0$ because of the one-step RSB [18].

In this paper, we present an examination of the phase transition of the $\pm J$ Heisenberg models with and without random anisotropies at a finite magnetic field $H \neq 0$. Special attention is devoted to an induced magnetic moment $\langle S_i \rangle$ at each site i . We consider an SG spin component, $\tilde{S}_i (\equiv S_i - \langle S_i \rangle)$, to examine cooperative phenomena of the system. Results suggest that, in the isotropic model, the ground-state stiffness and the scaling property of the SG correlation length suggest the presence of the SG (GT-like) phase transition which might be the KT-type transition similar to those at $H = 0$ [13]. On the other hand, in the anisotropic model, both the CG transition and the SG transition might disappear, although further investigations for larger sizes would be needed to clarify them.

We study the $\pm J$ Heisenberg SG models in three dimensions ($d = 3$) in a magnetic field H described using the Hamiltonian

$$\mathcal{H} = - \sum_{\langle ij \rangle} J_{ij} \mathbf{S}_i \mathbf{S}_j - \sum_{\langle ij \rangle} \sum_{\mu\nu} D_{ij}^{\mu\nu} S_i^\mu S_j^\nu - H \sum_i S_i^z, \quad (1)$$

where \mathbf{S}_i is the classical vector spin of $|\mathbf{S}_i| = 1$; $J_{ij} = +J$ or $-J$ with the same probability of $1/2$. The second term expresses the anisotropic energy; $D_{ij}^{\mu\nu} (= D_{ji}^{\mu\nu} = D_{ij}^{\nu\mu})$ ($\mu, \nu = x, y, z$) are symmetric random anisotropic constants uniformly distributed in the range $[-D : D]$. We consider two cases: $D = 0$ and $D \neq 0$.

2. The isotropic case of $D = 0$

First, we consider the ground-state stiffness of the model using a method proposed by Matsubara *et al* [5]. Here we consider lattices of $L \times L \times (L + 1)$ with open boundaries for the $(L + 1)$ direction and periodic boundary conditions for the other two directions. The

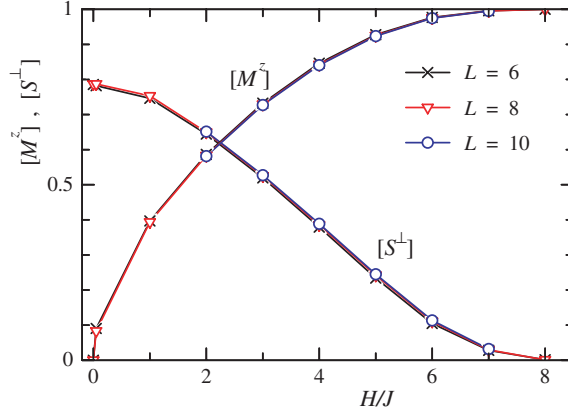


Figure 1. Magnetization $[M^z]$ and the transverse component $[S^\perp]$ for various lattices L as functions of H .

Table 1. Parameters of the genetic algorithm (the GAI method) described in [20]. N_{samp} is the number of samples, N_p is the number of local populations and N_q is the number of spin quench steps per spin. These parameters are almost independent of the value of the field H .

| L | N_{samp} | N_p | N_q |
|-----|-------------------|-------|-------|
| 4–8 | 1000 | 16 | 100 |
| 10 | ~500 | 64 | 100 |
| 12 | ~50 | 256 | 200 |

lattice has two opposite surfaces Ω_1 and Ω_{L+1} . We first determine the ground-state spin configuration $\{\mathcal{S}_i \equiv \mathcal{S}_i^\parallel + \mathcal{S}_i^\perp\}$ and its energy E_L^0 . Then, fixing all the spins on the surface Ω_1 , all the spins on the surface Ω_{L+1} are rotated by the same angle $\phi = \pi/2$ around the z -axis and fixed. Under this boundary condition, we calculate the minimum energy of the system, E_L^ϕ , which is always higher than E_L^0 . The stiffness of the system might be characterized by the excess energy $\Delta E_L (\equiv E_L^\phi - E_L^0)$. The stiffness exponent θ_s might be defined by the relation $\Delta E_L \propto L^{\theta_s}$.

We have calculated $[\Delta E_L]$ of the model up to $L = 12$, together with the parallel (the magnetization) and the transverse components of the spins, $[M^z (= |\sum_i \mathcal{S}_i^\parallel|/N)]$ and $[S^\perp (= \sum_i |\mathcal{S}_i^\perp|/N)]$, in which $[\dots]$ means a sample average. We have used a genetic algorithm [19, 20], in particular the GAI method in [20]. Detailed parameters of the method are given in table 1. The parameter set of (N_p, N_q) has been chosen such that the search ratio defined in [20] becomes greater than 0.90. Figure 1 shows $[M^z]$ and $[S^\perp]$ as functions of H . Those values depend little on L , suggesting that they are those for $L \rightarrow \infty$. In fact, $[M^z]$ exhibits a characteristic property of the SG, i.e., it increases rapidly with H and saturates gradually at high magnetic fields $H_s \sim 7J$. Consequently, $[S^\perp]$ has a considerable value up to H_s . Figure 2 shows $[\Delta E_L]$ for several H in a log–log form. Note that scattering of the data of ΔE_L is not large as compared with that of the conventional defect energy and becomes smaller as L increases (see also figures 1–3 in [21]). Using least-squares fitting with data for $L \geq 6$, we estimated the stiffness exponent as $\theta_s = 0.61 \pm 0.02, 0.63 \pm 0.03, 0.64 \pm 0.02, 0.62 \pm 0.06$ and -0.18 ± 0.15 , respectively, for $H/J = 0, 2, 4, 6$ and 7 . The value of $\theta_s \sim 0.61$ for $H = 0$ is almost the same as $\theta_s \sim 0.62$, which was estimated in smaller systems of

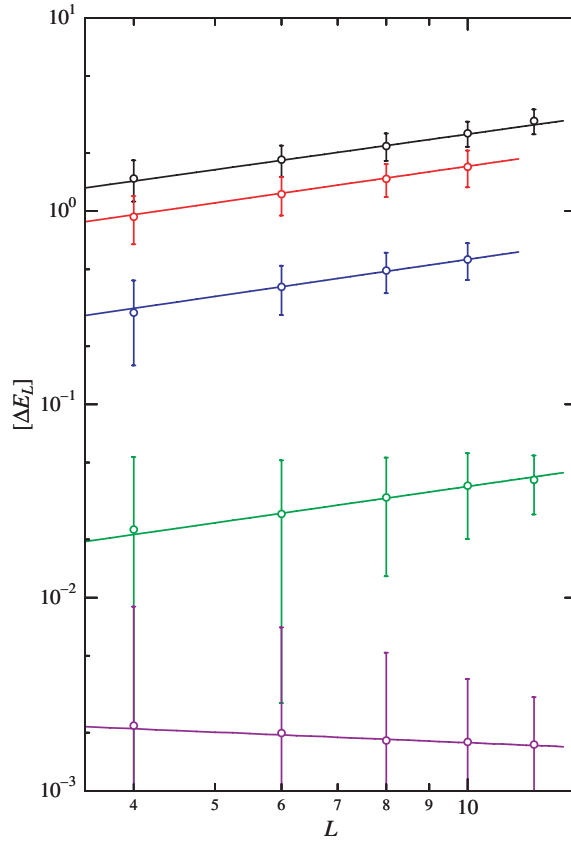


Figure 2. Excess energy $[\Delta E_L]$ for various lattices L . The symbols denote, from the above, those at $H/J = 0, 2, 4, 6$ and 7 . Lines are drawn using least-squares fitting with data for $L \geq 6$. The bar attached to each of the data denotes the standard deviation of the data, not the standard error (the standard deviation of the sample averaged value).

$L \leq 8$ [21]. θ_s are positive and almost equal for $H < H_s$. This result is analogous to that in the spin-flop (SP) phase of an antiferromagnetic Heisenberg (AFH) model, in which $\theta_s = 1$ for $H < H_s (\equiv H_c = 12J)$. Therefore, we expect that a phase transition occurs at $H \leq H_c (= 6.5 \pm 0.5J)$, where H_c denotes a critical field at zero temperature. Further investigations for larger sizes would be needed to confirm these results.

We next examine the phase transition of the model using the Monte Carlo (MC) method. We consider two replica systems with $\{S_i^\alpha\}$ and $\{S_i^\beta\}$. The lattice is 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. At $H \neq 0$, the spins are polarized to the z -direction: $m_i (\equiv \langle S_i^z \rangle^\alpha = \langle S_i^z \rangle^\beta) \neq 0$, where $\langle \dots \rangle$ means a thermal average. Magnitudes of m_i will vary from site to site. Figure 3 shows their distribution $P(m_i)$. In fact, m_i distributes in a very wide range. The slight size dependence of $P(m_i)$ reveals that m_i is purely magnetic-field induced. Then we subtract $\mathbf{m}_i (\equiv (0, 0, m_i))$ from the original spin [11]: $\tilde{S}_i^{\alpha,\beta} = S_i^{\alpha,\beta} - \mathbf{m}_i$. Hereafter, we call $\tilde{S}_i^{\alpha,\beta}$ SG components and consider their cooperative phenomena.

We consider the spin-glass correlation lengths ξ_L^η for the longitudinal ($\eta = \parallel$) and transverse ($\eta = \perp$) components. We calculate them using a formula [11]:

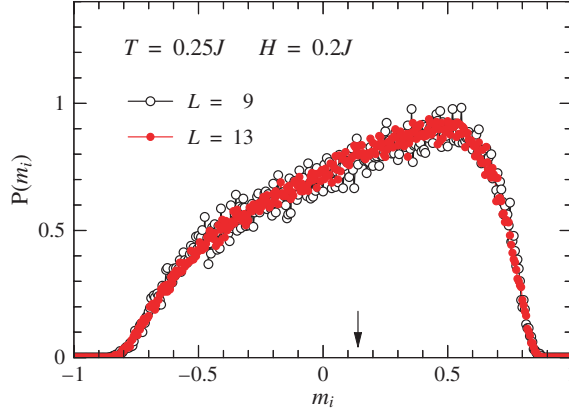


Figure 3. Distribution of the site magnetizations m_i of the model with $D = 0$ in a finite magnetic field. $T = 0.25J$ is slightly higher than $T_{SG}(\sim 0.2J)$ at $H = 0$. The arrow indicates the average value of m_i for $L = 13$.

$$\xi_L^\eta = \frac{1}{2 \sin(\mathbf{k}_{\min}/2)} \left(\frac{\tilde{\chi}_{SG}^\eta(\mathbf{0})}{\tilde{\chi}_{SG}^\eta(\mathbf{k}_{\min})} - 1 \right)^{1/2}, \quad (2)$$

where $\mathbf{k}_{\min} = (0, 0, 2\pi/(L+1))$. The \mathbf{k} -dependent SG susceptibility is given as $\tilde{\chi}_{SG}^\parallel(\mathbf{k}) = N[|\tilde{q}^{zz}(\mathbf{k})|^2]$, and $\tilde{\chi}_{SG}^\perp(\mathbf{k}) = N \sum_{\mu, \nu=x,y} [|\tilde{q}^{\mu\nu}(\mathbf{k})|^2]$, with $\tilde{q}^{\mu\nu}(\mathbf{k}) = \frac{1}{N} \sum_i \tilde{S}_i^{\alpha\mu} \tilde{S}_i^{\beta\nu} \exp(i\mathbf{k} \cdot \mathbf{R}_i)$. If an SG phase transition occurs, the correlation length divided by the system size L , ξ_L^η/L has the following scaling property:

$$\frac{\xi_L^\eta}{L} = \hat{\xi}^\eta(L^{1/\nu}(T - T_{SG}(H))), \quad (3)$$

where ν is the correlation length exponent, $T_{SG}(H)$ is the transition temperature at H and $\hat{\xi}^\eta$ represents a scaling function.

We performed a simulation of these two replica systems on the lattice with $L \leq 23$ having used a temperature exchange MC method [22] with an over-relaxation [13]. We show the details of the parameters in the MC simulations in table 2. Equilibration is checked by monitoring the stability of the results against runs at least twice as long. Figures 4(a) and (c) respectively show ξ_L^\perp/L and ξ_L^\parallel/L at $H = 0.2J$ as functions of T . These two quantities exhibit different size dependence. ξ_L^\perp/L for different L merges around $T = 0.22J$, suggesting the presence of the phase transition. This result is compatible with the ground-state study. In contrast, ξ_L^\parallel/L for larger sizes seems to merge at lower temperatures, which might suggest the crossover from a weak irreversible state to the strong one in the longitudinal component similar to that in the mean field model [15].

3. The anisotropic case of $D \neq 0$

Next we consider the anisotropic model ($D = 0.1J$) in a magnetic field ($H = 0.2J$). Imagawa and Kawamura (IK) [18] examined the same model with a smaller value of anisotropy ($D = 0.05J$) and suggested that the CG phase transition occurs because of the one-step-like RSB. They considered cooperative phenomena of the original spins $\{S_i^\alpha\}$ and $\{S_i^\beta\}$. We have

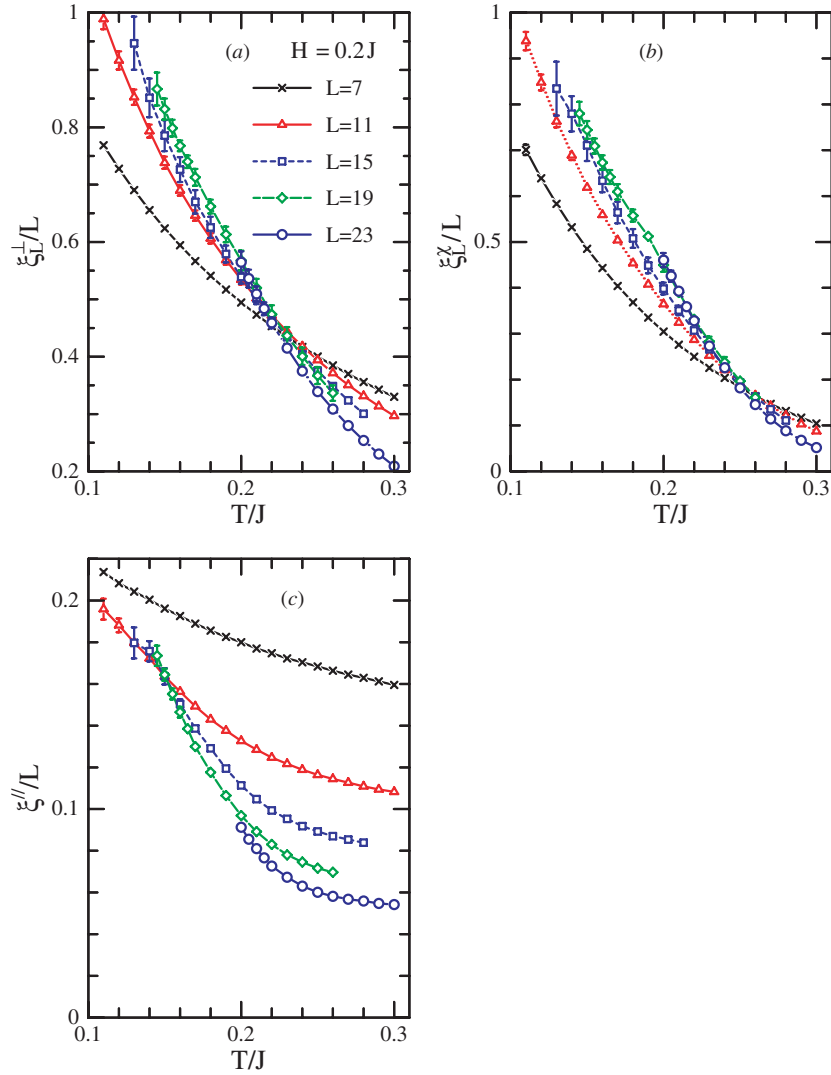


Figure 4. Plots of (a) ξ_L^\perp/L , (b) ξ_L^χ/L and (c) ξ_L^\parallel/L of the model with $D = 0$.

re-examined it³ using SG components $\{\tilde{S}_i^\alpha\}$ and $\{\tilde{S}_i^\beta\}$. Figure 5 shows ξ_L^\perp/L and ξ_L^χ/L as functions of T , where ξ_L^χ is the correlation length of the local chirality⁴. In stark contrast to the case of $D = 0$, it does not seem that the ξ_L^\perp/L for different L intersects at any temperature above $0.16J$. On the other hand, ξ_L^χ/L for larger sizes merges, similar to the IK results [18], though the results scatter rather strongly.

³ In this case, the results scatter rather strongly and the equilibration condition is relaxed. Therefore, results for the former 1/2 MC steps and those for the latter 1/2 MC steps coincide within an error of 1% at $D = 0$ and 2% at $D = 0.1J$.

⁴ A scalar chiral-overlap q_χ between the chiralities of the original spins of the two replicas, $\{S_i^\alpha\}$ and $\{S_i^\beta\}$, is given in [17]. Here we calculate it using the SG components $\{\tilde{S}_i^\alpha\}$ and $\{\tilde{S}_i^\beta\}$.

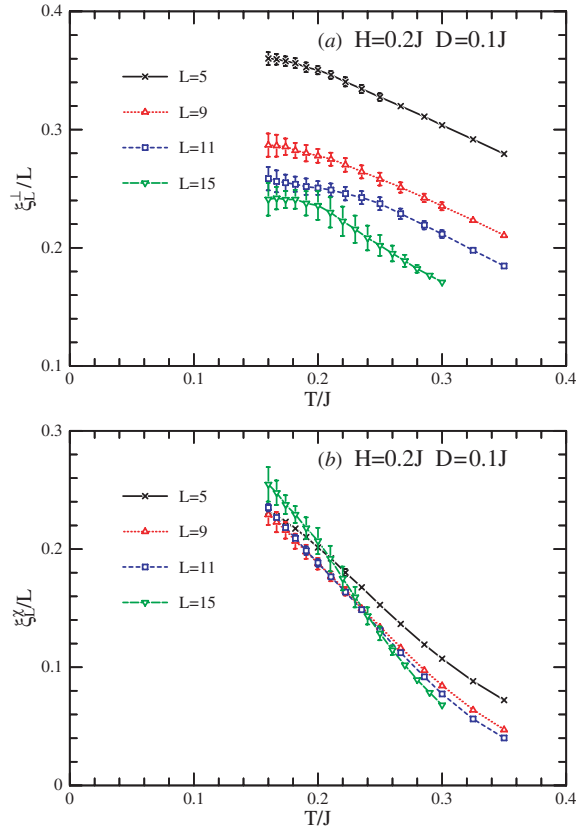


Figure 5. Plots of (a) ξ_L^\perp/L and (b) ξ_L^x/L of an anisotropic $\pm J$ model with $D = 0.1J$ at $H = 0.2J$.

Table 2. Parameters of the MC simulations at $D = 0$ and $D = 0.1J$. The over-relaxation sweep is repeated $(L + 1)/2$ times per every heat-bath sweep. N_{samp} is the number of samples, $MC S_{\text{equil}}$ is the number of MC sweeps for equilibration and $MC S_{\text{meas}}$ is the number of MC sweeps for measurement. The number of parallel tempering sweeps is equal to the number of heat-bath sweeps. T_{min} and T_{max} are the lowest and highest temperatures simulated.

| D/J | L | N_{samp} | $MC S_{\text{equil}}$ | $MC S_{\text{meas}}$ | T_{min}/J | T_{max}/J |
|-------|-----|-------------------|-----------------------|----------------------|--------------------|--------------------|
| 0 | 7 | 480 | 12 000 | 36 000 | 0.11 | 0.30 |
| 0 | 11 | 480 | 36 000 | 108 000 | 0.11 | 0.30 |
| 0 | 15 | 256 | 72 000 | 216 000 | 0.13 | 0.28 |
| 0 | 19 | 128 | 140 000 | 420 000 | 0.145 | 0.26 |
| 0 | 23 | 128 | 200 000 | 600 000 | 0.20 | 0.30 |
| 0.1 | 5 | 480 | 3 600 | 10 800 | 0.16 | 0.35 |
| 0.1 | 9 | 480 | 12 000 | 36 000 | 0.16 | 0.35 |
| 0.1 | 11 | 288 | 24 000 | 72 000 | 0.16 | 0.35 |
| 0.1 | 15 | 128 | 100 000 | 300 000 | 0.16 | 0.30 |

Does the CG phase transition occur at $D \neq 0$ and $H \neq 0$? We have also re-examined the chirality overlap distribution using the SG components $\{\hat{S}_i^\alpha\}$ and $\{\hat{S}_i^\beta\}$. Figure 6 shows

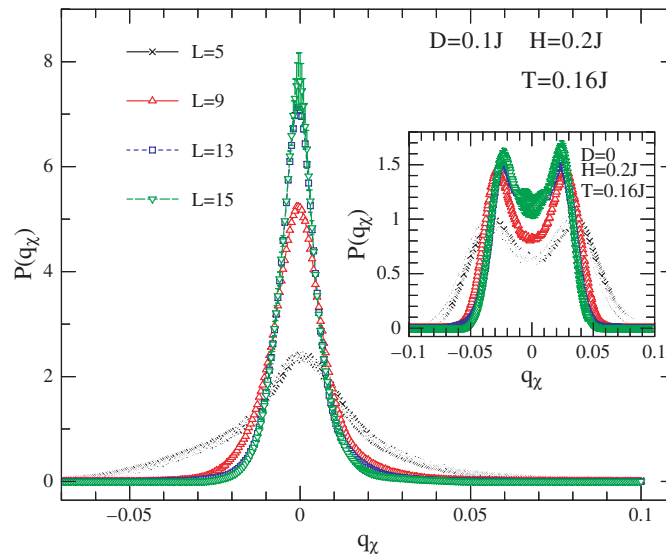


Figure 6. The chiral-overlap distribution functions at $T = 0.16J$ for $D = 0.1J$ at $H = 0.2J$. Inset: the case of $D = 0$ and $H = 0.2J$.

the chirality overlap distribution of $P(q_\chi)$ at a low temperature. In marked contrast to the IK results (see figure 8 in [18]), $P(q_\chi)$ at $T = 0.16J$ for $D = 0.1J$ exhibits a single peak at $q_\chi = 0$, which becomes sharper as L increases. This result suggests no freezing of the local chiralities in the anisotropic case. On the other hand, in the isotropic case ($D = 0$), $P(q_\chi)$ shows two-peak structures at low temperatures, similar to the IK results (see the inset of figure 6).

4. Conclusions

In summary, we have examined the phase transition of the three-dimensional $\pm J$ Heisenberg models at finite magnetic fields $H \neq 0$. When anisotropies are absent, our results suggest the occurrence of the SG (GT-like) phase transition. Of course, more extensive simulations for larger sizes would be needed to clarify the property of the phase transition, including the precise determination of transition temperatures. On the other hand, when they are present, the distribution of the chiral overlap suggests that a broken symmetry is lacking as soon as $D > 0$ for $T > 0.16J$, contrary to the IK results [18]. In order to get more confirmative results, further investigations for larger sizes and lower temperatures are strongly desired.

Acknowledgments

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