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Quantum Heisenberg spin-glass model with mixed-anisotropy interactions in applied magnetic fields

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Abstract. In the static replica symmetric approximation, a quantum Heisenberg $S = 1$ spin-glass model with single-ion uniaxial anisotropy and infinite-range random Dzyaloshinskii–Moriya (DM) interaction in applied magnetic fields is investigated. The local susceptibility and the corresponding order parameters are calculated numerically, and are found to be in good agreement with those of thermofield dynamics. The dependences of entropy and specific heat on temperature are studied numerically at various magnetic fields. It is shown that the entropy is always positive and the quantum fluctuation has a very strong effect on the specific heat. Especially, the typical crossover behaviour of the specific heat of a spin glass at various magnetic fields for mixed-anisotropy interactions is found.

1. Introduction

In recent years, it has been found that a number of hexagonal metallic spin-glass properties are strongly influenced by various types of anisotropies [1–3]. These systems can be described by a model in which, in addition to the random isotropic Heisenberg exchange interaction, a single spin uniaxial anisotropy energy $-I(S_z)^2$ is added [4, 5], where S_z is the z component of the spin operator. Theoretically, uniaxial anisotropy brings about several new features. The quantum Heisenberg spin-glass model with exchange randomness and uniaxial anisotropy has been investigated by many authors [6–10].

On the other hand, experiments on a canonical spin glass such as CuMn and AgMn in the presence of non-magnetic impurities (for example, Au or Pt) with strong spin–orbit coupling to the conduction electrons reveal the existence of an anisotropy, which can be explained by the Dzyaloshinskii–Moriya (DM) interaction [11, 12]. This interaction describes the scattering of the conduction electrons of the host (Cu) by Mn spins via the spin–orbit exchange of the non-magnetic impurity. The influence of the DM interaction has been investigated by Monte Carlo simulations for classical spin-glass system [13–15] as well as by analytical studies with random DM exchange [16–21]. Especially, it has been demonstrated that the specific heat versus temperature curve of CuMn alloys at various

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magnetic fields exhibits crossover behaviour [22]. In addition, the thermodynamic properties of classical spin-glass models have been studied by some authors [22, 23]. However, these investigations neglect the influence of quantum features of spin operators on the thermodynamic properties of spin-glass systems. Therefore, the investigation of various anisotropic agencies in quantum spin glasses constitutes a subject of current interest.

The purpose of this work is to extend the analysis of the Heisenberg $S = 1$ spin-glass model with single-ion uniaxial anisotropy and random DM anisotropy interactions in [24, 25]. Thermodynamic quantities, such as entropy and specific heat, are studied numerically at various magnetic fields. Special attention will be paid to the analysis of the crossover behaviour of specific heat–temperature curves at various magnetic fields. In order to compare with other methods, the temperature dependences of local susceptibilities and corresponding order parameters are also investigated numerically.

As emphasized earlier, a quantum spin glass in comparison with its classical counterpart is far from being a trivial one owing to the non-commutativity of the spin operators involved, which requires a special method of treatment [6, 10, 24–32]. Typically, quantum mechanics manifests itself via time-dependent self-interaction and order parameters, in contrast to the classical spin-glass systems, and the dynamics becomes an inherent feature of the problem, which significantly influences the calculation of critical lines and transition points, etc. The technique employed here to deal with both randomness and quantum features was introduced by some of us [24] and has been successfully implemented in another quantum spin-glass problem [25]. This theory allows one to treat both magnetic and thermodynamic problems.

2. Static imaginary-time replica symmetric formulation

The model Hamiltonian of the system is given by

$$H = -\sum_{ij} J_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j - \sum_{ij} \boldsymbol{D}_{ij} \cdot (\boldsymbol{S}_i \times \boldsymbol{S}_j) - \sum_i [I(S_{iz})^2 + hS_{iz}] \tag{1}$$

where $\boldsymbol{S} = (S_x, S_y, S_z)$ is the quantum spin operator associated with the local moment S. The first two sums are over all possible distinct pairs (i, j) of sites. The strengths of exchange interactions J_{ij} and $\boldsymbol{D}_{ij}$, the latter corresponding to the DM interaction, are quenched and independently distributed with symmetric Gaussian probability distributions

$$P(J_{ij}) = \left(\frac{N}{2\pi J^2}\right)^{1/2} \exp\left(-\frac{N J_{ij}^2}{2J^2}\right) \tag{2a}$$

and

$$W(\boldsymbol{D}_{ij}) = \left(\frac{N}{2\pi D^2}\right)^{3/2} \exp\left(-\frac{N \boldsymbol{D}_{ij}^2}{2D^2}\right) \tag{2b}$$

respectively. I is the strength of the single-ion uniaxial anisotropy . As usual, the scaling of the variances J/N and D/N ensures a sensible thermodynamic limit $N \to +\infty$. The external magnetic field h is supposed to be in the direction of the z axis.

The derivation of the free energy is a straightforward generalization of the work by Bray and Moore [26]. In order to average over the random couplings $\{J_{ij}\}$ and $\{\boldsymbol{D}_{ij}\}$, we apply the replica method and Matsubara imaginary-time functional-integral technique,

which allows us to treat the non-commuting spin operators as C numbers. The present calculation follows [24] closely; we therefore quote here only the final saddle-point free energy per spin. One gets

$$n\beta F[R,Q] = \left(\frac{J\beta}{2}\right)^2 \int_0^1 d\tau \int_0^1 d\tau' \left(\sum_\alpha \sum_{\mu\nu\sigma\rho} R^\alpha_{\mu\nu}(\tau,\tau') R^\alpha_{\sigma\rho}(\tau,\tau') P_{\mu\nu\sigma\rho} + \sum_{\alpha\neq\gamma} \sum_{\mu\nu\sigma\rho} Q^{\alpha\gamma}_{\mu\nu}(\tau,\tau') Q^{\alpha\gamma}_{\sigma\rho}(\tau,\tau') P_{\mu\nu\sigma\rho} \right) - \ln \mathrm{Tr}\, T_\tau \exp(-\beta H_{\mathrm{eff}}[R,Q]) \quad (3)$$

$$-\beta H_{\mathrm{eff}}[R,Q] = \tfrac{1}{2}(J\beta)^2 \int_0^1 d\tau \int_0^1 d\tau' \left(\sum_\alpha \sum_{\mu\nu\sigma\rho} R^\alpha_{\mu\nu}(\tau,\tau') P_{\mu\nu\sigma\rho} S^\alpha_\sigma(\tau) S^\alpha_\rho(\tau') + \sum_{\alpha\neq\gamma} \sum_{\mu\nu\sigma\rho} Q^{\alpha\gamma}_{\mu\nu}(\tau,\tau') P_{\mu\nu\sigma\rho} S^\alpha_\sigma(\tau) S^\gamma_\rho(\tau') \right) + \beta \int_0^1 d\tau \left(\sum_\alpha h S^\alpha_z(\tau) + I[S^\alpha_z(\tau)]^2 \right) \quad (4)$$

with

$$P_{\mu\nu\sigma\rho} = d^2 \delta_{\mu\nu}\delta_{\sigma\rho} + (1-d^2)\delta_{\mu\sigma}\delta_{\nu\rho} \qquad d = D/J \qquad \beta = 1/T \qquad (k_B = 1)$$

where T_τ denotes the 'time'-ordering operator, which rearranges the operators in the expansion of the exponent in the order of decreasing 'time' arguments τ. Functional differentiation with respect to $R^\alpha_{\mu\nu}(\tau,\tau')$ and $Q^{\alpha\gamma}_{\mu\nu}(\tau,\tau')$ yields

$$\begin{aligned} R^\alpha_{\mu\nu}(\tau,\tau') &= \langle T_\tau S^\alpha_\mu(\tau) S^\alpha_\nu(\tau') \rangle \\ Q^{\alpha\gamma}_{\mu\nu}(\tau,\tau') &= \langle T_\tau S^\alpha_\mu(\tau) S^\gamma_\nu(\tau') \rangle \end{aligned} \quad (5)$$

where S^α_μ is a Cartesian component of S^α; $\alpha, \gamma = 1, 2, \ldots, n$ are replica indices. The angular brackets denote an average with respect to the effective Hamiltonian in (4). Non-trivial solutions for these functions stand for the dynamic spin self-interaction and spin-glass order parameter, respectively. Furthermore, within the static replica symmetric approximation, these order parameters and self-interactions can be separated into longitudinal (L) and transverse (T) components by the decomposition

$$\begin{aligned} Q_{\mu\nu} &= \delta_{\mu\nu}[Q_L \delta_{\mu z} + Q_T(1-\delta_{\mu z})] \\ R_{\mu\nu} &= \delta_{\mu\nu}[R_L \delta_{\mu z} + R_T(1-\delta_{\mu z})]. \end{aligned} \quad (6)$$

After substituting these equations into the free energy (equations (3) and (4)) and applying Hubbard–Stratonovich transformation to linearize those quadratic forms in the effective Hamiltonian, the free-energy density becomes

$$\beta F[R,Q] = (J\beta/2)^2 \{ R_L^2 + 2(1+d^2)R_T^2 + 4d^2 R_L R_T - [Q_L^2 + 2(1+d^2)Q_T^2 + 4d^2 Q_L Q_T] \} - \int Dz \ln L(z) \quad (7)$$

$$L(z) = \int Dz_1 \Phi(z, z_1) \qquad \Phi(z, z_1) = \sum_{n=-s}^{s} \exp(-\beta\lambda_n) \quad (8)$$

where λ_n denotes the eigenvalue of the effective Hamiltonian in equation (4). The abbreviation

$$\int \mathrm{D}z \cdots = \int_{-\infty}^{+\infty} \frac{\mathrm{d}^3 z}{(2\pi)^{3/2}} \exp\left(-\frac{z^2}{2}\right) \cdots \tag{9}$$

is used.

The stationarity of the functional $F[R, Q]$ in equation (7) with respect to the spin self-interactions and spin-glass order parameters gives the following self-consistent equations [24]:

$$R_{\mathrm{L}} = \frac{1}{(a_4 J\beta)^2} \int \frac{\mathrm{D}z}{L(z)} \int \mathrm{D}z_1 \Phi(z, z_1)(z_1^2 - 1) \tag{10}$$

$$R_{\mathrm{T}} = \frac{1}{2(a_2 J\beta)^2} \int \frac{\mathrm{D}z}{L(z)} \int \mathrm{D}z_1 \Phi(z, z_1)(x_1^2 + y_1^2 - 2) \tag{11}$$

$$Q_{\mathrm{L}} = \frac{1}{(a_4 J\beta)^2} \int \mathrm{D}z \left(\frac{1}{L(z)} \int \mathrm{D}z_1 \Phi(z, z_1) z_1\right)^2 \tag{12}$$

$$Q_{\mathrm{T}} = \frac{1}{(a_2 J\beta)^2} \int \mathrm{D}z \left(\frac{1}{L(z)} \int \mathrm{D}z_1 \Phi(z, z_1) x_1\right)^2. \tag{13}$$

The corresponding parameters are defined by

$$a_1 = [d^2 Q_{\mathrm{L}} + (1 + d^2) Q_{\mathrm{T}}]^{1/2} \qquad a_2 = [d^2(R_{\mathrm{L}} - Q_{\mathrm{L}}) + (1 + d^2)(R_{\mathrm{T}} - Q_{\mathrm{T}})]^{1/2}$$

$$a_3 = [Q_{\mathrm{L}} + 2d^2 Q_{\mathrm{T}}]^{1/2} \qquad a_4 = [R_{\mathrm{L}} - Q_{\mathrm{L}} + 2d^2(R_{\mathrm{T}} - Q_{\mathrm{T}})]^{1/2}.$$

The unaveraged susceptibility is given by

$$\chi_{\mu\nu}(z) = -[\partial m_\mu(z)/\partial h_\nu]|_{h_\nu \to 0} \tag{14}$$

while

$$m_\mu(z) = -[1/\beta L(z)][\partial L(z)/\partial h_\mu]|_{h_\mu \to 0} \tag{15}$$

where h_θ ($\theta = \mu, \nu$) denotes an infinitesimal applied magnetic field. Furthermore, since the rotational symmetry with respect to the z axis (the direction of the fixed magnetic field) remains after the DM interaction has been averaged over, the matrix element of the local susceptibility tensor can be obtained readily as

$$\chi_{\mu\nu} = \frac{1}{a_\mu a_\nu \beta J^2} \int \mathrm{D}z \left(\frac{1}{L(z)} \int \mathrm{D}z_1 \Phi(z, z_1)(\mu_1 \nu_1 - \delta_{\mu\nu}) - \frac{1}{L^2(z)} \int \mathrm{D}z_1 \Phi(z, z_1)\mu_1 \int \mathrm{D}z_1 \Phi(z, z_1)\nu_1\right) \tag{16}$$

where $a_x = a_y = a_2$ and $a_z = a_4$.

For spin number $S = 1$, the eigenvalue λ_n of the exponent function in equation (8) can be specified explicitly as

$$\lambda_n = 2\tilde{I}/3 + 2r \cos\{\tfrac{1}{3}[\varphi + 2(n+1)\pi]\} \qquad (n = -1, 0, 1) \tag{17}$$

and

$$r = J\{\tfrac{1}{3}[(a_1x + a_2x_1)^2 + (a_1y + a_1y_1)^2 + (a_3z + a_4z_1 + h/J)^2] + \tilde{I}^2/9\}^{1/2} \tag{18}$$

$$\varphi = \cos^{-1}[-q/(2r^3)] \tag{19}$$

$$q = J^3\{(\tilde{I}/3)[(a_1x+a_2x_1)^2+(a_1y+a_2y_1)^2-2(a_3z+a_4z_1+h/J)^2]+2\tilde{I}^3/27\} \qquad \tilde{I} = I/J. \tag{20}$$

One of the advantages in the present static approximation is to calculate directly the thermodynamic quantities from the free energy in (7). Therefore, we will focus here on the entropy and the specific heat. The entropy of the system with fixed volume V can be determined by the following thermodynamic formula:

$$S_V = -\partial F[R, Q]/\partial T \tag{21}$$

and the corresponding specific heat is

$$C_V = T\partial S_V/\partial T. \tag{22}$$

Since the local susceptibility, entropy and specific heat are all functions of order parameters R and Q (which depend on temperature), they must be solved self-consistently by using equations (10)–(13).

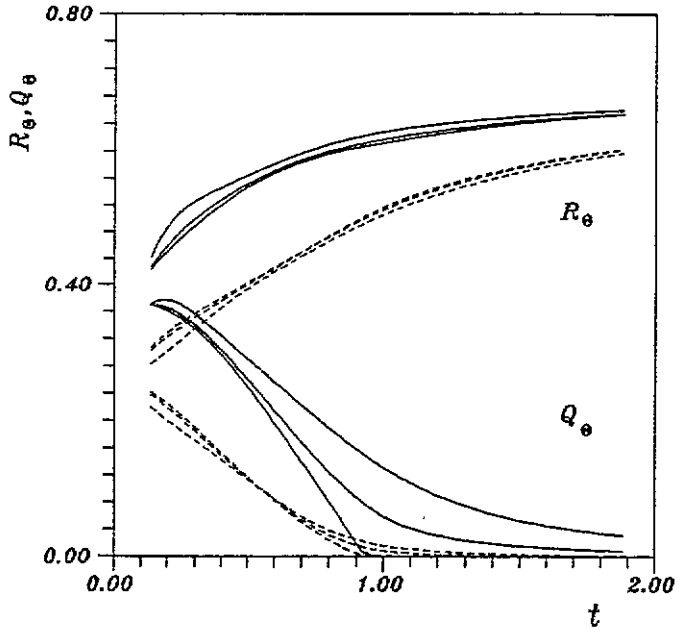

Figure 1. The temperature dependence of the longitudinal (R_L and Q_L; full curves) and transverse (R_T and Q_T; broken curves) spin-glass order parameters and spin self-interactions for different reduced magnetic fields $\tilde{h} = h/J$. The upper curves refer to R_θ and the lower ones refer to Q_θ; $\tilde{h} = 0.0$, 0.15 and 0.3 correspond to longitudinal components from top to bottom and to transverse from bottom to top, respectively, and $S = 1$, $d = 0.3$, $\tilde{I} = 0.2$.

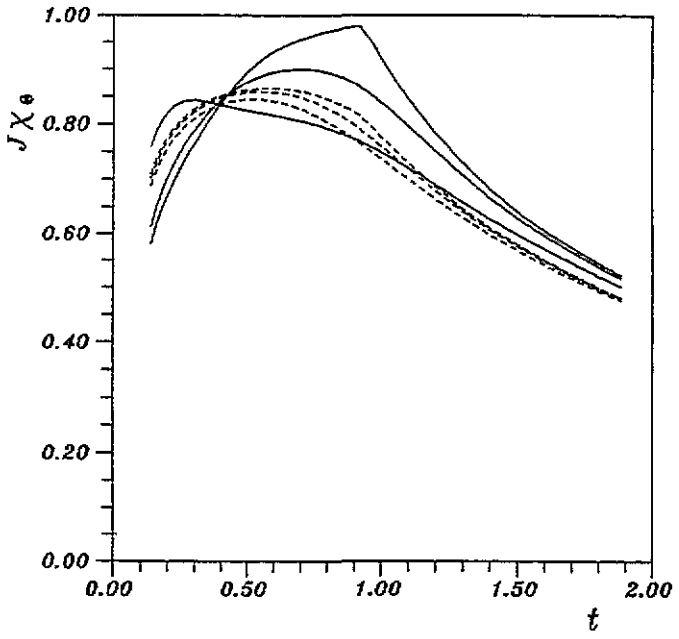

Figure 2. The local susceptibilities change with temperature for the same conditions as in figure 1. The longitudinal (full curves) and the transverse components (broken curves) correspond to the reduced magnetic fields $\tilde{h} = 0.0$, 0.15 and 0.3 from top to bottom (at high temperatures), respectively.

3. Numerical analysis

In order to avoid complications caused by mixing of various longitudinal and transverse modes in self-consistent equations, we restrict our consideration to weak anisotropies and take $d = 0.3$ and $\tilde{I} = 0.2$. However, it turns out that in this restricted case a great richness of thermodynamic features already occurs.

Figure 1 shows that spin self-interactions and spin-glass order parameters change with temperature [$t = 3T/(2J)$] for different magnetic fields for spin number $S = 1$. Obviously, the spin-glass order parameters and corresponding self-interactions tend to coincide as temperature decreases. The longitudinal components of spin self-interaction and spin-glass order parameter R_L, Q_L increase with magnetic field. Longitudinal spin-glass order parameters Q_L are always non-zero in external magnetic fields. Obviously, the spin self-interaction and the spin-glass order parameter for zero magnetic field are split into two parts, respectively. Figure 2 gives the longitudinal and transverse susceptibility–temperature curves for the same condition as in figure 1. It is found that the longitudinal and transverse susceptibilities are mixed strongly due to the two kinds of anisotropies. The result is in qualitative agreement with that of the thermofield dynamics by Kopeć and Büttner [10,21]. In addition, the longitudinal component of local susceptibility increases with magnetic field at low temperatures, while it decreases as the magnetic field increases. This behaviour describes characteristics of spin-glass systems with single-ion uniaxial anisotropy.

The entropy–temperature curves are plotted in figure 3. It has been demonstrated that the entropy has a weak dependence on the external magnetic fields. It is obvious that the entropy is positive at zero temperature. It is argued that, since two anisotropies suppress quantum fluctuation at low temperature, the replica symmetric solutions become stable [24]. Figure 4

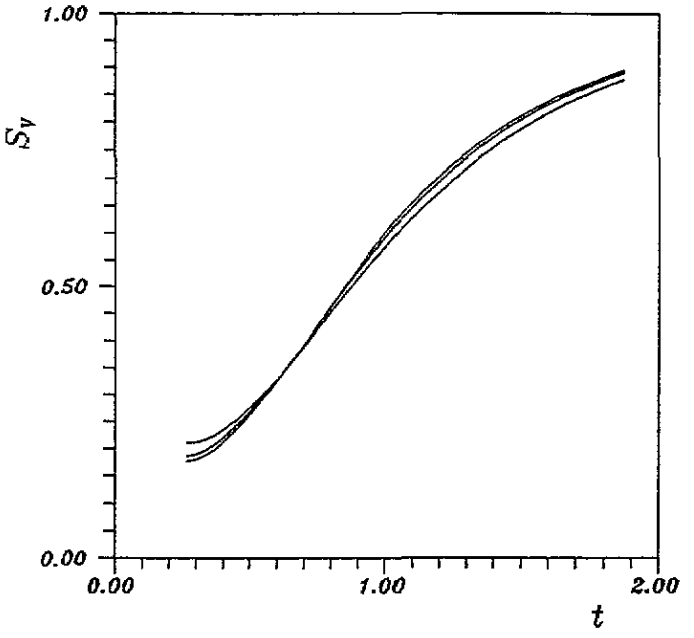

Figure 3. The entropy–temperature curves at reduced external magnetic fields $\tilde{h} = 0.0$, 0.15 and 0.3 (from bottom to top); the rest of the parameters are the same as in figure 1.

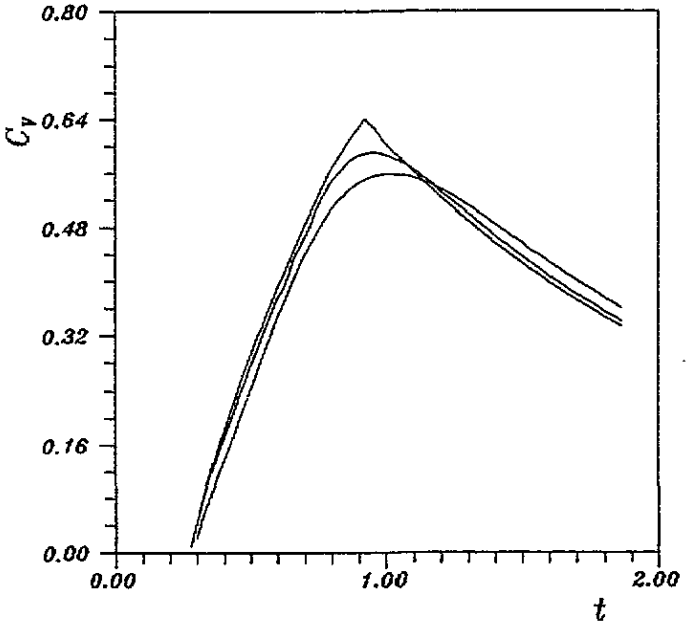

Figure 4. The specific heat–temperature curves for the same conditions as in figure 1. The curves from top to bottom are for $\tilde{h} = 0.0$, 0.15 and 0.3, respectively.

shows the temperature dependence of specific heat. It is found that cusps of specific-heat

curves are smoothed by the external magnetic field. Especially, the specific-heat curves for different magnetic fields exhibit a typical crossover behaviour, which has been observed by Brodale *et al* [22] in experiments on CuMn alloys. We found that this feature can appear even if there exist weak single-ion uniaxial anisotropy and random DM interaction.

It should be stressed that an exact calculation of the thermodynamic quantities for the quantum spin glass, such as specific heat and entropy, requires precise knowledge of the time dependence of the spin self-interaction involved. Therefore, this means that calculation of the exact thermodynamic quantities will depend on the detailed time dependence of $R(\tau)$ in the present Matsubara approach with replica method. It seems that the complexity of the problem prevents an analytically tractable approach. However, as was pointed out earlier [24], the static approximations will give a rather good result when the temperature is not too low. On the other hand, compared with that of the thermofield dynamics (TFD) [10, 21], the present calculations are in basic agreement with theirs. We argue that the reason may be that both the static and instantaneous approximations neglect the dependence of spin self-interaction on time.

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