Quantum Heisenberg spin glass with Dzyaloshinskii-Moriya interactions

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A theory of the quantum Heisenberg spin-glass model with Dzyaloshinskii-Moriya interactions is presented in external magnetic fields for arbitrary spin. The imaginary-time functional-integral technique and the replica method are used. The model is investigated numerically within the static approximation. The smallest eigenvalue of the Hessian matrix is obtained by a generalized Almeida-Thouless method and the stability conditions are found, which give the upper and lower critical lines, respectively. Anisotropy-temperature phase diagrams are evaluated for different spin numbers in the case of no applied field. Thermodynamic functions, such as the entropy and the specific heat, are studied. Additionally, we can show that the local susceptibilities for different spin numbers are stabilized on a plateau at low temperatures by a small amount of the anisotropy.

I. INTRODUCTION

In recent years, considerable research has been devoted to anisotropic spin-glass systems. Experimentally, macroscopic anisotropy is found in the hysteresis of the remanent magnetization in a lot of spin-glass systems.[1,2] The anisotropy is found to behave either uniaxially or unidirectionally. Spin glasses with uniaxial anisotropy behave either Ising-like or Heisenberg-like, depending on the magnitude of the single-spin anisotropy energy. This type of anisotropy has been the subject of some recent theoretical investigations.[3–7]

Additionally, unidirectional anisotropy has been found in otherwise isotropic spin glasses due to nonmagnetic impurities.[8] This kind of anisotropy can be explained by Dzyaloshinskii-Moriya[9] (DM) interactions in addition to the usual isotropic exchange interactions. The DM interaction has the form

$$H_{\mathrm{DM}} = \sum_{ij} \mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j) \tag{1}$$

with the vector coupling $\mathbf{D}_{ij} = -\mathbf{D}_{ji}$ between spins on lattice sites i and j. For example, in CuMn a conduction electron of the host (Cu) is first scattered by a Mn spin, then by a nonmagnetic impurity via spin-orbit interaction, and finally by a second Mn spin. Specifically, this anisotropy does not depend on the crystal directions, but on the field-induced remanent magnetization. As has been demonstrated recently,[10] in a magnetic field a strong crossover from an Ising-type or de Almeida–Thouless (AT) -type[11] to a Heisenberg or Gabay-Toulouse (GT) -type[12] transition is observed due to DM interactions.

Besides the experimental work, numerous theoretical studies have been devoted to spin-glass systems with DM interactions. Bray and Moore[13] considered a classical Heisenberg spin-glass model with dipolar and DM interactions and pointed out that the model exhibits the characteristic behavior of an Ising spin glass. Fischer[14] investigated a classical soft spin-glass model with DM anisotropy within the mean-field approximation and found the crossover behavior of the upper critical line. Dasgupta and Yao[15] studied the nature of the macroscopic anisotropy in a classical Ruderman-Kittel-Kasuya-Yosida (RKKY) spin glass with weak DM interactions by a Monte Carlo simulation. Their results reproduced several features observed in hysteresis and torque experiments qualitatively. Subsequently, Goldbart[16] investigated a classical vector spin glass with quenched random DM interactions and uniaxial anisotropy within the replica theory. He predicted spin-glass order below a critical temperature and established Parisi's[17] replica symmetry-breaking scheme. In the limit of infinite anisotropy its thermodynamic behavior becomes that of the Ising spin glass.

Since quantum fluctuations become important at low temperatures, it is desirable to extend these investigations to quantum models. Quantum spin glasses have been studied for the first time by Sommers[18] and by Bray and Moore[19] who deal with an isotropic quantum Heisenberg spin glass. The quantum nature of the spins is taken care of by introducing a local dependence of the dynamical variables on an imaginary time. The static approximation imposed by these authors is known to give rather good results at not too low temperatures, and it is applied to a large number of different spin-glass systems.[5,6,20–22] Going beyond the static approximation means to take the time dependence of the dynamic self-interactions into account explicitly. This is possible only for some basic quantum spin glasses without an applied field.[7,23,24]

So far the quantum Heisenberg spin glass with DM anisotropy has been studied only by Kopeć and Büttner[25] with the help of the thermofield dynamics. They have calculated numerically field-temperature phase diagrams and anisotropy-temperature phase diagrams for different values of the anisotropy and the applied magnetic field, respectively. These calculations are based on a rather crude approximation for the time dependence of the relevant Green's functions. It is therefore of great interest to study the same model with other methods.

In the present paper we investigate this model within the static approximation. We introduce time-dependent operators and the replica method in order to treat the quantum nature of the spins and the quenched average, respectively. The self-consistency equations are obtained in the general case. We calculate phase diagrams, order parameters, local susceptibilities, and thermodynamic quantities. The results are compared with those obtained in Ref. 25.

II. MODEL HAMILTONIAN AND REPLICA METHOD

The Hamilton operator for a Heisenberg spin glass with Sherrington-Kirkpatrick[26] (SK) exchange interactions and infinite-ranged random Dzyaloshinsky-Moriya interactions is given by

$$H = -\sum_{ij} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j - \sum_{ij} \mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j) - \sum_i \mathbf{h}\cdot\mathbf{S}_i, \tag{2}$$

where $\mathbf{h}$ denotes an external magnetic field. The sums extend over all distinct pairs of sites (ij) and the exchange interactions J_{ij} and $\mathbf{D}_{ij}$ are random parameters with symmetric Gaussian probability distributions

$$P(J_{ij}) = \left(\frac{N}{2\pi J^2}\right)^{1/2} \exp\left(-\frac{NJ_{ij}^2}{2J^2}\right) \tag{3}$$

and

$$W(\mathbf{D}_{ij}) = \left(\frac{N}{2\pi D^2}\right)^{3/2} \exp\left(-\frac{N\mathbf{D}_{ij}\cdot\mathbf{D}_{ij}}{2D^2}\right). \tag{4}$$

The spin operators $\mathbf{S}_i$ obey the standard spin-commutation relations. In order to carry out the average over random bonds we use the replica method, where the average of the n-time replica partition function Z is given by

$$\langle Z^n\rangle_{JD} = \int_{-\infty}^{+\infty} \prod_{ij} dJ_{ij} P(J_{ij}) \int_{-\infty}^{+\infty} \prod d\mathbf{D}_{ij} W(\mathbf{D}_{ij}) \times \mathrm{Tr}\, T_\tau \exp\left\{\beta \int_0^1 d\tau \sum_{\alpha=1}^{n} \left[\left(\sum_{ij} J_{ij}\mathbf{S}_i^\alpha(\tau)\cdot\mathbf{S}_j^\alpha(\tau) + \sum_{ij}\mathbf{D}_{ij}\cdot[\mathbf{S}_i^\alpha(\tau)\times\mathbf{S}_j^\alpha(\tau)]\right) + \sum_i \mathbf{h}\cdot\mathbf{S}_i^\alpha(\tau)\right]\right\}, \tag{5}$$

and where we introduce a formal dependence of the spin operators on the imaginary time τ in order to treat them as c numbers.[18,19] The imaginary time-ordering operator T_τ rearranges the operators in the expansion of the exponential in Eq. (5). Now, the integrals defining the J and D averages can be performed readily. The n-replica partition function may be rewritten as the following quadratic form:

$$\langle Z^n\rangle_{JD} = \mathrm{Tr}\, T_\tau \exp\left\{\frac{(\beta J)^2}{4N}\int_0^1 d\tau \int_0^1 d\tau' \left[(1-d^2)\sum_\alpha\sum_{\mu\nu}\left(\sum_i S_{i\mu}^\alpha(\tau)S_{i\nu}^\alpha(\tau')\right)^2 + d^2\sum_\alpha\left(\sum_{i\mu}S_{i\mu}^\alpha(\tau)S_{i\mu}^\alpha(\tau')\right)^2 + (1-d^2)\sum_{\alpha\neq\beta}\sum_{\mu\nu}\left(\sum_i S_{i\mu}^\alpha(\tau)S_{i\nu}^\beta(\tau')\right)^2 + d^2\sum_{\alpha\neq\beta}\left(\sum_{i\mu}S_{i\mu}^\alpha(\tau)S_{i\mu}^\beta(\tau')\right)^2\right] + \beta\int_0^1 d\tau\sum_{i\alpha}\mathbf{h}\cdot\mathbf{S}_i^\alpha(\tau)\right\}, \tag{6}$$

where we set $d = D/J$. The variable $S_{i\mu}^\alpha(\tau)$ is a Cartesian component of the operator $\mathbf{S}_i^\alpha(\tau)$. These terms can be linearized via a Hubbard-Stratonovich transformation

$$\langle Z^n\rangle_{JD} = \int\prod_\alpha \mathcal{D}\Delta^\alpha(\tau,\tau')\int\prod_{\mu\nu,\alpha}\mathcal{D}R_{\mu\nu}^\alpha(\tau,\tau')\int\prod_{\alpha\neq\beta}\mathcal{D}\Lambda^{\alpha\beta}(\tau,\tau')\int\prod_{\mu\nu,\alpha\neq\beta}\mathcal{D}Q_{\mu\nu}^{\alpha\beta}(\tau,\tau') \times \exp\left(-Nn\beta F[\mathbf{R},\boldsymbol{\Delta},\mathbf{Q},\boldsymbol{\Lambda}]\right), \tag{7}$$

where in the limit $N \to \infty$ the functional integrals can be evaluated by the method of steepest descents and the problem is reduced to a single-site problem. Due to the stationarity of the free energy one finds[16]

$$\Lambda^{\alpha\beta}(\tau,\tau') = \sum_{\mu} Q^{\alpha\beta}_{\mu\mu}(\tau,\tau'), \qquad \Delta^{\alpha}(\tau,\tau') = \sum_{\mu} R^{\alpha}_{\mu\mu}(\tau,\tau'). \tag{8}$$

The free energy and the effective Hamiltonian become

$$n\beta F[\mathbf{R},\mathbf{Q}] = \left(\frac{\beta J}{2}\right)^2 \int_0^1 d\tau \int_0^1 d\tau' \left[\sum_{\alpha} \sum_{\mu\nu\sigma\rho} R^{\alpha}_{\mu\nu}(\tau,\tau') R^{\alpha}_{\sigma\rho}(\tau,\tau') P_{\mu\nu\sigma\rho} + \sum_{\alpha\neq\beta} \sum_{\mu\nu\sigma\rho} Q^{\alpha\beta}_{\mu\nu}(\tau,\tau') Q^{\alpha\beta}_{\sigma\rho}(\tau,\tau') P_{\mu\nu\sigma\rho} \right] - \ln \mathrm{Tr}\, T_{\tau} \exp(-\beta H_{\mathrm{eff}}[\mathbf{R},\mathbf{Q}]), \tag{9}$$

$$-\beta H_{\mathrm{eff}}[\mathbf{R},\mathbf{Q}] = \tfrac{1}{2}(\beta J)^2 \int_0^1 d\tau \int_0^1 d\tau' \left[\sum_{\alpha} \sum_{\mu\nu\sigma\rho} R^{\alpha}_{\mu\nu}(\tau,\tau') P_{\mu\nu\sigma\rho} S^{\alpha}_{\sigma}(\tau) S^{\alpha}_{\rho}(\tau') + \sum_{(\alpha\neq\beta)} \sum_{\mu\nu\sigma\rho} Q^{\alpha\beta}_{\mu\nu}(\tau,\tau') P_{\mu\nu\sigma\rho} S^{\alpha}_{\sigma}(\tau) S^{\beta}_{\rho}(\tau') \right] + \beta \int_0^1 d\tau \sum_{\alpha} \mathbf{h}\cdot\mathbf{S}^{\alpha}(\tau), \tag{10}$$

with

$$P_{\mu\nu\sigma\rho} = d^2 \delta_{\mu\nu}\delta_{\sigma\rho} + (1-d^2)\delta_{\mu\sigma}\delta_{\nu\rho}. \tag{11}$$

III. THE STATIC APPROXIMATION IN THE REPLICA-SYMMETRIC APPROACH

We consider replica symmetry and the order parameters and self-interactions as independent of the times τ and τ'. Additionally, magnetic fields are applied in the z direction only. The order parameters and self-interactions may be separated now into longitudinal (L) and transverse (T) components by the decomposition

$$R_{\mu\nu} = \delta_{\mu\nu}\left[R_L \delta_{\mu z} + R_T(1-\delta_{\mu z})\right], \qquad Q_{\mu\nu} = \delta_{\mu\nu}\left[Q_L \delta_{\mu z} + Q_T(1-\delta_{\mu z})\right]. \tag{12}$$

After substituting these equations into the free energy [Eqs. (9) and (10)], Hubbard-Stratonovich transformations are applied to linearize the quadratic forms in the effective Hamiltonian. The free-energy density becomes

$$\beta F[\mathbf{R},\mathbf{Q}] = \left(\frac{\beta J}{2}\right)^2 \left\{ R_L^2 + 2(1+d^2)R_T^2 + 4d^2 R_L R_T - \left[Q_L^2 + 2(1+d^2)Q_T^2 + 4d^2 Q_L Q_T\right] \right\} - \int D\mathbf{z} \ln L(\mathbf{z}), \tag{13}$$

with

$$L(\mathbf{z}) = \int D\mathbf{z}_1 \mathrm{Tr} \exp\left\{ \beta J \left[a_1(xS_x + yS_y) + a_2(x_1 S_x + y_1 S_y) + a_3 z S_z + a_4 z_1 S_z\right] + \beta h S_z \right\} \tag{14}$$

$$= \int D\mathbf{z}_1 \frac{\sinh[(2S+1)\Omega(\mathbf{z},\mathbf{z}_1)]}{\sinh[\Omega(\mathbf{z},\mathbf{z}_1)]} \equiv \int D\mathbf{z}_1 \Phi_S(\Omega) \tag{15}$$

and

$$a_1 = \sqrt{d^2 Q_L + (1+d^2)Q_T}, \quad a_2 = \sqrt{d^2(R_L - Q_L) + (1+d^2)(R_T - Q_T)}, \quad a_3 = \sqrt{Q_L + 2d^2 Q_T}, \quad a_4 = \sqrt{R_L - Q_L + 2d^2(R_T - Q_T)}. \tag{16}$$

Throughout we use the abbreviation

$$\int D\mathbf{z}\, A(\mathbf{z}) = \int_{-\infty}^{+\infty} \frac{d^3 z}{(2\pi)^{3/2}} \exp(-\mathbf{z}^2/2) A(\mathbf{z}). \tag{17}$$

The function $\Omega(\mathbf{z}, \mathbf{z}_1)$ is given by

$$\Omega(\mathbf{z}, \mathbf{z}_1) = \frac{\beta J}{2} \sqrt{(a_1 x + a_2 x_1)^2 + (a_1 y + a_2 y_1)^2 + (a_3 z + a_4 z_1 + h/J)^2}. \tag{18}$$

The stationarity of the functional $F[\mathbf{R}, \mathbf{Q}]$ with respect to the spin self-interactions and spin-glass order parameters gives the following self-consistency equations:

$$\begin{aligned}
R_L &= -2d^2 R_T + \frac{1}{(\beta J)^2} \int \frac{D\mathbf{z}}{L(\mathbf{z})} \int D\mathbf{z}_1 \Phi_S(\Omega) \left[\frac{d^2}{a_2^2}(x_1^2 + y_1^2 - 2) + \frac{1}{a_4^2}(z_1^2 - 1)\right], \\
R_T &= \frac{-d^2}{1+d^2} R_L + \frac{1}{2(\beta J)^2 (1+d^2)} \int \frac{D\mathbf{z}}{L(\mathbf{z})} \int D\mathbf{z}_1 \Phi_S(\Omega) \left[\frac{1+d^2}{a_2^2}(x_1^2 + y_1^2 - 2) + \frac{2d^2}{a_4^2}(z_1^2 - 1)\right], \\
Q_L &= -2d^2 Q_T + \frac{1}{(\beta J)^2} \int \frac{D\mathbf{z}}{L(\mathbf{z})} \int D\mathbf{z}_1 \Phi_S(\Omega) \left[\frac{d^2}{a_2^2}(x_1^2 + y_1^2 - 2) + \frac{1}{a_4^2}(z_1^2 - 1)\right] \\
&\quad - \frac{1}{(\beta J)^2} \int D\mathbf{z} \left[\frac{d^2}{a_1^2}(x^2 + y^2 - 2) + \frac{1}{a_3^2}(z^2 - 1)\right] \ln L(\mathbf{z}), \\
Q_T &= -\frac{d^2}{1+d^2} Q_L + \frac{1}{2(\beta J)^2 (1+d^2)} \left[\int \frac{D\mathbf{z}}{L(\mathbf{z})} \int D\mathbf{z}_1 \Phi_S(\Omega) \left(\frac{1+d^2}{a_2^2}(x_1^2 + y_1^2 - 2) + \frac{2d^2}{a_4^2}(z_1^2 - 1)\right)\right. \\
&\quad \left. - \int D\mathbf{z} \left(\frac{1+d^2}{a_1^2}(x^2 + y^2 - 2) + \frac{2d^2}{a_3^2}(z^2 - 1)\right) \ln L(\mathbf{z})\right].
\end{aligned} \tag{19}$$

Now the susceptibility tensors can be determined by

$$\begin{aligned}
\chi_{\mu\nu} &= -\frac{\partial^2 f[\mathbf{R}, \mathbf{Q}]}{\partial h_\mu \partial h_\nu} \\
&= \frac{1}{a_\nu a_\mu \beta J^2} \int D\mathbf{z} \left[\frac{1}{L(\mathbf{z})} \int D\mathbf{z}_1 \Phi_S(\Omega)(\mu_1 \nu_1 - \delta_{\mu\nu}) - \frac{1}{L^2(\mathbf{z})} \int D\mathbf{z}_1 \Phi_S(\Omega) \mu_1 \int D\mathbf{z}_1 \Phi_S(\Omega) \nu_1\right] \\
&\equiv \int D\mathbf{z}\, \chi_{\mu\nu}(\mathbf{z}),
\end{aligned} \tag{20}$$

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

Let us now consider the special case with no applied field h. Due to symmetry one finds

$$R_T = R_L = R, \qquad Q_T = Q_L = Q \tag{21}$$

and the free-energy density [Eq. (14)] becomes

$$\beta F[R, Q] = 3 \left(\frac{\beta J}{2}\right)^2 (1 + 2d^2)(R^2 - Q^2) - \int D\mathbf{z} \ln L(\mathbf{z}). \tag{22}$$

It is now advantageous to introduce spherical coordinates where Ω is given by

$$\Omega = \frac{\beta J}{2} \sqrt{a_1^2 \rho^2 + a_2^2 \rho_1^2 + 2 a_1 a_2 \rho \rho_1 \cos\theta_1}, \tag{23}$$

since $a_1 = a_3$ and $a_2 = a_4$ in this special case $h = 0$. The corresponding self-consistency equations are

$$\begin{aligned}
R &= \frac{2}{3(\beta J)^2 (1+2d^2)(R-Q)} \int_0^\infty \frac{d\rho}{\sqrt{2\pi}} \rho^2 e^{-\rho^2/2} \frac{1}{L(\rho)} \int_0^\infty \frac{d\rho_1}{\sqrt{2\pi}} \int_{-1}^{1} d\cos\theta_1\, \rho_1^2 e^{-\rho_1^2/2}\, \Phi_S(\Omega)(\rho_1^2 - 3), \\
Q &= R + \frac{2}{3(\beta J)^2 (1+2d^2) Q} \int_0^\infty \frac{d\rho}{\sqrt{2\pi}} e^{-\rho^2/2} \rho^2 (3 - \rho^2) \ln L(\rho),
\end{aligned} \tag{24}$$

with

$$L(\rho) = \int_0^\infty \frac{d\rho_1}{\sqrt{2\pi}} \int_{-1}^1 d\cos\theta_1\, \rho_1^2\, e^{-\rho_1^2/2}\, \Phi_S(\Omega). \tag{25}$$

In the paramagnetic phase the order parameter vanishes. Since $a_1 = 0$, Ω becomes independent of θ_1 and the resulting equation for the self-interaction R reads

$$R = \frac{2}{3(\beta J)^2(1+2d^2)(R-Q)L(\rho=0)} \int_0^\infty \frac{d\rho_1}{\sqrt{2\pi}}\, \rho_1^2\, e^{-\rho_1^2/2}\, \Phi_S(\Omega)(\rho_1^2 - 3). \tag{26}$$

IV. STABILITY ANALYSIS AND PHASE DIAGRAMS

In order to evaluate conditions for the phase boundaries we analyze the stability of the replica-symmetric solution. We set

$$R_\mu^\alpha = R_\mu + \xi_\mu^\alpha, \qquad Q_\mu^{\alpha\beta} = Q_\mu + \eta_\mu^{\alpha\beta}, \tag{27}$$

where $\mu = x, y, z$, $R_x = R_y = R_T$, $R_z = R_L$, $Q_x = Q_y = Q_T$, and $Q_z = Q_L$. R_Θ and Q_Θ ($\Theta = L, T$) are the self-consistent solutions within the static approximation. The fluctuations are assumed to be small. The free energy $F[\mathbf{R}, \mathbf{Q}]$ has to be expanded up to the second order in the fluctuations, where its deviation from the stationary value should be positive definite for a stable solution. It turns out that the structure of the quadratic form is the one of the corresponding matrix of de Almeida and Thouless (AT) in their prior work on the stability of the SK solution.[11] Due to the inherent symmetry of the self-interactions in replica space, only those eigenvalues of the stability matrix which do not depend on self-interactions may lead to an instability. In the limit $n \to 0$ there remains the problem of finding the eigenvalues of the matrix

$$\lambda = P - 2\tilde{Q} + \tilde{R}, \tag{28}$$

which is a 3×3 matrix due to the three spatial components, and the matrices P, $\tilde{R}$, and $\tilde{Q}$ are defined in the Appendix. The following equation results:

$$\lambda_{\mu\nu} = d^2 + (1-d^2)\delta_{\mu\nu} - J^2 \sum_{\mu'\nu'} [d^2 + (1-d^2)\delta_{\mu\mu'}] \times [d^2 + (1-d^2)\delta_{\nu\nu'}]\chi^{(2)}_{\mu'\nu'}, \tag{29}$$

with the susceptibility correlation functions

$$\chi^{(2)}_{\mu\nu} = \int D\mathbf{z}[\chi_{\mu\nu}(\mathbf{z})]^2. \tag{30}$$

Because of rotational symmetry with respect to the z axis one can express the susceptibility correlation functions in matrix form as

$$\chi^{(2)} = \begin{pmatrix} \chi_T^{(2)} & \chi_{xy}^{(2)} & \chi_{xz}^{(2)} \\ \chi_{xy}^{(2)} & \chi_T^{(2)} & \chi_{xz}^{(2)} \\ \chi_{xz}^{(2)} & \chi_{xz}^{(2)} & \chi_L^{(2)} \end{pmatrix}. \tag{31}$$

The same symmetry argument applies to the matrix λ.

The condition for the occurrence of an instability is that the smallest of the eigenvalues κ of the matrix λ, defined by

$$\det[\lambda - \kappa 1] = 0, \tag{32}$$

vanishes at the critical temperature. The solutions of Eq. (32) are

$$\kappa_{1,2} = \tfrac{1}{2}(\lambda_L + \lambda_T + \lambda_{xy}) \mp \sqrt{\tfrac{1}{4}(\lambda_L + \lambda_T + \lambda_{xy})^2 + 2\lambda_{xz}^2 - \lambda_L(\lambda_T + \lambda_{xy})}. \tag{33}$$

Vanishing of the eigenvalue κ_1 determines the upper critical line — the so-called Gabay-Toulouse line[12] — at which transverse spin-glass ordering occurs. On the other hand, the lower critical line resulting from the condition $\kappa_2 = 0$ — the so-called Almeida-Thouless line[11] — describes the transition to longitudinal spin-glass ordering. Note that for $d = 0$ and $h = 0$ both of the eigenvalues vanish at the same critical temperature T_c.

In this paper we mainly consider the case of zero magnetic field but nonzero anisotropy d, where $\chi_L^{(2)} = \chi_T^{(2)} = \chi^{(2)}$ and $\chi_{xy}^{(2)} = \chi_{xz}^{(2)}$. The resulting eigenvalues become

$$\kappa_1 = \left(1 - J^2[\chi^{(2)} + 2\chi_{xy}^{(2)}][1+2d^2]\right)(1+2d^2), \qquad \kappa_2 = \left(1 - J^2[\chi^{(2)} - \chi_{xy}^{(2)}][1-d^2]\right)(1-d^2). \tag{34}$$

In the high-temperature phase the order parameter and the off-diagonal susceptibilities vanish while the diagonal susceptibility is related to the spin self-interaction by

$$\chi = \beta R. \tag{35}$$

The condition $\kappa_1 = 0$ reduces to

$$R_c = \frac{1}{\beta J\sqrt{1+2d^2}}. \tag{36}$$

In the case $S = \frac{1}{2}$ the self-consistency equation for R may be calculated analytically. The result is

$$R = \tfrac{1}{12}\left[1 + \frac{8}{4 + (\beta J)^2(1+2d^2)R}\right]. \tag{37}$$

Thus the transition temperature is given by

$$k_B T_c = \frac{1}{4\sqrt{3}} J(1+2d^2)^{1/2}. \tag{38}$$

It is enlarged due to anisotropy compared to the pure quantum Heisenberg spin glass[19] by a factor of $(1 + 2d^2)^{1/2}$. This result agrees with the thermofield calculations in Ref. 25, but the actual result shows a reduction of the transition temperature due to quantum fluctuations by a factor of $\sqrt{3}$ while the thermofield method did not. For strong DM interactions ($d \gg 1$) the transition temperature depends linearly on D.

In the opposite limit $S \gg 1$ the transition temperature approaches the classical limit[16]

$$k_B T_c = \frac{S(S+1)J}{3}(1+2d^2)^{1/2}. \quad (39)$$

We have solved the self-consistency equations (24) numerically to calculate the upper and lower critical lines for different spin numbers in the anisotropy-temperature plane. The results are displayed in Fig. 1. The corresponding classical upper critical line is shown for comparison. As expected, the upper critical lines in the static approximation approach the classical result with increasing spin number. In agreement with the thermofield calculations[25] the lower critical line terminates at a critical value of the anisotropy at zero temperature. But we find an enhancement with increasing spin number in the static approximation. Note that the lower critical lines are calculated with a Monte Carlo integration technique which explains the noise in the data.

Figure 2 shows the local susceptibilities as functions of the temperature for different anisotropy values at a fixed spin number $S = \frac{1}{2}$. We find a qualitative agreement with the thermofield results. Below the critical temperature both methods show a decreasing temperature-dependence with increasing anisotropy, but above the critical temperature the present curves do not coincide

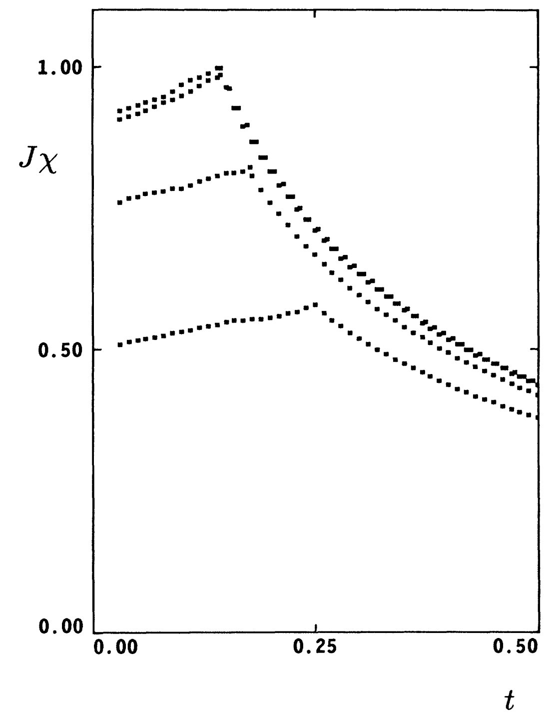

FIG. 2. Local static susceptibility vs temperature ($t = k_B T/J$) for $S = \frac{1}{2}$ and d =0.0, 0.2, 0.5, and 1.0 (from top to bottom, respectively).

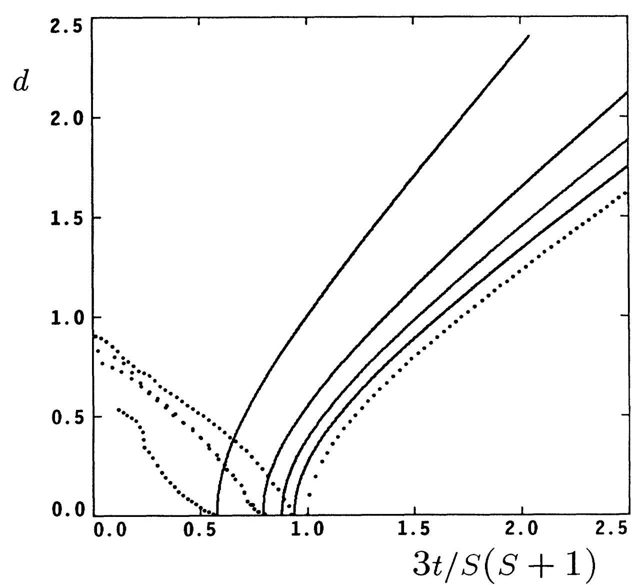

FIG. 1. The anisotropy-temperature ($t = k_B T/J$) phase diagram at $h = 0$, including upper (solid) and lower (dotted) critical lines for the spin numbers $S = \frac{1}{2}$, 1, $\frac{3}{2}$, and 2 (from left to right). The upper dotted line shows the corresponding phase boundary calculated in a classical treatment.

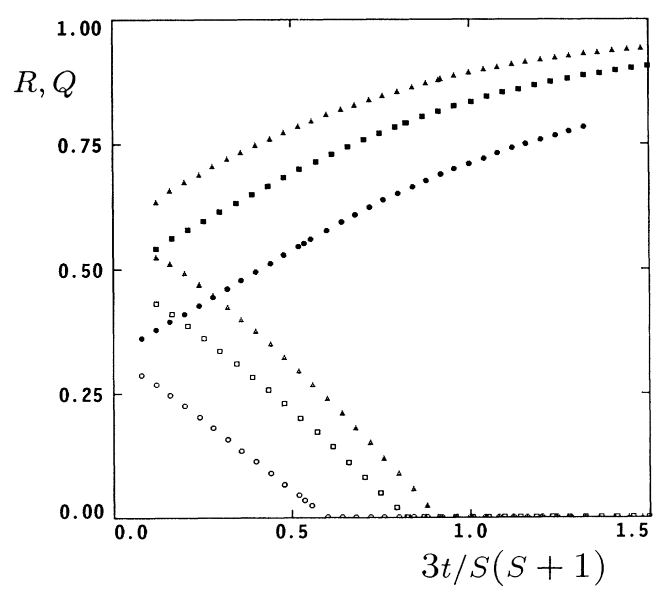

FIG. 3. Spin-glass order parameter q and self-interaction R as functions of the temperature ($t = k_B T/J$) for fixed anisotropy $d = 0.2$ but different spin numbers $S = \frac{1}{2}$, 1, and $\frac{3}{2}$ (circles, squares, and triangles, respectively). The self-interactions are given by the filled symbols.

for different anisotropy values. Figure 3 shows the spin-glass order parameter q and the self-interaction R as functions of the temperature for different spin numbers and for fixed anisotropy. In contrast to the thermofield results we find a rather linear decrease of the order parameter at low temperatures. Order parameter and self-interaction meet at zero temperature to ensure a finite free energy in this limit.

V. THERMODYNAMIC FUNCTIONS

The static approximation allows us to calculate thermodynamic quantities directly. We will focus here on the entropy and the specific heat in the case $h = 0$. With the free energy in Eq. (22) the entropy is given by

$$\mathcal{S}/k_B = \tfrac{3}{4}(\beta J)^2(1+2d^2)\left(R^2 - Q^2\right) + \int D\mathbf{z} \ln L(\mathbf{z}) - \int D\mathbf{z}\frac{1}{L(\mathbf{z})}\int D\mathbf{z}_1 \frac{\partial \Phi_S(\Omega)}{\partial \Omega}\Omega(\mathbf{z},\mathbf{z}_1) \tag{40}$$

and may be calculated if the self-consistent solutions of the self-interaction and the order parameter is known. The temperature dependence of the entropy for different spin numbers is shown in Fig. 4. The entropy remains positive at all temperatures though the replica-symmetric approach is used. This is presumably due to the static approximation which is known to become worse at very low temperatures and which has the tendency to increase the entropy rather strongly. Obviously, the entropy does not scale with the factor $S(S+1)$ like the transition temperature and the order parameter. In Fig. 4 the entropy is plotted against $\frac{t}{S(S+1)}$ which is the

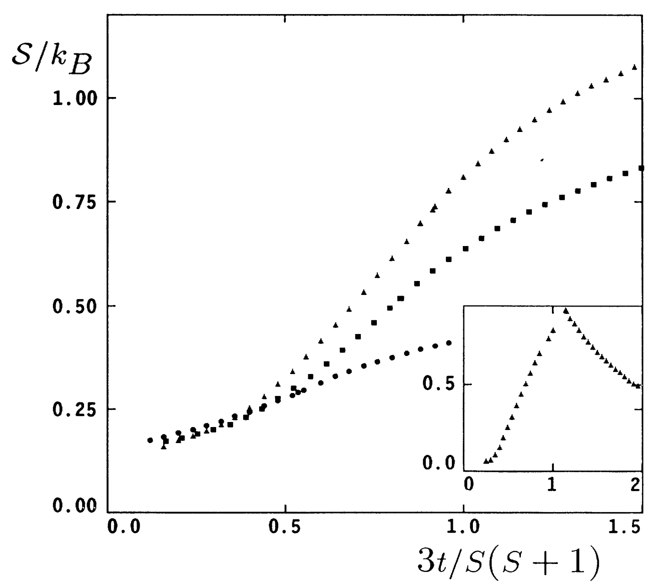

FIG. 4. temperature ($t = k_B T/J$) dependence of the entropy for fixed anisotropy $d = 0.2$ but different spin numbers $S = \frac{1}{2}$, 1, and $\frac{3}{2}$ (circles, squares, and triangles, respectively). The inset shows the specific heat in the case $S = \frac{3}{2}$.

correct temperature scale for a comparison of thermal quantities for different spin values. From this figure it is clearly seen that reducing the spin number S and thereby increasing the effect of quantum fluctuations results in a strong reduction of the entropy.

The specific heat can be readily obtained numerically as

$$C_v = T\,\frac{\partial \mathcal{S}}{\partial T}. \tag{41}$$

The inset in Fig. 4 shows a typical result for the specific heat. It depends quadratically on temperature at low temperatures and shows the typical mean-field cusp at T_c before it decreases at higher temperatures. The dependence on d is found to be very small.

VI. SUMMARY

A quantum vector spin-glass theory is presented in which the imaginary-time functional-integral technique and the replica method are used. The self-consistency equations for the spin-glass order parameters and self-interactions are set up in the general case of random exchange, random Dzyaloshinskii-Moriya interactions, and external magnetic field. These quite complicated equations have been solved numerically within the static approximation for the special case of the vanishing external field. We calculate phase diagrams, susceptibilities, and order parameters and find a rather good qualitative agreement with the thermofield calculations of Ref. 25, but we find some differences in detail. Additionally we calculate the entropy and specific heat which goes beyond the scope of the thermofield method.

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APPENDIX

The elements of the stability matrix appearing in the matrix λ are

$$P_{\mu\nu} = G_{\mu\nu}^{(\alpha\beta),(\alpha\beta)},$$
$$\tilde{Q}_{\mu\nu} = G_{\mu\nu}^{(\alpha,\beta),(\alpha,\gamma)}, \tag{A1}$$
$$\tilde{R}_{\mu\nu} = G_{\mu\nu}^{(\alpha,\beta),(\gamma,\delta)},$$

where distinct greek letters denote distinct replicas. The functions G are given by

$$G_{\mu\nu}^{(\alpha,\gamma),(\alpha',\gamma')} = \lim_{n\to 0} \left[d^2 + (1-d^2)\delta_{\mu\nu}\right] \delta_{(\alpha\gamma),(\alpha'\gamma')} - (\beta J)^2 \sum_{\mu'\nu'} \left[d^2 + (1-d^2)\delta_{\mu\mu'}\right] \left[d^2 + (1-d^2)\delta_{\nu\nu'}\right] \left(\langle S_{\mu'}^{\alpha} S_{\mu'}^{\gamma} S_{\nu'}^{\alpha'} S_{\nu'}^{\gamma'} \rangle - \langle S_{\mu'}^{\alpha} S_{\mu'}^{\gamma} \rangle \langle S_{\nu'}^{\alpha'} S_{\nu'}^{\gamma'} \rangle \right), \quad \text{(A2)}$$

where the thermal average has to be done with respect to the replica-symmetric effective Hamiltonian

$$-\beta H_{\text{eff}}[\mathbf{R},\mathbf{Q}] = \tfrac{1}{2}(\beta J)^2 \left[\sum_{\mu'\nu'} R_{\mu'} \left[d^2 + (1-d^2)\delta_{\mu'\nu'}\right] \sum_{\alpha} S_{\nu'}^{\alpha} S_{\nu'}^{\alpha} + \sum_{\mu'\nu'} Q_{\mu'} \left[d^2 + (1-d^2)\delta_{\mu'\nu'}\right] \sum_{(\alpha\neq\beta)} S_{\nu'}^{\alpha} S_{\nu'}^{\beta} \right] + \beta \sum_{\alpha} \mathbf{h}\cdot\mathbf{S}^{\alpha}. \quad \text{(A3)}$$

Due to replica symmetry this Hamiltonian may be linearized by introducing the Gaussian noises $\mathbf{z}$ and $\mathbf{z}_1$ where it becomes in the limit $n \to 0$ the argument of the exponential in Eq. (14). The expectation value of a spin operator then factorizes with respect to different replicas and finally results in

$$\lim_{n\to 0} \langle S_\mu \rangle = \int D\mathbf{z} \frac{1}{L(\mathbf{z})} \int D\mathbf{z}_1 \mathrm{Tr}\, S_\mu \exp\{\beta J [a_1(xS_x + yS_y) + a_2(x_1 S_x + y_1 S_y) + a_3 z S_z + a_4 z_1 S_z] + \beta h S_z\} = \int D\mathbf{z} \langle S_\mu \rangle_1 . \quad \text{(A4)}$$

The components of the eigenvalue matrix λ become

$$\lambda_{\mu\nu} = d^2 + (1-d^2)\delta_{\mu\nu} - (\beta J)^2 \sum_{\mu'\nu'} \left[d^2 + (1-d^2)\delta_{\mu\mu'}\right] \left[d^2 + (1-d^2)\delta_{\nu\nu'}\right] \times \int D\mathbf{z} \left[\langle S_{\mu'} S_{\nu'} \rangle_1^2 - 2\langle S_{\mu'} S_{\nu'} \rangle_1 \langle S_{\mu'} \rangle_1 \langle S_{\nu'} \rangle_1 + \langle S_{\mu'} \rangle_1^2 \langle S_{\nu'} \rangle_1^2 \right]$$
$$= d^2 + (1-d^2)\delta_{\mu\nu} - J^2 \sum_{\mu'\nu'} \left[d^2 + (1-d^2)\delta_{\mu\mu'}\right] \left[d^2 + (1-d^2)\delta_{\nu\nu'}\right] \int D\mathbf{z}\, \chi_{\mu'\nu'}^2(\mathbf{z}). \quad \text{(A5)}$$

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