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LETTER TO THE EDITOR

Phase diagrams of quantum spin glass models

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Abstract. Infinite-range quantum spin glass models with arbitrary spin are studied within the Matsubara time formalism. As an example the dynamic spin self-interaction $R(t, t')$ and the resulting phase diagrams are presented for the quantum Ising model in a transverse field. Some results, such as the phase transition temperatures, are also reported for the XY and the Heisenberg models.

In quantum spin glass models with infinite-range interactions [1–10] much attention has been paid to the description of the transition between the paramagnetic (P) and spin glass (SG) phases. For the quantum spin glass some of the quantum fluctuations persist in the paramagnetic phase in the form of the so-called dynamic spin self-interaction $R(t, t')$. This results in theories in which even this phase is not well described. However, some insight into the nature of the P phase can be achieved by an appropriate approximation of the spin self-interaction term of the paramagnetic free energy [2, 3]. The resulting form of $R(t, t')$ permits the construction of a line separating the P and SG phases.

In this work we present a method which enables us to obtain reliable approximations of the spin self-energy, regardless of the particular model or value of the spin.

The general formulation we use requires that the Hamiltonian H of the system of N interacting spins contains an exchange (two-site) part H_1, and a single-site part H_0. The single-site term may describe, for example, an external transverse field, or a single-ion anisotropy [4]. For the sake of clarity we restrict ourselves to the transverse quantum Sherrington–Kirkpatrick (SK) model [1], i.e. we outline the method using the example of the Ising model with arbitrary spin in the presence of an external transverse field. The generalization to other models is straightforward. Some results for the XY and the Heisenberg models are also given.

In our example H_1 and H_0 are

$$H_1 = -\tfrac{1}{2}\sum_{i\neq j}^{N} J_{ij}\sigma_{xi}\sigma_{xj} \qquad H_0 = -K\sum_{i=1}^{N}\sigma_{zi}. \tag{1}$$

The sum is over all pairs of spins and the exchange interactions J_{ij} are independent random variables governed by a symmetric Gaussian distribution with zero mean and variance $1/N$.

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In order to obtain the free energy averaged over the distribution of $\{J_{ij}\}$ we apply the replica method and Matsubara 'time' representation [2, 5], where the latter is based on the operator identity

$$T_\tau \exp\left[\int_{t_0}^{t} \mathrm{d}\tau\, B(\tau)\right] = \exp(-tA)\exp[(t-t_0)(A+B)]\exp(t_0 A)$$
$$B(t) = \exp(-tA)B\,\exp(tA). \tag{2}$$

Here the time ordering operator T_τ rearranges the operators in the expansion of the exponential, in order of decreasing time arguments. While the replica method handles the quenched disorder, the imaginary time representation enables us to avoid the problem of the non-commutativity of the spin operators and to treat them as c numbers. Applying (2) with $t = 1$ and $t_0 = 0$, the replica-symmetric free energy reads

$$F = q^2 - \int_0^1 \mathrm{d}\tau \int_0^1 \mathrm{d}\tau'\, R^2(\tau,\tau') + \int \mathrm{D}z \ln Q \tag{3a}$$

where

$$Q = Tr\exp(\beta K\sigma_z)T_\tau \exp\left[z\sqrt{2\beta q}\, I(\sigma_x) - q\beta^2 I^2(\sigma_x) + \Phi(R)\right] \tag{3b}$$

$$\Phi(R) = \beta\int_0^1 \mathrm{d}\tau \int_0^1 \mathrm{d}\tau'\, R(\tau,\tau')\sigma_x(\tau)\sigma_x(\tau') \tag{3c}$$

$$I(\sigma_x) = \int_0^1 \mathrm{d}\tau\, \sigma_x(\tau) \tag{3d}$$

$$\sigma_x(\tau) = \exp(-t\beta K\sigma_z)\sigma_x \exp(t\beta K\sigma_z) \qquad \mathrm{D}z = \left(\mathrm{d}z/\sqrt{2\pi}\right)\exp\left(-\tfrac{1}{2}z^2\right).$$

In equation (3b), the quantity q corresponds to the Edwards–Anderson spin glass order parameter and $R(t, t')$ is the dynamic spin self-interaction. Both q and $R(t, t')$ are determined from saddle-point equations. In the paramagnetic phase q vanishes and the phase transition takes place when the coefficient of q^2 in the free energy, equation (3a), becomes zero as a function of the temperature T. Thus, the spin-freezing temperature can be evaluated directly from an expression calculated in the high-temperature phase, and the equation of the phase transition line is

$$1 = 2\int_0^1 \mathrm{d}\tau \int_0^1 \mathrm{d}\tau'\, R(\tau,\tau') \qquad R(\tau,\tau') = (\beta/2)\langle T_\tau\sigma_x(\tau)\sigma_x(\tau')\rangle. \tag{4}$$

Here the angular bracket means the thermal average with respect to the effective Hamiltonian defined in the exponent in equation (3b). Since the exact solution of equation (4) for $R(t, t')$ is not known, a reasonable approximation is sought. Our approximation is made by separating $R(t, t')$ into a t-independent part R_0 and a variable part $C(t, t')$

$$R(t, t') = R_0 + C(t, t') \tag{5}$$

and treating the latter as a 'perturbing' term. In this way we rewrite equation (3*c*) as $\Phi(R) = \Phi_0 + V$, where

$$\Phi_0 = \beta R_0 I^2(\sigma_x) \qquad V = \int_0^1 \mathrm{d}\tau \int_0^1 \mathrm{d}\tau'\, C(\tau,\tau')\sigma_x(\tau)\sigma_x(\tau') \tag{6}$$

and $I(\sigma_x)$ is defined in equation (3*d*).

Using the standard cumulant expansion of $\ln Q$ in equation (3*a*), we can approximate the paramagnetic free energy by

$$F_{\mathrm{p}} = -\int_0^1 \mathrm{d}\tau \int_0^1 \mathrm{d}\tau' [R_0 + C(\tau,\tau')]^2 + \ln Q_0 + \langle V\rangle_0 + \tfrac{1}{2}\left(\langle V^2\rangle_0 - \langle V\rangle_0^2\right) + \ldots \tag{7}$$

where

$$Q_0 = Tr\, \exp(\beta K\sigma_z)T_\tau\, \exp\Phi_0 \tag{8}$$
$$\langle(\ldots)\rangle_0 = (1/Q_0)Tr\, \exp(\beta K\sigma_z)T_\tau(\ldots).$$

The approximation $C(t,\,t') = 0$ gives the so-called static approximation. Keeping only the first-order term in V we obtain

$$F_{\mathrm{p}}^1 = -\int_0^1 \mathrm{d}\tau \int_0^1 \mathrm{d}\tau' [R_0 + C(\tau,\tau')]^2 + \ln Q_0 + \beta\int_0^1 \mathrm{d}\tau \int_0^1 \mathrm{d}\tau'\, C(\tau,\tau')g_2(\tau,\tau') \tag{9}$$

where

$$g_2(\tau,\tau') = (\beta/2)\langle T_\tau\sigma_x(\tau)\sigma_x(\tau')\rangle_0. \tag{10}$$

The saddle-point equation $\delta F_{\mathrm{p}}^1/\delta C(\tau,\tau') = 0$ gives

$$R_0 + C(\tau,\tau') = (\beta/2)g_2(\tau,\tau') \tag{11}$$

i.e. the function $R(t,\,t')$ (5) is approximated by the correlation function of the static approximation (10). Using this relation the saddle-point equation for R_0 and the critical line equation are given by

$$\beta\int_0^1 \mathrm{d}\tau \int_0^1 \mathrm{d}\tau' [(\beta/2)g_2(\tau,\tau') - R_0]\partial g_2(\tau,\tau')/\partial R_0 = 0$$
$$1 = \beta\int_0^1 \mathrm{d}\tau \int_0^1 \mathrm{d}\tau'\, g_2(\tau,\tau') \tag{12}$$

respectively.

Now we show briefly how Q_0, g_2 and higher-order correlation functions may be calculated. Linearizing $I(\sigma_x)$ in $\exp(\Phi_0)$ by the Hubbard–Stratanovich transformation and then applying equation (2) we get for Q_0

$$Q_0 = \int \mathrm{D}x\, Tr\exp(\boldsymbol{h}\cdot\boldsymbol{\sigma}) = \int \mathrm{D}x \frac{\sinh[(h/2)(2\sigma+1)]}{\sinh(h/2)}$$
$$\boldsymbol{h} = \left(\sqrt{2\beta R_0 x}, 0, \beta K\right) \tag{13}$$

where h is the length of $\boldsymbol{h}$. Similarly, after the linearization we have

$$g_2(t, t') = \frac{1}{Q_0} \int \mathrm{D}x \, Tr \exp(\beta K \sigma_z) T_r \left\{ \sigma_x(t) \sigma_x(t') \exp\left[\sqrt{2\beta R_0} x I(\sigma_x) \right] \right\}. \tag{14}$$

Dividing the integral $I(\sigma_x)$ in the exponent of (14) (see also equation (3*d*)) into a sum of three parts, e.g. for $t > t'$, taking $[0,1) = [0,t') \cup [t', t) \cup [t, 1)$, and applying equation (2) for each time-ordered part yields

$$g_2(t, t') = \int \mathrm{D}x \, \rho_2(\boldsymbol{h}, t - t') \tag{15}$$

$$\rho_2(\boldsymbol{h}, t) = (1/Q_0) Tr \exp(\boldsymbol{h} \cdot \boldsymbol{\sigma}) \sigma_x^{\boldsymbol{h}}(t) \sigma_x^{\boldsymbol{h}}(0) \qquad t \in [0, 1) \tag{16}$$

$$\sigma_x^{\boldsymbol{h}}(t) = \exp[-(\boldsymbol{h} \cdot \boldsymbol{\sigma})t] \sigma_x \exp[(\boldsymbol{h} \cdot \boldsymbol{\sigma})t] \tag{17}$$

and

$$\rho_2(\boldsymbol{h}, -t) = \rho_2(\boldsymbol{h}, 1 - t). \tag{18}$$

Direct calculation of g_2 is straightforward but laborious. However, to see the qualitative behaviour of g_2 it suffices to derive a differential equation for $\rho_2(t)$:

$$\partial^2 \rho_2(\boldsymbol{h}, t) / \partial t^2 = \text{constant} + h^2 \rho_2(\boldsymbol{h}, t). \tag{19}$$

Because of the periodicity (18) of ρ_2, equation (19) has the solution

$$\rho_2(\boldsymbol{h}, t) = a(\boldsymbol{h}, \sigma) + b(\boldsymbol{h}, \sigma) \cosh(\tfrac{1}{2} h (1 - 2t)]. \tag{20}$$

For the Hamiltonian (1) the coefficients a and b are

$$a(h, \sigma) = [(h^2 - \beta^2 K^2)/h^2] \partial^2 Q_0(h) / \partial h^2$$

and

$$b(h, \sigma) = (\beta^2 K^2 / 2h^2) [\sigma(\sigma + 1) Q_0(h) - \partial^2 Q_0(h) / \partial h^2]. \tag{21}$$

The expressions (13), (20) and (21) for the functions $\rho^2(\boldsymbol{h}, t)$ and $Q_0(h)$ enable us, through equation (12), to construct the phase diagram for the Ising model, with arbitrary spin σ, in a transverse field. We present the phase diagrams for spin $\sigma = \frac{1}{2}$ and $\sigma = 1$ in figure 1. The results for $\sigma = \frac{1}{2}$ are equivalent to those obtained by Trotter–Suzuki formalism [11]. The *zero*-temperature limit of the critical field $K_c(T = 0)$ for arbitrary spin σ is given by

$$K_c(T = 0) = \sigma + \sqrt{\sigma(\sigma - 5/16)}$$

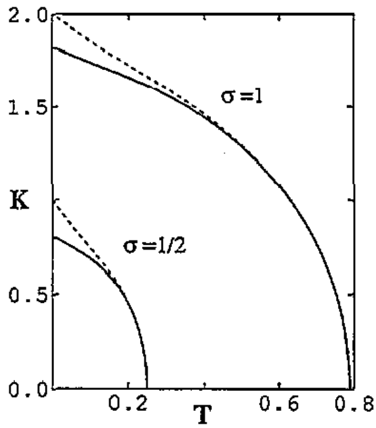

Figure 1. Phase transition lines for the Ising spin glass in a transverse field. T: temperature in units of $J = (\langle J_{ij}^2 \rangle / N)^{1/2}$; K: field in units of J; full curves: equation (12); broken curves: static approximation with $R_0 \neq 0$.

Table 1. Phase transition temperatures for the XY and Heisenberg models without external field for the spin number $\sigma = \frac{1}{2}$ using the temperature normalization of the numerical calculations.

	XY	Heisenberg
This work	0.762	0.588
Numerical calculation	0.763 [6]	0.593 [3]
Static approximation	0.756 [2, 5]	0.577 [2]
TFD	0.541 [12]	—

i.e. for large σ our approximation yields the static solution $K_c^{\text{static}}(T = 0) = 2\sigma$.

We conclude by noting that the set of equations (13, 20, 21), corresponding to the first-order approximation in $C(\tau)$, as well as the higher-order approximation [11], can also be obtained for other SK models. We have derived the first-order equations for the XY and the Heisenberg models without external field, but give here only the results. The calculation follows closely that of this paper and one can use the self-consistent supposition that the matrix $R_{nm}(t, t')(n, m = x, y, z)$ is diagonal [2]. The phase transition temperatures for $\sigma = \frac{1}{2}$ are reported in table 1.

The replica method combined with the Matsubara time representation has been used to construct a reliable approximation of the spin self-energy of the SK models. Spin freezing temperatures calculated for simpler models are in good agreement with the results of the numerical calculations [3, 6–10]. We believe that these relatively simple approximations can be successfully applied to more complicated models for which extensive numerical calculations are difficult.

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