Cluster-expansion method for the infinite-range quantum transverse Ising spin-glass model

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The infinite-range quantum Ising spin-glass model in a transverse field Γ is studied within the cluster-expansion method formulated originally for spin systems by Morita and Tanaka. With use of the pair approximation, the mean-field equation and condition for critical values of Γ_c and T_c are obtained including the case $T_c \to 0$.

The quantum transverse Ising spin-glass model has received much attention recently.[1-7] Most of the studies have been on the effect of a transverse field Γ on the spin-glass freezing temperature T_c using the static[5,6] and dynamic[7] approximation within the replica theory as well as the quantum version[3] of the Thouless, Anderson, and Palmer (TAP) method.[8]

Our model is described by the following Hamiltonian:

$$H = -\Gamma \sum_i \sigma_i^x - \tfrac{1}{2} \sum_{\substack{i,j \\ (i \neq j)}} J_{ij} \sigma_i^z \sigma_j^z \ ,$$

where σ_i^x, σ_i^z are the Pauli matrices referred to the ith site of the lattice and the random exchange J_{ij} obey the following Gaussian probability distribution

$$\rho(J_{ij}) = (Z/2\pi\tilde{J}^2)^{1/2} \exp(-ZJ_{ij}^2/2\tilde{J}^2) \ , \tag{2}$$

with a variance $\tilde{J}^2/Z$. Here Z denotes the number of neighbors of each spin satisfying the relation $N \gtrsim Z \gg 1$, where N is the total number of spins in the system. The exchange J_{ij} is assumed to be of the order $Z^{-1/2}$ which ensures a sensible thermodynamic limit.[8]

In the classical case ($\Gamma=0$) our model reduces to the one considered by Sherrington and Kirkpatrick.[9]

The TAP approach to the classical model[8] can be interpretated in terms of the cluster-expansion method, where the pair approximation leads to the TAP mean-field equation,[10] whereas the clusters consisting of three, four, and more spins correspond to the ring diagrams of the order N/Z.[8] The same interpretation is valid for the quantum case (1).

In this paper we report calculations on the mean-field equation and phase diagram of the infinite-range transverse Ising spin-glass model using the pair approximation, which is based on the cluster variation method formulated originally for spin systems by Morita and Tanaka.[11] Following this procedure we introduce the one- and two-lattice site density matrices denoted by $\rho(i)$ and $\rho(i,j)$, respectively, defined as follows:

$$\rho(i) = \exp\{\beta[f(i) - H(i)]\} \ , \tag{3}$$

$$\rho(i,j) = \exp\{\beta[f(i,j) - H(i,j)]\} \ , \tag{4}$$

where

$$H(i) = -\Gamma\sigma_i^x - h_i\sigma_i^z \tag{5}$$

and

$$H(i,j) = -\Gamma(\sigma_i^x + \sigma_j^x) - h_i'\sigma_i^z - h_j'\sigma_j^z - J_{ij}\sigma_i^z\sigma_j^z \tag{6}$$

are the effective Hamiltonians of the one- and two-site clusters, respectively, h_i, h_i', h_j' denote the effective fields defined as

$$h_i = \sum_{j \neq i} \lambda_{ij} \ , \tag{7}$$

$$h_i' = \sum_{k \neq i,j} \lambda_{ik} \ , \tag{8}$$

and

$$h_j' = \sum_{k \neq i,j} \lambda_{jk} \ , \tag{9}$$

and λ_{ij} is the variational parameter which is calculated from the following condition:

$$\frac{\partial f(i)}{\partial h_i} = \frac{\partial f(i,j)}{\partial h_i'} \ . \tag{10}$$

The normalization factors $f(i)$ and $f(i,j)$ have the following forms:

$$f(i) = -\left[\frac{1}{\beta}\right] \ln \mathrm{Tr} e^{-\beta H(i)}$$

$$= -\frac{\ln 2}{\beta} - \left[\frac{1}{\beta}\right] \ln\cosh[\beta(h_i^2 + \Gamma^2)^{1/2}] \tag{11}$$

and

$$f(i,j) = -\left[\frac{1}{\beta}\right] \ln \mathrm{Tr} \exp[-\beta H(i,j)] \ . \tag{12}$$

Our next step is to evaluate $f(i,j)$, Eq. (12). For this purpose we find the eigenvectors of the effective pair Hamiltonian $H(i,j)$ Eq. (6). After some calculations one obtains the following equation:

$$(\epsilon + J_{ij} + h_i' + h_j')(\epsilon + J_{ij} - h_i' - h_j')(\epsilon - J_{ij} - h_i' + h_j')(\epsilon - J_{ij} + h_i' - h_j') - 4\epsilon^2\Gamma^2 = 0 \ , \tag{13}$$

where the solutions $\epsilon=\epsilon_n(i,j)$ are the eigenenergies of $H(i,j)$, Eq. (6). However, $J_{ij}\sim Z^{-1/2}$, and according to the TAP idea[8] it is sufficient to resolve Eq. (13) up to the second order in J_{ij}. In the result we get

$$\epsilon_n(i,j)=\epsilon_n^{(0)}(i,j)+\epsilon_n^{(1)}(i,j)J_{ij}+\epsilon^{(2)}(i,j)J_{ij}^2+O(J_{ij}^3) , \quad (14)$$

where

$$\epsilon_1^{(0)}(i,j)=-E_i'-E_j' , \quad (15)$$

$$\epsilon_2^{(0)}(i,j)=-E_i'+E_j' , \quad (16)$$

$$\epsilon_3^{(0)}(i,j)=E_i'+E_j' , \quad (17)$$

$$\epsilon_4^{(0)}(i,j)=E_i'-E_j' , \quad (18)$$

with

$$E_i'=[(h_i')^2+\Gamma^2]^{1/2} , \quad (19)$$

$$\epsilon_n^{(1)}(i,j)=(-1)^n\frac{h_i'h_j'}{E_i'E_j'} , \quad (20)$$

and

$$\epsilon_n^{(2)}(i,j)=\frac{\Gamma^2}{2\epsilon_n^{(0)}(i,j)}\{(E_i')^{-1}(E_j')^{-1}-(-1)^n[(E_i')^2+(E_j')^2-\Gamma^2][(E_i')^2+(E_j')^2](E_i')^{-3}(E_j)^{-3}$$
$$+[(E_i')^2+(E_j')^2-\Gamma^2](E_i')^{-2}(E_j')^{-2}\} . \quad (21)$$

Hence, using the thermodynamic perturbation method we calculate (i,j) with the accuracy to J_{ij}^2.

In order to obtain λ_{ij} we note that

$$h_i'=h(m_i)-\lambda_{ij} , \quad (22)$$

where m_i is the mean spin on the ith site defined as follows:

$$m_i=m(h_i)=-\frac{\partial f(i)}{\partial h_i}=h_i(h_i^2+\Gamma^2)^{-1/2}\tanh[\beta(h_i^2+\Gamma^2)^{1/2}] , \quad (23)$$

and $h(m_i)$ denotes the inverse function to $m(h_i)$ Eq. (23). The variational condition (10) for λ_{ij} transforms now into the following condition:

$$m_i=\frac{\partial f(i,j;m_i,\lambda_{ij})}{\partial\lambda_{ij}} . \quad (24)$$

Taking into account Eq. (24) and the explicit form of m_i we obtain finally for λ_{ij} the following equation:

$$\lambda_{ij}=J_{ij}m_j-J_{ij}^2g(m_i,m_j)+O(J_{ij}^3) , \quad (25)$$

where

$$g(m_i,m_j)=\frac{1}{2}\frac{\partial\ln\chi_i}{\partial h(m_i)}m_j^2-m_i\chi_j-\beta m_im_j^2+\beta\Gamma^2\chi_i^{-1}h^{-2}(m_i)h^{-2}(m_j)E^{-4}(m_i)E^{-2}(m_j)$$
$$+\frac{2h(m_i)\chi_i^{-1}\Gamma^2}{[h^2(m_i)-h^2(m_j)]}\left[\frac{h^2(m_j)m_i}{h^2(m_i)E^2(m_i)}-\frac{h^2(m_i)m_j}{h^2(m_j)E^2(m_j)}\right]$$
$$-\frac{\Gamma^2}{h^2(m_i)-h^2(m_j)}\left[\frac{h^2(m_j)}{h(m_i)E^2(m_i)}\left[1-\frac{\chi_i^{-1}m_i}{h(m_i)}\right]-\frac{2h^2(m_j)\chi_i^{-1}m_i}{E^4(m_i)}-\frac{2\chi_i^{-1}h(m_i)m_j}{h(m_j)E^2(m_j)}\right] . \quad (26)$$

Here χ_i denotes the single-site susceptibility defined as

$$\chi_i=\chi(m_i)=\frac{\partial m_i}{\partial h_i}=E^{-1}(m_i)\tanh[\beta E(m_i)]-h^2(m_i)E^{-3}(m_i)\tanh[\beta E(m_i)]+\beta h^2(m_i)E^{-2}(m_i)\{1-\tanh^2[\beta E(m_i)]\} , \quad (27)$$

with

$$E(m_i)=[h^2(m_i)+\Gamma^2]^{1/2} . \quad (28)$$

Taking into account Eqs. (7) and (25) we get the self-consistent equation for m_i,

$$h(m_i)=\sum_j J_{ij}m_j-\sum_j J_{ij}^2g(m_i,m_j) . \quad (29)$$

It is easy to see that for the classical Ising spin-glass model ($\Gamma=0$) Eq. (29) takes the TAP form:[8]

$$\frac{1}{2\beta}\ln\left[\frac{1+m_i}{1-m_i}\right]=\sum_j J_{ij}m_i-\beta\sum_j J_{ij}^2 m_i(1-m_j^2) \ . \qquad (30)$$

The condition for the critical field Γ_c and temperature T_c can be obtained from linear terms (with the respect of the single-site magnetization) of Eq. (29). Using the maximum eigenvalue $(J_\lambda)_{\max}=2\tilde{J}$ of the Gaussian-random matrix $\|J_{ij}\|$,[8] we get

$$\partial\tilde{J}\chi_0-\tilde{J}^2\chi_0^2-1=-(\tilde{J}\chi_0-1)^2=0 \ , \qquad (31)$$

where

$$\chi_0=\lim_{m_i\to 0}\chi(m_i)=\Gamma^{-1}th\beta\Gamma \ , \qquad (32)$$

$$\Gamma_c\tanh^{-1}(\Gamma_c/T_c)=\tilde{J} \ . \qquad (33)$$

Contrary to the Ishii and Yamamoto result,[3] Eq. (33) gives a correct value of Γ_c if the freezing temperature $T_c\to 0$. Namely, for $T_c=0$ we obtain $\Gamma_c(T_c=0)=\tilde{J}$ in the accordance with previous calculations performed within the replica method.[6] In the classical case ($\Gamma_c=0$), Eq. (33) yields the known result.[8] In Fig. 1 the phase diagram obtained from Eq. (33) in the plane $T_c/\tilde{J}$ and $\Gamma_c/\tilde{J}$ is presented.

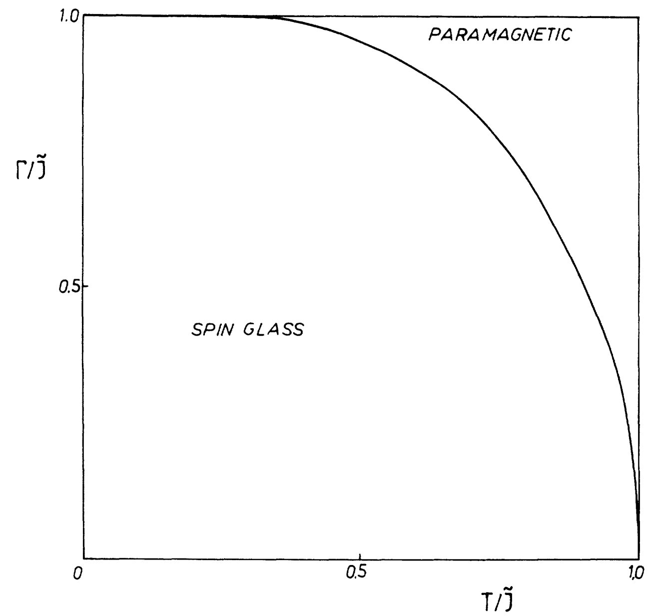

FIG. 1. The phase diagram caluclated from Eq. (33) for the infinite-range transverse Ising spin-glass model in the plane $\Gamma_c/\tilde{J}, T_c/\tilde{J}$.

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