AN EFFECTIVE EXPANSION FOR THE FREE ENERGY OF QUANTUM SPIN GLASS MODELS WITH INFINITE-RANGE INTERACTIONS

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Abstract. An expansion for the free energy functional of quantum spin models is build around diagonalisable single-ion term of the system's Hamiltonian. This expansion is obtained within the Matsubara time formalism by introducing recursive relations involving the spin correlation functions.

Introduction

Spin glass systems (SG) are collections of atoms or molecules with randomly distributed magnetic moments and frustrated interactions. They have gained much attentions of the scientific community since the seminal work by Edwards and Anderson [1]. Physical concepts and mathematical tools developed in the contest of SG are applicable not only in physics but also in biology, economy, informatics, e.g. in the study of optimization theory and neural networks.

In quantum spin glass models with infinite-range interactions attention has been paid to description of the transition between disordered (paramagnetic) and ordered spin glass phases. However, even an approximate description of the phase change involves an expansion of the free energy functional in terms of the powers of the order parameters. In this work we present a method to built such an expansion in a systematic way.

The general formulation requires that the Hamiltonian H of the system of interacting spins is composed of two parts: a single-site part H_0 and an exchange, two-site part H_1. The single-site term may represent an external magnetic field or single-ion anisotropies. The exchange two-site term we use is the quantum Sherrington-Kirkpatrick (SK) model [2]:

$$H_1 = -\frac{1}{2}\sum_{\alpha}\sum_{i \neq j}^{N} J_{ij} S_i^{\alpha} S_j^{\alpha} \tag{1}$$

where S_i^{α} are the spin operators - Pauli matrices - referred to the spin i of an ensemble of N spins $\alpha = x, y, z$ and $i = 1, \ldots, N$. The random exchange interactions

$\{J_{ij}\}$ are governed by independent probability distributions taken to be Gaussian with zero mean and variance $1/N$.

1. Free energy

In order to obtain the free energy averaged over the distribution of $\{J_{ij}\}$ we apply the replica trick and Matsubara "time" representation [3]. The replica trick is used to overcome the difficulties of averaging a logarithm and it employs the identity

$$[\ln Z]_J = \lim_{n \to 0} \frac{([Z^n]_J - 1)}{n} \tag{2}$$

where $[\ldots]_J$ means an averaging over the random exchange interactions J_{ij}.
The Matsubara "time" representation is based on the operator identity

$$T_\tau \exp\left[\int_{t_0}^{t} d\tau B(\tau)\right] = \exp(-tA) \cdot \exp[(t - t_0)(A + B)] \cdot \exp(t_0 A) \tag{3}$$

$$B(t) = \exp(-tA) \cdot B \cdot \exp(tA) \tag{4}$$

Here the time ordering operator T_τ rearranges the operator in the expansion of the exponential, in order of decreasing time arguments. This representation enables us to avoid the problem of the non-commutativity of the spin operators S^α and to treat them as numbers. Applying (2)-(4) to the Hamiltonian (1) the replica free energy has the following form [4, 5]

$$F = \int Dz_q \ln\left[\mathrm{Tr}\, e^{H_0} \cdot T_\tau \exp(\Phi)\right] = \int Dz_q \ln\left(\mathrm{Tr}\, e^{H_{\mathrm{eff}}}\right) \tag{5}$$

$$\Phi = z\Phi_1 + q\Phi_2 + \Phi_3 \tag{6}$$

$$\Phi_1 = \sqrt{2\beta} \int_0^1 d\tau \sum_n S^n(\tau) \tag{7}$$

$$\Phi_2 = -\beta \int_0^1 d\tau \int_0^1 d\tau' \sum_{n,m} S^n(\tau) \cdot S^m(\tau') \tag{8}$$

$$\Phi_3 = \beta \int_0^1 d\tau \int_0^1 d\tau' \sum_n S^n(\tau) R(\tau, \tau') S^n(\tau') \tag{9}$$

where $\beta = 1/T$ is the inverse temperature and the integration in Eq. (5) is over the field:

$$Dz_q = \frac{1}{\sqrt{2\pi}} d\left(z/\sqrt{q}\right) \exp\left[-\left(z/\sqrt{q}\right)^2/2\right] \tag{10}$$

In Equations (5)-(10), the quantity q is the Edwards-Anderson spin glass order parameter and $R(\tau, \tau')$ is the dynamic spin self-interaction. $R(\tau, \tau')$ describes the quantum fluctuations. The spin glass order parameter vanishes in the paramagnetic (disordered) phase whereas the dynamic spin self-interaction persists in both phases. In order to locate the phase change one needs to expand the free energy functional as a series in power of q. The phase transition takes place when the coefficient of q^2 becomes zero as a function of the temperature T and thus, one of the most useful information can be retrieve from an expansion of the functional F, Eqs. (5-9).

2. An expansion

Consider the free energy F given by Equations (5)-(10). Using these equations we can compute the thermal average with respect to the effective Hamiltonian H_{eff} defined in the exponent of Eq. (5). We denote this thermal average by the angular bracket, namely:

$$\left\langle T_\tau S^{n_1}(\tau_1) \cdots S^{n_p}(\tau_p) \right\rangle_{\text{eff}} = \frac{\text{Tr}\, e^{H_0} \cdot T_\tau S^{n_1}(\tau_1) \cdots S^{n_p}(\tau_p) \cdot \exp(\varPhi)}{\text{Tr}\, e^{H_0} \cdot T_\tau \exp(\varPhi)} \tag{11}$$

From Eq. (10) we see that

$$\frac{\partial^{(\nu)}}{\partial q^\nu} Dz_q = 2^{-\nu} \frac{\partial^{(2\nu)}}{\partial z^{2\nu}} Dz_q \tag{12}$$

Using Eqs. (11) and (12) we can compute the first derivative of F with respect to the order parameter q. First, we do this by direct computation. Direct computation involves the straightforward evaluation of multiple thermal averages of Eq. (11).

$$\partial_q F = \int \left(\partial_q Dz_q\right) \ln\left[\text{Tr}\, e^{H_0} \cdot T_\tau \exp(\varPhi)\right]$$
$$+ \int Dz_q \partial_q \ln\left[\text{Tr}\, e^{H_0} \cdot T_\tau \exp(z\varPhi_1 + q\varPhi_2 + \varPhi_3)\right] \tag{13}$$

The evaluation of the first term in Eq. (13) can be performed with the help of the equivalency (12)

$$\int Dz_q \frac{1}{2}\frac{\partial^2}{\partial z^2}\ln\left[\operatorname{Tr}e^{H_0}\cdot T_\tau \exp(z\Phi_1 + q\Phi_2 + \Phi_3)\right]$$

$$= \frac{\sqrt{2\beta}}{2}\int Dz_q \frac{\partial}{\partial z}\frac{\operatorname{Tr}e^{H_0}\cdot T_\tau \int_0^1 d\tau \sum_n S^n(\tau)\exp(z\Phi_1 + q\Phi_2 + \Phi_3)}{\operatorname{Tr}e^{H_0}\cdot T_\tau \exp(z\Phi_1 + q\Phi_2 + \Phi_3)} \qquad (14)$$

$$= \frac{\sqrt{2\beta}}{2}\int Dz_q \frac{\partial}{\partial z}\sum_n \int_0^1 d\tau \langle T_\tau S_n(\tau)\rangle_{\text{eff}}$$

The last line contains the derivative of the single spin thermal average $\langle T_\tau S_n(\tau)\rangle_{\text{eff}}$ with respect to z. This derivative can be evaluated directly yielding

$$\beta\int Dz_q \sum_{n,m}\int_0^1 d\tau_1 \int_0^1 d\tau_2 \left[\langle T_\tau S^n(\tau_1)S^m(\tau_2)\rangle_{\text{eff}} - \langle T_\tau S^n(\tau_1)\rangle_{\text{eff}}\langle T_\tau S^m(\tau_2)\rangle_{\text{eff}}\right] \quad (15)$$

The second term in Eq. (13) is directly related to the two-spin thermal average

$$\int Dz_q \partial_q \ln\left[\operatorname{Tr}e^{H_0}\cdot T_\tau \exp(z\Phi_1 + q\Phi_2 + \Phi_3)\right] = -\beta\int Dz_q \sum_{n,m}\int_0^1 d\tau_1 \int_0^1 d\tau_2 \langle T_\tau S^n(\tau_1)S^m(\tau_2)\rangle_{\text{eff}}$$
$$(16)$$

Comparing Eq. (13) to Eqs. (15) and (16) we get the final form of the first derivative of F

$$\partial_q F = -\beta\int Dz_q \left[\sum_n \int_0^1 d\tau \langle T_\tau S^n(\tau)\rangle_{\text{eff}}\right]^2 \qquad (17)$$

All above calculations can be easily performed with the help of the relations defined by Eqs. (11)-(12). For the sake of clarity we introduce the following notation

$$\frac{\partial^{(\nu)}}{\partial z^\nu}\equiv\partial_\nu,\ \frac{\partial^{(\nu)}}{\partial q^\nu}\equiv\Delta_\nu \qquad (18)$$

$$[p]=\sum_{\{n_i\}}\int_0^1 d\tau_1 \int_0^1 d\tau_2 \cdots \int_0^1 d\tau_p \langle T_\tau S^{n_1}(\tau_1)S^{n_2}(\tau_2)\cdots S^{n_p}(\tau_p)\rangle_{\text{eff}} \qquad (19)$$

Now we show briefly how to expand the functional F in powers of q in an efficient way. The first derivative of the free energy, Eq. (17) takes the following form

$$\Delta_1 F = -\beta\int Dz_q [1]^2 \qquad (20)$$

Using the above notation, Eqs. (18)-(19) and the properties given by Eqs. (11)-(12), we obtain a chain rule for the application of operators ∂_ν and Δ_ν on symbol $[p]$, i.e.

$$\partial_1[p] = \sqrt{2\beta}\left([p+1] - [p]\cdot[1]\right) \tag{21}$$

$$\Delta_1[p] = -\beta\left([p+2] - [p]\cdot[2]\right) \tag{22}$$

$$\partial_1[p]^k = k[p]^{k-1}\cdot\partial_1[p], \text{ similarly: } \Delta_1[p]^k = k[p]^{k-1}\cdot\Delta_1[p] \tag{23}$$

and

$$\partial_n[p] = \partial_1\partial_{n-1}[p], \quad \Delta_n[p] = \Delta_1\Delta_{n-1}[p] \tag{24}$$

As an example we compute the second and third derivatives of F with respect to q. They have the following forms

$$\Delta_2 F = -2\beta^2 \int Dz_q \left([2]^2 - 4[2]\cdot[1]^2 + 3[1]^4\right) \tag{25}$$

and

$$\Delta_3 F = -4\beta^3 \int Dz_q \left([3]^2 - 12[3]\cdot[2]\cdot[1] + 12[3]\cdot[1]^3 - 4[2]^3 + 45[2]^2\cdot[1]^2 \right. \\ \left. - 72[2]\cdot[1]^4 + 30[1]^6\right) \tag{27}$$

Above examples show that the expansion of the free energy can be obtained in the same way as when we solve recursion relations.

Conclusion

The replica method and the Matsubara time representation yield a reliable approximation of the free energy for the quantum spin system with random exchange interactions. If the system undergo the phase change the border line between two phases can be seen in the free energy expansion written as a series in power of the order parameter q. In this paper we presented a method to built the family of free energy derivatives with respect to q. We believe that this relatively simple scheme can be used to build appropriate free energy expansions for other spin models [6, 7].

References

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