Quantum phase transitions and dynamical correlations in spin-glass systems

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Abstract. We study effects of random fluctuations in quantum spin-glass systems. We show that the expression of the magnetic susceptibility is divided into the classical and quantum parts. The former can be analyzed by the standard replica method with the static approximation. The latter incorporates dynamical correlations and is determined by the energy gap distribution. By using the many-body interacting Ising spin-glass model with transverse field, we discuss possible mechanisms of the quantum phase transitions.

1. Introduction
Spin glasses have attracted interest for many years for their fundamental importance to the statistical mechanics and for a wide range of applications [1, 2, 3, 4]. Now the mean-field theory of the spin glasses has been well understood and the Sherrington-Kirkpatrick model [5], which is a typical mean-field spin-glass model, was solved exactly by using the replica method [6, 7, 8, 9].

However, once if we apply the transverse magnetic field, the quantum fluctuation effect becomes important and the model cannot be solved exactly [10]. Generally speaking, the quantum nature becomes important at low temperatures and the picture of the classical spin-glass transition can be changed significantly [11].

For classical thermodynamic systems, the phase transition is determined by the free energy $F = E - TS$. For a given temperature $T$, the state of the system is given by the configuration that gives the smallest free energy, which implies the state with low energy $E$ and large entropy $S$. However, they are not compatible with each other and the competition between them determines the state. When the temperature goes to zero, the entropy becomes irrelevant and the system takes its ground state. Therefore, the quantum phase transition at zero temperature can be found by looking at the energy gap between the ground and first excited states. In spite of this simple picture, the problem is not so simple to solve since the quantum fluctuation makes the ground state nontrivial. Concerning the Sherrington-Kirkpatrick model in a transverse field, there are many studies on the quantum phase transition [12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25]. However, due to the lack of the effective method, we do not even know the exact value of the transition point.

In this paper, we study the quantum phase transition of the mean-field spin-glass systems. Comparing several models, we discuss possible pictures of the transition. We pay special attention to the role of the quantum fluctuations and see how the effect affects the phase transition at zero temperature [26, 27].

In section 2, we discuss the role of the quantum effect from the expression of the susceptibility. Based on this observation, in section 3, we analyze the many-body interacting Ising spin-glass
model in a transverse field by using the replica method. The method used there is a classical one and we study the effect of the quantum fluctuations by the energy gap distribution in section 4. We discuss possible pictures of the quantum phase transition in section 5. Finally, section 6 is devoted to conclusions.

2. Susceptibility and quantum fluctuations

Magnetic properties of spin systems can be studied by the response of the system to the applied magnetic field. The magnetic field is included to the Hamiltonian $H$ as $H(h) = H - h \sum_{i=1}^{N} \sigma_{i}^{z}$ where $\sigma_{i}^{z}$ is the Pauli matrix on site $i$. The magnetization is given by the thermal average of the spin as $m = \frac{1}{N} \sum_{i=1}^{N} \langle \sigma_{i}^{z} \rangle / N$. It is expanded in $h$ as $m = \chi_{l} h - \chi_{nl} h^{3} + \cdots$ and the magnetic susceptibility is defined as the coefficients of each term. To study spin-glass systems, it is useful to treat not only the linear susceptibility $\chi_{l}$ but also the nonlinear one $\chi_{nl}$ [28, 29]. $\chi_{l}$ is calculated from the partition function $Z$ as

$$\chi_{l} = \frac{1}{N} \frac{\partial^2}{\partial h^2} \ln Z \bigg|_{h=0} = \frac{2N}{\beta} \int_{0}^{\beta} d\tau \int_{0}^{\tau} d\tau' \langle [\sigma(\tau)\sigma(\tau')] \rangle - \beta q, \quad (1)$$

where $\beta$ is the inverse temperature and the square bracket represents the ensemble average. In the last expression, we introduced the imaginary time representation

$$\sigma(\tau) = \frac{1}{N} \sum_{i=1}^{N} e^{\hat{H}\tau} \sigma_{i}^{z} e^{-\hat{H}\tau}, \quad (2)$$

and the spin-glass order parameter

$$q = \frac{1}{N} \left[ \left( \sum_{i=1}^{N} \sigma_{i}^{z} \right)^{2} \right]. \quad (3)$$

The nonlinear susceptibility can also be expressed in a similar way [26, 27].

The imaginary-time formulation clarifies the role of quantum fluctuations since $\tau$ does not appear in classical systems. To see the quantum effects explicitly, we utilize the spectral representation. We insert the completeness relation of eigenstates of the Hamiltonian to the imaginary-time representation. We have the expression

$$\chi_{l} = \beta (\chi - q) + \frac{2}{N} \left[ \frac{1}{Z} \sum_{m,n} e^{-\beta E_{n}} \left| \langle n | \sum_{i=1}^{N} \sigma_{i}^{z} | m \rangle \right|^{2} \right], \quad (4)$$

where $|n\rangle$ is the eigenstate with the eigenvalue $E_{n}$. The expression is divided into the classical and quantum parts. The first term represents the classical part and $\chi$ is equal to the spectral function

$$\chi(\omega) = \frac{1}{N} \left[ \frac{1}{Z} \sum_{nm} e^{-\beta E_{n}} \left| \langle n | \sum_{i} \sigma_{i}^{z} | m \rangle \right|^{2} \delta(\omega - (E_{m} - E_{n})) \right], \quad (5)$$

at $\omega = 0$. At zero temperature, the state $|n\rangle$ is restricted to the ground state, which means that the excited states do not contribute to the classical part. We note that in the classical system with $\Gamma = 0$, $\chi = 1$ and the linear susceptibility is given by $\chi_{l} = \beta (1 - q)$. It implies that the first term clarifies properties of the classical spin-glass state.
We take the ensemble average over random interaction $J$ where $\sigma$ is the Ising spin-glass model with transverse field assures the dynamical nature of the system. Thus, fluctuations in $\tau$ for the spin-glass transition. As the simplest possible model, we define the $p$-body interacting $\Phi(\tau) = \langle i\Phi(\tau) | (d/d\tau) | S(\tau) \rangle$ includes the derivative with respect to the imaginary time $\tau$, which assures the dynamical nature of the system. Thus, fluctuations in $\tau$ represent quantum effects.

In order to proceed further, we define the model. Our motivation is to discuss quantum effects for the spin-glass transition. As the simplest possible model, we define the $p$-body interacting Ising spin-glass model with transverse field

$$\hat{H} = - \sum_{i_1 < i_2 < \cdots < i_p} J_{i_1 i_2 \cdots i_p} \sigma^z_{i_1} \sigma^z_{i_2} \cdots \sigma^z_{i_p} - \Gamma \sum_{i=1}^N \sigma^x_i,$$

where $\sigma^x_i$ are Pauli matrices on site $i$, $N$ is the number of the site and $\Gamma$ is the transverse field. We take the ensemble average over random interaction $J_{i_1 i_2 \cdots i_p}$ with the Gaussian distribution

$$P(J_{i_1 \cdots i_p}) = \sqrt{\frac{N^{p-1}}{\pi p! J^2}} \exp \left\{ - \frac{N^{p-1}}{p! J^2} \left( J_{i_1 i_2 \cdots i_p} \right)^2 \right\}.$$

The model at $p = 2$ is known as the Sherrington-Kirkpatrick model [5] and $p = \infty$ as the Derrida’s random energy model [30, 31]. The reason why we study this mean-field model is that the model is solvable at the classical limit $\Gamma \to 0$ and the essential features of the spin-glass state can be found by analyzing this model. With the transverse field, the model cannot be solved exactly except the case of the limit $p \to \infty$ [32].

To handle the ensemble average, we use the replica method which is the standard prescription for the mean-field spin-glasses. We calculate the average of the $n$th power of the partition function and the average free energy per spin is obtained from the relation

$$f = -\frac{1}{N\beta} \ln Z = -\frac{1}{N\beta} \lim_{n \to 0} \frac{[Z^n] - 1}{n}.$$
The calculation of $[Z^n]$ goes along the same line as the classical case. The main difference is that the variables have the imaginary-time dependence. We obtain the expression

$$[Z^n] = \exp \left\{ -\frac{N J^2}{4} (p-1) \sum_{a,b=1}^n \int_0^\beta d\tau d\tau' \left( q_{ab}(\tau, \tau') \right)^p + N \ln \text{Tr} e^L \right\},$$

(11)

$$\text{Tr} e^L = \int D\mathbf{S} \exp \left\{ \sum_{a=1}^n \int_0^\beta d\tau (i\Phi_a(\tau) + \Gamma S_x^a(\tau)) \right. $$

$$+ \frac{J^2}{4} \sum_{a,b=1}^n \int_0^\beta d\tau d\tau' S_x^a(\tau) \left( q_{ab}(\tau, \tau') \right)^{p-1} S_x^b(\tau') \right\},$$

(12)

where $a$ and $b$ denote the replica indices and the order parameter $q$ is obtained from the saddle-point equation

$$q_{ab}(\tau, \tau') = \frac{\text{Tr} S_x^a(\tau) S_x^b(\tau') e^L}{\text{Tr} e^L}.$$  

(13)

3.2. Static approximation

To solve the saddle-point equation without imposing any ansatz is a formidable task and we need a reduction of the equation. If the transverse field is sufficiently large, the perturbative expansion is useful to find the imaginary-time dependence of the order parameter [33]. However, the perturbation is not an appropriate way to treat the spin-glass transition. The possible simplest approximation is to neglect the time dependence of the order parameter [34] as

$$q_{ab}(\tau, \tau') \to \begin{cases} \chi_a & a = b \\ q_{ab} & a \neq b \end{cases}.$$  

(14)

It was discussed in [25] that the static approximation is justified for $q_{ab}$ and not for $\chi_a$. On the other hand, we may drop the replica dependence of $\chi$ and not of $q$. The replica dependence of $q_{ab}$ is important when we find the replica symmetry breaking solution. However, it is known for the classical limit $\Gamma = 0$ at $p = 2$ that we can find the transition point from the replica symmetric solution replacing $q_{ab}$ by $q$. For $p \geq 3$, the one-step replica symmetry breaking solution is relevant and we use this ansatz in the following calculation. Using the static approximation and the one-step replica symmetry breaking ansatz, we can write the free energy

$$f = \frac{\beta J^2}{4} (p-1) (\chi^p - q^p + m q^p) - \frac{1}{\beta m} \ln \int Dz_1 \left\{ \int Dz_2 \left( e^{\beta h} + e^{-\beta h} \right) \right\}^m,$$

(15)

and the saddle-point equations

$$\chi = \frac{\int Dz_1 \left( \int Dz_2 \cosh \beta h \right)^{m-1} \int Dz_2 \left( \frac{M^2}{h^2} + \frac{\tanh \beta h}{\beta h} \right) \cosh \beta h}{\int Dz_1 \left( \int Dz_2 \cosh \beta h \right)^m},$$

(16)

$$q = \frac{\int Dz_1 \left( \int Dz_2 \cosh \beta h \right)^{m-2} \left( \int Dz_2 \frac{M}{h} \sinh \beta h \right)^2}{\int Dz_1 \left( \int Dz_2 \cosh \beta h \right)^m},$$

(17)

where

$$h = \sqrt{\Gamma^2 + M^2},$$

(18)

$$M = J \sqrt{\frac{p}{2}} \left( \sqrt{q^{p-1} z_1 + \sqrt{q^{p-1} z_2}} \right),$$

(19)

$$\int Dz_{1,2} (\cdots) = \int_{-\infty}^{\infty} \frac{dz_2}{\sqrt{2\pi}} e^{-z_2^2/2} (\cdots).$$

(20)
The Parisi parameter $m$ is also found from the saddle-point equation. The replica symmetric solution is given by setting $m = 0$.

Using this expression of the free energy, we can derive the linear susceptibility as $\chi_l = \beta(\chi - q)$. Therefore, the static approximation corresponds to neglecting the quantum part. If we can neglect the quantum fluctuation effects, the present approximation is justified and we can study the spin-glass state in the same way as the classical case. In fact, at the limit of $p \to \infty$, this approximation is justified. Using the static and one-step replica symmetry breaking ansatz, we can solve the model exactly [32].

At $p = 2$, the static approximation and the replica symmetric ansatz gives the transition point at zero temperature as $\Gamma/J = 2$. This value is larger than that estimated in the following studies. In figure 1, we plot the phase diagram in $\Gamma - T$ plane. The phase boundary separates the paramagnetic phase with $q = 0$ and the spin-glass one with $q \neq 0$.

We also plot the case of $p = 3$ in the figure. In this case, the static approximation and the one-step replica symmetry breaking ansatz is used. At temperatures lower than $T/J \sim 0.35$, the phase transition is of the first order.

![Figure 1](image-url)

**Figure 1.** Phase diagram at $p = 2$ (left) and $p = 3$ (right) obtained by the static approximation. The solid line denotes the second order phase transition between the paramagnetic (Para) and spin-glass (SG) phases. The dashed line in the left figure is the improved result mentioned in section 3.3. The dotted line in the right figure represents the first order transition. For the improved result at $p = 2$ and the static result at $p = 3$, the phase boundaries are not shown at low temperatures due to numerical problems.

### 3.3. Renormalization of dynamical fluctuations

The static approximation seems to give a reasonable result for the phase structure, at least, qualitatively. In principle, we can examine the validity of the approximation by using the stability analysis. We write the order parameter as

$$q_{ab}(\tau, \tau') = \begin{cases} 
\chi + \tilde{\chi}_a(\tau - \tau') & a = b \\
q + \tilde{q}_{ab}(\tau, \tau') & a \neq b
\end{cases}, \quad (21)$$

and expand the free energy with respect to the dynamical parts $\tilde{\chi}$ and $\tilde{q}$.

Here, for practical purpose, we consider the renormalization of the static free energy [25]. We write the order parameter as (21) and integrate over the dynamical part as

$$[Z^n] = \int D\tilde{\chi} D\tilde{q} \exp \{-Nn/\beta f[\chi, q, \tilde{\chi}, \tilde{q}]\} = \exp \{-Nn/\beta f_{\text{eff}}[\chi, q]\}. \quad (22)$$

The resultant effective static free energy $f_{\text{eff}}$ includes the dynamical fluctuation effect and can be analyzed by the classical picture. The static order parameters $\chi$ and $q$ are determined from
the saddle-point equation. Of course, it is difficult to perform the integrations exactly and we expand the dynamical variables up to second order. Then, using the Gaussian integration, we obtain $f_{\text{eff}}$ [25]. Since the expansion incorporates the factor $\beta J$, it is not justified at low temperatures.

We plot the improved result in figure 1. We see that the result is significantly modified at low temperatures. Since we are using the perturbative approximation, the saddle-point equation has no solution at low-$T$. We need a more reliable method. However, the extrapolation to the zero temperature limit implies the transition point $\Gamma/J \sim 1.5$, which is consistent with the results in [14, 21, 23, 24, 26, 27].

4. Energy gap and quantum effects

Next, we study the quantum part of the susceptibility (6). We easily see that this term diverges when the energy gap $E_n - E_0$ goes to zero. This is consistent with the picture that the quantum phase transition occurs when the gap goes to zero. However, in random systems, the location of energy levels depends on the sample and it is not clear how the spin-glass transition point is specified. It should be checked whether the self-averaging property holds for the energy gap distribution.

We calculate the average gap as a function of the transverse field at $p = 2, 3, 4$ and $\infty$ which is obtained by diagonalizing the quantum Hamiltonian numerically. We also consider the magnetization in $x$-direction at $T = 0$ defined as

$$m_x = -\frac{1}{N} \frac{\partial F}{\partial \Gamma}.$$  \hfill (23)

This is not an order parameter since there is not spontaneous symmetry breaking in the $x$-direction. Rather, this can be understood a kind of entropy at zero temperature. The thermodynamic entropy is defined as $S = -\partial F/\partial T$. Replacing $T$ by $\Gamma$, we obtain $m_x$.

![Figure 2](image)

**Figure 2.** Average energy gap (solid line with dots) and magnetization in the transverse direction $m_x$ (dotted line) for $p = 2, 3, 4$ and $\infty$. The size of the system is $N = 20$ and the average is taken over 20000 samples.

We plot the results in figure 2. At $p = 2$, the average gap is an increasing function with respect to the transverse field. The gap vanishing point is around $\Gamma/J \sim 0.7$ which is considerably smaller than the result obtained in the previous section. $m_x$ is also a smooth function and does not show any singular behavior. This result implies that the quantum phase transition cannot be obtained from the average quantity. On the other hand, the results at $p = 3, 4$ and $\infty$ show notable features. At some point, $m_x$ shows a discontinuous change and the energy gap shows a significant change ($p = 4$) or becomes minimum ($p = 3$ and $\infty$). This discontinuous change implies the first order phase transition.
The form of the average energy gap shows a difference between even and odd $p$. In fact, the Hamiltonian commutes with $\prod_{i=1}^{N} \sigma_x^i$ for even $p$ and not for odd $p$ and $p = \infty$. This spin flip symmetry is important to see whether the quantum effect is important or not. Equation (6) includes the matrix element $\langle n | \sigma_z^i | 0 \rangle$. This quantity measures how much excited states are contained in the ground state multiplied by $\sigma_z^i$. To study this, we calculate the inverse participation ratio

$$I = \sum_n |\langle n | \sigma_z^i | 0 \rangle|^4. \quad (24)$$

This quantity measures the inverse number of states included in $\sigma_z^i | 0 \rangle$ [35]. We plot the result in figure 3, which shows that when $\Gamma$ is small, the state $\sigma_z^i | 0 \rangle$ is almost equal to the first excited state (even $p$) or the ground state (odd $p$). Therefore, for odd $p$, there are not excitations to the higher states and the quantum part gives a small contribution.

5. Quantum phase transitions for random systems

Combining the results in the previous sections, we can discuss possible pictures of the quantum spin-glass phase transitions in each case.

- $p = 2$
  
  In this case, the quantum effect is important to find the phase transition at zero temperature. The second term of the susceptibility (4) dominates the critical behavior and the average gap is not useful to find the transition point.
  
  The distribution function of the energy gap has a power-law tail $P(\Delta) \sim \Delta^k$ at small $\Delta$ and the power index $k$ determines the nature of the phase transition since the quantum part of the linear susceptibility is written as $\chi^{(q)}_1 \sim \int d\Delta P(\Delta)/\Delta$. The spin-glass transition can be found by the divergence of the spin-glass susceptibility $\chi_{sg}$. In classical systems, it is directly related to the nonlinear susceptibility $\chi_{nl}$. However, this is not the case for quantum systems. The spectral representation shows that their quantum parts are written as $\chi_{sg} \sim \int d\Delta P(\Delta)/\Delta^2$ and $\chi_{nl} \sim \int d\Delta P(\Delta)/\Delta^3$. Thus, these three susceptibilities diverge at different points [26, 27]. In fact, it was also found in finite dimensional systems that the nonlinear susceptibility is divergent within the paramagnetic phase [36, 37, 38, 39, 40, 41]. Thus, the critical behavior of the model is determined by the rare event of samples. In classical systems, such rare configurations of disorder give a weak singularity which is known as the Griffiths-McCoy singularity [42, 43]. The main difference in the present case is that
it is crucial to find the phase transition. In addition to that, such effect is considered not to appear in mean-field systems since such a weak singularity comes from the ordered clusters in a disordered state. In our mean-field system, cluster can be formed in the imaginary time direction. This quantum Griffiths singularity is a purely quantum effect and is considered the main factor of the quantum phase transition of the present model.

- $p = 3$

The analysis of the inverse participation ratio shows that the quantum part of the susceptibility is small compared to the classical part. Therefore, the classical static approximation is expected to be justified for the replica analysis. At low temperatures, the analysis gives the first order transition at $\Gamma/J \sim 1.18$ while the gap analysis in figure 2 implies a smaller value $\Gamma/J \sim 0.8$. The numerical analysis of the gap was done for a finite size system and we need a more detailed analysis to clarify this small discrepancy.

- $p = 4$

In this case, the quantum part gives a relevant contribution and the gap fluctuation can be important. However, we see from figure 2 that the behavior of the average gap is related to a discontinuous change of $m_x$ implying a classical first order transition. Although the classical static approximation is not justified, the nature of the phase transition can be classical. We consider that the quantum fluctuation effect is hidden by the abrupt change of the ground state.

- $p = \infty$

This corresponds to the random energy model and can be solved exactly. The transition point at zero temperature is given by $\Gamma/J = \sqrt{\ln 2} \sim 0.83$. This value can also be found from figure 2. The property of the system can be determined by the ground state and the static approximation is justified in the replica analysis.

6. Conclusions

We have discussed quantum fluctuation effects on spin-glass transitions by using the $p$-body interacting Ising spin-glass model in a transverse field. The spectral representation of the susceptibility clarifies the role of quantum fluctuations to determine the state of the system.

The quantum effect can be best seen in the case of $p = 2$ where the gap distribution plays a crucial role for the phase transition at zero temperature. The average gap cannot be any help to characterize the state of the system, which means that the quantum system must be analyzed by a totally different way as the classical one.

For $p \geq 3$, the order parameter shows a discontinuous change. The existence of the quasi-stationary state implies a different type of quantum effects since the tunneling between different states is possible due to the quantum fluctuation.

Thus, compared to the classical spin-glass transitions, we see that the quantum spin-glass systems display different pictures for the phase transition. Our analysis is only for the Ising system with the transverse field and it is interesting to study other quantum systems. Such an analysis is left for future studies.

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