Classical-quantum crossover in the critical behavior of the transverse field S-K spin glass model

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We study the critical behavior of Sherrington-Kirkpatrick model in transverse field (at finite temperature) using Monte Carlo simulation and exact diagonalization (at zero temperature). We determine the phase diagram of the model by estimating the Binder cumulant. We also determine the correlation length exponent from the collapse of the scaled data. Below a non-zero temperature, we find the critical Binder cumulant (indicating the universality class of the transition behavior) and the correlation length exponent cross over from their ‘classical’ to ‘quantum values.

The motivation of this work is to study the phase diagram and critical behavior of the Sherrington-Kirkpatrick (S-K) spin glass model in transverse field using Monte Carlo and exact diagonalization techniques at finite and zero temperature respectively. Several approximate theoretical and numerical studies (see Refs. 3–7) have already been made on S-K model to get some isolated features of the quantum phase transition of this model. We report here a detailed numerical study. Using both Monte Carlo and exact diagonalization we determine the critical Binder cumulant which is an indicator of the nature of critical fluctuation. It also provides critical transverse field and/or temperature. We study the scaling behavior of the Binder cumulants with respect to the system sizes and the scaling fit gives the value(s) of the correlation length exponent. We find critical Binder cumulant and correlation length exponent cross over from a ‘classical’ value (corresponding to the classical S-K model) for high temperature and low transverse field, to a ‘quantum’ value for low temperature and high transverse field.

The Hamiltonian of quantum S-K model of $N$ spins is given by

$$H = H_0 + H_I; \quad H_0 = - \sum_{(i,j)} J_{ij} \sigma_i^z \sigma_j^z; \quad H_I = -\Gamma \sum_{i=1}^{N} \sigma_i^x,$$

where $\sigma_i^z, \sigma_i^x$ are the $z$ and $x$ components of Pauli spin matrices respectively and $\Gamma$ is the transverse field. For $\Gamma = 0$ the Hamiltonian in Eq. (1) reduces to the classical S-K spin glass Hamiltonian ($H_0$). In this model spin-spin interactions ($J_{ij}$) are distributed following Gaussian distribution $\rho(J_{ij}) = \left(\frac{N}{2\pi}J^2\right)^{-\frac{1}{2}} \exp\left(-\frac{N J^2}{2J^2}\right)$. The mean of Gaussian distribution is zero and the variance is $J/\sqrt{N}$. We work with $J = 1$. The effective classical Hamiltonian $H_{eff}$ of the Hamiltonian in Eq. (1) can be obtained by using Suzuki-Trotter formalism (see e.g., 2):

$$H_{eff} = -\sum_{n=1}^{M} \frac{1}{M} \sum_{(i,j)} J_{ij} \sigma_i^n \sigma_j^n - \sum_{i=1}^{N} \sum_{n=1}^{M} \frac{1}{\beta} \log \coth \frac{\beta \sigma_i^n \sigma_i^{n+1}}{M},$$

where $\sigma_i^n = \pm 1$ is the classical Ising spin and $\beta$ is the inverse of temperature $T$. The additional dimension appears in Eq. (2) is often called Trotter direction (theoretically $M \to \infty$).

We accomplish Monte Carlo simulation using Hamiltonian in Eq. (2) to find the critical transverse field for a fix temperature. We take $t_0$ Monte Carlo steps to equilibrate the system and then we make Monte Carlo averaging within next $t_1$ Monte Carlo steps. To study the critical behavior of the model, we take replica overlap $g$, which is defined as $g = 1 - \frac{1}{N M} \sum_{i=1}^{N} \sum_{n=1}^{M} \langle \sigma_i^n(t) \rangle^\phi \langle \sigma_i^n(t) \rangle^\theta$, where $\langle \sigma_i^n \rangle^\phi$ and $\langle \sigma_i^n \rangle^\theta$ are the spins of two different replicas $\phi$ and $\theta$ corresponding to the same realization of disorder. We study the variation of average Binder cumulant $\langle g \rangle$ with $\Gamma$ and $T$ for different system sizes. For our study we define the average Binder cumulant $\langle g \rangle$ given by:

$$g = \frac{1}{2} \left[ 3 - \frac{\langle \phi \rangle^2}{\langle \theta \rangle^2} \right],$$

where $\langle . \rangle$ and overhead bar indicate thermal and configuration averages respectively. It may be noted that with another definition for disorder averaging $g = \frac{1}{2} \left[ 3 - \frac{\langle \phi \rangle^2}{\langle \langle \phi \rangle \rangle^2} \right]$ one obtains huge fluctuation and bad statistics (see e.g., 8). We therefore work with the above definition (4) of $g$ to make a consistent study through out the entire range of temperature.

In our simulation we take the Trotter size $M = 10$ and work with the system sizes $N = 20, 60, 180$. The equilibrium time of the system is $t_0 = 75000$ and we take $25000$ ($t_1$) Monte Carlo steps for thermal averaging. 500 samples are averaged over to get the configuration average. The intersection of the $g$ vs. $\Gamma$ curves for different system sizes gives the values of the critical transverse field $\Gamma_c$ and critical Binder cumulant $g_c$. We observe some finite size effects in the $g$ vs. $\Gamma$ curves (see Fig. 11 (a, c, e)). For a pair of two different system sizes $N$ and $N'$, we evaluate the values of $\Gamma_c(N, N')$ and $g_c(N, N')$ from the interaction of the $g$ vs. $\Gamma$ curves for these two system sizes. The same procedure is followed in case of $\Gamma = 0$ (and here $g$ vs. $T$ curves). Since $g = g(L/\xi)$ where $L$ denotes the linear size of the system and $\xi$ represents the correlation length, $\xi \sim (T - T_\xi)^{-\nu_T}$ or $(\Gamma - \Gamma_c)^{-\nu_T}$ with correlation exponents $\nu_T$ or $\nu_T$. Hence close to critical
region we can write,
\[ g \sim g((T - T_c)N^{x_T}) \text{ or } g((\Gamma - \Gamma_c)N^{x_T}) \]  \hspace{1cm} (4)
where \( x_T = 1/\nu d \) and \( x_T = 1/\nu d \) with \( L = N^{1/d} \). Accounting every possible pair, we extrapolate \( T_c(N, N') \) and \( \Gamma_c(N, N') \) with \( (N N')^{-x_T/2} \) and \( (N N')^{-x_T/2} \) to get \( T_c \) or \( \Gamma_c \) for infinite system size. In absence of a finite size scaling behavior of the \( g \) we fit its finite size variations of \( g(N, N') \) to \( 1/\sqrt{NN'} \) to evaluate \( g_c \) in the thermodynamic limit. We also try to collapse the \( g \) curves for two different system sizes following the Eq. 4. From a pair of system sizes, we get \( \Gamma_c(N, N') \) and merge their \( g \) curves by suitably scaling the tuning parameters with chosen values of the exponents \( x_T \) and \( x_T \).

We notice that in the range starting from the classical S-K model at \( \Gamma = 0 \) to almost \( T \approx 0.50 \) (\( \Gamma \approx 1.36 \)), the \( g \) takes a constant value 0.22 ± 0.02 (see insets of Fig. 1 (a, c, e)) and we find good fitting of \( T_c(N, N') \) and \( \Gamma_c(N, N') \) for \( x_T = x_T = 0.33 \). In this region of the phase diagram, we also find good pairwise data collapse of \( g \) curves (to Eq. 4) for \( x_T = x_T = 0.31±0.02 \) (see Fig. 1 (b, d, f)). From insets of Fig. 1 (a, c) we observe that, in the range \( T = 0.40 \) (\( \Gamma \approx 1.50 \)) to \( T = 0.25 \) (\( \Gamma \approx 1.59 \)), the value of \( g_c \) is nearly equal to zero. In this region, we get the best fit of \( \Gamma_c(N, N') \) for \( x_T = 0.66 \) while pairwise collapses of \( g \) curves (see Fig. 1 (b, d)) are made with \( x_T = 0.66 ± 0.02 \). Such a crossover in \( g \) or the exponent value \( x_T (\approx x_T) \) with \( \Gamma \) (or \( T \)) values within this range (0.5 < \( T < 0.4 \), 1.36 < \( \Gamma < 1.50 \)) may be abrupt. Our numerical analysis is not very accurate here and gradual changes within this range cannot be ruled out.

We explore the other extreme limit of the spin glass phase diagram (i.e., the system at temperature \( T = 0 \)) through the Binder cumulant analysis of the system using an exact diagonalization technique. We have performed exact diagonalization of the Hamiltonian for rather small system sizes (up to \( N = 22 \)) using Lanczos algorithm. Here, we are interested to show the continuity of our Monte Carlo result of nearly zero value of critical Binder cumulant even at zero temperature. We construct the Hamiltonian \( H \) in spin basis states i.e., the eigenstates of the spin operators \( (\sigma_i^z, i = 1,..,N) \) for performing the diagonalization. Then the \( n \)-th eigenstate of the Hamiltonian in Eq. 4 is represented as \( |\psi_n\rangle = \sum_{\alpha=0}^{2^N-1} a_n^{\alpha} |\varphi_\alpha\rangle \), where \( |\varphi_\alpha\rangle \) are the eigenstates of the Hamiltonian \( H_0 \) and \( a_n^{\alpha} = \langle \varphi_\alpha |\psi_n\rangle \). As we are interested in the zero temperature analysis, our main focus is confined on the ground state \( |\psi_0\rangle \) averaging of different quantities. In this case the order parameter of the system can be defined as \( Q = (1/N) \sum_i \langle \sigma_i^z |\psi_0\rangle^2 \). The configuration average is again indicated by the overhead bar. To calculate Binder cumulant, the various moments can be calculated.
extrapolated values (with best fit scaling exponent value for the various moments can be determined using Eq. (5). The extrapolated value of $\Gamma$ signifying finite size effect of the system. (b) shows the Binder cumulant curves for different pair of system sizes ($N$ and $N'$) collapse following the scaling fit (to Eq. 4) with the exponent $x_{\Gamma} = 0.67 \pm 0.02$ (see the inset).

Using Refs. [113],

$$Q_k = \frac{1}{N^k} \sum_{i_1} \cdots \sum_{i_k} \langle \psi_0 | \sigma_{i_1}^x \cdots \sigma_{i_k}^x | \psi_0 \rangle^2. \quad (5)$$

Here $Q_{k,s}$ are actually $k$-spin correlation functions for a particular disorder configuration. One can easily realize that order parameter $Q = Q_1$. If we know the ground state at different parameter values of the Hamiltonian the various moments can be determined using Eq. [13].

In this context the average Binder cumulant is defined as

$$g = \frac{1}{2} \left[ 3 - \frac{Q_2}{Q_1^2} \right]$$

(note the difference with the Eq. (13)).

The variations of $g$ as a function of $\Gamma$ is shown in Fig. [3] (c) for different system sizes. To study the finite size effects, we follow the same technique as described earlier for determining the point of intersection $\Gamma_c(N, N')$. The extrapolated value of $\Gamma_c(N, N')$ is
the critical behaviors are indicated (\(g_c \approx 0\), \(\nu \approx 1/4\) for low \(T\)-high \(\Gamma\) region and \(g_c \approx 0.22\), \(\nu \approx 1/2\) for high \(T\)-low \(\Gamma\) region). The crossover point is around \(T \approx 0.45\) and \(\Gamma \approx 1.46\).

In summary, we estimate the entire phase diagram of the quantum S-K spin glass using Monte Carlo simulation and exact diagonalization results (see Fig. 5). The estimated phase diagram compares well with some earlier estimates for isolated parts (Refs. [6,7]). The pure quantum fluctuation driven transition (at \(T = 0\)) of the model is also studied using an exact diagonalization method. Zero temperature results also provide the vanishing value of \(g_c\) that support our Monte Carlo results. During the exploration of phase diagram by varying \(T\) or \(\Gamma\), we find that \(g_c\) drops (from a value about 0.22) to a very low value (< 0.02) below a certain point (\(T \approx 0.45, \Gamma \approx 1.46\)): \(g_c\) remains fairly constant (at value 0.22 ± 0.02) from classical transition point (\(\Gamma = 0, T = 1.0\)) to almost \(T = 0.45, \Gamma = 1.46\) and assumes a very low value (< 0.02) or vanishes (with Gaussian fluctuations) beyond this point and remains the same up to \(\Gamma \approx 1.62, T = 0\) (see also [10]). The scaling fits to Eq. (4) give \(x_T = x_T \approx 1/3\) for high \(T\) and low \(\Gamma\) values, while \(x_T = x_T \approx 2/3\) for low \(T\) and high \(\Gamma\) values.

We believe, these two values of \(g_c\) indicate two different universality classes and our observation indicates that the universality class of classical fluctuation dominated transitions (at low \(\Gamma\) and high \(T\)) is quite different from that for the quantum fluctuation dominated transitions (for high \(\Gamma\) and \(T\)). Existence of such distinct universality classes appears more reasonable when compared with the observation that the correlation length exponent \(\nu\) also has two different values in these two regions of the phase diagram (having two different values of \(g_c\)). As mentioned earlier, in the classical fluctuation dominated region we find \(x_T\) or \(x_T \approx 0.31 ± 0.2\). If we take critical dimension of the classical spin glass \(d_c = 6\), then from the relation \(x_T = x_T = 1/d_c\nu\) (Eq. (4), see also [13]) we get \(\nu = 1/2\), which is consistent with the earlier estimates[14]. Similarly for quantum fluctuation dominated transitions we find (considering again \(d_c = 6\) for the quantum glass as well) \(\nu \approx 1/4\), which agrees with earlier estimates[14]. Such changes in the values of \(g_c\) and \(\nu\) at a non-vanishing temperature clearly indicate the classical to quantum fluctuation dominated critical behavior crossover occurs there.

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