Classical-to-quantum crossover in the critical behavior of the transverse-field Sherrington-Kirkpatrick spin glass model

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We study the critical behavior of the 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. Our numerical studies here indicate that critical Binder cumulant (indicating the universality class of the transition behavior) and the correlation length exponent cross over from their "classical" to "quantum" values at a finite temperature (unlike the cases of pure systems, where such crossovers occur at zero temperature). We propose a qualitative argument supporting such an observation, employing a simple tunneling picture.

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I. INTRODUCTION

The motivation of this work is to study the phase diagram and critical behavior of the Sherrington-Kirkpatrick (SK) spin glass model [1] in transverse field [2] using Monte Carlo and exact diagonalization techniques at finite and zero temperature, respectively, and investigate the crossover behavior from classical to quantum fluctuation dominated phase transitions. Several approximate theoretical and numerical studies (see Refs. [3–9]) have already been made on SK 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 [10], which is an indicator of the nature of critical fluctuation. It also provides critical transverse field 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 SK model) for high temperature and low transverse field, to a "quantum" value for low temperature and high transverse field at a finite temperature.

II. MODEL

The Hamiltonian of quantum SK model of N spins is given by

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

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

$$H_{\rm eff} = -\sum_{n=1}^{M}\sum_{i<j}\frac{J_{ij}}{M}\sigma_i^n\sigma_j^n - \sum_{i=1}^{N}\sum_{n=1}^{M}\frac{1}{2\beta}\log\coth\frac{\beta\Gamma}{M}\sigma_i^n\sigma_i^{n+1}, \quad (2)$$

where $\sigma_i^n = \pm 1$ is the classical Ising spin and β is the inverse of temperature T. The additional dimension appears in Eq. (2), is often called Trotter direction; $M \to \infty$ as $T \to 0$.

III. MONTE CARLO RESULTS

We accomplish Monte Carlo simulation using Hamiltonian in Eq. (2) to find the critical transverse field for a fixed temperature. We also perform Monte Carlo simulation on Hamiltonian H_0 to extract the critical behavior of the classical SK model. We take t_0 Monte Carlo steps to equilibrate the system and make Monte Carlo averaging over next t_1 steps. To study the critical behavior of the model, we take replica overlap $q(t)$, which is defined as $q(t) = \frac{1}{NM}\sum_{i=1}^{N}\sum_{n=1}^{M}[\sigma_i^n(t)]^{\phi}[\sigma_i^n(t)]^{\theta}$, where $(\sigma_i^n)^{\phi}$ and $(\sigma_i^n)^{\theta}$ are the spins of two different replicas ϕ and θ corresponding to the same realization of disorder. We study the variation of average Binder cumulant (g) with Γ and T for different system sizes. For our study we define the average Binder cumulant [11,12] given by

$$g = \frac{1}{2}\left[3 - \overline{\left(\frac{\langle q^4\rangle}{(\langle q^2\rangle)^2}\right)}\right]; \quad \langle q^n\rangle = \frac{1}{t_1}\sum_{t=t_0}^{t_0+t_1} q^n(t), \quad (3)$$

where $\langle . \rangle$ and overhead bar indicate thermal and configuration averages, respectively. It may be noted that with another definition for disorder averaging [11] $g = \frac{1}{2}[3 - \frac{\overline{\langle q^4\rangle}}{(\overline{\langle q^2\rangle})^2}]$ one obtains huge fluctuation and bad statistics (see, e.g., Ref. [11]). We therefore work with the above definition of g [Eq. (3)] to make a consistent study throughout the entire range of temperature.

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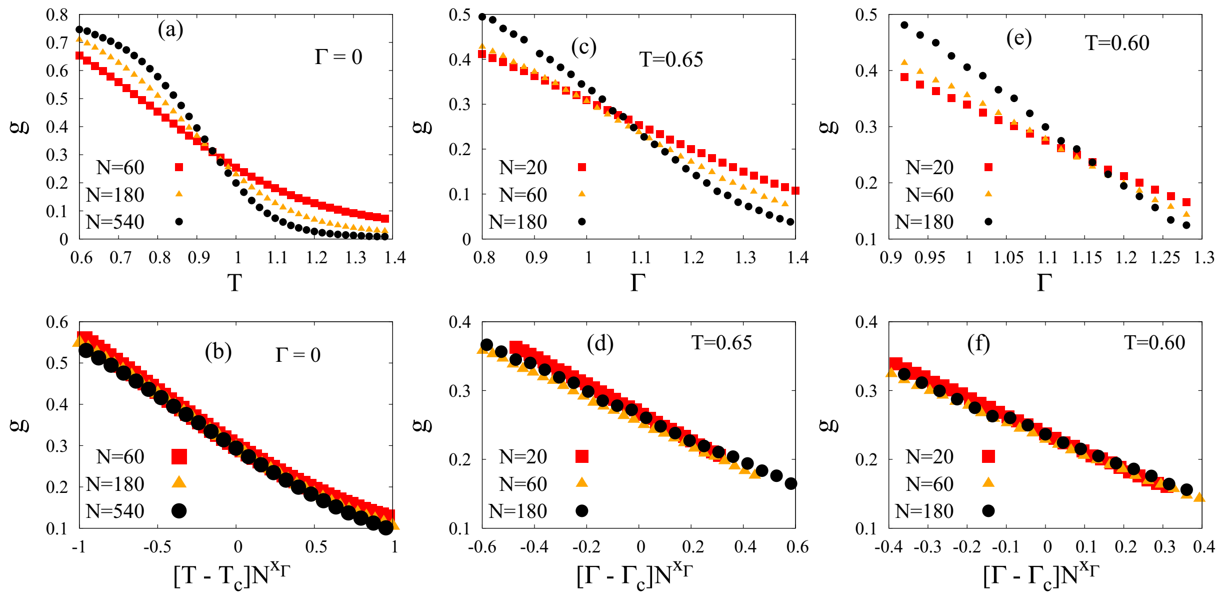

FIG. 1. (Color online) Monte Carlo results for the Binder cumulant (g) plotted as function of temperature T and transverse field Γ are shown: (a) for classical SK model (at $\Gamma = 0$) and (c) and (e) for $T = 0.65$ and 0.60, respectively. The crossing points give the estimate for T_c or Γ_c. The statistical errors are indicated by the symbol sizes. Figures (b), (d), and (f) show the collapses of g curves of (a), (c), and (e), respectively, when the variations of g are plotted against $[T - T_c]N^{x_T}$ or $[\Gamma - \Gamma_c]N^{x_\Gamma}$ [see Eq. (4)]. The scaling collapses give the values x_T or $x_\Gamma = 0.31 \pm 0.02$.

Near critical point g scales as $g = g(L/\xi, M/L^z)$ [11], where L denotes the linear size of the system and M is the Trotter size. The dynamical exponent is symbolized by z. ξ represents the correlation length, which scales as $\xi \sim (T - T_c)^{-\nu_T}$ or $(\Gamma - \Gamma_c)^{-\nu_\Gamma}$ with correlation exponents ν_T or ν_Γ. Hence, close to critical region we can write

$$g \sim g[(T - T_c)N^{x_T}, M/N^{z/d_c}] \quad \text{or} \quad g[(\Gamma - \Gamma_c)N^{x_\Gamma}, M/N^{z/d_c}], \tag{4}$$

where $x_T = 1/\nu_T d_c$ and $x_\Gamma = 1/\nu_\Gamma d_c$ with $L = N^{1/d_c}$. The critical transverse field or temperature are denoted by Γ_c or T_c, respectively. Here d_c denotes the effective dimension of the system, which helps to extract the linear size L ($\sim N^{1/d_c}$) and Trotter size M ($\sim L^z \sim N^{z/d_c}$) for a N spin system, thereby allowing the scaling properties of $g = g(N^{1/d_c}/\xi, M/N^{z/d_c})$ with the correlation length ξ. The intersection of the g versus Γ curves for different system sizes (keeping M/L^z fixed) gives the estimate of values of Γ_c and critical Binder cumulant g_c. We try to collapse the g curves by following Eq. (4). Such collapses of the g curves are made by suitably scaling the tuning parameters with chosen values of the exponents x_T and x_Γ.

To simulate $H_{\rm eff}$ we take system sizes $N = 20, 60, 180$. We work with $d_c = 6$ and $z = 4$ [13] (these values are associated with classical SK model). To keep M/L^z fixed, we start with $M = 10$ for the system size $N = 20$ and take $M = 21,43$ for system sizes $N = 60, 180$, respectively. Due to the absence of any additional dimension (Trotter dimension) in the Hamiltonian H_0, we are able to take larger system sizes $N = 60, 180, 540$ in the Monte Carlo simulation of the classical SK model. The equilibrium time of the system is $t_0 = 75\,000$ and we take $25\,000$ (t_1) Monte Carlo steps for thermal averaging. We averaged 1000 samples to get the configuration average. We notice that in the range starting from the classical SK model at $\Gamma = 0$ to almost $T \simeq 0.50$ ($\Gamma \simeq 1.30$), the g_c takes a constant value 0.22 ± 0.02 [see Figs. 1(a), 1(c), and 1(e)] and we find good data collapse of g curves [to Eq. (4)] for $x_T = x_\Gamma = 0.31 \pm 0.02$ [see Figs. 1(b), 1(d), and 1(f)]. This result ($x_T = x_\Gamma$ or $\nu_T = \nu_\Gamma$) is also consistent with analytic nature of the $T-\Gamma$ phase boundary of the model (see Sec. V). In the range $T = 0.30$ ($\Gamma \simeq 1.50$) to $T = 0.20$ ($\Gamma \simeq 1.54$), we observe that the value of g_c is nearly equal to zero but in this range we do not get decent collapses of g curves for any one chosen value of x_Γ. We repeat our simulation in this range with $d_c = 8$ and $z = 2$ [14,15] (these values correspond to quantum SK model). With these values of d_c and z we take Trotter sizes $M = 10, 13, 17$ for the system sizes $N = 20, 60, 180$, respectively, to keep M/L^z constant. Again we find vanishingly small value of g_c [see Figs. 2(a) and 2(c)]. This time we get good data collapse of g curves [see Figs. 2(b) and 2(d)] for $x_\Gamma = 0.50 \pm 0.02$. However, we are not able to get good collapse of the g curves in the entire range of classical critical behavior for ($\Gamma = 0$, $T \simeq 1.0$) to ($\Gamma \simeq 1.30$, $T \simeq 0.50$). As we observe a change in the value of x_Γ at low temperature, we also evaluate the variation of g with T keeping Γ fixed at 1.5. This variation is shown in Fig. 3(a) and corresponding collapse of g curves [see Fig. 3(b)] provides $x_T = 0.49$ which confirms $x_T \simeq x_\Gamma \simeq 0.50$. Such a crossover in g_c or the exponent value x_Γ (=x_T) with Γ (or T) values within this range ($0.5 < T < 0.35$, $1.30 < \Gamma < 1.45$) may be abrupt. From our numerical studies here it is not possible to rule out that this crossover is gradual and not abrupt. It requires further studies.

IV. ZERO-TEMPERATURE DIAGONALIZATION RESULTS

We explore the pure quantum critical behavior of the spin glass (i.e., the system at temperature $T = 0$) through

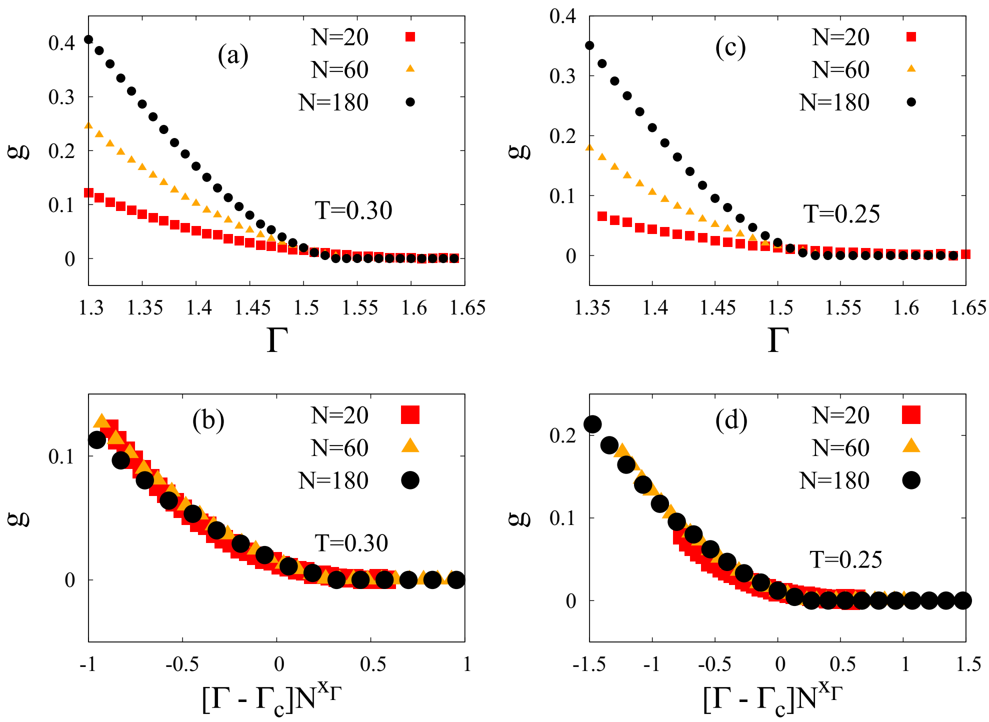

FIG. 2. (Color online) Monte Carlo results for the Binder cumulant (g) plots with transverse field Γ at temperatures 0.30 and 0.25 are shown in (a) and (c), respectively. The statistical errors are of the order of the symbol sizes. Figures (b) and (d) show the collapses of g curves in (a) and (c), respectively. Again the variations of g are plotted according to the scaling relation Eq. (4) and the collapses give the value $x_\Gamma = 0.50 \pm 0.02$.

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 [16]. 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 of Eq. (1) in spin basis states, i.e., the eigenstates of the spin operators (σ_i^z, $i = 1, \ldots, N$) for performing the diagonalization. Then the nth eigenstate of the Hamiltonian in Eq. (1) is represented as $|\psi_n\rangle = \sum_{\alpha=0}^{2^N-1} a_\alpha^n |\varphi_\alpha\rangle$, where $|\varphi_\alpha\rangle$ are the eigenstates of the Hamiltonian H_0 and $a_\alpha^n = \langle\varphi_\alpha|\psi_n\rangle$. 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 $Q = (1/N)\sum_i \overline{\langle\psi_0|\sigma_i^z|\psi_0\rangle^2}$. The configuration average is again indicated by the overhead bar. To calculate Binder cumulant, the various moments can be calculated using Refs. [1,18],

$$Q_k = \frac{1}{N^k}\sum_{i_1}^{N}\ldots\sum_{i_k}^{N}\langle\psi_0|\sigma_{i_1}^z\ldots\sigma_{i_k}^z|\psi_0\rangle^2. \tag{5}$$

Here Q_ks are actually k-spin correlation functions for a particular disorder configuration. One can easily realize that order parameter $Q = \overline{Q_1}$. If we know the ground state at different parameter values of the Hamiltonian the various

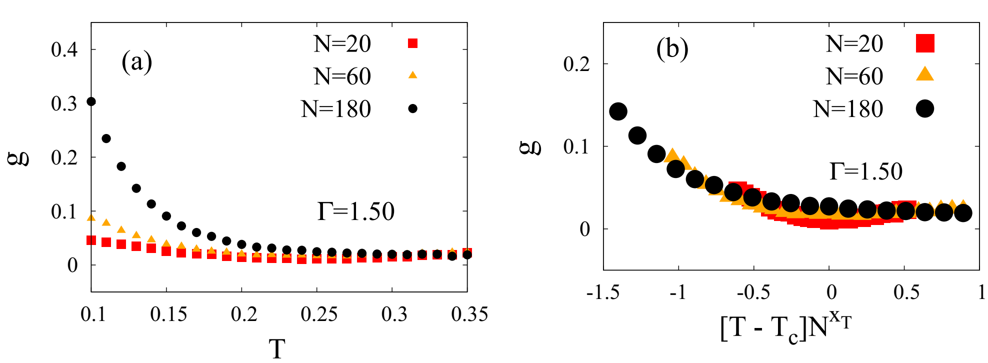

FIG. 3. (Color online) (a) The plot shows the Monte Carlo results for the variation of Binder cumulant (g) as a function of temperature T at the transverse field $\Gamma = 1.5$. (b) The plot shows collapse of g curves in (a) with $x_T = 0.49$. The statistical errors of the data points are of the order of the symbol sizes.

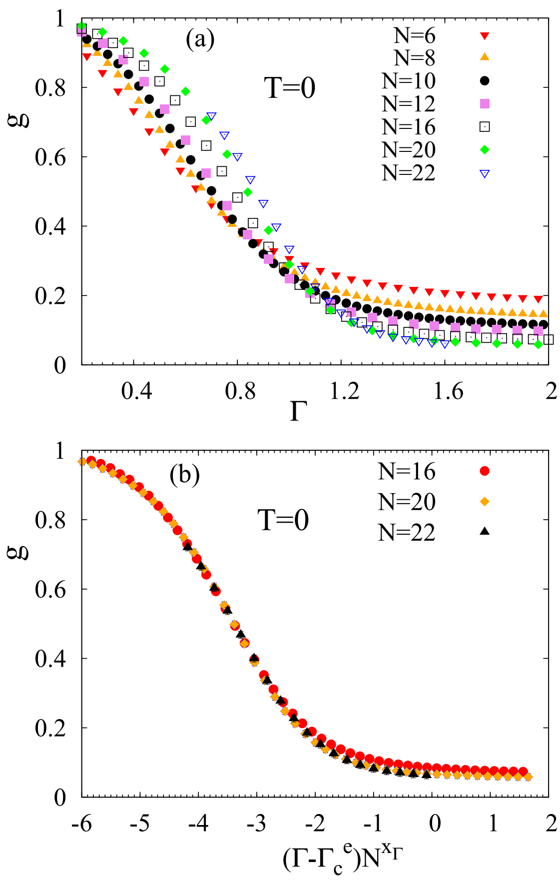

FIG. 4. (Color online) The plot (a) shows the variation of Binder cumulant g as a function of Γ for different system sizes for quantum SK model at $T = 0$ (exact diagonalization results). The larger system sizes intersect at higher values of Γ signifying finite-size effect of the system. (b) The Binder cumulant curves for different system sizes (N) collapse following the scaling fit [to Eq. (4) for $M = 0$] with an estimated $\Gamma_c^e = 1.62$ and exponent $x_\Gamma = 0.5$.

moments can be determined using Eq. (5). In this context the average Binder cumulant is defined as $g = \frac{1}{2}[3 - (\overline{\frac{Q_4}{\langle Q_2 \rangle^2}})]$ [note the difference with the Eq. (3)].

The variations of g as a function of Γ is shown in Fig. 4(a) for different system sizes. To study the finite-size effects, we consider a pair of two different system sizes N and N' and evaluate the values of $\Gamma_c(N,N')$ and $g_c(N,N')$ from the intersection of the g versus Γ curves for these two system sizes. Accounting every possible pair, we extrapolate $\Gamma_c(N,N')$ with $(NN')^{-x_\Gamma/2}$ to get Γ_c for infinite system size. In the absence of an established finite-size scaling behavior of g, we fit its finite-size variations of $g_c(N,N')$ to $1/\sqrt{NN'}$ to evaluate g_c in the thermodynamic limit. The extrapolated value of $\Gamma_c(N,N')$ is 1.62 ± 0.03 in the limit of $N,N' \to \infty$, which is indicated in Fig. 5(a). Here the best fit value of the scaling exponent x_Γ for getting the extrapolated value of $\Gamma_c(N,N')$ is 0.51, which is consistent with that obtained from collapse of g curves for different system sizes [see Fig. 4(b)]. One can also see that the extrapolated value of $\Gamma_c(N,N')$ is nearly equal to the estimated value $\Gamma_c^e = 1.62$, which is required for getting a good collapse of Binder cumulant curves for different system sizes [see

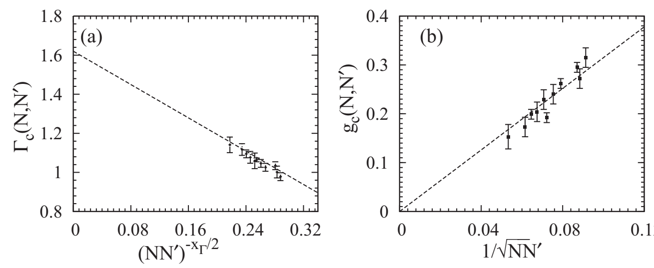

FIG. 5. The plot shows critical transverse field $[\Gamma_c(N,N')]$ and critical Binder cumulant $[g_c(N,N')]$ as a function of $(NN')^{-x_\Gamma/2}$ and $1/\sqrt{NN'}$, respectively, where N and N' are two system sizes, obtained from exact diagonalization: (a) The extrapolated value of Γ_c is found to be 1.62 and (b) g_c tends to a null value for a infinite size system. For these two plots best fit line is also shown.

Fig. 5(b)]. On the other hand, g_c takes nearly a zero value in the limit of $N,N' \to \infty$ [see Fig. 5(b)], and this is consistent with our Monte Carlo results at the low temperatures. These indicate that starting from around $T = 0.35$ to $T = 0$ the values of g_c as well as of x_Γ remain practically unchanged at its quantum fluctuation dominated value ($g_c \simeq 0$, $x_\Gamma \simeq 0.50$).

V. SUMMARY AND DISCUSSIONS

In summary, we estimate the entire phase diagram (see Fig. 6) of the quantum SK spin glass using Monte Carlo simulation and exact diagonalization results to determine the Binder cumulants g, which allows accurate estimate of the phase diagram and extraction of the correlation length exponent value. We use system sizes $N = 20, 60, 180$ with moderately chosen M values (to keep M/L^z constant) for Monte Carlo simulation, whereas for exact diagonalization the maximum system size limit is $N = 22$. The estimated

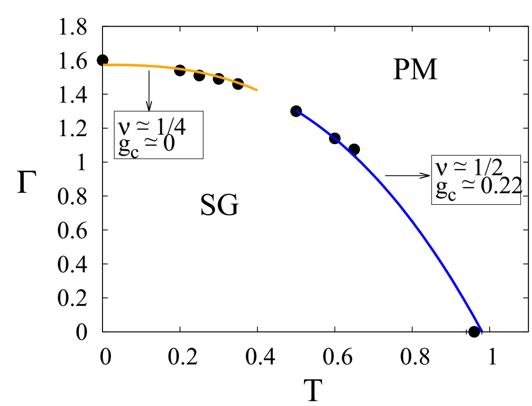

FIG. 6. (Color online) Consolidated phase diagram of the SK spin glass model in transverse field, obtained from the Monte Carlo simulation and exact diagonalization. The statistical errors are indicated if they are more than the symbol sizes. Here SG and PM denote, respectively, the spin glass and paramagnetic phases. The points at $T = 0$ and $\Gamma = 0$ correspond to purely quantum and classical cases, respectively. The obtained critical behaviors are indicated ($g_c \simeq 0$, $\nu \simeq 1/4$ for low T-high Γ region, and $g_c \simeq 0.22$, $\nu \simeq 1/2$ for high T-low Γ region). The crossover point is around $T \simeq 0.45$ and $\Gamma \simeq 1.33$.

phase diagram compares well with some earlier estimates for isolated parts (Refs. [6,7]), which fall in the high-temperature (classical) critical-behavior region of the of SK model. The earlier studies, therefore, could not address the classical-quantum crossover phenomena observed here.

During the exploration of phase diagram by varying T or Γ, we find that g_c remains fairly constant (at value 0.22 ± 0.02) from classical transition point ($\Gamma = 0$, $T \simeq 1.0$) to almost $\Gamma = 1.33$, $T = 0.45$ and assumes a very low value (less than 0.03; see Fig. 3), or vanishes (with Gaussian fluctuations) beyond this point and remains the same up to $\Gamma \simeq 1.62$, $T = 0$ (see also Ref. [17]). It may be mentioned that even with nontrivial (non-Gaussian) fluctuations, the critical Binder cumulant value can effectively vanish for fluctuation induced discontinuous transitions (see, e.g., Binder *et al.* [19]). The scaling fits to Eq. (4) give x_T or $x_\Gamma = 0.31 \pm 0.02$ for high T and low Γ values, while $x_T = x_\Gamma = 0.50 \pm 0.02$ for low T and high Γ values. We should mention that we performed the same Monte Carlo simulations on infinite range pure ferromagnetic system. In this case, g_c and x_Γ values remain almost the same for any finite temperature we considered (up to $T = 0.1$), indicating that the crossover to quantum behavior occurs only at zero temperature, as theoretical analysis for such pure systems clearly suggests (see, e.g., Ref. [2]).

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 Γ and high T) is quite different from that for the quantum fluctuation-dominated transitions (for high Γ and T). Existence of such distinct universality classes appears more reasonable when compared with the observation that the correlation length exponent ν also has two different values in these two parts of the phase boundary (having two different values of g_c). If we take effective dimension $d_c = 6$ [13] and $x_T = x_\Gamma = 1/3$ for entire classical fluctuation-dominated transitions, then using the relation $x_\Gamma = x_T = 1/d_c\nu$ (Eq. (4); see also Refs. [14,18]) we get $\nu = 1/2$, which is consistent with the earlier estimate [13]. Similarly, for quantum fluctuation dominated transitions we find $\nu = 1/4$ for $x_\Gamma = 1/2$ (considering $d_c = 8$ [14,15]), which agrees with earlier estimates [14,15]. As mentioned already, any other combinations of d_c and x_Γ values did not give good collapse for g. Such changes in the values of g_c and ν for the different regions of the phase diagram (Fig. 6) clearly indicate that, in contrast to the pure case, the crossover between classical and quantum fluctuation-dominated critical behaviors for the transverse Ising SK model occurs at a nonvanishing temperature.

Due to random and competing spin-spin interactions, the free-energy landscape of SK spin glass is highly rugged. Such uneven free-energy landscape contains high ($[O(N)]$ free-energy barriers, which separate several local free-energy minima. For low T, unlike in the pure case (where the landscape is inclined smoothly toward the minima), the thermal fluctuations become ineffective in helping such systems to cross tall barriers to reach the paramagnetic state by flipping finite fractions of N spins. On the other hand, due to the presence of high Γ, tunneling through such tall but narrow barriers becomes highly probable [20,21]. Quantum fluctuations, therefore, induce the phase transition and determine the transition behavior. Such effectiveness of quantum (over thermal) fluctuations at low T in such frustrated systems might, therefore, be responsible for a classical-quantum crossover at a finite (but low) temperature (and large transverse field) in the quantum SK model. In fact, our study establishes that the critical value of the Binder cumulant (with associated scaling exponents) and its crossover behavior gives a quantitative measure of the relative importance of classical versus quantum fluctuations in determining the nature of the phases in such frustrated systems.

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