Sherrington-Kirkpatrick model in a transverse field: Absence of replica symmetry breaking due to quantum fluctuations

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The Sherrington-Kirkpatrick model under a transverse field is studied here employing the Suzuki-Trotter formula to map the model to an equivalent classical one. The effective Thouless-Anderson-Palmer free energy is used to study the stability of the system, and Monte Carlo computer simulations of the effective classical model are performed to obtain the phase diagram and the magnetization overlap distribution. Our results indicate a trivial overlap distribution due to quantum fluctuations. The phase diagram shows a slight initial increase in the glass transition temperature T_g as the transverse field is switched on, confirming that obtained by Yokota.

I. INTRODUCTION

The infinite-range Ising spin-glass model proposed by Sherrington and Kirkpatrick (SK),[1] in the context of a mean-field solution of the magnetic spin-glass transitions, has revealed many intriguing features[2] of the disordered systems involving frustration. One such feature is the loss of replica symmetry and the consequent breaking of ergodicity beyond the de Almeida–Thouless (AT) line.[3] As a consequence, one gets a broad pure state overlap distribution $W(q)$ (from a Parisi order function[4]) below the AT line even in the thermodynamic limit.[5,2] It is not clear, however, how far this feature is universal for disordered frustrated systems. For example, detailed analysis[6] of the decay of the connected correlation function at large distances for short-range Ising (and other classical) spin-glass models has indicated a trivial overlap distribution function $W(q)$, in contrast to that for the long-range (SK) model.

We have studied here the SK model under a transverse field employing the Suzuki-Trotter formula[7] to reduce the model to an equivalent classical one and using Thouless-Anderson-Palmer (TAP) free energy[2] analysis and also Monte Carlo simulations for this effective classical model. Our results indicate a trivial overlap distribution function $W(q)$, even for this long-range SK model due to quantum fluctuations. We also obtain the temperature (T) –transverse field (Γ) phase diagram for the model, which shows an interesting feature for small Γ, namely a slight increase in T_g (the glass transition point) with Γ, due to an initial suppression[8] of the random reaction field by quantum effects.

It is known that quantum fluctuations in general do not affect the normal critical behavior for second-order (continuous) transitions at $T \neq 0$. The additional quantum dynamics only effectively increases the lattice dimensionality by unity for the zero-temperature-transition critical behavior.[9] The situation is very different in the case of spin glasses, where quantum fluctuations along with frustrations play an important role in determining the glass ground-state properties and the transition processes. The numerical calculations of Marland and Betts[10] indicated that frustration in such cases does not produce any macroscopic entropy in the ground state because of quantum motions between the degenerate classical states. The approximate mean-field-type calculations of Klemm,[11] in particular, indicated that the quantum fluctuations may be strong enough for a spin-$\frac{1}{2}$ Heisenberg system to destroy completely the spin-glass state. However, Bray and Moore[12] showed, using the replica theory, the existence of a phase transition even in the presence of quantum motions, and calculated the depression of transition temperature T_g due to quantum fluctuations in the mean-field approximation. Chakrabarti studied[13] the short-range Ising spin-glass models in a transverse field, where similar quantum effects, as in ordinary transitions, were shown by exact analysis for the unfrustrated Mattis model and by an approximate renormalization-group treatment for the frustrated case. Dos Santos *et al.* studied the effect of disorder correlation in the equivalent "time" dimension using the real-space renormalization-group method, and Walasek and Lukierska-Walasek obtained the phase diagram of the same short-range model using mean-field-type approximation.[14] The mean-field results for the model were used by Iida and Terrauchi and Aksenov *et al.* for analyzing the experimental results on structural glass transitions in order-disorder-type ferroelectric systems with random competing interactions.[15]

The phase diagram for the long-range SK model in a transverse field has recently been studied by Ishii and Yamamoto, Federov and Shender, and Usadel using replica theory and by Walasek and Lukierska-Walasek using cluster expansion methods.[16] Yokota[8] employed the TAP method to study the equivalent classical Hamiltonian obtained using the Suzuki-Trotter[7] formula. His study indicates an interesting feature of the phase diagram in that the glass transition temperature T_g initially increases slightly with the transverse field Γ because of an initial cancellation of the TAP reaction field. This contrasts with the phase diagram of the system obtained[16] using methods other than the TAP method, so that the feature might appear as an artifact of the TAP analysis. Our Monte Carlo study, however, confirms this feature of the phase diagram. Our interest, in fact, has essentially been in the overlap distribution $W(q)$ for such a quantum SK model. The results obtained by us using the effective TAP free energy and Monte Carlo simulations indicate (simulations have been performed up to a maximum number of spins $N=32$) that the breaking of ergodicity or the replica symmetry[2] that occurs in the classical SK model below the AT line does not take place in the presence of transverse fields.

II. EFFECTIVE CLASSICAL HAMILTONIAN

We consider the system described by the following Hamiltonian:

$$H=-\Gamma\sum_i S_i^x-\sum_{\langle i,j\rangle} J_{ij}S_i^zS_j^z , \tag{1}$$

where S_i are the Pauli matrices for the ith spin and the notation $\langle i,j\rangle$ denotes the distinct pairs. Γ represents the transverse field, and the random exchange interaction J_{ij} among, say, N spins is assumed to have a Gaussian distribution (centered at zero),

$$P(J_{ij})=(N/2\pi\tilde{J})^{1/2}\exp(-NJ_{ij}^2/2\tilde{J}^2) . \tag{2}$$

Applying the Suzuki-Trotter formula[7] to the partition function, the effective classical Hamiltonian (with an added dimension) is obtained in the Mth approximation as

$$H_{\text{eff}}=-(1/M)\sum_m \sum_{\langle i,j\rangle} J_{ij}S_{im}S_{jm}-(1/2\beta)\log[\coth(\beta\Gamma/M)]\sum_i\sum_m S_{im}S_{im+1}-(M/2)\log[\tfrac{1}{2}\sinh(2\beta\Gamma/M)] . \tag{3}$$

Here S_{im} denotes the Ising spin defined on the lattice (i,m), i is the position in the original SK model, and m is the index for the extra dimension introduced due to the quantum dynamics. The summation over m along the Trotter direction goes from 1 to M in the Mth approximation, and the quantum to classical mapping is exact only for infinite M. In Eq. (3), $\beta=1/kT$ and the exchange distribution is as given in Eq. (2).

III. TAP FREE ENERGY AND AT STABILITY

We use the TAP method[2] to find the approximate free energy in terms of local magnetic moments ($\mu_i\equiv\langle S_i\rangle$, where i is any site on the effective classical system) and their reaction fields [averaged over $P(J)$]. In the limit $x=\beta\Gamma\ll 1$ the free energy expanded up to second order in $\beta\Gamma$ gives[8]

$$\begin{aligned}\beta F_{\text{TAP}}=&\sum_i[(\tfrac{1}{2}+\tfrac{1}{8}x^2)\mu_i^2+(\tfrac{1}{12}+\tfrac{1}{32}x^2)\mu_i^4+(\tfrac{1}{30}+\tfrac{1}{64}x^2)\mu_i^6]\\&+\sum_{\langle i,j\rangle}\{-\beta J_{ij}\mu_i\mu_j+\tfrac{1}{2}(\beta J_{ij})^2[(1-\tfrac{3}{8}x^2)(\mu_i^2+\mu_j^2)+\tfrac{1}{8}x^2(\mu_i^4+\mu_j^4)\\&\qquad-(1-\tfrac{1}{2}x^2)\mu_i^2\mu_j^2-\tfrac{1}{64}x^2(\mu_i^6+\mu_j^6)+\tfrac{9}{32}x^2(\mu_i^4\mu_j^2+\mu_i^2\mu_j^4)]\} .\end{aligned} \tag{4}$$

The extremum condition $\partial F_{\text{TAP}}/\partial\mu_i=0$ leads to the TAP equation for the system (the limit $\Gamma\to 0$ recovers the original TAP equation[2] for the SK model), giving the phase diagram in the T-Γ plane.[8]

To study the AT stability[3,2] of this TAP solution, we look at the Hessian matrix $A_{ij}=\partial^2F_{\text{TAP}}/\partial\mu_i\partial\mu_j$ formed from the second derivative of F_{TAP}. Stability condition is satisfied by Trace $A\geq 0$, which gives

$$[1+\beta^2\Gamma^2(\tfrac{1}{4}+\tfrac{3}{8}q+\tfrac{15}{32}r)]-\beta^2\tilde{J}^2[(1+\tfrac{3}{8}\beta^2\Gamma^2)-(2+\tfrac{9}{4}\beta^2\Gamma^2)q+(1-\tfrac{255}{64}\beta^2\Gamma^2)r]\geq 0 , \tag{5}$$

where $q\equiv 1/N\sum\mu_i^2$ is the spin-glass order parameter and $r\equiv 1/N\sum\mu_i^4$. From the above inequality, it is clear that in the absence of any transverse field Γ, stability can be maintained from infinite temperature (where $q=r=0$) to transition temperature $T_g(0)=\tilde{J}$. For nonzero Γ, stability is achieved for all temperatures down to $T=T_g(\Gamma)-\Gamma/2\sqrt{2}+\frac{7}{16}\Gamma^2\tilde{J}^2$, where

$$T_g(\Gamma)=T_g(0)+\Gamma/2\sqrt{2}-\tfrac{3}{8}\Gamma^2/\tilde{J}^2$$

(in the limit $\Gamma\to 0$) is the glass transition temperature, obtained from[8] $\partial F_{\text{TAP}}/\partial\mu_i=0$, in the presence of Γ. Thus, unlike in the classical SK model where the AT stability can be maintained only above $T_g[=T_g(0)]$, here this approximate calculation indicates a stability even below $T_g[=T_g(\Gamma)]$ when the system is already in spin-glass phase. It is to be noted that in the presence of a longitudinal field instead of a transverse one, the SK model exhibits AT stability[3] only above the AT line with ferromagnetic spin ordering along the applied (longitudinal) field. The quantum SK system, on the other hand, like the short-ranged systems,[6] is found to exhibit stability and hence a trivial order-parameter distribution while remaining in the spin-glass phase at the same time.

IV. MONTE CARLO SIMULATION

Monte Carlo computer simulations of the SK model in the presence of a transverse field are performed using the Metropolis heat-bath method[17] for the classical spin system given by Hamiltonian (3) with finite M. We take a two-dimensional $(N \times M)$ lattice having Ising spins on lattice sites. N spins along the x direction in each of the M trotter rows are the spins of the classical SK model interacting with each other (within the row) with interaction strength J_{ij} having a Gaussian probability distribution [Eq. (2)] of width $(N-1)^{-1}$. The y direction represents the Trotter axis, and each of M spins along this axis in each of the N columns interacts only with its two nearest-neighbor spins along the Trotter axis with strength $\zeta=(T/2)\log[\coth(\Gamma/MT)]$. We use the periodic boundary condition along the Trotter direction. The Suzuki-Trotter approximation becomes better with increasing M, and for finite M, a correction[18] of the order of M^{-2} is needed to the thermodynamic quantities. However, with M, the interaction strength ζ increases logarithmically whereas J_{ij}/M weakens. For $M \gg \Gamma/T$, the singular behavior of ζ tends to arrange the spins parallel along the Trotter direction whereas vanishingly small J_{ij}/M makes the interaction among the Trotter chains almost zero. This imbalance in the two cooperative interactions invalidates[19] the Monte Carlo process to work as an important sampling. For certain values of T and Γ, M is to be selected such that $M \ll \Gamma/T$, and we have taken $(\Gamma/MT)=0.06$ throughout the simulation. This has been found to be the optimal value of the ratio in the Monte Carlo simulation study[19] of the transverse Ising model. In determining the phase diagram in the Γ-T plane, we find that as Γ is increased, T_g is lowered and the condition on Γ/MT demands large M values, which virtually takes into account the enhanced quantum effects. However, a large amount of computer time forces us to limit the study in the range $\Gamma \ll 0.6\tilde{J}$.

We determine the overlap distribution[5] $W(q)$ simulating two "identical" (having the same J distribution and starting spin configuration) Monte Carlo samples independently and taking the magnetization overlap between the samples. The spins are flipped by the "heat-bath" Monte Carlo procedure and time is measured in units of Monte Carlo steps per spin. To equilibrate, the samples are simulated at a certain temperature T up to a time t_0 before determining any magnetization overlap between them. It is difficult to ascertain equilibrium as the finite size of the system prevents the symmetry breaking associated with the transition, and the system flips between two degenerate time-reversed states with a finite frequency.[20,21] This hinders any thermal averaging processes. The equilibrium is then determined by studying the time evolution of the function $P(t)$ defined[21] at time t by

$$P(t)=(1/NM)\sum_{\alpha,\beta}^{N}\sum_{\gamma,\delta}^{M} s_{\alpha\gamma}(0)s_{\beta\delta}(0)s_{\alpha\gamma}(t)s_{\beta\delta}(t) ,$$

where $s_{\alpha\gamma}(t)$ is the state of the (α,γ)th spin at the tth step. $P(t)$ falls sharply at first and subsequently attains a nonzero constant value (with fluctuations) in the spin-glass phase after a time t_0, which determines the equilibrium situation. The relaxation time t_0 is found to increase with N initially but decreases with M, and for $N=32$, $M=5$, we find that equilibrium is achieved typically after 3000 to 4000 Monte Carlo steps per spin.

For $t > t_0$, we determine the magnetization overlap

$$Q(t)=(1/NM)\sum_{\alpha=1}^{N}\sum_{\gamma=1}^{M} s^1_{\alpha\gamma}(t_0+t)s^2_{\alpha\gamma}(t_0+t) , \tag{6}$$

where the superscripts 1 and 2 refer to the two "identical" samples. The overlap distribution $W(q)$ is determined from

$$W(q)=\langle (1/\tau)\sum_{t=1}^{\tau}\delta[q-Q(t)]\rangle_J .$$

Here, $\langle \ldots \rangle_J$ denotes the average over various J configurations. In our simulation, $\tau \simeq 500$ and the J averaging is done over 30 to 40 samples. The distribution function $W(q)$ for $T=0.4\tilde{J}$ and $\Gamma=0.15\tilde{J}$, as obtained from the simulation, is shown in Fig. 1 for $N=16$, 24, and 32. Since the model given by the Hamiltonian (3) has a time-reversal symmetry, we expect $W(q)$ to be symmetric in q and plot the distribution against $|q|$.

It is interesting to note that unlike the classical case,[5] $W(q)$ turns out to have an oscillatory dependence on q with a frequency linear in N. Moreover, analysis of the results for $W(q)$ at differnt J configurations reveals that this oscillatory dependence of $W(q)$ on q is statistically independent. The positions of the maxima or minima and their numbers remain the same in any J configuration and hence invariance over sample averages. We think that this behavior of $W(q)$ is an artifact of the finite size of the system. In fact, as frequency increases with N, the amplitude of oscillation decays and the entire distribution profile appears to merge with its upper boundary shown by the dashed curve in Fig. 1. The nature of the distribution $W(q)$, thus, would be given by this dashed curve in the thermodynamic limit, and henceforth we would refer to this dashed curve as $W(q)$ in this paper.

When $T < T_g(\Gamma)$, the system is in the spin-glass phase characterized by a continuous distribution (for a finite system) of $W(q)$ from $q=0$ to 1 with a peak at nonzero value of q depending on Γ. In the presence of Γ, as T is increased, the position of the peak is shifted towards smaller q values and centered around $q=0$ in the paramagnetic phase. For the finite paramagnetic system, $W(q)$ is expected to be a Gaussian distribution centered at zero and of width of order $(NM)^{1/2}$, which goes over to a delta function only in the thermodynamic limit. The temperature at which the peak first touches the $q=0$ axis gives the transition temperature $T_g(\Gamma)$. However, the determination of this temperature introduces some uncertainty. We determine $T_g(\Gamma)$ for various values of $\Gamma \le 0.6$ with an accuracy of 4%–5%. The phase diagram is shown in Fig. 2. The phase diagram clearly indicates an initial small increase of $T_g(\Gamma)$ with Γ, in accordance with the findings of Yokota.[8] For $\Gamma > 0.6\tilde{J}$, our results are inadequate for good statistics, and we have not shown the results. However, the results indeed indicate a sharp lowering of $T_g(\Gamma)$ which has been shown in Fig. 2 by the dashed line. Such a sharp fall of $T_g(\Gamma)$ with large Γ was obtained in almost all the theoretical studies[16] of the phase diagram of the model, and has also been supported

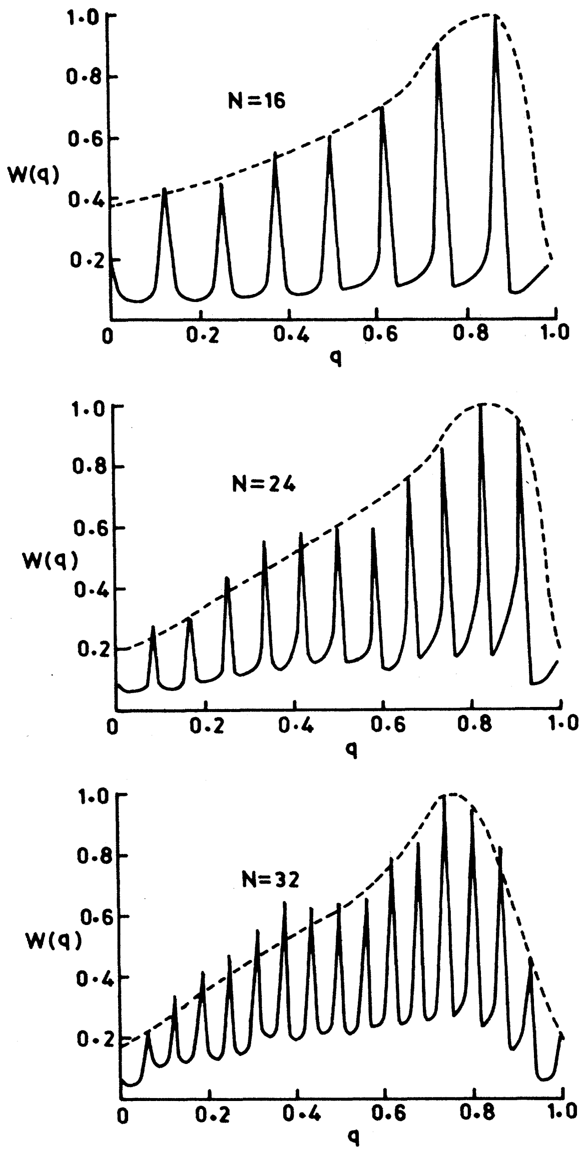


FIG. 1. Simulation results for the overlap distribution for the SK model in the transverse field $\Gamma=0.15$ ($\tilde{J}=1$) and temperature $T=0.4$ for system sizes $N=16$, 24, and 32. Here the distribution is normalized to its maximum value. The upper profiles denoted by the dashed curves give $W(q)$.

in a Monte Carlo simulation study[21] by Ishii and Yamamoto. For any Γ, we get somewhat higher values of $T_g(\Gamma)$: $T_g(0)$ turns out to be 1.08 ± 0.02 instead of unity. This, we think, is again due to the finite size of the system, and a run for $T_g(0)$ for $N=64$ actually gives $T_g(0)$ very close to unity. Due to the finite size of the system the entire phase diagram has been shifted along the positive T direction. Nevertheless, we expect the nature of the curve to remain the same in the thermodynamic limit.

The dependence of $W(q)$ on N for $T=0.4\tilde{J}$ and

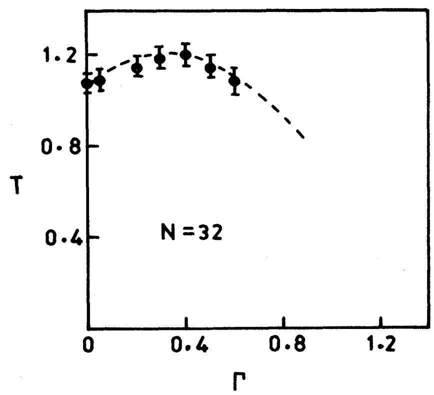
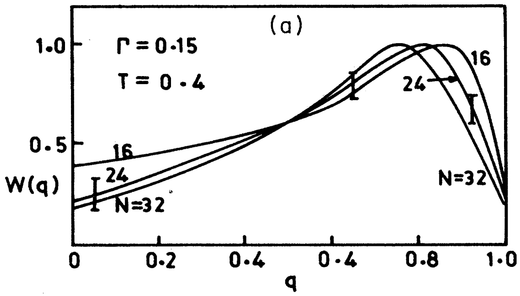


FIG. 2. Phase diagram for the SK model in the transverse field in the T-Γ plane ($\tilde{J}=1$).

$\Gamma=0.15\tilde{J}$ is shown in Fig. 3(a) for $N=16$, 24, and 32. A corresponding classical ($\Gamma=0$) result for $W(q)$, as has been obtained from our simulation (with $M=1$), is shown in Fig. 3(b). In the classical SK system we do not get any oscillatory dependence of $W(q)$ on q, and our results for the classical system agree with the simulation results obtained earlier by Young.[5] It may be noted that we have plotted $W(q)$ normalized to its maximum value rather than with normalized integrated probability as in Young.[5] In contrast to the classical case where, in addition to a peak at large q, we also get a long tail extending to $q=0$ with a finite weight $W(0)$ independent of N, the quantum SK model exhibits a peak at large q along with a tail, but the weight $W(0)$ at $q=0$ falls off with increasing N. The tail in the presence of finite Γ falls [see Fig. 3(a)] almost linearly with q near $q=0$, and does not show any indication of going to a constant value with a slight upturn that is expected[5] in the classical ($\Gamma=0$) case, and as obtained in our simulation with identical system sizes [see Fig. 3(b)]. On the low-q side of the peak, the entire distribution appears to shrink down as N is increased. Contrary to this, in the classical case, the low-q part of $W(q)$ is rather flat and appears with much weight which even increases with N. On the high-q side, we find a rapid fall of $W(q)$ as is seen in the classical case. However, in the presence of the transverse field, this fall is much faster and goes to zero much more rapidly. Detailed computation with various large N and M values and much better statistics (regarding time averaging and configurational entropy), involving a very large amount of computer time, is needed for any quantitative study of the situation. However, our simulation clearly shows a narrowing of the distribution on both low- and high-q regions as N is increased, indicating that $W(q)$ might go over to a delta function $W(q)=\delta(q-q_{\mathrm{Tr}})$ in the thermodynamic limit. This means the system is ergodic and there is a definite spin-glass order parameter q_{Tr} depending upon the transverse field. A comparison of the peak positions for different N in Figs. 3(a) and 3(b) suggests that $q_{\mathrm{Tr}} < q_{\mathrm{Cl}}$, where the classical spin-glass order param-



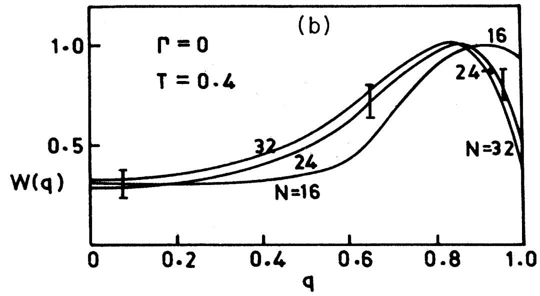


FIG. 3. Variation of the overlap distribution $W(q)$ with system size N ($\tilde{J}=1$): (a) for the quantum case ($\Gamma=0.15$, $T=0.4$); (b) for the corresponding classical case ($\Gamma=0$, $T=0.4$).

eter q_{Cl} is the q value averaged over the distribution $W(q)$ for $\Gamma=0$. This, we expect to be due to quantum fluctuations.

V. DISCUSSIONS

We have studied the SK model under a transverse field, reducing the model to an equivalent classical one employing the Suzuki-Trotter formula. The TAP formalism is used to study the stability of the system, and Monte Carlo simulation is performed to obtain the phase diagram and the magnetization overlap distribution. The phase diagram indicates a slight initial increase of the glass transition temperature T_g with transverse field Γ due to an initial suppression of the TAP reaction field by quantum effects, as was shown by Yokota.[8] Our stability analysis shows that, unlike the classical system, the transverse SK model is stable well below the glass transition temperature T_g. This is supported by the overlap distribution, obtained in our Monte Carlo simulation, which appears to go over a Gaussian form (reducing to a delta function in the thermodynamic limit), indicating an ergodic spin-glass phase characterized by a definite (single) order parameter q_{Tr} like that found in short-ranged Ising spin-glass models. Of course, these indications from our simulation results are only for $N=16$, 24, and 32. We attribute the ergodicity of the transverse SK model to the quantum fluctuations due to the transverse field. Quantum tunneling between the classical "trap" states, separated by infinite (but narrow) barriers in the free-energy surface,[2] is possible, as quantum tunneling probability is proportional to the barrier area which is finite. We expect that any amount of transverse field Γ would lead to the collapse of the distribution $W(q)$ to a delta function; only the relaxation time depends on Γ, such that with smaller Γ the system would take more time to relax to the equilibrium state. Detailed study is needed to find the effect of transverse field Γ on relaxation time and the equilibrium state thus attained.

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