Reaching the ground state of a quantum spin glass using a zero-temperature quantum Monte Carlo method

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Here we discuss the annealing behavior of an infinite-range $\pm J$ Ising spin glass in the presence of a transverse field using a zero-temperature quantum Monte Carlo method. Within the simulation scheme, we demonstrate that quantum annealing not only helps finding the ground state of a classical spin glass, but can also help simulating the ground state of a quantum spin glass, in particular, when the transverse field is low, much more efficiently.

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Quantum annealing (QA) [1–10] is a method of finding the ground state (minimum energy state) of a given classical Hamiltonian $\mathcal{H}$ employing external quantum fluctuations [by adding a time-dependent kinetic part $\mathcal{H}'(t)$ which does not commute with $\mathcal{H}$] and subsequent adiabatic reduction of them [by reducing the strength of $\mathcal{H}'(t)$ from a very high initial value to zero finally]. If the evolution is slow enough and the initial state is the ground state of the total Hamiltonian [which is effectively given by the dominating kinetic part $\mathcal{H}'(t=0)$], then according to adiabatic theorem of quantum mechanics the state of the system will always remain close to the ground state and thus, at the end of the annealing, the system will be found in the ground state of the classical Hamiltonian (at the end only the original classical part is retained) with a high probability [4]. Based on this principle, algorithms can be framed to anneal complex physical systems like spin glasses as well as the objective functions of hard combinatorial optimization problems [like the traveling salesman problem] mapped to glasslike Hamiltonians, towards their ground (optimal) states. So far, the successful QA Monte Carlo schemes are mostly based on finite temperature Monte Carlo methods [1,11]. Here we study the annealing behavior of an infinite-range $\pm J$ Ising spin glass in a transverse field, using a zero-temperature quantum Monte Carlo method. We show here, with the above-mentioned Monte Carlo scheme, one cannot only find the classical ground state with the help of QA, but one can also simulate the low-kinetic energy ground states of the quantum Hamiltonian much more efficiently with the help of QA.

The model and the basic QA scheme for it are introduced in Sec I. In Sec. II we discuss at length the zero-temperature quantum Monte Carlo method used here. We discuss the results of QA employed to reach the ground state of the classical spin glass in Sec. III. We demonstrate in Sec. IV how QA can be utilized to simulate the ground state of a quantum spin glass. We conclude with a short summary.

I. MODEL

We consider an infinite range Ising spin system whose Hamiltonian is given by

$$\mathcal{H} = -\sum_{i,j(>i)}^{N} J_{ij}\sigma_i^z\sigma_j^z, \tag{1}$$

where σ_i^z is the z component of Pauli spin, representing a classical Ising spin at site i and J_{ij}'s are random variables taking up values either $+1$ or -1 with equal probabilities. The above Hamiltonian describes a cluster of N Ising spins, each connected to all others through exchange interactions of equal strength ($J=1$) but random signs. To make the energy extensive in system-size, one has to scale the energy with a factor of $N^{3/2}$, as done in the rest of the paper. The system is heavily frustrated (i.e., no spin configuration can satisfy all the bonds) due to the presence of both ferromagnetic and antiferromagnetic bonds in random fashion. The high degree of connectivity (i.e., the infinite range of the interactions) adds to the complexity of the problem. For such a system, finding the ground state spin configuration for any arbitrarily given realization of interactions (the set of J_{ij}'s) is known to be a nondeterministic-polynomial-time-hard (NP-hard) problem [13]. In the thermodynamic limit the system becomes a nonergodic spin glass below some spin glass temperature T_G.

The eigenstates of $\mathcal{H}$ (the basis states) are the direct products of the eigenstates of σ_i^z's. Each basis state represents a distinct spin configuration of the system. To perform zero-temperature quantum annealing of this $\pm J$ Ising system, we add a transverse field term $\mathcal{H}' = \Omega(t)\Sigma_{i=1}^{N}\sigma_i^x$, where σ_i^x's are x components of Pauli spins which introduce probability of tunneling between the basis states (classical configurations), and $\Omega(t)$ is the strength of the transverse field. The total Hamiltonian is thus given by

$$\mathcal{H}_{tot} = \mathcal{H} + \mathcal{H}'(t) = -\sum_{i,j(>i)}^{N} J_{ij}\sigma_i^z\sigma_j^z - \Omega(t)\sum_{i=1}^{N}\sigma_i^x. \tag{2}$$

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We start with a high enough value of Ω initially (at $t=0$) and sample the ground state of $\mathcal{H}_{tot}$ using a zero-temperature quantum Monte Carlo algorithm (discussed below). During sampling, we reduce the strength $\Omega(t)$ of the transverse field following a linear annealing schedule

$$\Omega(t) = \Omega_0(1 - t/\tau), \tag{3}$$

where t denotes evolution time. At the end of the simulation ($t=\tau$) we are left with the classical Hamiltonian $\mathcal{H}$ and if τ is large enough, the simulated system is finally found to be in one of its ground state configurations. For low values of τ, one generally ends up with a higher energy configuration.

II. ZERO-TEMPERATURE QUANTUM MONTE CARLO METHOD

To simulate the ground state of $\mathcal{H}_{tot}$, we use a zero-temperature quantum Monte Carlo technique [12]. This Monte Carlo method projects out the ground state (at zero temperature) of a given quantum Hamiltonian unlike the path integral Monte Carlo method (also projective in nature) which samples the thermal state of a quantum system at some nonzero temperature. The path integral Monte Carlo method becomes exceedingly inefficient as the temperature is lowered, and comes to a halt at $T=0$. We describe the method to some detail here, since it is not broadly known, and has been implemented so far only to simulate pure systems with short-ranged interactions. Here we generalize the implementation for an infinite-range system with disorders.

In this method one makes a linear transformation of the form

$$\mathcal{W} = C\mathcal{I} - \mathcal{H}_{tot}, \tag{4}$$

where C is a suitable real constant and $\mathcal{I}$ is the identity operator, such that the matrix representation of $\mathcal{W}$ in the eigenbasis of $\mathcal{H}$ is non-negative and irreducible (if such a transformation could not be done for an $\mathcal{H}_{tot}$, then this method would not be applicable for it). One can then consider $\mathcal{W}$ to be the transfer-matrix of a uniform chain [with periodic boundary condition (PBC)] of classical clusters, where each cluster is nothing but a classical cluster of N mutually interacting Ising spins represented by $\mathcal{H}$.

Now the key point is that one can simulate the chain of classical clusters using the elements of its transfer-matrix $\mathcal{W}$ and in this simulation the equilibrium average of any observable (say, energy) related to a single cluster is approximately equal to the expectation value of the observable over the dominant eigenstate of $\mathcal{W}$. The dominant eigenstate of $\mathcal{W}$ in turn is the ground state of $\mathcal{H}_{tot}$ (due to the form of the linear transformation between them). Thus we actually simulate the ground state properties of $\mathcal{H}_{tot}$ by simulating the chain. In the next section we establish the scheme in detail.

A. Simulation of a chain of classical clusters using transfer matrix

In this section we demonstrate that the equilibrium averages for a single member of a uniform classical chain (with PBC) is approximately equal to the respective averages (expectation values) over the dominant eigenstate of the transfer matrix of the chain. Let us consider a uniform chain of L identical classical spin clusters (or any localized discrete degrees of freedom in general) μ_i's, as shown in Fig. 1. Each of the μ_i's can be in, say, p different states. One may note here that if each cluster μ is a spin cluster embedded in dimension d, then the chain is actually a $d+1$-dimensional object. Since the chain is uniform, its Hamiltonian will be of the form

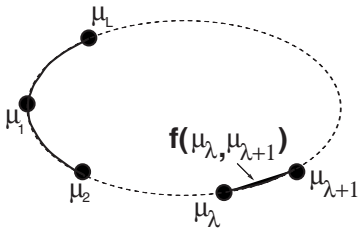

FIG. 1. The uniform chain of clusters (with periodic boundary condition) used to simulate the ground state of $\mathcal{H}_{tot}$ [Eq. (2)]. A cluster (solid circle) in the chain is basically the cluster of N Ising spins with a given realization of J_{ij}'s, represented by $\mathcal{H}$ in Eq. (2). The interactions $f(\mu_\lambda, \mu_{\lambda+1})$ between any two nearest-neighbor clusters are determined by the relation $\mathcal{W}_{\mu_\lambda\mu_{\lambda+1}} = e^{-\beta f(\mu_\lambda,\mu_{\lambda+1})}$, where $\mathcal{W}$ is obtained from $\mathcal{H}_{tot}$ by the linear transformation [Eq. (4)]. If the dimension of each cluster is d, then the dimension of the resulting chain is $d+1$.

$$\mathcal{H}_{d+1} = \sum_{\lambda=1}^{L} f(\mu_\lambda, \mu_{\lambda+1}),$$

where $f(\mu_\lambda, \mu_{\lambda+1})$ is a $p \times p$ matrix whose elements are the possible contributions to the Hamiltonian from a pair of neighboring spins, as each of them takes up p different values independently. The partition function of the chain is thus given by

$$\begin{aligned} Z &= \sum_{\mu_1=1}^{p} \sum_{\mu_L=1}^{p} \exp\left[-\beta \sum_{\lambda=1}^{L} f(\mu_\lambda, \mu_{\lambda+1}) \right] \\ &= \sum_{\mu_1=1}^{p} \sum_{\mu_L=1}^{p} e^{-\beta f(\mu_1,\mu_2)} e^{-\beta f(\mu_2,\mu_3)} \cdots e^{-\beta f(\mu_L,\mu_1)} \\ &= \sum_{\mu_1=1}^{p} \sum_{\mu_L=1}^{p} \mathcal{W}_{\mu_1\mu_2} \mathcal{W}_{\mu_2\mu_3} \cdots \mathcal{W}_{\mu_L\mu_1}, \end{aligned} \tag{5}$$

where $\mathcal{W}_{\mu_\lambda\mu_{\lambda+1}} = e^{-\beta f(\mu_\lambda,\mu_{\lambda+1})}$, β being the temperature inverse, and $p=2^N$, N being the number of spin in each cluster. Here, many of the elements $\mathcal{W}_{\mu_\lambda\mu_{\lambda+1}}$'s are zero, which might be viewed as some additional external constraints on the dynamics. Again, since each of μ_λ and $\mu_{\lambda+1}$ can take up p independent values (i.e., can be in p independent states), $\mathcal{W}_{\mu_\lambda\mu_{\lambda+1}}$ defines a $p \times p$ matrix $\mathcal{W}$. Hence summing over all the indices from μ_2 to μ_L and recalling the rule of matrix multiplication one gets

$$Z = \sum_{\mu_1=1}^{p} (\mathcal{W}^L)_{\mu_1\mu_1} = \mathrm{Tr}(\mathcal{W}^L).$$

The matrix $\mathcal{W}$ is a transfer matrix for the chain. If the matrix $\mathcal{W}$ is symmetric then (it is not the necessary but the sufficient condition) one can write

$$Z = \sum_{r=1}^{p} (\theta_r)^L, \tag{6}$$

where θ_r are the eigenvalues of $\mathcal{W}$ ordered by the index r, so that $|\theta_i| \geqslant |\theta_j|$ if $i < j$. Here a few points are to be noted. Since the matrix $\mathcal{W}$ is both non-negative and primitive (i.e., there exists some finite n, such that $\mathcal{W}^n$ is strictly positive), according to Perron-Frobenius theorem (see [14]) the dominant eigenvalue θ_1 is strictly positive and nondegenerate. Thus

$$Z = (\theta_1)^L \left[1 + \sum_{r=2}^{p} \left(\frac{\theta_r}{\theta_1} \right)^L \right] \approx (\theta_1)^L.$$

Here, the leading order error is $(\theta_2/\theta_1)^L$ and since θ_1 is nondegenerate,

$$\lim_{L\to\infty} \left(\frac{\theta_i}{\theta_1} \right)^L = 0 \tag{7}$$

for any $i \neq 1$.

Now, to see how one can simulate the chain using $\mathcal{W}$, one has to note that the probability that the chain be in a given state A, in which $\mu_1 = \mu_1(A), \mu_2 = \mu_2(A), \ldots$ etc., is

$$\begin{aligned} P(A) &= (e^{-\beta f[\mu_1(A),\mu_2(A)]} \cdots e^{-\beta f[\mu_L(A),\mu_1(A)]})/Z \\ &= (\mathcal{W}_{\mu_1(A)\mu_2(A)} \cdots \mathcal{W}_{\mu_L(A)\mu_1(A)})/Z. \end{aligned} \tag{8}$$

Thus using the conditions of detailed balance, one obtains transition probability from a state A to another state B given by

$$P(A \to B) = \frac{\mathcal{W}_{\mu_1(B)\mu_2(B)} \cdots \mathcal{W}_{\mu_L(B)\mu_1(B)}}{\mathcal{W}_{\mu_1(A)\mu_2(A)} \cdots \mathcal{W}_{\mu_L(A)\mu_1(A)}}, \tag{9}$$

where of course, the move is always accepted if $P(A \to B) > 1$. Thus if $\mathcal{W}$ is given, we can simulate the equilibrium properties (thermal average) of any physical quantity related to a cluster μ in the chain. To obtain that, we require to know the probabilities for the cluster μ to be in its different possible states when the chain is in equilibrium. Let $P(\mu = k)$ denote the probability that the cluster is found in its kth state when the chain is at thermal equilibrium (at a given β). If the kth state is represented by a column vector $|k\rangle$, then these column vectors satisfy the matrix relation

$$\langle i|\mathcal{W}|j\rangle = \mathcal{W}_{ij},$$

where $\langle i|$ is the transpose of $|i\rangle$ and the sequence of matrices implies the proper multiplications between them.

On the other hand, if $|E_1\rangle$ is the dominant (normalized) eigenvector of $\mathcal{W}$ corresponding to the dominant eigenvalue θ_1, and if $\mathcal{W}$ is Hermitian then one can expand $|E_1\rangle$ linearly in terms of the basis vectors as

$$|E_1\rangle = \sum_{k=1}^{p} \gamma_k^1 |k\rangle, \tag{10}$$

where γ_k^1 is the amplitude of the basis state $|k\rangle$ in $|E_1\rangle$. Thus in the sampling of $|E_1\rangle$ using the basis states $|k\rangle$'s, the probability of occurrence of the state $|k\rangle$ will be $|\gamma_k^1|^2$. Now, one can show that

$$P(\mu = k) = |\gamma_k^1|^2 + O((\theta_2/\theta_1)^L). \tag{11}$$

The above equation says that one can sample the dominant eigenstate $|E_1\rangle$ of the matrix $\mathcal{W}$ just by sampling its basis states (classical configurations of a cluster in the chain) according to the probability of their occurrence in the simulation of the cluster at equilibrium in the chain [using the elements of $\mathcal{W}$ itself, as prescribed in Eq. (9)].

To prove Eq. (11), we take any cluster in the chain and call it μ_1. The probability that μ_1 is found in the state $|k\rangle$ is

$$\begin{aligned} P(\mu_1 = k) &= \frac{1}{Z} \left[\sum_{\mu_2} \sum_{\mu_3} \cdots \sum_{\mu_L} \mathcal{W}_{\mu_1\mu_2} \mathcal{W}_{\mu_2\mu_3} \cdots \mathcal{W}_{\mu_L\mu_1} \right]_{\mu_1=k} \\ &= \frac{1}{Z} (\mathcal{W})^L_{kk} = \frac{\langle k|(\mathcal{W})^L|k\rangle}{\mathrm{tr}\{(\mathcal{W})^L\}}. \end{aligned} \tag{12}$$

Above, we have summed up the probabilities of all the configurations of the chain, in which $\mu_1 = k$. Now let $|\theta_i\rangle$ $(i = 1, 2, \ldots, p)$ denote the normalized eigenvector of $\mathcal{W}$ corresponding to the eigenvalue θ_i. Then one may have a linear transformation between $|\theta_i\rangle$'s and $|k\rangle$ of the form

$$|\theta_i\rangle = \sum_k \gamma_k^j |\mu_k\rangle$$

and the reverse transformation

$$|k\rangle = \sum_i (\gamma^\dagger)_i^k |\theta_i\rangle = \sum_i \gamma_k^{i*} |\theta_i\rangle,$$

γ being a unitary matrix. Hence

$$\mathcal{W}^L|k\rangle = \sum_i \gamma_k^{i*} \theta_i^L |\theta_i\rangle \Rightarrow \langle k|\mathcal{W}^L|k\rangle = \sum_i |\gamma_k^j|^2 \theta_i^L,$$

using orthonormality of $|\theta_i\rangle$'s. Thus from Eq. (12) we get

$$\begin{aligned} P(\mu_1 = k) &= \frac{\langle k|\mathcal{W}^L|k\rangle}{\mathrm{tr}\{\mathcal{W}^L\}} = \frac{\Sigma_i |\gamma_k^j|^2 \theta_i^L}{\Sigma_i \theta_i^L} = \frac{\Sigma_i |\gamma_k^j|^2 (\theta_i/\theta_1)^L}{1 + \Sigma_{i\neq 1} (\theta_i/\theta_1)^L} \\ &\approx |\gamma_k^1|^2 + O((\theta_2/\theta_1)^L), \end{aligned}$$

which proves Eq. (11).

Thus one can in fact simulate the dominant eigenstate of any given suitable (Hermitian, non-negative, and primitive) $N \times N$ matrix up to a good approximation using the above results. One has to define a uniform chain (with PBC) of classical clusters, each having N possible configurations. The ith state of a cluster corresponds to the ith vector of the basis in which the given matrix is represented. One then views the given matrix as the transfer matrix for a cluster in the chain and simulates the chain using its elements [as prescribed in Eq. (9)]. At equilibrium, the probability of getting a cluster in its ith state is equal to the modulus square of the weight of

the ith basis vector in the representation of the dominant eigenstate of the given matrix (up to an error of the form discussed above).

B. Implementation of the Monte Carlo method

We now illustrate the implementation of the above Monte Carlo scheme by employing it to simulate the ground state of $\mathcal{H}_{tot}$ given in Eq. (2). Here basis vector $|k\rangle$'s are the eigenvectors of $\mathcal{H}$, and a classical cluster is the cluster of N Ising spins with exchange interaction described by $\mathcal{H}$. Now we make a linear transformation of the form given in Eq. (4), with $C=N(N-1)/2$. The resulting $\mathcal{W}$ matrix is clearly non-negative [since none of its diagonal elements are all smaller than $N(N-1)/2$ and off-diagonal elements are either 0 or $\Omega(t)$, which we always take to be positive]. Since $\mathcal{H}_{tot}$ connects a basis state to all other basis states that can be obtained by a single spin flip from it, there is no closed subspace for $\mathcal{H}_{tot}$. Thus $\mathcal{W}$ is also irreducible. It can be shown that for a non-negative irreducible matrix, all the results of the Perron-Frobenius theorem we have used here hold good [14]. Besides, $\mathcal{W}$ is of course Hermitian. Hence we can take $\mathcal{W}$ as a transfer matrix for the chain. It corresponds to some interaction $f(\mu_\lambda, \mu_{\lambda+1})$ between two neighboring (μ_λ and $\mu_{\lambda+1}$) and some inverse temperature β (not explicitly important here), given by

$$\mathcal{W}(\mu_\lambda, \mu_{\lambda+1}) = e^{-\beta f(\mu_\lambda, \mu_{\lambda+1})}.$$

To simulate the ground state of $\mathcal{H}_{tot}$ at a given Ω for a particular realization of J_{ij}'s, we construct a uniform chain of L clusters with PBC. Each cluster is a cluster of N classical Ising spins (described by cooperative term of $\mathcal{H}_{tot}$) connected through the given particular realization of J_{ij}'s [see Eq. (1)]. We start with an arbitrary spin configuration (same for all clusters) and a given value of Ω. In one Monte Carlo step we randomly visit L clusters. At each such visit we make an allowed move (a move whose probability is not trivially zero), such that the chain goes from a state A, say, to a new state, say B. The probability of acceptance of the move is nothing but the transition probability $P(A \to B)$ calculated following Eq. (9) (using the elements of $\mathcal{W}$). While sampling, one can easily avoid moves whose probabilities are trivially zero (due to the sparsity of the matrix $\mathcal{W}$) by constructing a more restricted Markov process to do the sampling [12].

For doing quantum annealing of the same system, we start with a high enough value of Ω and reduce it very slowly with time t (Monte Carlo step) following a linear schedule. During visiting different clusters in a given Monte Carlo step, Ω is, however, held fixed. The linear schedule $\Omega(t) = \Omega_{in}(1-t/\tau)$ is specified by $\Omega(t=0)=\Omega_{in}$ and the annealing time τ. We keep τ of the order of 95% of the total number of Monte Carlo steps executed—we allow the system to equilibrate at $\Omega=0$ in the remaining 5% of the steps.

To prepare the initial state, we start with a uniform state with all spins in the same (up, say) direction and run the Monte Carlo method for the fixed value of Ω, namely for $\Omega=\Omega_{in}$, until it reaches a steady state. The state thus prepared is the Monte Carlo realization of the initial ground state in the Markovian sense.

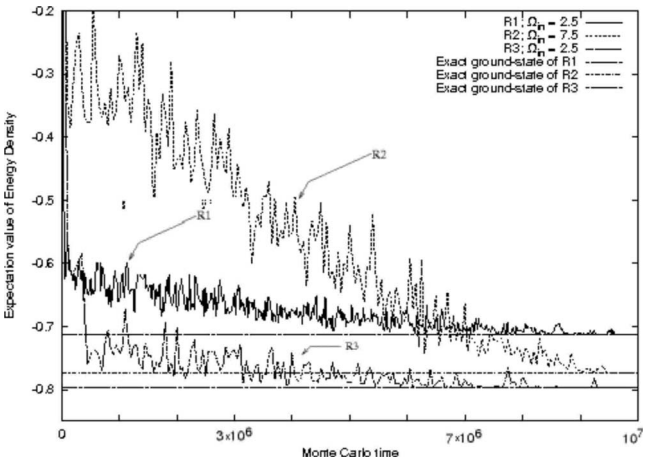

FIG. 2. Annealing behavior of three different randomly generated realizations (R1, R2, and R3) of J_{ij}'s is shown for $N=30$ and plotted with respect to the Monet Carlo time t. In each case the system goes to the exact ground state (shown by respective horizontal lines) at the end of the annealing. In each case the annealing time is 10^7 Monte Carlo steps, the number of clusters in the chain is $L=600$, and each Monte Carlo step consists of visiting L clusters randomly and making a random spin-flip trial there. In each case, the transverse field has been reduced to zero from its initial value $\Omega_{in}=5$ following a linear schedule, within the Monte Carlo steps.

III. ANNEALING TO THE CLASSICAL GROUND STATE

We have studied the relaxation behavior of several random J_{ij} samples with $N=30$ for a linear annealing schedule (we start with an initial transverse field Ω_{in} and reduce it linearly with a Monte Carlo step, so that it becomes zero before the last few, 5%, steps. We observe that for an annealing of $\sim 10^7$ Monte Carlo steps, the system reaches the true ground state (determined by an extensive search method) in almost every case, for a suitably large initial transverse field Ω_{in}. We calculate the average exchange energy of the chain (over L clusters) in each Monte Carlo step and average that over a few, ~500, Monte Carlo steps. The exchange energy [as given by $\mathcal{H}$ of Eq. (2)] is not linear in N and we have to scale it by a factor $N^{3/2}$ to obtain the intensive energy density. In the thermodynamic limit, this intensive energy density approaches the value −0.7633 [16] (our finite size results show some fluctuations about that). In Fig. 2 the relaxation behavior of three typical random realizations (R1, R2, and R3) during their annealing are shown. We found that for doing annealing of a given sample within a given number of steps, there is a suitable range of Ω_{in}. If Ω_{in} falls below the range, then the transition probabilities are too low to be able to anneal the system within the given time. On the other hand, if Ω_{in} is above the range, then the rate of change of $\Omega(t)$ is not slow enough to ensure the convergence to the ground state finally (i.e., the evolution in no more adiabatic). In Fig. 2, the values of respective Ω_{in}'s belong to the lower end of the respective ranges. The ranges are generally wide enough, and one can find a Ω_{in} within the range, just by a few trials.

The relaxation behavior is found to be typically "linear" in the sense that the long-time averages decrease linearly

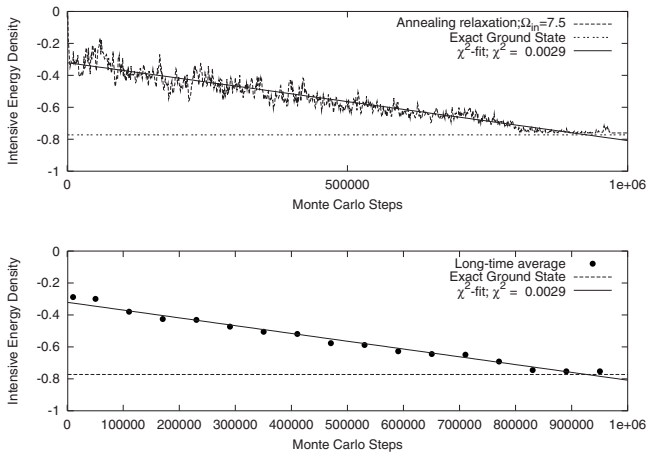

FIG. 3. In this figure the annealing relaxation (N=30, L=600, and Ω_{in}=7.5) for a particular realization is shown. Here the annealing time τ=10^6 Monte Carlo steps. The upper frame shows the relaxation of intensive energy density with time, when averaged over small (~500) Monte Carlo steps. The lower frame shows the same relaxation, when the averaging is done over a much larger number of (~10^4) Monte Carlo steps. A linear χ^2 fit for the longer time average is shown in the lower part of the figure.

with time (see lower part of Fig. 3). The relaxation observed in shorter time scale of course shows fluctuations around that linear behavior (shown in the upper part of Fig. 3). This linear nature of relaxation is typically seen independent of the details of the particular realizations.

In Fig. 4, the (disorder averaged) variation of the final energy with the annealing time τ is shown. When the annealing time τ is small, a small increment in τ allows one to improve the final result substantially. For large $\tau(\tau > 10^6)$, the improvement in the final energy is much slower with the increment in τ. This is because for small τ, the search is

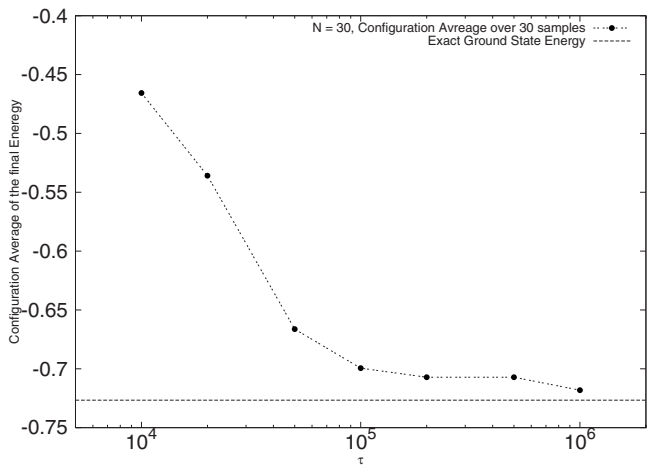

FIG. 4. Here the variation of the final energy with the annealing time τ is shown for the sample size N=30. Each data point is averaged over the same set of 30 disorder configurations. The transverse field Ω is reduced linearly from Ω_{in}=1.5 and the number of replica (clusters) is taken to be L=600. The horizontal line denotes the exact ground state (averaged over the same set of configurations) obtained by an exhaustive search algorithm.

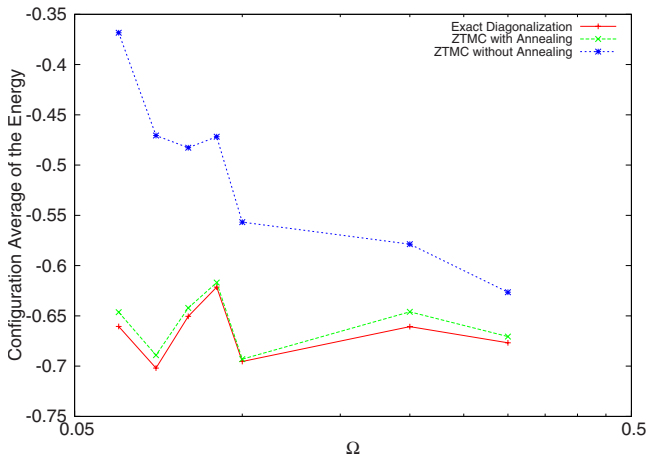

FIG. 5. (Color online) In this figure a comparison between the results of simulation (with and without pre-annealing) of the ground state of the Hamiltonian (2) for different static values of Ω and the corresponding exact results obtained by numerical exact diagonalization for the same set of samples. Each data point represents an average over the same set of 40 randomly generated samples of size N=20. The total number of Monte Carlo steps is 10^5 for each Monte Carlo simulation (including the annealing period for the annealed simulations). In the figure, the results of simulations with annealing are seen to be much closer to the exact diagonalization results than those without annealing, for lower values of Ω.

mostly confined among the higher energy configurations, which are highly degenerate. Thus a relatively lower energy configuration (but still quite high in energy) is much easier to find with a moderate increment in τ; but as τ is increased, the search goes down in energy, where the degeneracy is much lower, and hence it becomes difficult to find a lower energy configuration even by increasing τ substantially.

IV. BETTER SIMULATION OF LOW KINETIC-ENERGY QUANTUM STATES USING QUANTUM ANNEALING

In a glassy system, where the potential energy landscape has valleys separated by huge energy barriers, simulating the ground states (and possibly other low-lying states) for low kinetic energy (such as the ground state for a low value of the transverse of a transverse Ising spin glass) using a zero-temperature quantum Monte Carlo method may be very difficult and time-consuming. This is because, for a small kinetic term, the acceptance probability may become very small for higher potential energy states, and the system may take a very long time to get out of a local potential energy minimum in order to visit other equally relevant lower-potential-energy valleys. Thus if one gets stuck in a local minimum far above the ground state, at an early stage of the simulation, then one would not be able to reach the low lying valleys (the classical Ising spin configurations with lower potential energy), whose contributions to the ground state are much more significant. This can be remedied to some extent by annealing the sample quantum mechanically starting with a high value of the kinetic energy, and then reducing it slowly up to the low value at which the simulation is desired.

For the Hamiltonian given by Eq. (2), simulation of the ground state for a small fixed value of the transverse field Ω (using the zero-temperature transfer-matrix Monte Carlo algorithm described here) is found to be much closer to the exact result (obtained using exact diagonalization [15]) when the simulation is done following an annealing (reducing Ω from a high value to the low value at which the simulation is desired) than that done directly keeping the value of Ω fixed to the low value from the onset. We compare the results of both kinds of simulations (with and without annealing) for several random samples of the spin glass for $N=20$ with the respective exact diagonalization results for them (see Fig. 5).

We conclude summarizing a few points regarding the performance of the algorithm described here. The algorithm discussed here is quite general (applicable to any disordered spin system in any dimension) and may be used for simulating small system sizes quite satisfactorily. However, the moves are very restricted, since each spin flip in a cluster requires the two nearest-neighboring clusters to be either in the same configuration with it, or differ by a single spin flip [see Eq. (9)]. For large system sizes, this is too restrictive a condition to move freely enough through the configuration space to procure a satisfactory sampling rate. In addition, since the acceptance probability for higher potential energy configurations (like most other zero-temperature quantum Monte Carlo algorithms [17]) depends on the magnitude of the kinetic term, it is hard to simulate the ground state for low values of the kinetic term. We have shown how quantum annealing can be utilized in overcoming this difficulty (at least partially). This remedy is expected to work also for other zero-temperature quantum Monte Carlo methods in principle.

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