Quantum annealing in a kinetically constrained system

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Classical and quantum annealing is discussed in the case of a generalized kinetically constrained model, where the relaxation dynamics of a system with trivial ground state is retarded by the appearance of energy barriers in the relaxation path, following a local kinetic rule. Effectiveness of thermal and quantum fluctuations in overcoming these kinetic barriers to reach the ground state are studied. It has been shown that for certain barrier characteristics, quantum annealing might by far surpass its thermal counter part in reaching the ground state faster.

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I. INTRODUCTION

Here we demonstrate the effectiveness of quantum annealing [1] in the context of a certain generalized kinetically constrained systems (KCS) [2]. KCS's are simple model systems having trivial ground state structures and static properties, but a complex relaxation behavior due to some explicit constraints introduced in the dynamics of the system [2]. These systems are very important in understanding how much of the slow and complex relaxation behavior of a glass can be attributed to its constrained dynamics alone, leaving aside any complexity of its energy landscape structure. In KCS's one can view the constraints to be represented by infinitely high energy barriers appearing dynamically. To study annealing, we generalize such models by allowing the height of such kinetically occurring barriers to be finite but large.

It has been demonstrated in certain models with energy barriers [1,3] that one can effectively appoint quantum fluctuations (instead of thermal ones) to anneal a glassy system toward its ground state. In the method of quantum annealing, one introduces quantum fluctuations by including a term in the Hamiltonian due to tunneling field, that does not commute with the original (classical) Hamiltonian, and thus generate transition probabilities between the eigenstates (classical configurations) of the original (classical) Hamiltonian. The introduction of such a quantum tunneling is supposed to make the energy barriers in the landscape transparent to the system. This allows transitions between different configurations classically trapped between even infinite barriers, if the barriers are narrow enough. In other words, it is expected that application of a quantum tunneling term will make the free energy landscape completely ergodic, i.e., the system will consequently be able to visit any configuration with finite probability (Ray *et al.* [1]). Finally, of course, the quantum tunneling term is to be tuned to zero to get back the ground state of the classical Hamiltonian. In case of thermal annealing as well, the energy landscape is made almost ergodic to thermal transitions at the initial stage of the annealing by starting with a high enough temperature (which is slowly reduced to zero and the system becomes nonergodic as the temperature falls below some glass transition point). But it has been argued that when the barriers are very high but narrow enough, quantum annealing would be the better choice, since probability of quantum tunneling across a barrier increases with the decrease of barrier width, while thermal transition probability in such a case has no such dependence on barrier width. However, quantum and thermal fluctuations are inherently different in nature (as reflected in the functional forms of the transition probabilities in respective cases), giving rise to nontrivial differences in their effectiveness in performing annealing. In fact, unlike the classical glasses below the glass transition point, quantum spin glasses (transverse Ising spin glasses in particular) may remain ergodic even in the glass phase (for low enough tunneling fields [1,5]).

Here we study quantum annealing in the context of a kinetically constrained system, which can be represented by a generalized version of the East model [4] (a one-dimensional KCS). We also compare the results with that of thermal annealing done in the same system. The original East model is basically a one-dimensional chain of noninteracting classical Ising ("up-down") spins in a longitudinal field h, say, in the downward direction. The ground state of such a system is trivially given by all spins down. A kinetic constraint is introduced in the model by putting the restriction that the ith spin cannot flip if the $(i-1)$-th spin is down. Such a kinetic constraint essentially changes the topology of the configuration space, since the shortest path between any two configurations differing by one or more forbidden flips, is increased in a complicated manner owing to the blockage of the "straight" path consisting of direct flips of the dissimilar spins. Further, the constraint becomes more limiting as more spins turn down, as happens in the late approach to equilibrium. As a result, the relaxation processes have to follow more complex and lengthier paths, giving rise to exponentially large timescale ($\sim e^{1/T^2}$, where T is the temperature) [4].

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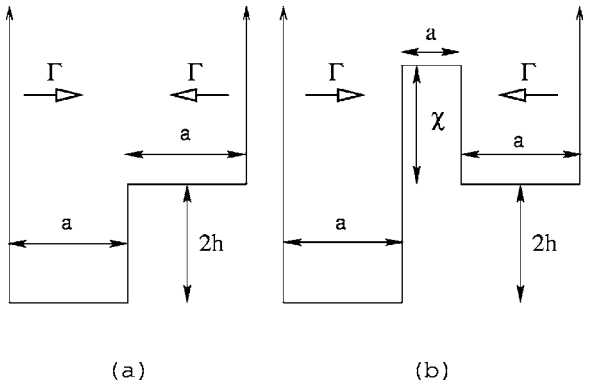

FIG. 1. Potential energy wells for the spin at site i, when $(i-1)$-th spin is (a) up and (b) down, with the external field h in the downward direction and barrier height χ very large and the width a small. For the classical generalized East model, flipping across the barrier in (b) is a thermal jump (at any finite T). In the quantum model considered here, probability for crossing the barrier in (b) is due to quantum tunneling through it at a finite Γ.

II. MODEL

Our model is a chain of asymmetric double wells (each with infinite boundary walls), with a particle localized within each of them. The asymmetry is due to an energy difference of $2h$ between the two wells of a double well. The particle in one of the two (asymmetric) wells can change its location to the other well stochastically, either due to the thermal fluctuation or due to quantum fluctuation present in the system. The generalized kinetic constraint is introduced by assuming that if the particle in the $(i-1)$-th double well resides in the lower one of the two wells, then there appears a barrier of height χ and width a between the two wells of the ith double well. In such a situation the particle in the ith double well has to cross the barrier in order to change its location from one well to the other [Fig. 1(b)]. On the other hand, if the particle of the $(i-1)$-th is in its upper well, there is no such barrier to cross for [Fig. 1(a)]. Following the approximate mapping done in case of symmetric double well [5], this model can be approximately represented by a generalized version of the East model, where each Ising spin is in a local longitudinal field h in the downward direction. The spin at the ith site sees a barrier of height χ and width a between its two energy states when the $(i-1)$-th spin is down [Fig. 1(b)], where as no such barrier occurs for the ith spin when the $(i-1)$-th spin is up [Fig. 1(a)]. This kinetic constraint is the same in both cases irrespective of whether the dynamics is classical or quantum.

When dynamics of the particle is due to quantum fluctuations, the tunneling probabilities come from the following semiclassical picture of scattering of a particle in a double well with infinitely remote outer boundaries ($a \to \infty$ in Fig. 1). If a particle is put in one of the wells of such a double well with some kinetic energy (actually the expectation value) Γ, then it will eventually be scattered by the separator (a barrier or step) between the two wells. In such a scattering, there is a finite probability P that the particle manages to go to the other well. We calculate P from the simple picture of scatterings of a particle by one-dimensional potentials as prescribed below. In the thermal case we take simple Boltzmann probabilities for crossing the same barriers. The minimum of the energy of the Ising chain (equivalent to the potential energy of the chain of the double wells) trivially corresponds to the state with all the spins down, i.e., aligned along the longitudinal field h (where all the particles are in their respective lower wells). To reach the ground state in the quantum case, we start with a very large initial value of Γ and then reduce it following an exponential schedule given by $\Gamma=\Gamma_0 \exp(-t/\tau_Q)$. Here t denotes the time, and τ_Q sets the effective time scale of annealing. At zero temperature the spin flip dynamics occurs only due to the tunneling (kinetic energy) term Γ, and hence the system ceases to have any relaxation dynamics in the limit $\Gamma \to 0$. It may be mentioned here that in the absence of any analytical expression for the tunneling probability in the asymmetric case of the type discussed here, (see e.g., [6]), we employ the asymmetric barrier tunneling probabilities available [7]. Similarly, in the thermal case, we start with a high initial temperature T_0 and reduce it eventually following an exponentially decreasing temperature schedule given by $T=T_0 \exp(-t/\tau_C)$; τ_C being the time constant for the thermal annealing schedule. Here, when $(i-1)$-th spin is down, the flipping probability for the i-th spin [$\sim \exp-(\chi/T)$]. Otherwise, it flips with probability $P=1$ if it were in the up state, and with Boltzmann probability $P=\exp(-h/T)$ if it were in the down state.

III. SIMULATION AND RESULTS

We have employed the quantum transmission (flipping) probabilities (cf. [7]) from a very elementary scattering picture which is qualitatively adequate, though not strictly valid for the asymmetric double well [shown in Fig. 1(b)] because the states within it are bounded by its finite width a. Following are the flipping probabilities (P) for the ith spin in different possible situations used in our Monte Carlo simulation:

(1) If the $(i-1)$-th spin is up and the ith spin is also up then $P=1$.

(2) If the $(i-1)$-th spin is up and the ith spin is down then (a) $P=0$ for $\Gamma < 2h$ and (b) $P=\min\{1, 4[\Gamma(\Gamma-2h)]^{1/2}/(\sqrt{\Gamma}+\sqrt{\Gamma-2h})^2\}$ for $\Gamma \geq 2h$.

(3) If the $(i-1)$-th spin is down and the ith spin is up then $P=\min\{1, 4[\Gamma(\Gamma+2h)]^{1/2}/[(\sqrt{\Gamma}+\sqrt{\Gamma+2h})^2+g^2]\}$.

(4) If the $(i-1)$-th spin is down and the ith spin is down then (a) $P=0$ for $\Gamma < 2h$, and (b) $P=\min\{1, 4[\Gamma(\Gamma-2h)]^{1/2}/[(\sqrt{\Gamma}+\sqrt{\Gamma-2h})^2+g^2]\}$ for $\Gamma \geq 2h$ (h and Γ denoting the magnitudes only).

Here $g=\chi a$, χ and a being, respectively, the height and width of the barrier representing the kinetic constraint. The above expressions for P are actually the transmission coefficients in respective cases of one-dimensional scattering across asymmetric barrier or step (according to the form of the potential encountered in passing from one well to the other, see, e.g., [7]). Application of the above scattering picture, even for the double wells in Fig. 1(b) (which our simulation is based on) as discussed before, is of course an ap-

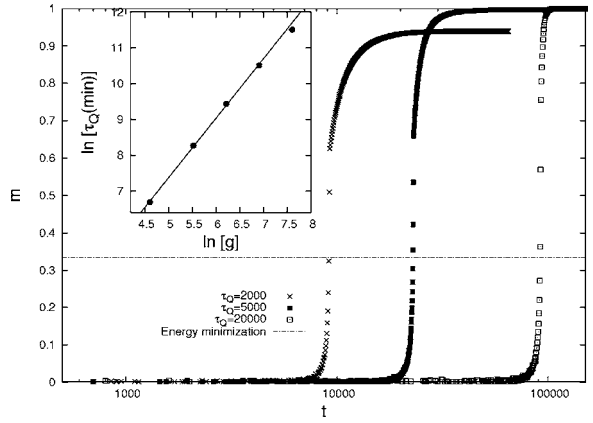

FIG. 2. Quantum annealing ($T=0$) for $g=100$, $\Gamma_0=100$, and $h=1$ is shown for different values of τ_Q, for a chain of 5×10^4 spins (m averaged over the same set of ten initial configurations for each τ_Q). The horizontal (dashed) line indicates the average (over the same set $\mathcal{C}$) value of m that could be reached from the initial configurations by simply minimizing the energy following the downhill principle (a single step is enough to get there). In the inset, variation of $\ln[(\tau_Q)_{\min}]$ with $\ln[g]$ is shown (by the points) for one given configuration. The error in $(\tau_Q)_{\min}$ is typically less than 0.5% in each case. The continuous line in the inset shows a fit of the data by the continuous line $(\tau_Q)_{\min}\sim g^{\kappa}$; $\kappa\approx1.67$ (obtained by linear least-square fitting).

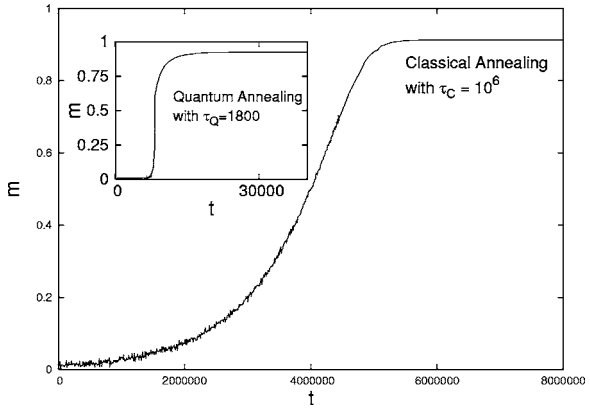

FIG. 3. Comparison between classical and quantum annealing for a chain of 5×10^4 spins (for the same initial disordered configuration with $m_i\sim10^{-3}$). We show the results for $\tau_Q=1.8\times10^3$ (for quantum) and $\tau_C=10^6$ (for classical) with $h=1$; a lower τ_C would not produce substantial annealing. Starting from the same initial values $\Gamma_0=T_0=100$, (and $g=100$ in the quantum case) we observe that classical annealing requires about 10^7 steps, whereas quantum annealing takes about 10^4 steps for achieving the same final order $m_f\sim0.92$.

proximation. It may be noted that our flipping probabilities used here do not satisfy the condition of detailed balance, though the evolution matrix has got the required stochastic structure (see Sec. IV for details).

In our simulation, we take N Ising spins ($\sigma_i=\pm1$, $i=1,\ldots,N$) on a linear chain with periodic boundary condition. The initial spin configuration is taken to be random such that magnetization $m=(1/N)\Sigma_i\sigma_i$ is practically negligible ($m_i\approx0$). We then start with a tunneling field Γ_0 and follow the zero temperature (semiclassical) Monte Carlo scheme as mentioned above, using the spin flip probabilities P's appropriate for the four cases (1)–(4). Each complete run over the entire lattice is taken as one time unit, and as time progresses, Γ is decreased from its initial value Γ_0 according to $\Gamma=\Gamma_0e^{-t/\tau_Q}$. The results are shown in Fig. 2. It shows that for $N=50\,000$, $g=100$ and $\Gamma_0=100$ the system freezes before reaching the ground state ($m_f=1$) for low values of τ_Q; say for $\tau_Q=2000$. For a somewhat greater value, e.g., $\tau_Q=5000$, the system is completely annealed to the ground state within about 4×10^4 time steps. However, for a much greater τ_Q, like $\tau_Q=20\,000$, the system of course anneals completely but consumes more time unnecessarily. These generic features remain the same for other higher values of g. We have also studied the dependence of annealing behavior with the parameter g, which is actually a measure of how impenetrable is the infinite barrier representing the kinetic constraint. Computations were carried out to locate, for a given value of g, the minimum value of τ_Q for which the system just anneals up to $m_f=0.8$ (complete annealing requires prohibitively longer computer time for this comparative study).

We call this minimum value $(\tau_Q)_{\min}$. A bisection scheme was used to locate $(\tau_Q)_{\min}$ for different values of g starting for the same initial configuration. The inset in Fig. 2 shows that $(\tau_Q)_{\min}$ increases fairly sharply with g (an empirical analysis shows $(\tau_Q)_{\min}\sim g^{1.67}$, for $g\leqslant1000$. This variation with g depends on the specific functional forms of P occurring in the quantum case. In contrast to this, in classical case, $(\tau_C)_{\min}$ grows exponentially with the barrier height χ and is independent of the barrier width a. However, for even higher values of g, the slope is expected to decrease, and finally in the asymptotic limit $g\to\infty$, the relaxation behavior should converge to that of one with an unsurpassed kinetic constraint (like the classical East model). This asymptotic convergence could not however be explored, since the required computational time becomes prohibitively long as g is increased further.

We compare the results of thermal and quantum annealing for the same order of initial value and time constant for Γ and T (barrier height χ is taken to be 1000 in both cases while g was taken to be 100 in the quantum annealing case, or equivalently the barrier width a is taken to be of the order of 0.1). We observe that to achieve a similar degree of annealing (attaining a certain final magnetization m_f), starting from the same disordered configuration, one typically requires much smaller τ_Q compared to τ_C; typically, $\tau_C\sim10^3\times\tau_Q$ for equivalent annealing (for similar optimal values of final order $m_f\sim0.92$). This comparison of course depends on the barrier characteristics (value of g) as shown in the inset of Fig. 2.

IV. SUMMARY AND DISCUSSION

We have discussed here the annealing of a generalized kinetically constrained chain of N double wells with a particle in each, starting from a disordered state (with negligible initial order), to its (external field induced) fully ordered ground state. In our model kinetic retardations are repre-

sented by barriers of finite height and width. We have shown that for certain barrier characteristics, namely, very high but thin barriers quantum annealing can be far superior to its thermal counter part in reaching the ground state. The noise necessary for the annealing are introduced by temperature T in the thermal case and by a quantum mechanical kinetic energy term Γ in the quantum case. The introduced noise is reduced following an exponential schedule in both cases: $T=T_0e^{-t/\tau_C}, \Gamma=\Gamma_0e^{-t/\tau_Q}$, with $T_0 \approx \Gamma_0$. For our simulation for the quantum case, we have taken the tunneling probabilities P (for cases (1)–(4)) and employed them in a semiclassical fashion for the one-dimensional spin chain considered. We observe that for similar achievement in final order ($m_f \simeq 0.92$ starting from $m_i=10^{-3}$), $\tau_C \sim 10^3 \tau_Q$ for $N=5\times10^4$. For even larger order ($m_f \sim 1$), quantum annealing works even better ($\tau_C \sim 10^3 \tau_Q$, for the same value of N). These comparisons are for $g=10^2$ and $\chi=10^3$ for the constraint barriers.

In this picture, we considered the collective dynamics of a many particle system, where each one is confined in a (field) induced asymmetric double-well potential for which we considered only the low lying two states (the wave packet localized in one well or the other), representing the two states (up and down) of an Ising spin discussed above. The tunneling of the wave packet from one well to the other was taken into account by employing a scattering picture and we used the tunneling probabilities as the flip probabilities for the quantum Ising spins. As such, the reported simulation for the one-dimensional quantum East model is a semiclassical one.

Here a few words regarding the absence of detailed balance in our flipping probabilities will be in order. Detailed balance (e.g., using rates which are ratios of Boltzmann probabilities) is indeed the simplest way of ensuring the approach of a nonequilibrium system to the simplest types of steady state (e.g., the thermal equilibrium state's corresponding to a canonical ensemble). But the study of the approach of nonequilibrium systems to steady states typically (and necessarily, in the case of nonproduct states) involves a more general set of dynamic rules, captured, for example, by an evolution operator involving a (typically non-Hermitian) Hamiltonian which has the usual stochastic structure which ensures conservation of probability, and ensures eigenvalues, one of which is zero, having non-negative real parts. Tunneling is one among many possible processes (usually captured by transition rates in a master equation) which can satisfy these requirements, and is clearly more appropriate than, e.g., Arrhenius rates in a quantum system at zero temperature.

It may be noted that, because of the absence of interspin interaction, the dimensionality actually plays no role in this model except for the fact that the kinetic constraints on any spin depend only on the left nearest neighbor (directedness in one dimension). Hence the semiclassical one-dimensional simulation, instead of a proper quantum Monte Carlo simulation (equivalent to a higher-dimensional classical one [5]), is quite appropriate here. Additionally, even for interacting (finite range) one-dimensional system order is always completely destroyed at any finite temperature ($T=0$ is the critical point). Thus it is difficult to reach the ground state efficiently by employing thermal annealing in such systems in the presence of competing interactions [5]. However, quantum critical points in such systems exists at the finite value of the tunneling (disordering) field Γ, and one can utilize the order below the critical point while annealing, and reach the ground state more efficiently.

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