Quantum Annealing in a Kinetically Constrained System

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Classical and quantum annealing is discussed for a kinetically constrained chain of $N$ non-interacting asymmetric double wells, represented by Ising spins in a longitudinal field $h$. It is shown that in certain cases, where the kinetic constraints may arise from infinitely high but vanishingly narrow barriers appearing in the relaxation path of the system, quantum annealing exploiting the quantum-mechanical penetration of sufficiently narrow barriers may be far more efficient than its thermal counterpart. We have used a semiclassical picture of scattering dynamics to do our simulation for the quantum system.

Keywords: Quantum Annealing; Kinetically Constrained Systems; East model

I. INTRODUCTION

Here we demonstrate the effectiveness of quantum annealing \cite{1} in the context of Kinetically Constrained System (KCS) \cite{2}. These KCSs are simple model systems which have trivial ground state structures and static properties, but a complex relaxation behaviour due to some explicit constraints introduced in the dynamics of the system \cite{2}. Such systems are very important to understand how much of the slow and complex relaxation behaviour of a glass can be attributed to its constrained dynamics alone, leaving aside any complexity of its energy landscape structure.

It has been demonstrated in certain models with energy barriers \cite{1,3} that one can effectively appoint quantum fluctuations (instead of thermal ones) to anneal a glassy system towards its ground state. In the method of quantum annealing, one introduces quantum fluctuations by including a term in the Hamiltonian due to tunnelling field, that does not commute with the original (classical) Hamiltonian, and thus generate tunnelling probabilities between the eigenstates (classical configurations) of the original (classical) Hamiltonian. The introduction of such a quantum tunnelling is supposed to make the infinitely high but infinitesimally narrow barriers transparent to the system. This allows transitions between different configurations classically trapped between such infinite barriers. In other words, it is expected that application of a quantum tunnelling term will make the free energy landscape ergodic, i.e., the system will consequently be able to visit any configuration with finite probability (Ray et al \cite{1}). Finally, of course, the quantum tunnelling term is to be tuned to zero to get back the ground state of the classical Hamiltonian.

To study quantum annealing \cite{1,3} in a representative KCS it has to be appropriately generalised. The KCSs studied so far are all classical and the constraints are absolutely unsurpassable. To incorporate the quantum effect we first visualize that these constraints originate from infinitely high energy barriers, so that the classical system remains unable to jump over such a barrier at any finite temperature. Then in the quantum version of such a system we consider the possibility of tunnelling through such barriers quantum mechanically in certain cases when the barrier width approaches zero fast enough so that the barrier becomes integrable. We specifically define here a quantum version of a classical one-dimensional directed KCS, known as the East model \cite{4}, and study the quantum relaxational behaviour and consequent annealing (to the ground state in the classical limit).

The classical East model is basically a one-dimensional chain of non-interacting Ising (‘up-down’) spins in a longitudinal field $h$, say, in 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 $i$-th 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) \cite{4}.

II. MODEL

To introduce the possibility of quantum tunnelling through infinite but integrable barriers representing classical constraints, we start with a chain of asymmetric double wells, each with a particle localized within it. When the barrier (or step) between the two wells is penetrable, then if we initially prepare a wave packet in one well with sufficiently high expectation value of kinetic en-
ergy \(\Gamma\), it will eventually tunnel to the other well. If there is no dissipation, then such to and fro motion between the two wells will persist, following successive elastic reflections from the infinitely high outer boundaries of the double well. In the corresponding Ising spin representation this tunnelling dynamics of a particle (wave packet) between the two wells is represented by a quantum mechanical spin flip dynamics introduced in the model through the inclusion of a transverse field term in the Hamiltonian. Clearly, the value of the transverse field \(\Gamma\) depends upon the height and width of the energy barrier between the wells and the kinetic energy \(\Gamma\) of the wave packets [5]. In such a representation, our model reduces to a chain of non-interacting Ising spins (double wells) in the presence of a downward field \(h\) (proportional to the well asymmetry). The spin flip dynamics (flipping probabilities) in this model will however be calculated directly from a semiclassical picture of the motion of a particle in a bounded double well. The kinetic constraint is introduced by assuming that the \(i\)-th spin faces an infinitely high energy barrier between its two states (up and down), when the \((i-1)\)-th spin is down. As in the classical model, this barrier is absent when the \((i-1)\)-th spin is up (see Fig. 1). When the dynamics is classical, the barriers are impenetrable and the spin at \(i\)-th site has to wait until the \((i-1)\)-th spin flips to the up state. In the quantum version of the model considered here, we allow for tunnelling through such (classically impenetrable) infinite barriers for the flip of the \(i\)-th spin even when the \((i-1)\)-th spin is down. The tunnelling probabilities come from the following semiclassical picture of scattering of a particle in a double well with infinitely remote outer boundaries \((w \to \infty\) 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 \(\Gamma\), 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. 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). However, if one starts with a random configuration and kinetic energy \(\Gamma\) is not sufficient for tunnelling to the upper well, then the system, more or less, will exhibit the zero temperature (energy minimization) relaxation behaviour of the classical East model, and will extremely slowly approach the ground state (i.e., the minimum of the potential energy). For sufficiently high \(\Gamma\), the system occasionally tunnels through the infinite barriers corresponding to the constraints and thus can take up some of the relaxation paths forbidden classically. However, at any nonzero \(\Gamma\), the ground state (lowest potential energy state) will be mixed with higher potential energy eigenstates. To reach the ground state, we start with a very large initial value of \(\Gamma\) and then reduce it following an exponential schedule given by \(\Gamma = \Gamma_0 \exp(-t/\tau_\Omega)\). Here \(t\) denotes the time, and \(\tau_\Omega\) sets the effective time scale of annealing. At zero temperature the slow spin flip dynamics occurs only due to the tunnelling (kinetic energy) term \(\Gamma\), and hence the system ceases to have any relaxational dynamics in the limit \(\Gamma \to 0\). It may be mentioned here that in absence of any analytical expression for the tunnelling probability in asymmetric case of the type discussed here, (see e.g., [6]), we employ the asymmetric barrier tunnelling probabilities available [7].

**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 of its bound states and finite \(w\). Following are the flipping probabilities \((P\) for the \((i-1)\)-th spin in different possible situations used in our Monte Carlo simulation:

I. If the \((i-1)\)-th spin is up and the \(i\)-th spin is also up, then \(P = 1\).

II. If the \((i-1)\)-th spin is up and the \(i\)-th 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 \(\Gamma \geq 2h\).

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

IV. If the \((i-1)\)-th spin is down and the \(i\)-th spin is up 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 \(\Gamma\) denoting the magnitudes only).

Here \(g = \chi^2 a, \chi\) 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. 1b (which our simulation is based on) as discussed before, is of course an approximation.

In our simulation, we take \(N\) Ising spins \((\sigma_i = \pm 1, \ i = 1, ..., N)\) on a linear chain with periodic boundary condition. The initial spin configuration is taken to be random such that magnetization \(m = (1/N)\sum_i \sigma_i\) is practically negligible \((m_i \approx 0)\). We then start with a tunnelling field \(\Gamma_0\) and follow the zero temperature (semi-classical) Monte Carlo scheme as mentioned above, using the spin flip probabilities \(P\)'s appropriate for the four cases I-IV. Each complete run over the entire lattice is taken as one time unit and as time progresses, \(\Gamma\) is decreased from its initial value \(\Gamma_0\) according to \(\Gamma = \Gamma_0 e^{-t/\tau_\Omega}\). The results are shown in Fig. 2. It
Here, when \((i - 1)\)-th spin is (a) up and (b) down, with the external field \(h\) in the downward direction and barrier height \(\chi \to \infty\). For the classical East model, flipping to right well in (b) is impossible (at any finite \(T\)). In the quantum model considered here, although \(\chi \to \infty\), the well width \(a \to 0\) in such a way that \(\chi^2a (\equiv g)\) is finite, giving a finite tunnelling probability for going to the right well in (b). The limit \(w \to \infty\) helps utilising the scattering picture employed here.

\[
\begin{align*}
\Gamma & \quad \text{w} \\
2h & \quad \chi \\
\end{align*}
\]

(a)

\[
\begin{align*}
\Gamma & \quad w \\
2h & \quad \chi \\
\end{align*}
\]

(b)

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 \(\chi \to \infty\). For the classical East model, flipping to right well in (b) is impossible (at any finite \(T\)). In the quantum model considered here, although \(\chi \to \infty\), the well width \(a \to 0\) in such a way that \(\chi^2a (\equiv g)\) is finite, giving a finite tunnelling probability for going to the right well in (b). The limit \(w \to \infty\) helps utilising the scattering picture employed here.

shows that for \(g = 100\) and \(\Gamma_0 = 100\) the system freezes before reaching the ground state \((m_f = 1)\) for low values of \(\tau_Q\); 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 \(4 \times 10^4\) time steps. However, for a much greater \(\tau_Q\), like \(\tau_Q = 20000\), 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 behaviour 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 \(\tau_Q\) for which the system just anneals upto \(m_f = 0.8\) (complete annealing requires prohibitively longer computer time for this comparative study). We call this minimum value \((\tau_Q)_{\text{min}}\). A bisection scheme was used to locate \((\tau_Q)_{\text{min}}\) for different values of \(g\) starting for the same initial configuration. The inset in Fig. 2 shows that \((\tau_Q)_{\text{min}}\) increases fairly sharply with \(g\) (an empirical analysis shows \((\tau_Q)_{\text{min}} \approx ag^2 + b\), where \(a\) and \(b\) are constants) for \(g \leq 1000\). This quadratic variation with \(g\) might be due to the specific functional form of \(P\) we have used. However, for even higher values of \(g\), the slope is expected to decrease, and finally in the asymptotic limit \(g \to \infty\), the relaxation behaviour should converge to that of one with an unsurpassable 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 have also studied thermal annealing of the same (classical East) model for \(\Gamma = 0\), following an exponentially decreasing temperature schedule given by \(T = T_0 \exp \left(-t/\tau_C\right); \tau_C\) being the time constant for the thermal annealing schedule and \(T_0\) the initial temperature. Here, when \((i - 1)\)-th spin is down, the flipping probability for the \(i\)-th spin \((\sim \exp \left(-\chi/T\right))\) is negligible since \(\chi\) is very large. Otherwise, it flips with probability \(P = 1\) if it were in the up state, and with Boltzmann probability \(P = \exp \left(-h/T\right)\) if it were in the down state. In Fig. 3 we compare the results for the same order of initial value and time constant for \(\Gamma\) and \(T\) (barrier height \(\chi\) is taken to be 1000 in both the 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 \(10^{-4}\)). 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 \(\tau_Q\) compared to \(\tau_C\); typically, \(\tau_C \approx 10^3 \times \tau_Q\) for equivalent annealing (for similar optimal values of final order \(m_f \approx 0.92\)). For annealing with final order \(m_f \approx 1\), we find \(\tau_C \approx 10^4 \times \tau_Q\). This comparison of course depends on the value of \(g\) used (for the barriers) as shown in the inset of Fig. 2.

IV. SUMMARY

We have discussed here the annealing of a kinetically constrained Ising spin chain of \(N\) spins, starting from a disordered state (with negligible initial magnetization), to its (external field induced) fully ordered ground state. At any finite temperature \(T\) (in the classical model) the system takes an exponentially long time to relax to the ordered state because of the kinetic constraints, which act like an infinite potential barrier, depending on the neighbouring spin configurations. Quantum mechanically, this infinite barrier is taken to be penetrable, i.e. with finite tunnelling probability, depending on the barrier height \(\chi\) and width \(a\) \((a \to 0\) faster than \(\chi^{-2}\)). The introduced noise, required for the annealing, is reduced following an exponential schedule in both the cases: \(T = T_0 e^{-t/\tau_C}\), \(\Gamma = \Gamma_0 e^{-t/\tau_0}\), with \(T_0 \approx \Gamma_0\). For our simulation for the quantum case, we have taken the tunnelling probabilities \(P\) (for cases I-IV) and employed them in a semi-classical
We observe that for similar achievement in final order \(m_f \sim 0.92\) starting from \(m_i = 10^{-3}\), \(\tau_C \sim 10^3\tau_Q\) for \(N = 5 \times 10^4\). 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 comparison 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 tunnelling of the wave packet from one well to the other was taken into account by employing a scattering picture and we used the tunnelling 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. It may be noted however that, because of the absence of inter-spin 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 neighbour (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.

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