Quantum annealing in the transverse Ising model

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We introduce quantum fluctuations into the simulated annealing process of optimization problems, aiming at faster convergence to the optimal state. Quantum fluctuations cause transitions between states and thus play the same role as thermal fluctuations in the conventional approach. The idea is tested by the transverse Ising model, in which the transverse field is a function of time similar to the temperature in the conventional method. The goal is to find the ground state of the diagonal part of the Hamiltonian with high accuracy as quickly as possible. We have solved the time-dependent Schrödinger equation numerically for small size systems with various exchange interactions. Comparison with the results of the corresponding classical (thermal) method reveals that the quantum annealing leads to the ground state with much larger probability in almost all cases if we use the same annealing schedule. [S1063-651X(98)02910-9]

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I. INTRODUCTION

The technique of simulated annealing (SA) was first proposed by Kirkpatrick *et al.* [1] as a general method to solve optimization problems. The idea is to use thermal fluctuations to allow the system to escape from local minima of the cost function so that the system reaches the global minimum under an appropriate annealing schedule (the rate of decrease of temperature). If the temperature is decreased too quickly, the system may become trapped in a local minimum. Too slow annealing, on the other hand, is practically useless although such a process would certainly bring the system to the global minimum. Geman and Geman proved a theorem on the annealing schedule for a generic problem of combinatorial optimization [2]. They showed that any system reaches the global minimum of the cost function asymptotically if the temperature is decreased as $T=c/\ln t$ or slower, where c is a constant determined by the system size and other structures of the cost function. This bound on the annealing schedule may be the optimal one under generic conditions although a faster decrease of the temperature often gives satisfactory results in practical applications for many systems.

Thermal fluctuations were introduced in the optimization problem so that transitions between states take place in the process of search for the global minimum among many states. Thus there seems to be no reason to avoid use of other mechanisms for state transitions if these mechanisms may lead to better convergence properties. One such possibility is the generalized transition probability of Tsallis [3], which is a generalization of the conventional Boltzmann-type transition probability appearing in the master equation and thus used in Monte Carlo simulations (see also [4]). In the present paper we seek another possibility of making use of quantum tunneling processes for state transitions, which we call quantum annealing (QA). In particular we would like to learn how effectively quantum tunneling processes possibly lead to the global minimum in comparison to temperature-driven processes used in the conventional method of SA.

In the virtual absence of previous studies along such a line of consideration, it seems better to focus our attention on a specific model system, rather than to develop a general argument, to gain insight into the role of quantum fluctuations in the situation of optimization problem. Quantum effects have been found to play a very similar role to thermal fluctuations in the Hopfield model in a transverse field in thermal equilibrium [5]. This observation motivates us to investigate dynamical properties of the Ising model under quantum fluctuations in the form of a transverse field. We therefore discuss in this paper the transverse Ising model with a variety of exchange interactions. The transverse field controls the rate of transition between states and thus plays the same role as the temperature does in SA. We assume that the system has no thermal fluctuations in the QA context and the term ''ground state'' refers to the lowest-energy state of the Hamiltonian without the transverse field term.

Static properties of the transverse Ising model have been investigated quite extensively for many years [6]. There have, however, been very few studies on the dynamical behavior of the Ising model with a transverse field. We refer to the work by Sato *et al.* who carried out quantum Monte Carlo simulations of the two-dimensional Gaussian spin glass model in an infinitesimal transverse field, showing a reasonably fast approach to the ground state [7].

We present here a point of view that compares the efficiency of QA directly with that of classical SA in reaching the ground state. We solve the time-dependent Schrödinger equation and the classical master equation numerically for small-size systems with the same exchange interactions under the same annealing schedules. Calculations of probabilities that the system is in the ground state at each time for both classical and quantum cases give important implications on the relative efficiency of the two approaches.

In the next section we explain the model and define the measure of closeness of the system in QA to the desired ground state. This measure is compared with the corresponding classical probability that the system is in the ground state, the definition of which is also given there. In Sec. III numerical results for QA and SA are shown for various types of annealing schedules and interactions. The data suggest that QA generally gives a larger probability to lead to the ground state than SA under the same conditions on the an-

nealing schedule and interactions. Section IV deals with the analytical solutions for the one-spin case, which turns out to be quite nontrivial. Explicit solutions yield very useful information to clarify several subtle aspects of the problem. The final section is devoted to summary and discussions.

II. TRANSVERSE ISING MODEL

Let us consider the following Ising model with longitudinal and transverse fields:

$$\mathcal{H}(t)=-\sum_{ij} J_{ij}\sigma_i^z\sigma_j^z-h\sum_i \sigma_i^z-\Gamma(t)\sum_i \sigma_i^x \tag{1}$$

$$\equiv\mathcal{H}_0-\Gamma(t)\sum_i \sigma_i^x, \tag{2}$$

where the types of interactions will be specified later. The term of longitudinal field was introduced to remove the trivial degeneracy in the exchange interaction term coming from the overall up-down symmetry that effectively reduces the available phase space by half. The $\Gamma(t)$ term causes quantum tunneling between various classical states (the eigenstates of the classical part $\mathcal{H}_0$). By decreasing the amplitude $\Gamma(t)$ of the transverse field from a very large value to zero, we hopefully drive the system into the optimal state, the ground state of $\mathcal{H}_0$.

The natural dynamics of the present system is provided by the Schrödinger equation

$$i\frac{\partial|\psi(t)\rangle}{\partial t}=\mathcal{H}(t)|\psi(t)\rangle. \tag{3}$$

We solve this time-dependent Schrödinger equation numerically for small-size systems. The representation to diagonalize $\mathcal{H}_0$ (the z representation) will be used throughout the paper. The corresponding classical SA process is described by the master equation

$$\frac{dP_i(t)}{dt}=\sum_j \mathcal{L}_{ij}P_j(t), \tag{4}$$

where $P_i(t)$ represents the probability that the system is in the ith state. We consider single-spin flip processes with the transition matrix elements given as

$$\mathcal{L}_{ij}=\begin{cases}\{1+\exp[(E_i-E_j)/T(t)]\}^{-1} & \text{(single-spin difference)}\\ -\sum_{k\neq i}\mathcal{L}_{ki} & (i=j)\\ 0 & \text{(otherwise)}.\end{cases} \tag{5}$$

In SA, the temperature $T(t)$ is first set to a very large value and then is gradually decreased to zero. The corresponding process in QA should be to change $\Gamma(t)$ from a very large value to zero. The reason is that the high-temperature state in SA is a mixture of all possible states with almost equal probabilities, and the corresponding state in QA is the linear combination of all states with equal amplitude in the z representation, which is the lowest eigenstate of the Hamiltonian (1) for very large Γ. The low-temperature state after a successful SA is the ground state of $\mathcal{H}_0$, which should also be the eigenstate of $\mathcal{H}(t)$ as $\Gamma(t)$ is reduced to zero sufficiently slowly in QA. Another justification of identification of Γ and T comes from the fact that the $T=0$ phase diagram of the Hopfield model in a transverse field has almost the same structure as the equilibrium phase diagram of the conventional Hopfield model at finite temperature if we identify the temperature axis of the latter phase diagram with the Γ axis in the former [5]. We therefore change $\Gamma(t)$ in QA and $T(t)$ in SA from infinity to zero with the same functional forms $\Gamma(t)=T(t)=c/t, c/\sqrt{t}, c/\ln(t+1)$ $(t{:}0\to\infty)$ or $-ct$ $(t{:}-\infty\to 0)$. The reason for choosing these functional forms is that they allow either for analytical solutions in the single-spin case as shown in Sec. IV or for comparison with the Geman-Geman bound mentioned in Sec. I.

To compare the performance of the two methods QA and SA, we calculate the probabilities $P_{\mathrm{QA}}(t)=|\langle g|\psi(t)\rangle|^2$ for QA and $P_{\mathrm{SA}}(t)=P_g(t)$ for SA, where $P_g(t)$ is the probability to find the system in the ground state at time t in SA and $|g\rangle$ is the ground-state wave function of $\mathcal{H}_0$. Note that we treat only small-size systems (the number of spins $N=8$) and thus the ground state can be picked out explicitly. In the ideal situation $P_{\mathrm{QA}}(t)$ and $P_{\mathrm{SA}}(t)$ will be very small initially and increase towards 1 as $t\to\infty$.

It is useful to introduce another set of quantities $P_{\mathrm{SA}}^{\mathrm{st}}(T)$ and $P_{\mathrm{QA}}^{\mathrm{st}}(\Gamma)$. The former is the Boltzmann factor of the ground state of $\mathcal{H}_0$ at temperature T while the latter is defined as $|\langle g|\psi_\Gamma\rangle|^2$, where the wave function ψ_Γ is the lowest-energy stationary state of the full Hamiltonian (1) for a given fixed value of Γ. In the quasistatic limit, the system follows equilibrium in SA and thus $P_{\mathrm{SA}}(t)=P_{\mathrm{SA}}^{\mathrm{st}}(T(t))$. Correspondingly for QA, $P_{\mathrm{QA}}(t)=P_{\mathrm{QA}}^{\mathrm{st}}(\Gamma(t))$ when $\Gamma(t)$ changes sufficiently slowly. Thus the differences between both sides of these two equations give measures of how closely the system follows quasistatic states during dynamical process of annealing.

III. NUMERICAL RESULTS

We now present numerical results on P_{SA} and P_{QA} for various types of exchange interactions and transverse fields. All calculations were performed with a constant longitudinal field $h=0.1$ to remove trivial degeneracy.

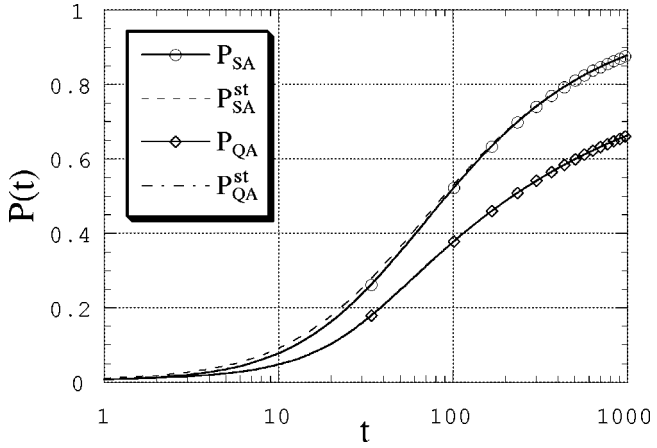

FIG. 1. Time dependence of the overlaps $P_{SA}(t)$, $P_{QA}(t)$, $P^{st}_{SA}(T(t))$ and $P^{st}_{QA}(\Gamma(t))$ of the ferromagnetic model with $\Gamma(t)=T(t)=3/\ln(t+1)$.

A. Ferromagnetic model

Let us first discuss the ferromagnetic Ising model with $J=$const for all pairs of spins. Figure 1 shows the overlaps for the case of $\Gamma(t)=T(t)=3/\ln(t+1)$. It is seen that both QA and SA follow stationary (equilibrium) states during dynamical processes rather accurately. In SA the theorem of Geman and Geman [2] guarantees that the annealing schedule $T(t)=c/\ln(1+t)$ assures convergence to the ground state ($P_{SA}\rightarrow 1$ in our notation) if c is adjusted appropriately. Our choice $c=3$ is somewhat arbitrary but the tendency is clear for $P_{SA}\rightarrow 1$ as $t\rightarrow\infty$, which is also clear from approximate satisfaction of the quasiequilibrium condition $P_{SA}(t)=P^{st}_{SA}(T(t))$. Although there are no mathematically rigorous arguments for QA corresponding to the Geman-Geman bound, the numerical data indicate convergence to the ground state under the annealing schedule $\Gamma(t)=3/\ln(t+1)$ at least for the ferromagnetic system. It should be remembered that the unit of time is arbitrary since we have set $\hbar=1$ in the Schrödinger equation (3) and the unit of time $\tau=1$ in the master equation (4). Thus the fact that the curves for QA in Fig. 1 lie below those for SA at any given time does not have any positive significance.

If we decrease the transverse field and the temperature faster, $\Gamma(t)=T(t)=3/\sqrt{t}$, there appears a qualitative difference between QA and SA as shown in Fig. 2. The quantum method clearly gives better convergence to the ground state while the classical counterpart gets stuck in a local minimum with a non-negligible probability. To see the rate of approach of P_{QA} to 1, we have plotted $1-P_{QA}$ in a log-log scale in Fig. 3. It is seen that $1-P_{QA}$ behaves as const/t in the time region between 100 and 1000.

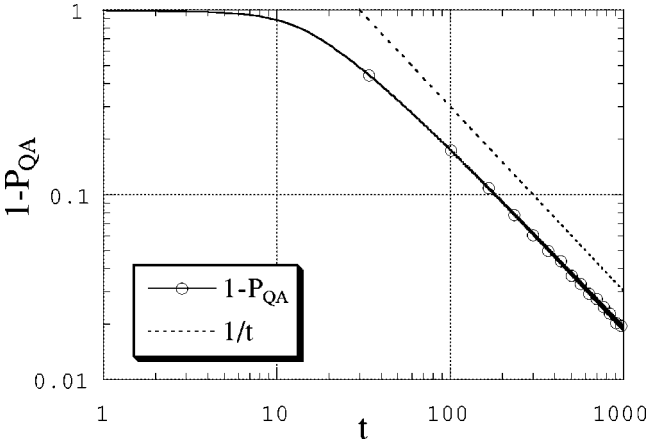

FIG. 3. Time dependence of $1-P_{QA}(t)$ of the ferromagnetic model with $\Gamma(t)=3/\sqrt{t}$. The dotted line represents t^{-1} to guide the eye.

By a still faster annealing schedule $\Gamma(t)=T(t)=3/t$, the system becomes trapped in intermediate states both in QA and SA as seen in Fig. 4.

B. Frustrated model

We next analyze the interesting case of a frustrated system shown in Fig. 5. The full lines indicate ferromagnetic interactions while the broken line is for an antiferromagnetic interaction with the same absolute value as the ferromagnetic ones. If the temperature is very high in the classical case, the spins 4 and 5 are changing their states very rapidly and hence the effective interaction between spins 3 and 6 via spins 4 and 5 will be negligibly small. Thus the direct antiferromagnetic interactions between spins 3 and 6 is expected to dominate the correlation of these spins, which is clearly observed in Fig. 6 as the negative value of the thermodynamic corre-

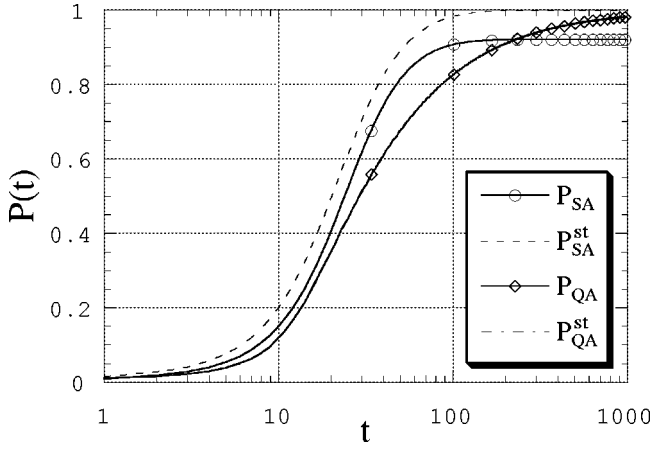

FIG. 2. Time dependence of the overlaps of the ferromagnetic model with $\Gamma(t)=T(t)=3/\sqrt{t}$.

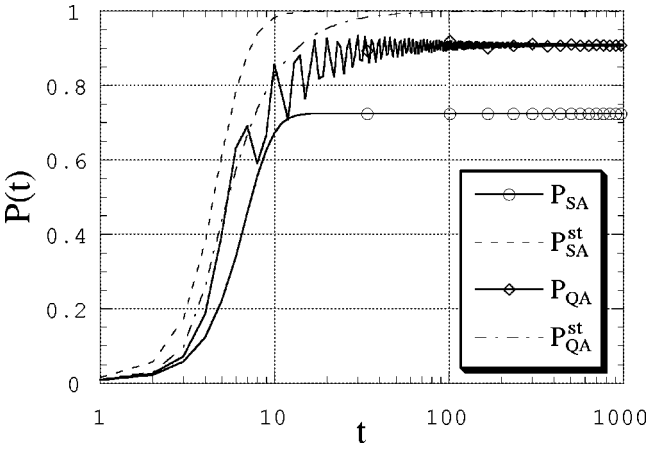

FIG. 4. Time dependence of the overlaps of the ferromagnetic model with $\Gamma(t)=T(t)=3/t$.

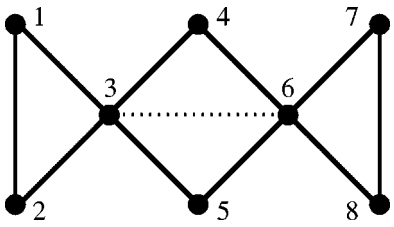

FIG. 5. The frustrated model where the solid lines denote ferromagnetic interactions and the broken line is for an antiferromagnetic interaction.

lation function $\langle \sigma_3^z \sigma_6^z \rangle_c$ in the high-temperature side. At low temperatures, on the other hand, the spins 4 and 5 tend to be fixed in some definite direction and consequently the effective ferromagnetic interactions between spins 3 and 6 are roughly twice as large as the direct antiferromagnetic interaction. This argument is justified by the positive value of the correlation function at low temperatures in Fig. 6. Therefore the spins 3 and 6 must change their relative orientation at some intermediate temperature. This means that the free-energy landscape goes under significant restructuring as the temperature is decreased and therefore the annealing process should be performed with sufficient care.

If the transverse field in QA plays a similar role to the temperature in SA, we expect similar dependence of the correlation function $\langle \sigma_3^z \sigma_6^z \rangle_q$ on the transverse field Γ. Here the expectation value is evaluated by the stationary eigenfunction of the full Hamiltonian (1) with the lowest eigenvalue at a given Γ. The broken curve in Fig. 6 clearly supports this idea. We therefore expect that the frustrated system of Fig. 5 is a good test ground for comparison of QA and SA in the situation with a significant change of spin configurations in the dynamical process of annealing.

The results are shown in Fig. 7 for the annealing schedule $\Gamma(t)=T(t)=3/\sqrt{t}$. The time scale τ is normalized as $\tau = tT_c^2$ in SA and $\tau = t\Gamma_c^2$ in QA. The values, T_c and Γ_c, are the points where the correlation functions vanish in Fig. 6. Thus both classical and quantum correlation functions vanish at $\tau = 1$. The tendency is clear that QA is better suited for ground-state search in the present system.

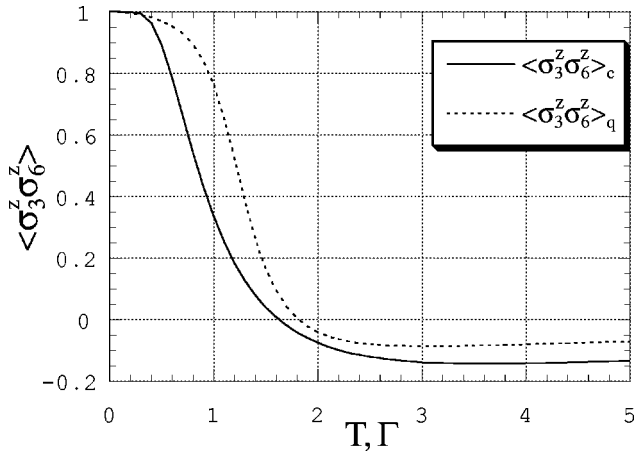

FIG. 6. Correlation functions of spins 3 and 6 in Fig. 5 for the classical and quantum cases. In the classical model (full line) the correlation is shown as a function of temperature while the quantum case (dotted line) is regarded as a function of the transverse field.

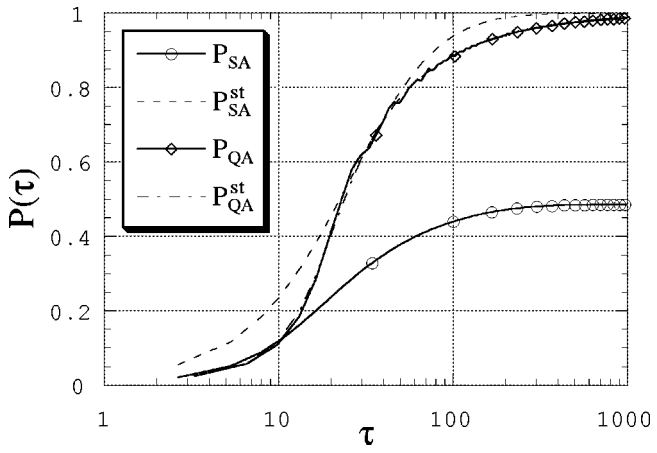

FIG. 7. Time dependence of the overlaps of the frustrated model under $\Gamma(t)=T(t)=3/\sqrt{t}$. Here the time scale τ is normalized by Γ_c and T_c (the points where the correlation functions vanish in Fig. 6).

C. Random interaction model

The third and final example is the Sherrington-Kirkpatrick (SK) model of spin glasses [8]. Interactions exist between all pairs of spins and are chosen from a Gaussian distribution with vanishing mean and variance $1/N$ ($N=8$ in our case). Figure 8 shows a typical result on the time evolution of the probabilities under the annealing schedule $\Gamma(t)=T(t)=3/\sqrt{t}$. We have checked several realizations of exchange interactions under the same distribution function and have found that the results are qualitatively the same. Figure 8 again suggests that QA is better suited than SA for the present optimization problem.

IV. SOLUTION OF THE SINGLE-SPIN PROBLEM

It is possible to solve the time-dependent Schrödinger equation explicitly when the problem involves only a single spin and the functional form of the transverse field is $\Gamma(t) = -ct, c/t$, or $c/\sqrt{t}$. We note that the single-spin problem is trivial in SA because there are only two states involved (up and down) and thus there are no local minima. This does not mean that the same single-spin problem is also trivial in the quantum mechanical version. In QA with a single spin, the

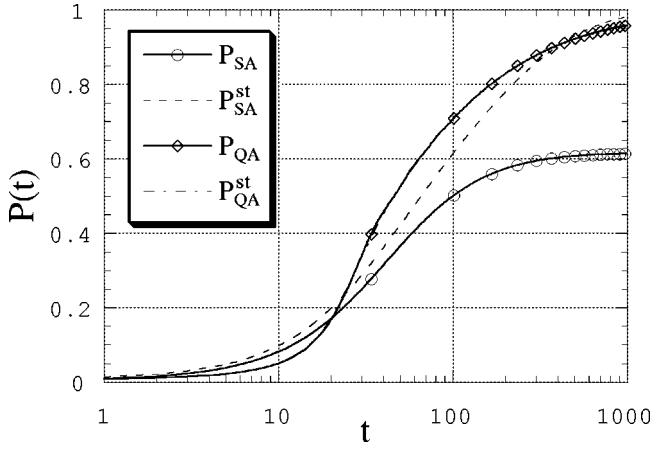

FIG. 8. Time dependence of the overlaps for the SK model with $\Gamma(t)=T(t)=3/\sqrt{t}$.

transition between the two states is caused by a finite transverse field. The system goes through tunneling processes to reach the other state, and an approximate annealing schedule is essential to reach the ground state. On the other hand, in SA, the transition from the higher state to the lower state takes place even at $T=0$ and thus the system always reaches the ground state.

Let us first discuss the case of $\Gamma(t)=-ct$ with t changing from $-\infty$ to 0. This is the well-known Landau-Zener model and the explicit solution of the time-dependent Schrödinger equation is available in the literature [9–13]. With the notation $a(t)=\langle +|\psi(t)\rangle$ and $b(t)=\langle -|\psi(t)\rangle$ and the initial condition $a(-\infty)=b(-\infty)=1/\sqrt{2}$ (the lowest eigenstate), the solution for $b(t)$ is found to be (see the Appendix)

$$b(t)=\frac{he^{-\pi h^2/8c}}{2\sqrt{c}}\left\{-\frac{2ct+h}{h}D_{-\lambda-1}(-iz)-\frac{ih^2+2c}{\sqrt{2c}h}e^{3/4\pi i}D_{-\lambda-2}(-iz)\right\}, \tag{6}$$

where $D_{-\lambda-1}, D_{-\lambda-2}$ represent the parabolic cylinder function (or Weber function) and z and λ are given as

$$z=\sqrt{2c}e^{-\pi i/4}t, \tag{7}$$

$$\lambda=\frac{ih^2}{2c}. \tag{8}$$

The final value of $b(t)$ at $t=0$ is

$$b(0)=-\frac{h\sqrt{\pi}2^{-ih^2/4c}e^{-\pi h^2/8c}}{2\sqrt{2c}}\left\{\frac{1}{\Gamma(1+ih^2/4c)}+\frac{\sqrt{c}e^{3/4\pi i}(1+ih^2/2c)}{h\Gamma(3/2+ih^2/4c)}\right\}. \tag{9}$$

The probability to find the system in the ground state at $t=0$ is, when $h^2/c\gg 1$,

$$P_{\mathrm{QA}}(0)=|a(0)|^2=1-|b(0)|^2\sim 1-\frac{c^2}{16h^4}. \tag{10}$$

Thus the probability $P_{\mathrm{QA}}(t)$ does not approach 1 for finite c.

We next present the solution for $\Gamma(t)=c/t$ with t changing from 0 to ∞ under the initial condition $a=b=1/\sqrt{2}$ (see Appendix):

$$b(t)=\frac{1}{\sqrt{2}}e^{iht}t^{ic}F(1+ic,1+2ic;-2iht), \tag{11}$$

where F is the confluent hypergeometric function. The asymptotic form of $b(t)$ as $t\to\infty$ is

$$b(t)\sim\frac{\sqrt{2}(2h)^{-ic}\Gamma(2ic)}{\Gamma(ic)}\{e^{-iht-\pi c/2}+ce^{iht+\pi c/2}(2ht)^{-1}\}. \tag{12}$$

The probability of finding the system in the target ground state behaves asymptotically as

$$P_{\mathrm{QA}}(t)=|a(t)|^2 \tag{13}$$

$$=1-|b(t)|^2 \tag{14}$$

$$\sim 1-\frac{\sinh(\pi c)}{\sinh(2\pi c)}\left\{e^{-\pi c}+\frac{c\cos(2ht)}{ht}+\frac{c^2e^{\pi c}}{4h^2t^2}\right\} \tag{15}$$

$$\sim 1-e^{-2\pi c}, \tag{16}$$

the last approximation being valid for $c\gg 1$ after $t\to\infty$. The system does not reach the ground state as $t\to\infty$ as long as c is finite. Larger c gives a more accurate approach to the ground state, which is reasonable because it takes a longer time to reach a given value of $\Gamma(=c/t)$ for larger c, implying slower annealing.

The final example of the solvable model concerns the annealing schedule $\Gamma(t)=c/\sqrt{t}$. The solution for $b(t)$ is derived in the Appendix under the initial condition $a=b=1/\sqrt{2}$ as

$$b(t)=\frac{1}{\sqrt{2}}e^{iht}F\left(\frac{1}{2}-i\gamma,\frac{1}{2};-2iht\right)+\frac{c}{\sqrt{h}}e^{(3/4)\pi i}e^{iht}(-2iht)^{1/2}F\left(1-i\gamma,\frac{3}{2};-2iht\right), \tag{17}$$

where $\gamma=c^2/2h$. The large-t behavior is found to be

$$b(t)\sim\sqrt{\pi}e^{-\pi c^2/4h}\left[e^{-iht}(2ht)^{-i\gamma}\left\{\frac{1}{\sqrt{2}\Gamma\left(\frac{1}{2}-i\gamma\right)}+\frac{\sqrt{h}e^{(5/4)\pi i}}{c\Gamma(-i\gamma)}\right\}+e^{iht}(2ht)^{-1/2+i\gamma}\left\{\frac{e^{-(1/4)\pi i}}{\sqrt{2}\Gamma(i\gamma)}+\frac{c}{2\sqrt{h}\Gamma\left(\frac{1}{2}+i\gamma\right)}\right\}\right], \tag{18}$$

and the probability $P_{\mathrm{QA}}(\infty)$ for $c^2/h \gg 1$ is obtained as

$$P_{\mathrm{QA}}(\infty) = 1 - |b(\infty)|^2 \sim 1 - \frac{h^2}{64c^4}. \tag{19}$$

This equation indicates that the single-spin system does not reach the ground state under the present annealing schedule $\Gamma(t) = c/\sqrt{t}$ for which the numerical data in the previous section suggested an accurate approach. We therefore conclude that the asymptotic value of $P_{\mathrm{QA}}(t)$ in the previous section may not be exactly equal to 1 for $\Gamma(t) = 3/\sqrt{t}$ although it is very close to 1.

The annealing schedule $\Gamma(t) = c/\sqrt{t}$ has a feature that distinguishes this function from the other ones $-ct$ and c/t. As we saw in the previous discussion, the final asymptotic value of $P_{\mathrm{QA}}(t)$ is not 1 if the initial condition corresponds to the ground state for $\Gamma \to \infty$, $a = b = 1/\sqrt{2}$. However, as shown in the Appendix, by an appropriate choice of the initial condition, it is possible to drive the system to the ground state if $\Gamma(t) = c/\sqrt{t}$. This is not possible for any initial conditions in the case of $\Gamma(t) = -ct$ or c/t.

V. SUMMARY AND DISCUSSIONS

We have proposed the idea of quantum annealing (QA) in which quantum tunneling effects cause transitions between states in optimization problem, in contrast to the usual thermal transitions in simulated annealing (SA). The idea was tested in the transverse Ising model obeying the time-dependent Schrödinger equation. The transverse field term was controlled so that the system approaches the ground state. The numerical results on the probability to find the system in the ground state were compared with the corresponding probability derived from the numerical solution of the master equation representing the SA processes. We have found that QA shows convergence to the optimal (ground) state with larger probability than SA in all cases if the same annealing schedule is used. The system approaches the ground state rather accurately in QA for the annealing schedule $\Gamma = c/\sqrt{t}$ but not for a faster decrease of the transverse field.

We have also solved the single-spin model exactly for QA in the cases of $\Gamma(t) = -ct, c/t$, and $c/\sqrt{t}$. The results showed that the ground state is not reached perfectly for all these annealing schedules. Therefore the asymptotic values of $P_{\mathrm{QA}}(t)$ in numerical calculations are probably not exactly 1 although they seem to be quite close to the optimal value 1.

The rate of approach to the asymptotic value close to 1, $1 - P_{\mathrm{QA}}(t)$, was found to be proportional to $1/t$ in Fig. 3 for the ferromagnetic model. On the other hand, the single-spin solution shows the existence of a term proportional to $1/\sqrt{t}$; see Eq. (18). Probably the coefficient of the $1/\sqrt{t}$ term is very small in the situation of Fig. 3 and the next-order contribution dominates in the time region shown in Fig. 3.

A simple argument using perturbation theory yields useful information about the asymptotic form of the probability function if we assume that the system follows quasistatic states during dynamical processes. The probability to find the system in the ground state is expressed using the perturbation in terms of $\Gamma (\ll 1)$ as

$$P_{\mathrm{QA}}(\Gamma) \sim 1 - \Gamma^2 \sum_{i \neq 0} \frac{1}{(E_0^{(0)} - E_i^{(0)})^2}, \tag{20}$$

where $E_i^{(0)}$ is the energy of the ith state of the nonperturbed (classical) system and $E_0^{(0)}$ is the ground-state energy. If we set $\Gamma = c/\sqrt{t}$, we have

$$P_{\mathrm{QA}}(\Gamma) \sim 1 - \frac{1}{t} \sum_{i \neq 0} \left(\frac{c}{E_0^{(0)} - E_i^{(0)}} \right)^2. \tag{21}$$

Thus the approach to the asymptotic value is proportional to $1/t$ as long as the system stays in quasistatic states. The corresponding probability for SA is

$$P_{\mathrm{SA}}(T) \sim \frac{e^{-E_0/T}}{\sum_i e^{-E_i/T}} \sim 1 - \sum_{i \neq 0} e^{-(E_i - E_0)/T}, \tag{22}$$

which shows absence of universal ($1/t$-like) dependence on time.

The present method of QA bears some similarity to the approach by the generalized transition probability in which the dynamics is described by the master equation but the transition probability has power-law dependence on the temperature in contrast to the usual exponential form of the Boltzmann factor [3]. This power-law dependence on the temperature allows the system to search for a wider region in the phase space because of larger probabilities of transition to higher-energy states at a given $T(t)$, which may be the reason for faster convergence to the optimal states [3,4]. The transverse field term Γ in our QA represents the rate of transition between states which is larger than the transition rate in SA [see Eq. (5)] at a given small value of the control parameter $\Gamma(t) = T(t)$. This larger transition probability may lead to a more active search in wider regions of the phase space, leading to better convergence similarly to the case of the generalized transition probability.

We have solved the Schrödinger equation and the master equation directly by numerical methods for the purpose of comparison of QA and SA. This method faces difficulties for larger N because the number of states increases exponentially as 2^N. The classical SA solves this problem by exploiting stochastic processes, Monte Carlo simulations, which have the computational complexity growing as a power of N. The corresponding reduction of the computational complexity is lacking in QA, and it is an important future problem in practical implementation of the idea of QA. Another future problem is to devise implementations of QA in other optimization problems such as the traveling salesman problem or the graph bipartitioning for which there seems to be no direct analog of the transverse field to cause quantum transitions.

ACKNOWLEDGMENTS

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APPENDIX: SINGLE-SPIN PROBLEM

In this Appendix we explain some technical aspects to deriving the exact solution of the time-dependent Schrödinger equation for the transverse Ising model with a single spin. The three cases of $\Gamma(t)=-ct, c/t$, and $c/\sqrt{t}$ will be discussed.

1. Case of $\Gamma(t)=-ct$ (Landau-Zener model) [9–13]

Let us express the solution of the Schrödinger equation at time t by the parameters $a=\langle+|\psi(t)\rangle$ and $b=\langle-|\psi(t)\rangle$. The Schrödinger equation (3) with $\mathcal{H}=-h\sigma^z-\Gamma\sigma^x$ is expressed as a set of first order differential equations for a and b. It is convenient to change the variables as

$$\tilde{a}=\frac{1}{\sqrt{2}}(a+b), \quad \tilde{b}=\frac{1}{\sqrt{2}}(a-b), \tag{A1}$$

by which the Schrödinger equation is now

$$\frac{d^2\tilde{b}(t)}{dt^2}+(-ic+h^2+c^2t^2)\tilde{b}(t)=0. \tag{A2}$$

By using the notation

$$z=\sqrt{2c}e^{-\pi i/4}t, \tag{A3}$$

$$\lambda=\frac{ih^2}{2c}, \tag{A4}$$

we find

$$\frac{d^2\tilde{b}(t)}{dz^2}+\left(\lambda+\frac{1}{2}-\frac{1}{4}z^2\right)\tilde{b}(t)=0. \tag{A5}$$

The initial state is specified as $a=b=1/\sqrt{2}$ or $\tilde{b}=0$ as $t\to-\infty$. The solution of Eq. (A5) satisfying this condition is the parabolic cylinder function $D_{-\lambda-1}(-iz)$ [14]. Thus, we obtain the solution as

$$\tilde{a}(t)=\frac{1}{h}\left(-ct\tilde{b}(t)-i\frac{d\tilde{b}(t)}{dt}\right), \tag{A6}$$

$$\tilde{b}(t)=C_1D_{-\lambda-1}(iz), \tag{A7}$$

where C_1 is a constant. To fix C_1, we use the condition

$$|\tilde{a}(-\infty)|=\frac{2C_1ce^{\pi h^2/8c}}{h\sqrt{2c}}=1. \tag{A8}$$

Then we have

$$C_1=\frac{h}{\sqrt{2c}}e^{-\pi h^2/8c}. \tag{A9}$$

The wave function of this system is given in Eq. (6).

2. Case of $\Gamma(t)=c/t$

We next consider the case of $\Gamma(t)=c/t$. By eliminating a from the Schrödinger equation, we obtain

$$\frac{d^2b(t)}{dt^2}-\frac{1}{\Gamma(t)}\frac{d\Gamma(t)}{dt}\frac{db(t)}{dt}+\left(h^2+\Gamma^2(t)-\frac{ih}{\Gamma(t)}\frac{d\Gamma(t)}{dt}\right)b(t)=0. \tag{A10}$$

Substituting $\Gamma(t)=c/t$, we have

$$\frac{d^2b(t)}{dt^2}-\frac{1}{t}\frac{db(t)}{dt}+\left(h^2+\frac{ih}{t}+\frac{c^2}{t^2}\right)b(t)=0. \tag{A11}$$

The solutions of this equation are expressed by the confluent P function [14]

$$\tilde{P}\left\{\begin{array}{cccc} \infty & & 0 & \\ \overbrace{ih \quad 1} & & ic & t \\ -ih & 0 & -ic & \end{array}\right\} = e^{iht}t^{ic}\tilde{P}\left\{\begin{array}{cccc} \infty & & 0 & \\ \overbrace{0 \quad 1+ic} & & 0 & -2iht \\ 1 & ic & -2ic & \end{array}\right\}, \tag{A12}$$

the right-hand side of which has two independent expressions in terms of the confluent hypergeometric function

$$f(t)=e^{iht}t^{ic}F(1+ic,1+2ic;-2iht), \tag{A13}$$

$$g(t)=e^{iht}t^{ic}(-2iht)^{-2ic}F(1-ic,1-2ic;-2iht). \tag{A14}$$

The general solution is $b(t)=C_1f(t)+C_2g(t)$. Using the initial condition

$$b(0)=C_1+C_2=\frac{1}{\sqrt{2}}, \tag{A15}$$

$$a(0)=C_1-C_2=\frac{1}{\sqrt{2}}, \tag{A16}$$

we find

$$b(t)=\frac{1}{\sqrt{2}}e^{iht}t^{ic}F(1+ic,1+2ic;-2iht). \tag{A17}$$

The asymptotic forms of $b(t)$ and $|b(t)|^2$ are then given as

$$b(t)\sim\frac{\sqrt{2}(2h)^{-ic}\Gamma(2ic)}{\Gamma(ic)}\{e^{-iht-\pi c/2}+ce^{iht+\pi c/2}(2ht)^{-1}\}, \tag{A18}$$

$$|b(t)|^2 \sim \frac{\sinh(\pi c)}{\sinh(2\pi c)}\left\{ e^{-\pi c} + \frac{c\cos(2ht)}{ht} + \frac{c^2 e^{\pi c}}{4h^2 t^2}\right\}. \tag{A19}$$

Case of $\Gamma(t)=c/\sqrt{t}$

The final solvable model has $\Gamma(t)=c/\sqrt{t}$. The Schrödinger equation (A10) is then expressed as

$$\frac{d^2 b(t)}{dt^2} - \frac{1}{2t}\frac{db(t)}{dt} + \left(h^2 + \frac{2c^2+ih}{2t}\right) b(t) = 0. \tag{A20}$$

The solution is the confluent P function [14]

$$\tilde{P}\left\{ \begin{array}{cccc} & \overbrace{\qquad\qquad}^{\infty} & & 0 \\ ih & & \tfrac{1}{2}-i\gamma & 0 \quad t \\ -ih & & i\gamma & \tfrac{1}{2} \end{array} \right\} = e^{iht}\tilde{P}\left\{ \begin{array}{cccc} & \overbrace{\qquad\qquad}^{\infty} & & 0 \\ 0 & & \tfrac{1}{2}-i\gamma & 0 \quad -2iht \\ 1 & & i\gamma & \tfrac{1}{2} \end{array} \right\}, \tag{A21}$$

where $\gamma = c^2/2h$. The two independent solutions are thus [14]

$$f(t) = e^{iht} F\left(\frac{1}{2} - i\gamma, \frac{1}{2}; -2iht \right), \tag{A22}$$

$$g(t) = e^{iht}(-2iht)^{1/2} F\left(1 - i\gamma, \frac{3}{2}; -2iht \right). \tag{A23}$$

The general solution of Eq. (A20) is therefore the linear combination of the above two functions

$$b(t) = C_1 f(t) + C_2 g(t). \tag{A24}$$

The constants C_1 and C_2 are fixed by the requirement

$$b(0) = C_1 = \frac{1}{\sqrt{2}}, \tag{A25}$$

$$a(0) = \frac{\sqrt{h}}{\sqrt{2}c} e^{(5/4)\pi i} C_2 = \frac{1}{\sqrt{2}}. \tag{A26}$$

Substituting C_1 and C_2 into Eq. (A24), we find

$$b(t) = \frac{1}{\sqrt{2}} e^{iht} F\left(\frac{1}{2} - i\gamma, \frac{1}{2}; -2iht \right) + \frac{c}{\sqrt{h}} e^{(3/4)\pi i} \times e^{iht}(-2iht)^{1/2} F\left(1 - i\gamma, \frac{3}{2}; -2iht \right). \tag{A27}$$

The asymptotic form is

$$b(t) \sim \sqrt{\pi} e^{-\pi c^2/4h} \left[e^{-iht}(2ht)^{-i\gamma} \left\{ \frac{1}{\sqrt{2}\Gamma\left(\frac{1}{2} - i\gamma \right)} + \frac{\sqrt{h} e^{(5/4)\pi i}}{c\Gamma(-i\gamma)} \right\} + e^{iht}(2ht)^{-1/2+i\gamma} \left\{ \frac{e^{-(1/4)\pi i}}{\sqrt{2}\Gamma(i\gamma)} + \frac{c}{2\sqrt{h}\Gamma\left(\frac{1}{2} + i\gamma \right)} \right\} \right]. \tag{A28}$$

The probability $|b(\infty)|^2$ that the system remains in the excited state can be calculated as the asymptotic form of Eq. (A28) with the condition $c^2/h \gg 1$

$$|b(\infty)|^2 = \frac{\pi e^{-\gamma\pi}}{2} \left| \frac{1}{\Gamma\left(\frac{1}{2} - i\gamma \right)} + \frac{\gamma^{-1/2} e^{(5/4)\pi i}}{\Gamma(-i\gamma)} \right|^2 \tag{A29}$$

$$\sim \frac{e^{-\gamma\pi}}{4} \left| e^{1/2} \left(\frac{1}{2} - i\gamma \right)^{i\gamma} + \gamma^{-1/2} e^{(5/4)\pi i} (-i\gamma)^{i\gamma + 1/2} \right|^2 \tag{A30}$$

$$\sim \frac{e^{-\gamma\pi}}{4} \left| (-i\gamma)^{i\gamma} \frac{i}{8\gamma} \right|^2 = \frac{1}{256\gamma} = \frac{h^2}{64c^4}. \tag{A31}$$

3. Dependence of the final value on the initial condition

We show that we can choose the initial condition so that the final state is the ground state when $\Gamma = c/\sqrt{t}$. This is not possible for $\Gamma = -ct$ or c/t. From Eq. (A24), the asymptotic form of the solution as $t \to \infty$ is

$$b(t) \sim C_1 \frac{\sqrt{\pi} e^{-\pi c^2/4h - iht}(2ht)^{-ic^2/2h}}{\Gamma(1/2 - ic^2/2h)} + C_2 \frac{i\sqrt{\pi h} e^{-\pi c^2/4h - iht}(2ht)^{-ic^2/2h}}{c^2 \Gamma(-ic^2/2h)}. \tag{A32}$$

The coefficients C_1 and C_2 are fixed under the conditions $b(\infty) = 0$ and $|a(0)|^2 + |b(0)|^2 = 1$ as

$$C_1 = \left\{ 1 + \frac{\sinh(\pi c^2/h)}{2\sinh^2(\pi c^2/2h)} \right\}^{-1/2}, \tag{A33}$$

$$C_2 = \frac{ic^2 \Gamma(-ic^2/2h)}{h\Gamma(1/2 - ic^2/2h)} C_1. \tag{A34}$$

This solution is not the ground state of the Hamiltonian $\mathcal{H}(0)$.

The reason one cannot obtain such a solution for the other schedules ($\Gamma = c/t, -ct$) is the following: The general solution for $\Gamma = c/t$ also has two coefficients, and the initial state is represented as the linear combination of two terms whose phases are indefinite:

$$a(0)=C_1 t^{ic}|_{t\to 0}-C_2 t^{-ic}|_{t\to 0}, \tag{A35}$$

$$b(0)=C_1 t^{ic}|_{t\to 0}+C_2 t^{-ic}|_{t\to 0}. \tag{A36}$$

The lowest-energy state at $t=0$ corresponds to $a(0)=b(0)=1/\sqrt{2}$ (times an arbitrary phase factor), which is realized by choosing $C_2=0$ in Eqs. (A35) and (A36). The indefiniteness of t^{ic} as $t\to 0$ is irrelevant because this is only the overall phase factor. Such a situation does not happen for other values of $a(0)$ and $b(0)$, leading to a serious difficulty in determining the wave function at $t=0$. Thus we cannot choose an initial condition other than $a(0)=b(0)=1/\sqrt{2}$. A similar fact exists in the case of $\Gamma=-ct$.

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