Convergence of Quantum Annealing with Real-Time Schrödinger Dynamics

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Convergence conditions for quantum annealing are derived for optimization problems represented by the Ising model of a general form. Quantum fluctuations are introduced as a transverse field and/or transverse ferromagnetic interactions, and the time evolution follows the real-time Schrödinger equation. It is shown that the system stays arbitrarily close to the instantaneous ground state, finally reaching the target optimal state, if the strength of quantum fluctuations decreases sufficiently slowly, in particular inversely proportionally to the power of time in the asymptotic region. This is the same condition as the other implementations of quantum annealing, quantum Monte Carlo and Green's function Monte Carlo simulations, in spite of the essential difference in the type of dynamics. The method of analysis is an application of the adiabatic theorem in conjunction with an estimate of a lower bound of the energy gap based on the recently proposed idea of Somma *et. al.* for the analysis of classical simulated annealing using a classical-quantum correspondence.

KEYWORDS: quantum annealing, annealing schedule, adiabatic theorem, optimization problem, transverse-field Ising model

Quantum annealing (QA) recently attracts much attention as a novel algorithm for optimization problems.[1–4] A factitious kinetic energy of quantum nature is introduced to the classical system which represents the cost function to be minimized. The resulting system searches the phase space by means of quantum transitions, which are gradually decreased as time proceeds. If the initial state is the ground state of the initial quantum Hamiltonian, the system is expected to keep track of the ground state of the instantaneous Hamiltonian under a slow decrease of quantum fluctuations. From this viewpoint, QA is also called quantum adiabatic evolution.[5] Most of the numerical studies[1–3,6–15] showed that QA is more efficient in solving optimization problems than the well-known classical algorithm, simulated annealing (SA).[16,17]

Convergence theorems for stochastic implementations of QA have been proved for the transverse-field Ising model.[18] A power-law decrease of the transverse field has been shown to be sufficient to guarantee convergence to the optimal state for generic optimization problems. This power-law annealing schedule is faster than that of the inverse-log law for SA given in the theorem of Geman and Geman.[17,19] However, these theorems for QA were proved for stochastic processes to realize QA. It has been unknown so far what annealing schedule would

guarantee the convergence of QA following the real-time Schrödinger equation. We have solved this problem on the basis of the idea of Somma *et. al.*[20] These authors found that the inverse-log law condition for SA can be derived from the adiabatic theorem for a quantum system obtained from the original classical system through a classical-quantum mapping. Although they also discussed some aspects of QA, their interest was to use quantum mechanics to simulate finite-temperature classical statistical mechanics. We point out in the present article that the convergence condition of genuine quantum annealing, in which the system follows the real-time Schrödinger equation without temperature, can also be derived by a similar analysis.

Let us suppose that the optimization problem one wants to solve can be represented as the ground-state search of an Ising model of general form

$$H_{\rm pot} \equiv -\sum_{i=1}^{N} J_i \sigma_i^z - \sum_{ij} J_{ij} \sigma_i^z \sigma_j^z - \sum_{ijk} J_{ijk} \sigma_i^z \sigma_j^z \sigma_k^z - \cdots , \tag{1}$$

where σ_i^z denotes the z component of the Pauli matrix at site i. Quantum annealing is realized typically by the addition of a time-dependent transverse field

$$H_{\rm kin}(t) \equiv -\Gamma(t) \sum_{i=1}^{N} \sigma_i^x, \tag{2}$$

which may be regarded as the quantum kinetic energy to be compared with the potential energy (1). Initially the coefficient of the kinetic term $\Gamma(t)$ is chosen to be very large, and the total Hamiltonian

$$H(t) = H_{\rm pot} + H_{\rm kin}(t) \tag{3}$$

is dominated by the second kinetic term. The coefficient $\Gamma(t)$ is then decreased gradually toward 0, leaving eventually only the potential term. Accordingly the state vector $|\psi(t)\rangle$, which follows the real-time Schrödinger equation

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = H(t)|\psi(t)\rangle, \tag{4}$$

is expected to evolve from the trivial initial ground state of the transverse field (2) to finally the non-trivial ground state of eq. (1). The problem of central concern in the present paper is how slowly we should decrease $\Gamma(t)$ to keep the state vector arbitrarily close to the instantaneous ground state of the total Hamiltonian (3), namely the adiabaticity condition, to achieve the goal of minimization of eq. (1).

The adiabatic theorem[21] provides the excitation probability at time t as

$$|\langle n(t)|\psi(t)\rangle|^2 \simeq \left| \frac{\left\langle n(t) \left| \dfrac{\partial H(t)}{\partial t} \right| 0(t) \right\rangle}{\left(\varepsilon_n(t) - \varepsilon_0(t)\right)^2} \right|^2 , \tag{5}$$

where $|n(t)\rangle$ is the nth instantaneous eigenstate of $H(t)$ with the eigenvalue $\varepsilon_n(t)$. We assume that $|0(t)\rangle$ is the ground state of $H(t)$ and $|\psi(0)\rangle = |0(0)\rangle$. The probability (5) needs to be

arbitrarily small for the success of QA. We therefore evaluate an upper bound of

$$\frac{\left|\left\langle n(t)\left|\frac{\partial H(t)}{\partial t}\right|0(t)\right\rangle\right|}{\left(\varepsilon_n(t)-\varepsilon_0(t)\right)^2}. \tag{6}$$

For this purpose we estimate the numerator and the denominator on the left-hand side of eq. (6). As for the numerator, it is straightforward to see

$$\left|\left\langle n(t)\left|\frac{\partial H(t)}{\partial t}\right|0(t)\right\rangle\right| \le -N\frac{\mathrm{d}\Gamma}{\mathrm{d}t}, \tag{7}$$

since the time dependence of $H(t)$ lies only in the kinetic term, which has N terms. Note that $\mathrm{d}\Gamma/\mathrm{d}t$ is negative.

A lower bound on the denominator of eq. (6) can be evaluated using an inequality for a strictly positive operator.[22] First we recall that the Perron-Frobenius theorem states that a non-negative square matrix M has a real eigenvalue λ_0 satisfying $|\lambda| \le \lambda_0$ for any other eigenvalue λ. If all the elements of M are strictly positive, $M_{ij} > 0$, its eigenvalues satisfy the stronger inequality,[22]

$$|\lambda| \le \frac{\kappa-1}{\kappa+1}\lambda_0, \tag{8}$$

where κ is defined by

$$\kappa = \max_{i,j,k}\frac{M_{ik}}{M_{jk}}. \tag{9}$$

We apply the above inequality (8) to the operator $M \equiv (E_{\max} - H(t))^N$, where $E_{\max}$ is the largest eigenvalue of H_{pot}. All the elements of the matrix M are strictly positive in the representation to diagonalize σ_i^z because $E_{\max} - H(t)$ is non-negative and irreducible (that is, any state can be reached from any other state within N steps at most). In the asymptotic region $t \gg 1$ where $\Gamma(t) \ll 1$, the minimum element of M, which is between two states having all spins in mutually opposite directions, is equal to $N!\Gamma(t)^N$, where $N!$ comes from the ways of permutation to flip spins. Replacement of H_{kin} by $-N$ shows that the maximum matrix element of M has the upper bound $(E_{\max} - E_{\min} + N)^N$, where $E_{\min}$ is the lowest eigenvalue of H_{pot}. Thus we have

$$\kappa \le \frac{(E_{\max} - E_{\min} + N)^N}{N!\Gamma(t)^N}. \tag{10}$$

Since the eigenvalue of $H(t)$ is denoted by $\varepsilon_n(t)$, eq. (8) is rewritten as

$$(E_{\max} - \varepsilon_n(t))^N \le \frac{\kappa-1}{\kappa+1}(E_{\max} - \varepsilon_0(t))^N. \tag{11}$$

Substitution of eq. (10) into the above inequality yields

$$\varepsilon_n(t) - \varepsilon_0(t) \ge \frac{2(E_{\max} - \varepsilon_0(t))N!}{N(E_{\max} - E_{\min} + N)^N}\Gamma(t)^N \equiv A\Gamma(t)^N, \tag{12}$$

where we used $\kappa \gg 1$ in the asymptotic time region where $\Gamma(t)$ is very small. The coefficient A is estimated using the Stirling formula as

$$A \simeq \frac{2\sqrt{2\pi N}(E_{\max} - \varepsilon_0(t))}{N\mathrm{e}^N} \left(\frac{N}{E_{\max} - E_{\min} + N} \right)^N, \tag{13}$$

which demonstrates that A is exponentially small for large N.

Now, by the combination of the above estimates (7) and (12), we find that the sufficient condition for convergence is that the upper bound of eq. (6)

$$-\frac{N}{A^2 \Gamma(t)^{2N}} \frac{\mathrm{d}\Gamma}{\mathrm{d}t} \tag{14}$$

is arbitrarily small. By equating eq. (14) to a small constant δ and integrating the resulting differential equation, we find

$$\Gamma(t) = (\alpha\, t)^{-1/(2N-1)}, \tag{15}$$

where α is exponentially small for large N and is proportional to δ. The transverse field should be decreased following this functional form or slower. Therefore the asymptotic power decay of the transverse field guarantees that the excitation probability is bounded by the arbitrarily small constant δ^2 at each time.

The same discussions apply to quantum annealing using transverse ferromagnetic interactions in addition to a transverse field,

$$\tilde{H}_{\mathrm{kin}}(t) = -\tilde{\Gamma}(t) \left(\sum_{i=1}^{N} \sigma_i^x + \sum_{ij} \sigma_i^x \sigma_j^x \right). \tag{16}$$

A recent study showed the effectiveness of this type of quantum kinetic energy.[23] A modification of the strictly positive operator to $(E_{\max} - H(t))^{N/2}$ in the above argument leads to a lower bound of the energy gap as a quantity proportional to $\tilde{\Gamma}(t)^{N/2}$. The resulting asymptotic annealing schedule is

$$\tilde{\Gamma}(t) \propto t^{-1/(N-1)}, \tag{17}$$

which is faster than the case with the transverse field only, eq. (15). This result implies that the additional non-zero off-diagonal elements of $H(t)$ would widen the energy gap and accelerate the convergence of QA.

In this paper, we have derived conditions for convergence of QA under the real-time Schrödinger dynamics using the adiabatic theorem. The asymptotic power-law annealing schedule (15) guarantees the adiabatic evolution during the annealing process at its final stage $t \gg 1$. This condition coincides with our previous results for stochastic implementations of QA.[18] It is remarkable that essentially different types of dynamics share the same condition for convergence. Note that the power decay derived above applies to the asymptotic region

$t \gg 1$. At the initial stage, $\Gamma(t)$ must be tuned following a different functional form to satisfy the adiabatic condition.

For the adiabatic theorem to be applicable, the energy gap between the ground state and the first excitation state should be finite. The inequality (12) implies that this condition is always satisfied in the transverse-field Ising model as long as the system size is finite. In the thermodynamic limit, of course, the gap may vanish at the critical point. We emphasize that the system size N is kept finite in the present paper because our purpose is to study optimization problems in which the number of elements is always finite.

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