

Mathematical foundation of quantum annealing

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Quantum annealing is a generic name of quantum algorithms that use quantum-mechanical fluctuations to search for the solution of an optimization problem. It shares the basic idea with quantum adiabatic evolution studied actively in quantum computation. The present paper reviews the mathematical and theoretical foundations of quantum annealing. In particular, theorems are presented for convergence conditions of quantum annealing to the target optimal state after an infinite-time evolution following the Schrödinger or stochastic (Monte Carlo) dynamics. It is proved that the same asymptotic behavior of the control parameter guarantees convergence for both the Schrödinger dynamics and the stochastic dynamics in spite of the essential difference of these two types of dynamics. Also described are the prescriptions to reduce errors in the final approximate solution obtained after a long but finite dynamical evolution of quantum annealing. It is shown there that we can reduce errors significantly by an ingenious choice of annealing schedule (time dependence of the control parameter) without compromising computational complexity qualitatively. A review is given on the derivation of the convergence condition for classical simulated annealing from the view point of quantum adiabaticity using a classical-quantum mapping. © 2008 American Institute of Physics.

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I. INTRODUCTION

An optimization problem is a problem to minimize or maximize a real single-valued function of multivariables called the cost function.^{1,2} If the problem is to maximize the cost function f , it suffices to minimize f . It thus does not lose generality to consider minimization only. In the present paper we consider combinatorial optimization, in which variables take discrete values. Well-known examples are satisfiability problems, exact cover, maximum cut, Hamilton graph, and traveling salesman problem. In physics, the search of the ground state of spin systems is a typical example, in particular, systems with quenched randomness such as spin glasses.

Optimization problems are classified roughly into two types, easy and hard ones. Loosely speaking, easy problems are those for which we have algorithms to solve in steps (=time) polynomial in the system size (polynomial complexity). In contrast, for hard problems, all known algorithms take exponentially many steps to reach the exact solution (exponential complexity). For these latter problems it is virtually impossible to find the exact solution if the problem size exceeds a moderate value. Most of the interesting cases as exemplified above belong to the latter hard class.

It is therefore important practically to devise algorithms which give approximate but accurate solutions efficiently, i.e., with polynomial complexity. Many instances of combinatorial optimization problems have such approximate algorithm. For example, the Lin–Kernighan algorithm is often used to solve the traveling salesman problem within a reasonable time.³

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In the present paper we will instead discuss generic algorithms, simulated annealing (SA) and quantum annealing (QA). The former was developed from the analogy between optimization problems and statistical physics.^{4,5} In SA, the cost function to be minimized is identified with the energy of a statistical-mechanical system. The system is then given a temperature, an artificially introduced control parameter, which, by reducing slowly from a high value to zero, we hope to drive the system to the state with the lowest value of the energy (cost function), reaching the solution of the optimization problem. The idea is that the system is expected to stay close to thermal equilibrium during time evolution if the rate of decrease in temperature is sufficiently slow, and is thus led in the end to the zero-temperature equilibrium state, the lowest-energy state. In practical applications SA is immensely popular due to its general applicability, reasonable performance, and relatively easy implementation in most cases. SA is usually used as a method to obtain an approximate solution within a finite computation time since it needs an infinitely long time to reach the exact solution by keeping the system close to thermal equilibrium.

Let us now turn our attention to QA (see Refs. 6–11).¹ In SA, we make use of thermal (classical) fluctuations to let the system hop from state to state over intermediate energy barriers to search for the desired lowest-energy state. Why then not try quantum-mechanical fluctuations (quantum tunneling) for state transitions if such may lead to better performance? In QA we introduce artificial degrees of freedom of quantum nature, noncommutative operators, which induce quantum fluctuations. We then ingeniously control the strength of these quantum fluctuations so that the system finally reaches the ground state, just like SA in which we slowly reduce the temperature. More precisely, the strength of quantum fluctuations is first set to a very large value for the system to search for the global structure of the phase space, corresponding to the high-temperature situation in SA. Then the strength is gradually decreased to finally vanish to recover the original system hopefully in the lowest-energy state. Quantum tunneling between different classical states replaces thermal hopping in SA. The physical idea behind such a procedure is to keep the system close to the instantaneous ground state of the quantum system, analogously to the quasiequilibrium state to be kept during the time evolution of SA. Similarly to SA, QA is a generic algorithm applicable, in principle, to any combinatorial optimization problem and is used as a method to reach an approximate solution within a given finite amount of time.

The reader may wonder why one should invent yet another generic algorithm when we already have the powerful SA. A short answer is that QA outperforms SA in most cases, at least theoretically. Analytical and numerical results indicate that the computation time needed to achieve a given precision of the answer is shorter in QA than in SA. Also, the magnitude of error is smaller for QA than for SA if we run the algorithm for a fixed finite amount of time. We shall show some theoretical bases for these conclusions in this paper. Numerical evidence is found in Refs. 9–11 and 14–22.

A drawback of QA is that a full practical implementation should rely on the quantum computer because we need to solve the time-dependent Schrödinger equation with a very large scale. Existing numerical studies have been carried out either for small prototype examples or for large problems by Monte Carlo simulations using the quantum-classical mapping by adding an extra [Trotter or imaginary-time (IT)] dimension.^{23–25} The latter mapping involves approximations, which inevitably introduces additional errors as well as the overhead caused by the extra dimension. Nevertheless, it is worthwhile to clarify the usefulness and limitations of QA as a theoretical step toward a new paradigm of computation. This aspect is shared by quantum computation in general whose practical significance will be fully exploited on the quantum computer.

The idea of QA is essentially the same as quantum adiabatic evolution (QAE), which is now actively investigated as an alternative paradigm of quantum computation.²⁶ It has been proved that QAE is equivalent to the conventional circuit model of quantum computation,²⁷ but QAE is sometimes considered more useful than the circuit model for several reasons including robustness

¹The term quantum annealing first appeared in Refs. 12 and 13 in which the authors used quantum transitions for state search and the dynamical evolution of control parameters were set by hand as an algorithm. QA in the present sense using natural Schrödinger dynamics was proposed later independently in Refs. 6 and 7.

against external disturbance. In the literature of quantum computation, one is often interested in the computational complexity of the QAE-based algorithm for a given specific problem under a fixed value of acceptable error. QAE can also be used to find the final *quantum* state when the problem is not a classical optimization.

In some contrast to these situations on QAE, studies of QA are often focused not on computational complexity but on the theoretical convergence conditions for infinite-time evolution and on the amount of errors in the final state within a fixed evolution time. Such a difference may have led some researchers to think that QA and QAE are to be distinguished from each other. We would emphasize that they are essentially the same and worth investigations by various communities of researchers.

The structure of the present paper is as follows. Section II discusses the convergence condition of QA, in particular, the rate of decrease in the control parameter representing quantum fluctuations. It will be shown there that a qualitatively faster decrease in the control parameter is allowed in QA than in SA to reach the solution. This is one of the explicit statements of the claim more vaguely stated above that QA outperforms SA. In Sec. III we review the performance analysis of SA using quantum-mechanical tools. The well-known convergence condition for SA will be re-derived from the perspective of quantum adiabaticity. The methods and results in this section help us strengthen the interrelation between QA, SA, and QAE. The error rate of QA after a finite-time dynamical evolution is analyzed in Sec. IV. There we explain how to reduce the final residual error after evolution of a given amount of time. This point of view is unique in the sense that most references of QAE study the time needed to reach a given amount of tolerable error, i.e., computational complexity. The results given in this section can be used to qualitatively reduce residual errors for a given algorithm without compromising computational complexity. Convergence conditions for stochastic implementation of QA are discussed in Sec. V. The results are surprising in that the rate of decrease in the control parameter for the system to reach the solution coincides with that found in Sec. II for the pure quantum-mechanical Schrödinger dynamics. The stochastic (and therefore classical) dynamics shares the same convergence conditions as fully quantum dynamics. Summary and outlook are described in Sec. VI.

The main parts of this paper (Secs. II, IV, and V) are based on the Ph.D. thesis of Morita²⁸ as well as several original papers of the present and other authors as will be referred to appropriately. The present paper is not a comprehensive review of QA since an emphasis is given almost exclusively to the theoretical and mathematical aspects. There exists an extensive body of numerical studies and the reader is referred to Refs. 9–11 for reviews.

II. CONVERGENCE CONDITION OF QA: REAL-TIME SCHRÖDINGER EVOLUTION

The convergence condition of QA with the real-time (RT) Schrödinger dynamics is investigated in this section, following Ref. 29. We first review the proof of the adiabatic theorem³⁰ to be used to derive the convergence condition. Then introduced is the Ising model with a transverse field as a simple but versatile implementation of QA. The convergence condition is derived by solving the condition for adiabatic transition with respect to the strength of the transverse field.

A. Adiabatic theorem

Let us consider the general Hamiltonian which depends on time t only through the dimensionless time $s=t/\tau$,

$$H(t) = \tilde{H}\left(\frac{t}{\tau}\right) \equiv \tilde{H}(s). \quad (1)$$

The parameter τ is introduced to control the rate of change in the Hamiltonian. In natural quantum systems, the state vector $|\psi(t)\rangle$ follows the RT Schrödinger equation,

$$i \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle, \quad (2)$$

or, in terms of the dimensionless time,

$$i \frac{d}{ds} |\tilde{\psi}(s)\rangle = \tau \tilde{H}(s) |\tilde{\psi}(s)\rangle, \quad (3)$$

where we set $\hbar=1$. We assume that the initial state is chosen to be the ground state of the initial Hamiltonian $H(0)$ and that the ground state of $\tilde{H}(s)$ is not degenerate for $s \geq 0$. We show in Sec. III that the transverse-field Ising model (TFIM), to be used as $H(t)$ in most parts of this paper, has no degeneracy in the ground state (except possibly in the limit of $t \rightarrow \infty$). If τ is large, the Hamiltonian changes slowly and it is expected that the state vector keeps track of the instantaneous ground state. The adiabatic theorem provides the condition for adiabatic evolution. To see this, we derive the asymptotic form of the state vector with respect to the parameter τ .

Since we wish to estimate how close the state vector is to the ground state, it is natural to expand the state vector by the instantaneous eigenstates of $\tilde{H}(s)$. Before doing so, we derive useful formulas for the eigenstates. The k th instantaneous eigenstate of $\tilde{H}(s)$ with the eigenvalue $\varepsilon_k(s)$ is denoted as $|k(s)\rangle$,

$$\tilde{H}(s) |k(s)\rangle = \varepsilon_k(s) |k(s)\rangle. \quad (4)$$

We assume that $|0(s)\rangle$ is the ground state of $\tilde{H}(s)$ and that the eigenstates are orthonormal, $\langle j(s) | k(s) \rangle = \delta_{jk}$. From differentiation of (4) with respect to s , we obtain

$$\left\langle j(s) \left| \frac{d}{ds} \right| k(s) \right\rangle = \frac{-1}{\varepsilon_j(s) - \varepsilon_k(s)} \left\langle j(s) \left| \frac{d\tilde{H}(s)}{ds} \right| k(s) \right\rangle, \quad (5)$$

where $j \neq k$. In the case of $j=k$, the same calculation does not provide any meaningful result. We can, however, impose the following condition:

$$\left\langle k(s) \left| \frac{d}{ds} \right| k(s) \right\rangle = 0. \quad (6)$$

This condition is achievable by the time-dependent phase shift: If $|\tilde{k}(s)\rangle = e^{i\theta(s)} |k(s)\rangle$, we find

$$\left\langle \tilde{k}(s) \left| \frac{d}{ds} \right| \tilde{k}(s) \right\rangle = i \frac{d\theta}{ds} + \left\langle k(s) \left| \frac{d}{ds} \right| k(s) \right\rangle. \quad (7)$$

The second term on the right-hand side is purely imaginary because

$$\left[\left\langle k(s) \left| \frac{d}{ds} \right| k(s) \right\rangle \right]^* + \left\langle k(s) \left| \frac{d}{ds} \right| k(s) \right\rangle = \frac{d}{ds} \langle k(s) | k(s) \rangle = 0. \quad (8)$$

Thus, condition (6) can be satisfied by tuning the phase factor $\theta(s)$ even if the original eigenstate does not satisfy it.

Theorem 2.1: *If the instantaneous ground state of the Hamiltonian $\tilde{H}(s)$ is not degenerate for $s \geq 0$ and the initial state is the ground state at $s=0$, i.e., $|\tilde{\psi}(0)\rangle = |0(0)\rangle$, the state vector $|\tilde{\psi}(s)\rangle$ has the asymptotic form in the limit of large τ as*

$$|\tilde{\psi}(s)\rangle = \sum_j c_j(s) e^{-i\tau\phi_j(s)} |j(s)\rangle, \quad (9)$$

$$c_0(s) \approx 1 + \mathcal{O}(\tau^{-2}), \quad (10)$$

$$c_{j \neq 0}(s) \approx \frac{i}{\tau} [A_j(0) - e^{i\tau[\phi_j(s) - \phi_0(s)]} A_j(s)] + \mathcal{O}(\tau^{-2}), \quad (11)$$

where $\phi_j(s) \equiv \int_0^s ds' \varepsilon_j(s')$, $\Delta_j(s) \equiv \varepsilon_j(s) - \varepsilon_0(s)$, and

$$A_j(s) \equiv \frac{1}{\Delta_j(s)^2} \left\langle j(s) \left| \frac{d\tilde{H}(s)}{ds} \right| 0(s) \right\rangle. \quad (12)$$

Proof: Substitution of (9) into Schrödinger equation (3) yields the equation for the coefficient $c_j(s)$ as

$$\frac{dc_j}{ds} = \sum_{k \neq j} c_k(s) \frac{e^{i\tau[\phi_j(s) - \phi_k(s)]}}{\varepsilon_j(s) - \varepsilon_k(s)} \langle j(s) | \frac{d\tilde{H}(s)}{ds} | k(s) \rangle, \quad (13)$$

where we used (5) and (6). Integration of this equation yields

$$c_j(s) = c_j(0) + \sum_{k \neq j} \int_0^s d\tilde{s} c_k(\tilde{s}) \frac{e^{i\tau[\phi_j(\tilde{s}) - \phi_k(\tilde{s})]}}{\varepsilon_j(\tilde{s}) - \varepsilon_k(\tilde{s})} \langle j(\tilde{s}) | \frac{d\tilde{H}(\tilde{s})}{d\tilde{s}} | k(\tilde{s}) \rangle. \quad (14)$$

Since the initial state is chosen to be the ground state of $H(0)$, $c_0(0) = 1$ and $c_{j \neq 0}(0) = 0$. The second term on the right-hand side is of the order of τ^{-1} because its integrand rapidly oscillates for large τ . In fact, the integration by parts yields the τ^{-1} factor. Thus, $c_{j \neq 0}(0)$ is of order τ^{-1} at most. Hence only the $k=0$ term in the summation remains up to the order of τ^{-1} ,

$$c_{j \neq 0}(s) \approx \int_0^s d\tilde{s} \frac{e^{i\tau[\phi_j(\tilde{s}) - \phi_0(\tilde{s})]}}{\Delta_j(\tilde{s})} \langle j(\tilde{s}) | \frac{d\tilde{H}(\tilde{s})}{d\tilde{s}} | 0(\tilde{s}) \rangle + \mathcal{O}(\tau^{-2}), \quad (15)$$

and the integration by parts yields (11). \square

Remark: The condition for the adiabatic evolution is given by the smallness of the excitation probability. That is, the right-hand side of (11) should be much smaller than unity. This condition is consistent with the criterion of the validity of the above asymptotic expansion. It is represented by

$$\tau \gg |A_j(s)|. \quad (16)$$

Using the original time variable t , this adiabaticity condition is written as

$$\frac{1}{\Delta_j(t)^2} \left| \langle j(t) | \frac{dH(t)}{dt} | 0(t) \rangle \right| = \delta \ll 1. \quad (17)$$

This is the usual expression of the adiabaticity condition.

B. Convergence conditions of quantum annealing

In this section, we derive the condition which guarantees the convergence of QA. The problem is what annealing schedule (time dependence of the control parameter) would satisfy adiabaticity condition (17). We solve this problem on the basis of the idea of Somma *et al.*³¹ developed for the analysis of SA in terms of quantum adiabaticity as reviewed in Sec. III.

1. Transverse-field Ising model

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

$$H_{\text{Ising}} \equiv - \sum_{i=1}^N J_i \sigma_i^z - \sum_{ij} J_{ij} \sigma_i^z \sigma_j^z - \sum_{ijk} J_{ijk} \sigma_i^z \sigma_j^z \sigma_k^z - \cdots, \quad (18)$$

where the σ_i^α ($\alpha=x,y,z$) are the Pauli matrices, components of the spin $\frac{1}{2}$ operator at site i . The eigenvalue of σ_i^z is $+1$ or -1 , which corresponds the classical Ising spin. Most combinatorial optimization problems can be written in this form by, for example, mapping binary variables (0 and 1) to spin variables (± 1). Another important assumption is that Hamiltonian (18) is extensive, i.e., proportional to the number of spins N for large N .

To realize QA, a fictitious kinetic energy is introduced typically by the time-dependent transverse field

$$H_{\text{TF}}(t) \equiv - \Gamma(t) \sum_{i=1}^N \sigma_i^x, \quad (19)$$

which induces spin flips, quantum fluctuations, or quantum tunneling between the two states $\sigma_i^z = 1$ and $\sigma_i^z = -1$, thus allowing a quantum search of the phase space. Initially the strength of the transverse field $\Gamma(t)$ is chosen to be very large, and the total Hamiltonian

$$H(t) = H_{\text{Ising}} + H_{\text{TF}}(t) \quad (20)$$

is dominated by the second kinetic term. This corresponds to the high-temperature limit of SA. The coefficient $\Gamma(t)$ is then gradually and monotonically decreased toward 0, leaving eventually only the potential term H_{Ising} . Accordingly the state vector $|\psi(t)\rangle$, which follows the RT Schrödinger equation, is expected to evolve from the trivial initial ground state of transverse-field term (19) to the nontrivial ground state of (18), which is the solution of the optimization problem. An important issue is how slowly we should decrease $\Gamma(t)$ to keep the state vector arbitrarily close to the instantaneous ground state of total Hamiltonian (20). The following theorem provides a solution to this problem as a sufficient condition.

Theorem 2.2: *Adiabaticity (17) for TFIM (20) yields the time dependence of $\Gamma(t)$ as*

$$\Gamma(t) = a(\delta t + c)^{-1/(2N-1)} \quad (21)$$

for $t > t_0$ (for a given positive t_0) as a sufficient condition of convergence of QA. Here a and c are constants of $\mathcal{O}(N^0)$ and δ is a small parameter to control adiabaticity appearing in (17).

The following theorem proved by Hopf³² will be useful in proving this theorem. See Appendix A for the proof.

Theorem 2.3: *If all the elements of a square matrix M are strictly positive, $M_{ij} > 0$, its maximum eigenvalue λ_0 and any other eigenvalues λ satisfy*

$$|\lambda| \leq \frac{\kappa - 1}{\kappa + 1} \lambda_0, \quad (22)$$

where κ is defined by

$$\kappa \equiv \max_{i,j,k} \frac{M_{ik}}{M_{jk}}. \quad (23)$$

Proof of Theorem 2.2: We show that power decay (21) satisfies adiabaticity condition (17) which guarantees convergence to the ground state of H_{Ising} as $t \rightarrow \infty$. For this purpose we estimate the energy gap and the time derivative of the Hamiltonian. As for the latter, it is straightforward to see

$$\left| \langle j(t) | \frac{dH(t)}{dt} | 0(t) \rangle \right| \leq -N \frac{d\Gamma(t)}{dt} \quad (24)$$

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

To estimate a lower bound for the energy gap, we apply Theorem 2.3 to the operator $M \equiv (E_+ - H(t))^N$. We assume that the constant E_+ satisfies $E_+ > E_{\text{max}} + \Gamma_0$, where $\Gamma_0 \equiv \Gamma(t_0)$ and E_{max} is the maximum eigenvalue of the potential term H_{Ising} . All the elements of the matrix M are strictly positive in the representation that diagonalizes $\{\sigma_i^z\}$ because $E_+ - H(t)$ is non-negative and irreducible, that is, any state can be reached from any other state within at most N steps.

For $t > t_0$, where $\Gamma(t) < \Gamma_0$, all the diagonal elements of $E_+ - H(t)$ are larger than any nonzero off-diagonal element $\Gamma(t)$. Thus, the minimum element of M , which is between two states having all the 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 $H_{\text{TF}}(t)$ by $-N\Gamma_0$ shows that the maximum matrix element of M has the upper bound $(E_+ - E_{\text{min}} + N\Gamma_0)^N$, where E_{min} is the lowest eigenvalue of H_{Ising} . Thus, we have

$$\kappa \leq \frac{(E_+ - E_{\text{min}} + N\Gamma_0)^N}{N! \Gamma(t)^N}. \quad (25)$$

If we denote the eigenvalue of $H(t)$ by $\varepsilon_j(t)$, (22) is rewritten as

$$[E_+ - \varepsilon_j(t)]^N \leq \frac{\kappa - 1}{\kappa + 1} [E_+ - \varepsilon_0(t)]^N. \quad (26)$$

Substitution of (25) into the above inequality yields

$$\Delta_j(t) \geq \frac{2[E_+ - \varepsilon_0(t)]N!}{N(E_+ - E_{\text{min}} + N\Gamma_0)^N} \Gamma(t)^N \equiv A \Gamma(t)^N, \quad (27)$$

where we used $1 - ((\kappa - 1)/(\kappa + 1))^{1/N} \geq 2/N(\kappa + 1)$ for $\kappa \geq 1$ and $N \geq 1$. The coefficient A is estimated using the Stirling formula as

$$A \approx \frac{2\sqrt{2\pi N}[E_+ - \varepsilon_0^{\text{max}}]}{Ne^N} \left(\frac{N}{E_+ - E_{\text{min}} + N\Gamma_0} \right)^N, \quad (28)$$

where $\varepsilon_0^{\text{max}}$ is $\max_{t > t_0} \{\varepsilon_0(t)\}$. This expression implies that A is exponentially small for large N .

Now, by combination of estimates (24) and (27), we find that the sufficient condition for convergence for $t > t_0$ is

$$-\frac{N}{A^2 \Gamma(t)^{2N}} \frac{d\Gamma(t)}{dt} = \delta \ll 1, \quad (29)$$

where δ is an arbitrarily small constant. By integrating this differential equation, we obtain (21). \square

Remark: The asymptotic power decay of the transverse field guarantees that the excitation probability is bounded by the arbitrarily small constant δ^2 at each instant. This annealing schedule is not valid when $\Gamma(t)$ is not sufficiently small because we evaluated the energy gap for $\Gamma(t) < \Gamma_0$ ($t > t_0$). If we take the limit $t_0 \rightarrow 0$, Γ_0 increases indefinitely and the coefficient a in (21) diverges. Then result (21) does not make sense. This is the reason why a finite positive time t_0 should be introduced in the statement of Theorem 2.2.

2. Transverse ferromagnetic interactions

The same discussions as above apply to QA using the transverse ferromagnetic interactions in addition to a transverse field,

$$H_{\text{TI}}(t) \equiv -\Gamma_{\text{TI}}(t) \left(\sum_{i=1}^N \sigma_i^x + \sum_{ij} \sigma_i^x \sigma_j^x \right). \quad (30)$$

The second summation runs over appropriate pairs of sites that satisfy extensiveness of the Hamiltonian. A recent numerical study shows the effectiveness of this type of quantum kinetic energy.¹⁸ The additional transverse interaction widens the instantaneous energy gap between the ground state and the first excited state. Thus, it is expected that an annealing schedule faster than (21) satisfies the adiabaticity condition. The following theorem supports this expectation.

Theorem 2.4: *The adiabaticity for the quantum system $H_{\text{Ising}} + H_{\text{TI}}(t)$ yields the time dependence of $\Gamma(t)$ for $t > t_0$ as*

$$\Gamma_{\text{TI}}(t) \propto t^{-1/(N-1)}. \quad (31)$$

Proof: The transverse interaction introduces nonzero off-diagonal elements to the Hamiltonian in the representation that diagonalizes σ_i^z . Consequently, any state can be reached from any other state within $N/2$ steps at most. Thus, the strictly positive operator is modified to $(E_+ - H_{\text{Ising}} - H_{\text{TI}}(t))^{N/2}$, which leads to the lower bound for the energy gap as a quantity proportional to $\Gamma_{\text{TI}}(t)^{N/2}$. The rest of the proof is the same as that of Theorem 2.2. \square

The above result implies that additional nonzero off-diagonal elements of the Hamiltonian accelerate the convergence of QA. It is thus interesting to consider the many-body transverse interaction of the form

$$H_{\text{MTI}}(t) = -\Gamma_{\text{MTI}}(t) \prod_{i=1}^N (1 + \sigma_i^x). \quad (32)$$

All the elements of H_{MTI} are equal to $-\Gamma_{\text{MTI}}(t)$ in the representation that diagonalizes σ_i^z . In this system, the following theorem holds.

Theorem 2.5: *The adiabaticity for the quantum system $H_{\text{Ising}} + H_{\text{MTI}}(t)$ yields the time dependence of $\Gamma(t)$ for $t > t_0$ as*

$$\Gamma_{\text{MTI}}(t) \propto \frac{2^{N-2}}{\delta t}. \quad (33)$$

Proof: We define the strictly positive operator as $M = E_+ - H_{\text{Ising}} - H_{\text{MTI}}(t)$. The maximum and minimum matrix elements of M are $E_+ - E_{\min} + \Gamma_{\text{MTI}}(t)$ and $\Gamma_{\text{MTI}}(t)$, respectively. Thus we have

$$\kappa = \frac{E_+ - E_{\min} + \Gamma_{\text{MTI}}(t)}{\Gamma_{\text{MTI}}(t)}, \quad (34)$$

$$\frac{\kappa - 1}{\kappa + 1} = \frac{E_+ - E_{\min}}{E_+ - E_{\min} + 2\Gamma_{\text{MTI}}(t)} \geq 1 - \frac{2\Gamma_{\text{MTI}}(t)}{E_+ - E_{\min}}, \quad (35)$$

The inequality for strictly positive operator (22) yields

$$\Delta_j(t) \geq \frac{2\Gamma_{\text{MTI}}(t)(E_+ - \varepsilon_0^{\max})}{E_+ - E_{\min}} \equiv \tilde{A}\Gamma_{\text{MTI}}(t), \quad (36)$$

where \tilde{A} is $\mathcal{O}(N^0)$. Since the matrix element of the derivative of the Hamiltonian is bounded as

$$\left| \langle j(t) | \frac{dH(t)}{dt} | 0(t) \rangle \right| \leq -2^N \frac{d\Gamma_{\text{MTI}}}{dt}, \quad (37)$$

we find that the sufficient condition for convergence with the many-body transverse interaction is

$$-\frac{2^N}{\tilde{A}^2 \Gamma_{\text{MTI}}(t)^2} \frac{d\Gamma_{\text{MTI}}}{dt} = \delta \ll 1. \quad (38)$$

Integrating this differential equation yields annealing schedule (33). \square

3. Computational complexity

The asymptotic power-law annealing schedules guarantee the adiabatic evolution during the annealing process. The power-law dependence on t is much faster than the log-inverse law for the control parameter in SA, $T(t) = pN / \log(\alpha t + 1)$, to be discussed in Sec. III, first proved by Geman and Geman.³³ However, it does not mean that QA provides an algorithm to solve NP (non-deterministic polynomial) problems in polynomial time. In the case with the transverse field only, the time for $\Gamma(t)$ to reach a sufficiently small value ϵ (which implies that the system is sufficiently close to the final ground state of H_{Ising} whence H_{TF} is a small perturbation) is estimated from (21) as

$$t_{\text{TF}} \approx \frac{1}{\delta} \left(\frac{1}{\epsilon} \right)^{2N-1}. \quad (39)$$

This relation clearly shows that the QA needs a time exponential in N to converge.

For QA with many-body transverse interactions, the exponent of t in annealing schedule (33) does not depend on the system size N . Nevertheless, it also does not mean that QA provides a polynomial-time algorithm because of the factor 2^N . The characteristic time for Γ_{MTI} to reach a sufficiently small value ϵ is estimated as

$$t_{\text{MTI}} \approx \frac{2^{N-2}}{\delta \epsilon}, \quad (40)$$

which again shows exponential dependence on N .

These exponential computational complexities do not come as a surprise because Theorems 2.2, 2.4, and 2.5 all apply to any optimization problem written in generic form (18), which includes the worst cases of most difficult problems. Similar arguments apply to SA.³⁴

Another remark is on the comparison of $\Gamma(t) (\propto t^{-1/(2N-1)})$ in QA with $T(t) (\propto N / \log(\alpha t + 1))$ in SA to conclude that the former schedule is faster than the latter. The transverse-field coefficient Γ in a quantum system plays the same role qualitatively and quantitatively as the temperature T does in a corresponding classical system at least in the Hopfield model in a transverse field.³⁵ When the phase diagram is written in terms of Γ and α (the number of embedded patterns divided by the number of neurons) for the ground state of the model, the result has precisely the same structure as the T - α phase diagram of the finite-temperature version of the Hopfield model without a transverse field. This example serves as a justification of the direct comparison of Γ and T at least as long as the theoretical analyses of QA and SA are concerned.

III. CONVERGENCE CONDITION OF SA AND QUANTUM ADIABATICITY

We next study the convergence condition of SA to be compared with QA. This problem was originally solved by Geman and Geman³³ using the theory of the inhomogeneous Markov chain as described in the quantum Monte Carlo context in Sec. V. It is quite surprising that their result is reproduced using the quantum adiabaticity condition applied after a classical-quantum mapping.³¹ This approach is reviewed in this section, following Ref. 31, to clarify the correspondence between the quasiequilibrium condition for SA in a classical system and the adiabaticity condition in the corresponding quantum system. The analysis will also reveal an aspect related to the equivalence of QA and QAE.

A. Classical-quantum mapping

The starting point is an expression of a classical thermal expectation value in terms of a quantum ground-state expectation value. A well-known mapping between quantum and classical systems is to rewrite the former in terms of the latter with an extra IT (or Trotter) dimension.²⁴ The mapping discussed in the present section is a different one, which allows us to express the thermal expectation value of a classical system in terms of the ground-state expectation value of a corresponding quantum system *without* an extra dimension.

Suppose that the classical Hamiltonian, whose value we want to minimize, is written as an Ising spin system as in (18):

$$H = - \sum_{i=1}^N J_i \sigma_i^z - \sum_{ij} J_{ij} \sigma_i^z \sigma_j^z - \sum_{ijk} J_{ijk} \sigma_i^z \sigma_j^z \sigma_k^z - \cdots . \quad (41)$$

The thermal expectation value of a classical physical quantity $Q(\{\sigma_i^z\})$ is

$$\langle Q \rangle_T = \frac{1}{Z(T)} \sum_{\{\sigma\}} e^{-\beta H} Q(\{\sigma_i\}), \quad (42)$$

where the sum runs over all configurations of Ising spins, i.e., over the values taken by the z components of the Pauli matrices, $\sigma_i^z = \sigma_i(\pm 1)$ ($\forall i$). The symbol $\{\sigma_i\}$ stands for the set $\{\sigma_1, \sigma_2, \dots, \sigma_N\}$.

An important element is the following theorem.

Theorem 3.1: *Thermal expectation value (42) is equal to the expectation value of Q by the quantum wave function*

$$|\psi(T)\rangle = e^{-\beta H/2} \sum_{\{\sigma\}} |\{\sigma_i\}\rangle, \quad (43)$$

where $|\{\sigma_i\}\rangle$ is the basis state diagonalizing each σ_i^z as σ_i . The sum runs over all such possible assignments.

Assume $T > 0$. Wave function (43) is the ground state of the quantum Hamiltonian

$$H_q(T) = -\chi \sum_j H_q^j(T) \equiv -\chi \sum_j (\sigma_x^j - e^{\beta H_j}), \quad (44)$$

where H_j is the sum of the terms of Hamiltonian (41) involving site j ,

$$H_j = -J_j \sigma_j^z - \sum_k J_{jk} \sigma_j^z \sigma_k^z - \sum_{kl} J_{jkl} \sigma_j^z \sigma_k^z \sigma_l^z - \cdots . \quad (45)$$

The coefficient χ is defined by $\chi = e^{-\beta p}$ with $p = \max_j |H_j|$.

Proof: The first half is trivial:

$$\frac{\langle \psi(T) | Q | \psi(T) \rangle}{\langle \psi(T) | \psi(T) \rangle} = \frac{1}{Z(T)} \sum_{\{\sigma\}} e^{-\beta H} \langle \{\sigma_i\} | Q | \{\sigma_i\} \rangle = \langle Q \rangle_T. \quad (46)$$

To show the second half, we first note that

$$\sigma_x^j \sum_{\{\sigma\}} |\{\sigma_i\}\rangle = \sum_{\{\sigma\}} |\{\sigma_i\}\rangle \quad (47)$$

since the operator σ_x^j just changes the order of the above summation. It is also easy to see that

$$\sigma_x^j e^{-\beta H/2} = e^{\beta H_j} e^{-\beta H/2} \sigma_x^j \quad (48)$$

because

$$\sigma_x^j e^{-\beta H/2} \sigma_x^j = e^{-\beta(H-H_j)/2} \sigma_x^j e^{-\beta H_j/2} \sigma_x^j = e^{-\beta(H-H_j)/2} e^{\beta H_j/2} = e^{\beta H_j} e^{-\beta H/2} \quad (49)$$

as both H and H_j are diagonal in the present representation and $H-H_j$ does not include σ_j^z , so $[H-H_j, \sigma_j^x]=0$. We therefore have

$$H_q^j(T) |\psi(T)\rangle = (\sigma_x^j - e^{\beta H_j}) e^{-\beta H/2} \sum_{\{\sigma\}} |\{\sigma_i\}\rangle = 0. \quad (50)$$

Thus $|\psi(T)\rangle$ is an eigenstate of $H_q(T)$ with eigenvalue 0. In the present representation, the nonvanishing off-diagonal elements of $-H_q(T)$ are all positive and the coefficients of $|\psi(T)\rangle$ are also all positive as one sees in (43). Then $|\psi(T)\rangle$ is the unique ground state of $H_q(T)$ according to the Perron–Frobenius theorem.³⁶ \square

A few remarks are in order. In the high-temperature limit, the quantum Hamiltonian is composed just of the transverse-field term,

$$H_q(T \rightarrow \infty) = - \sum_j (\sigma_x^j - 1). \quad (51)$$

Correspondingly the ground-state wave function $|\psi(T \rightarrow \infty)\rangle$ is the simple summation over all possible states with equal weight. In this way the thermal fluctuations in the original classical system are mapped to the quantum fluctuations. The low-temperature limit has, in contrast, the purely classical Hamiltonian

$$H_q(T \approx 0) \rightarrow \chi \sum_j e^{\beta H_j} \quad (52)$$

and the ground state of $H_q(T \approx 0)$ is also the ground state of H as is apparent from definition (43). Hence the decrease in thermal fluctuations in SA is mapped to the decrease in quantum fluctuations. As explained below, this correspondence allows us to analyze the condition for quasiequilibrium in the classical SA using the adiabaticity condition for the quantum system.

B. Adiabaticity and convergence condition of SA

The adiabaticity condition applied to the quantum system introduced above leads to the condition of convergence of SA. Suppose that we monotonically decrease the temperature as a function of time, $T(t)$, to realize SA.

Theorem 3.2: *The adiabaticity condition for the quantum system of $H_q(T)$ yields the time dependence of $T(t)$ as*

$$T(t) = \frac{pN}{\log(\alpha t + 1)} \quad (53)$$

in the limit of large N . The coefficient α is exponentially small in N .

A few lemmas will be useful to prove this theorem.

Lemma 3.3: *The energy gap $\Delta(T)$ of $H_q(T)$ between the ground state and the first excited state is bounded below as*

$$\Delta(T) \geq a \sqrt{N} e^{-(\beta p + c)N}, \quad (54)$$

where a and c are N -independent positive constants in the asymptotic limit of large N .

Proof: The analysis of Sec. II B 1 applies with the replacement of $\Gamma(t)$ by $\chi = e^{-\beta p}$ and $\varepsilon_0(t) = 0$. This latter condition comes from $H_q(T) |\psi(T)\rangle = 0$. The condition $\Gamma(t) < \Gamma_0(t > t_0)$ is unnecessary here because the off-diagonal element χ can always be chosen smaller than the diagonal elements by adding a positive constant to the diagonal. Equation (27) gives

$$\Delta_j(t) \geq A e^{-\beta p N} \quad (55)$$

and A satisfies, according to (28),

$$A \approx b\sqrt{2\pi N}e^{-cN}, \quad (56)$$

with b and c positive constants of $\mathcal{O}(N^0)$. \square

Lemma 3.4: *The matrix element of the derivative of $H_q(T)$, relevant to the adiabaticity condition, satisfies*

$$\langle \psi_1(T) | \partial_T H_q(T) | \psi(T) \rangle = - \frac{\Delta(T) \langle \psi_1(T) | H | \psi(T) \rangle}{2k_B T^2}, \quad (57)$$

where $\psi_1(T)$ is the normalized first excited state of $H_q(T)$.

Proof: By differentiating the identity

$$H_q(T) | \psi(T) \rangle = 0, \quad (58)$$

we find

$$\left(\frac{\partial}{\partial T} H_q(T) \right) | \psi(T) \rangle = - H_q(T) \frac{\partial}{\partial T} | \psi(T) \rangle = H_q(T) \left(- \frac{1}{2k_B T^2} H \right) | \psi(T) \rangle. \quad (59)$$

This relation immediately proves the lemma if we notice that the ground-state energy of $H_q(T)$ is zero and therefore $H_q(T) | \psi_1(T) \rangle = \Delta(T) | \psi_1(T) \rangle$. \square

Lemma 3.5: *The matrix element of H satisfies*

$$|\langle \psi_1(T) | H | \psi(T) \rangle| \leq pN\sqrt{Z(T)}. \quad (60)$$

Proof: There are N terms in $H = \sum_j H_j$, each of which is of norm of at most p . The factor $\sqrt{Z(T)}$ appears from normalization of $|\psi(T)\rangle$. \square

Proof of Theorem 3.2: The condition of adiabaticity for the quantum system $H_q(T)$ reads

$$\frac{1}{\Delta(T)^2 \sqrt{Z(T)}} \left| \langle \psi_1(T) | \partial_T H_q(T) | \psi(T) \rangle \frac{dT}{dt} \right| = \delta, \quad (61)$$

with sufficiently small δ . If we rewrite the matrix element by Lemma 3.4, the left-hand side is

$$\frac{|\langle \psi_1(T) | H | \psi(T) \rangle|}{2k_B T^2 \Delta(T) \sqrt{Z(T)}} \left| \frac{dT}{dt} \right|. \quad (62)$$

By replacing the numerator by its bound in Lemma 3.5 we have

$$\frac{pN}{2k_B T^2 \Delta(T)} \left| \frac{dT}{dt} \right| = \tilde{\delta} \ll 1 \quad (63)$$

as a sufficient condition for adiabaticity. Using the bound of Lemma 3.3 and integrating the above differential equation for $T(t)$ noticing $dT/dt < 0$, we reach the statement of Theorem 3.2. \square

C. Remarks

Equation (53) reproduces the Geman–Geman condition for convergence of SA.³³ Their method of proof is to use the theory of the classical inhomogeneous (i.e., time-dependent) Markov chain representing nonequilibrium processes. It may thus be naively expected that the classical system under consideration may not stay close to equilibrium during the process of SA since the temperature always changes. It therefore comes as a surprise that the adiabaticity condition, which is equivalent to the quasiequilibrium condition according to Theorem 3.1, leads to Theorem 3.2. The rate of temperature change in this latter theorem is slow enough to guarantee the quasiequilibrium condition even when the temperature keeps changing.

Also, Theorem 3.2 is quite general, covering the worst cases, as it applies to any system written as the Ising model of (41). This fact means that one may apply a faster rate of temperature decrease to solve a given specific problem with small errors. The same comment applies to the QA situation in Sec. II.

Another remark is on the relation of QA and QAE. Mathematical analyses of QA often focus their attention to the generic convergence conditions in the infinite-time limit as seen in Secs. II and V as well as in an earlier paper,⁷ although the residual energy after finite-time evolution has also been extensively investigated mainly in numerical studies. This aspect may have led some researchers to think that QA is different from QAE since the studies using the latter mostly concern the computational complexity of finite-time evolution for a given specific optimization problem using adiabaticity to construct an algorithm of QAE. As has been shown in the present and the previous sections, the adiabaticity condition also leads to the convergence condition in the infinite-time limit for QA and SA. In this sense QA, QAE, and even SA share essentially the same mathematical background.

IV. REDUCTION IN ERRORS FOR FINITE-TIME EVOLUTION

In Sec. II, we discussed the convergence condition of QA implemented for the TFIM. The power decrease in the transverse field guarantees the adiabatic evolution. This annealing schedule, however, does not provide practically useful algorithms because an infinitely long time is necessary to reach the exact solution. An approximate algorithm for finite annealing time τ should be used in practice. Since such a finite-time algorithm does not satisfy the generic convergence condition, the answer includes a certain amount of errors. An important question is how the error depends on the annealing time τ .

Suzuki and Okada¹⁶ showed that the error after adiabatic evolution for time τ is generally proportional to τ^{-2} in the limit of large τ with the system size N kept finite. In this section, we analyze their results in detail and propose new annealing schedules which show smaller errors proportional to τ^{-2m} ($m > 1$).³⁷ This method allows us to reduce errors by orders of magnitude without compromising the computational complexity apart from a possibly moderate numerical factor.

A. Upper bound for excitation probability

Let us consider general time-dependent Hamiltonian (1). The goal of this section is to evaluate the excitation probability (closely related with the error probability) at the final time $s=1$ under adiabaticity condition (16).

This task is easy because we have already obtained the asymptotic form of excitation amplitude (11). The upper bound for the excitation probability is derived as

$$|\langle j(1)|\tilde{\psi}(1)\rangle|^2 = |c_{j \neq 0}(1)|^2 \lesssim \frac{1}{\tau^2} [|A_j(0)| + |A_j(1)|]^2 + \mathcal{O}(\tau^{-3}). \quad (64)$$

This formula indicates that the coefficient of the τ^{-2} term is determined only by the state of the system at $s=0$ and 1 and vanishes if $A_j(s)$ is zero at $s=0$ and 1.

When the τ^{-2} term vanishes, a similar calculation yields the next order term of the excitation probability. If $\tilde{H}'(0)=\tilde{H}'(1)=0$, the excitation amplitude $c_{j \neq 0}(1)$ is at most of order τ^{-2} and then $c_0(1) \approx 1 + \mathcal{O}(\tau^{-3})$. Therefore we have

$$c_{j \neq 0}(1) \approx \int_0^1 ds \frac{e^{i\tau[\phi_j(s)-\phi_0(s)]}}{\Delta_j(s)} \langle j(s) | \frac{d\tilde{H}(s)}{ds} | 0(s) \rangle + \mathcal{O}(\tau^{-3}) \approx \frac{1}{\tau^2} [A_j^{(2)}(0) - e^{i\tau[\phi_j(s)-\phi_0(s)]} A_j^{(2)}(1)] + \mathcal{O}(\tau^{-3}), \quad (65)$$

where we defined

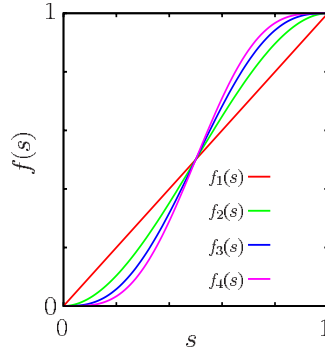


FIG. 1. (Color online) Examples of annealing schedules with reduced errors listed in (70)–(73).

$$A_j^{(m)}(s) \equiv \frac{1}{\Delta_j(s)^{m+1}} \langle j(s) | \frac{d^m \tilde{H}(s)}{ds^m} | 0(s) \rangle. \quad (66)$$

To derive the second line of (65), we used integration by parts twice and (5) and (6). The other τ^{-2} terms vanish because of the assumption $\tilde{H}'(0) = \tilde{H}'(1) = 0$. Thus the upper bound of the next order for the excitation probability under this assumption is obtained as

$$|\langle j(1) | \tilde{\psi}(1) \rangle|^2 \lesssim \frac{1}{\tau^4} [|A_j^{(2)}(0)| + |A_j^{(2)}(1)|]^2 + \mathcal{O}(\tau^{-5}). \quad (67)$$

It is easy to see that the τ^{-4} term also vanishes when $\tilde{H}''(0) = \tilde{H}''(1) = 0$. It is straightforward to generalize these results to prove the following theorem.

Theorem 4.1: *If the k th derivative of $\tilde{H}(s)$ is equal to zero at $s=0$ and 1 for all $k = 1, 2, \dots, m-1$, the excitation probability has the upper bound*

$$|\langle j(1) | \tilde{\psi}(1) \rangle|^2 \lesssim \frac{1}{\tau^{2m}} [|A_j^{(m)}(0)| + |A_j^{(m)}(1)|]^2 + \mathcal{O}(\tau^{-2m-1}). \quad (68)$$

B. Annealing schedules with reduced errors

Although we have so far considered the general time-dependent Hamiltonian, the ordinary Hamiltonian for QA with finite annealing time is composed of the potential term and the kinetic energy term,

$$\tilde{H}(s) = f(s)H_{\text{pot}} + [1 - f(s)]H_{\text{kin}}, \quad (69)$$

where H_{pot} and H_{kin} generalize H_{Ising} and H_{TF} in Sec. II, respectively. The function $f(s)$, representing the annealing schedule, satisfies $f(0) = 0$ and $f(1) = 1$. Thus $\tilde{H}(0) = H_{\text{kin}}$ and $\tilde{H}(1) = H_{\text{pot}}$. The ground state of H_{pot} corresponds to the solution of the optimization problem. The kinetic energy is chosen so that its ground state is trivial. The above Hamiltonian connects the trivial initial state and the nontrivial desired solution after evolution time τ .

The condition for the τ^{-2m} term to exist in the error is obtained straightforwardly from the results of Sec. V because Hamiltonian (69) depends on time only through the annealing schedule $f(s)$. It is sufficient that the k th derivative of $f(s)$ is zero at $s=0$ and 1 for $k=1, 2, \dots, m-1$. We note that $f(s)$ should belong to C^m , that is, $f(s)$ is an m th differentiable function whose m th derivative is continuous.

Examples of the annealing schedules $f_m(s)$ with the τ^{-2m} error rate are the following polynomials (Fig. 1):

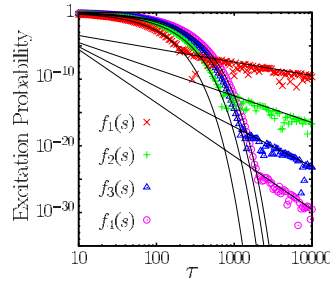


FIG. 2. (Color online) The annealing-time dependence of the excitation probability for two-level system (74) using schedules (70)–(73). The curved and straight lines show (75) and (76) for each annealing schedule, respectively. The parameters in (74) are chosen to be $h=2$ and $\alpha=0.2$.

$$f_1(s) = s, \quad (70)$$

$$f_2(s) = s^2(3 - 2s), \quad (71)$$

$$f_3(s) = s^3(10 - 15s + 6s^2), \quad (72)$$

$$f_4(s) = s^4(35 - 84s + 70s^2 - 20s^3). \quad (73)$$

The linear annealing schedule $f_1(s)$, which shows the τ^{-2} error, has been used in the past studies. Although we here list only polynomials symmetrical with respect to the point $s=1/2$, this is not essential. For example, $f(s)=(1-\cos(\pi s^2))/2$ also has the τ^{-4} error rate because $f'(0)=f'(1)=f''(0)=0$ but $f''(1)=-2\pi^2$.

C. Numerical results

1. Two-level system

To confirm the upper bound for the excitation probability discussed above, it is instructive to study the two-level system, the Landau–Zener problem, with the Hamiltonian

$$H_{\text{LZ}}(t) = - \left[\frac{1}{2} - f\left(\frac{t}{\tau}\right) \right] h\sigma^z - \alpha\sigma^x. \quad (74)$$

The energy gap of $H_{\text{LZ}}(t)$ has the minimum 2α at $f(s)=1/2$. If the annealing time τ is not large enough to satisfy (16), nonadiabatic transitions occur. The Landau–Zener theorem^{38,39} provides the excitation probability $P_{\text{ex}}(\tau) = |\langle 1(1) | \tilde{\psi}(1) \rangle|^2$ as

$$P_{\text{ex}}(\tau) = \exp \left[- \frac{\pi\alpha^2\tau}{f'(s^*)h} \right], \quad (75)$$

where s^* denotes the solution of $f(s^*)=1/2$. On the other hand, if τ is sufficiently large, the system evolves adiabatically. Then the excitation probability has upper bound (68), which is estimated as

$$P_{\text{ex}}(\tau) \leq \frac{4h^2\alpha^2}{\tau^2m(h^2 + 4\alpha^2)^{m+2}} \left[\left| \frac{d^m f}{ds^m}(0) \right| + \left| \frac{d^m f}{ds^m}(1) \right| \right]^2. \quad (76)$$

We numerically solved Schrödinger equation (2) for system (74) with the Runge–Kutta method.⁴⁰ Figure 2 shows the result for the excitation probability with annealing schedules (70)–(73). The initial state is the ground state of $H_{\text{LZ}}(0)$. The parameters are chosen to be $h=2$ and $\alpha=0.2$. The curved and straight lines show (75) and (76), respectively. In the small and large τ regions, the excitation probability perfectly fits to those two expressions.

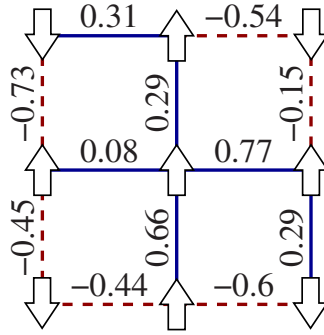


FIG. 3. (Color online) Configuration of random interactions $\{J_{ij}\}$ on the 3×3 square lattice which we investigated and spin configuration of the target state. The solid and dashed lines indicate ferromagnetic and antiferromagnetic interactions, respectively.

2. Spin-glass model

We next carried out simulations of a rather large system, the Ising spin system with random interactions. The quantum fluctuations are introduced by the uniform transverse field. Thus, the potential and kinetic energy terms are defined by

$$H_{\text{pot}} = - \sum_{\langle ij \rangle} J_{ij} \sigma_i^z \sigma_j^z - h \sum_{i=1}^N \sigma_i^z, \quad (77)$$

$$H_{\text{kin}} = - \Gamma \sum_{i=1}^N \sigma_i^x. \quad (78)$$

The initial state, namely, the ground state of H_{kin} , is the all-up state along the x axis.

The difference between the obtained approximate energy and the true ground-state energy (exact solution) is the residual energy E_{res} . It is a useful measure of the error rate of QA. It has the same behavior as the excitation probability because it is rewritten as

$$E_{\text{res}} \equiv \langle \tilde{\psi}(1) | H_{\text{pot}} | \tilde{\psi}(1) \rangle - \varepsilon_0(1) \quad (79)$$

$$= \sum_{j>0} \Delta_j(1) |\langle j(1) | \tilde{\psi}(1) \rangle|^2. \quad (80)$$

Therefore E_{res} is expected to be asymptotically proportional to τ^{-2m} using the improved annealing schedules.

We investigated the two-dimensional square lattice of size 3×3 . The quenched random coupling constants $\{J_{ij}\}$ are chosen from the uniform distribution between -1 and $+1$, as shown in Fig. 3. The parameters are $h=0.1$ and $\Gamma=1$. Figure 4 shows the τ dependence of the residual energy using annealing schedules (70)–(73). Straight lines representing τ^{-2m} ($m=1,2,3,4$) are also shown for comparison. The data clearly indicate the τ^{-2m} law for large τ . The irregular behavior around $E_{\text{res}} \approx 10^{-25}$ comes from numerical rounding errors.

3. Database search problem

As another example, we apply the improved annealing schedule to the database search problem of an item in an unsorted database. Consider N items, among which one is marked. The goal of this problem is to find the marked item in a minimum time. The pioneering quantum algorithm proposed by Grover⁴¹ solves this task in time of order \sqrt{N} , whereas the classical algorithm tests $N/2$ items on average. Farhi *et al.*²⁶ proposed a QAE algorithm and Roland and Cerf⁴² found a

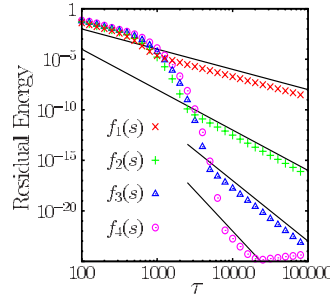


FIG. 4. (Color online) The annealing-time dependence of the residual energy for the two-dimensional spin-glass model with improved annealing schedules. The solid lines denote functions proportional to τ^{-2m} ($m=1,2,3,4$). The parameter values are $h=0.1$ and $\Gamma=1$.

QAE-based algorithm with the same computational complexity as Grover's algorithm. Although their schedule is optimal in the sense that the excitation probability by the adiabatic transition is equal to a small constant at each time, it has the τ^{-2} error rate. We show that annealing schedules with the τ^{-2m} error rate can be constructed by a slight modification in their optimal schedule.

Let us consider the Hilbert space which has the basis states $|i\rangle$ ($i=1,2,\dots,N$), and the marked state is denoted by $|m\rangle$. Suppose that we can construct Hamiltonian (69) with two terms,

$$H_{\text{pot}} = 1 - |m\rangle\langle m|, \quad (81)$$

$$H_{\text{kin}} = 1 - \frac{1}{N} \sum_{i=1}^N \sum_{j=1}^N |i\rangle\langle j|. \quad (82)$$

The Hamiltonian H_{pot} can be applied without the explicit knowledge of $|m\rangle$, the same assumption as in Grover's algorithm. The initial state is a superposition of all basis states,

$$|\psi(0)\rangle = \frac{1}{\sqrt{N}} \sum_{i=1}^N |i\rangle, \quad (83)$$

which does not depend on the marked state. The energy gap between the ground state and the first excited state,

$$\Delta_1(s) = \sqrt{1 - 4 \frac{N-1}{N} f(s)[1-f(s)]}, \quad (84)$$

has a minimum at $f(s)=1/2$. The highest eigenvalue $\varepsilon_2(s)=1$ is $(N-2)$ -fold degenerate.

To derive the optimal annealing schedule, we briefly review the results reported by Roland and Cerf.⁴² When the energy gap is small [i.e., for $f(s) \approx 1/2$], nonadiabatic transitions are likely to occur. Thus we need to change the Hamiltonian carefully. On the other hand, when the energy gap is not very small, too slow a change wastes time. Thus the speed in parameter change should be adjusted adaptively to the instantaneous energy gap. This is realized by tuning the annealing schedule to satisfy adiabaticity condition (16) in each infinitesimal time interval, that is,

$$\frac{|A_1(s)|}{\tau} = \delta, \quad (85)$$

where δ is a small constant. In the database search problem, this condition is rewritten as

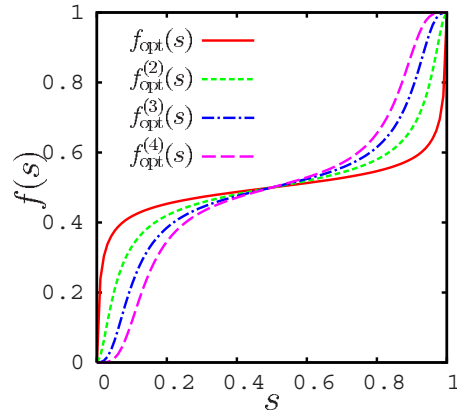


FIG. 5. (Color online) The optimal annealing schedules for the database search problem ($N=64$). The solid line denotes original optimal schedule (87) and the dashed lines are for the modified schedules.

$$\frac{\sqrt{N-1}}{\tau N \Delta_1(s)^3} \frac{df}{ds} = \delta. \quad (86)$$

After integration under boundary conditions $f(0)=0$ and $f(1)=1$, we obtain

$$f_{\text{opt}}(s) = \frac{1}{2} + \frac{2s-1}{2\sqrt{N-(N-1)(2s-1)^2}}. \quad (87)$$

As plotted by a solid line in Fig. 5, this function changes most slowly when the energy gap takes the minimum value. It is noted that the annealing time is determined by the small constant δ as

$$\tau = \frac{\sqrt{N-1}}{\delta}, \quad (88)$$

which means that the computation time is of order \sqrt{N} , similarly to Grover's algorithm.

Optimal annealing schedule (87) shows the τ^{-2} error rate because its derivative is nonvanishing at $s=0$ and 1. It is easy to see from (87) that the simple replacement of s with $f_m(s)$ fulfills the condition for the τ^{-2m} error rate. We carried out numerical simulations for $N=64$ with such annealing schedules, $f_{\text{opt}}^{(m)}(s) \equiv f_{\text{opt}}(f_m(s))$, as plotted by dashed lines in Fig. 5. As shown in Fig. 6, the residual energy with $f_{\text{opt}}^{(m)}(s)$ is proportional to τ^{-2m} . The characteristic time τ_c for the τ^{-2m} error

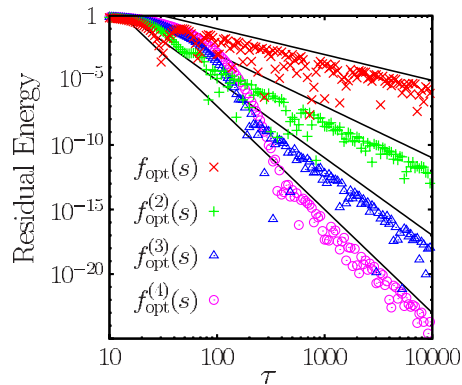


FIG. 6. (Color online) The annealing-time dependence of the residual energy for the database search problem ($N=64$) with the optimal annealing schedules described in Fig. 5. The solid lines represent functions proportional to τ^{-2m} ($m=1, 2, 3, 4$).

rate to show up increases with m : Since the modified optimal schedule $f_{\text{opt}}^{(m)}(s)$ has a steeper slope at $s=1/2$ than $f_{\text{opt}}(s)$, a longer annealing time is necessary to satisfy adiabaticity condition (86). Nevertheless, the difference in slopes of $f_{\text{opt}}^{(m)}(s)$ is only a factor of $\mathcal{O}(1)$, and therefore τ_c is still scaled as \sqrt{N} . Significant qualitative reduction in errors has been achieved without compromising computational complexity apart from a numerical factor.

D. Imaginary-time Schrödinger dynamics

So far, we have concentrated on QA following the RT Schrödinger dynamics. From the point of view of physics, it is natural that the time evolution of a quantum system obeys the RT Schrödinger equation. Since our goal is to find the solution of optimization problems, however, we need not stick to physical reality. We therefore investigate QA following the IT Schrödinger dynamics here to further reduce errors.

The IT evolution tends to filter out the excited states. Thus, it is expected that QA with the IT dynamics can find the optimal solution more efficiently than RT-QA. Stella *et al.*²⁰ investigated numerically the performance of IT-QA and conjectured that (i) the IT error rate is not larger than in the RT and that (ii) the asymptotic behavior of the error rate for $\tau \rightarrow \infty$ is identical for IT-QA and RT-QA. We prove their conjectures through the IT version of the adiabatic theorem.

1. Imaginary-time Schrödinger equation

The IT Schrödinger equation is obtained by the transformation $t \rightarrow -it$ in the time derivative of the original RT Schrödinger equation:

$$-\frac{d}{dt}|\Psi(t)\rangle = H(t)|\Psi(t)\rangle. \quad (89)$$

The time dependence of the Hamiltonian does not change. If the Hamiltonian is time independent, we easily see that the excitation amplitude decreases exponentially relative to the ground state,

$$|\Psi(t)\rangle = \sum_j c_j e^{-it\epsilon_j}|j\rangle \rightarrow \sum_j c_j e^{-t\epsilon_j}|j\rangle = e^{-t\epsilon_0} \sum_j c_j e^{-t(\epsilon_j - \epsilon_0)}|j\rangle. \quad (90)$$

However, it is not obvious that this feature survives in the time-dependent situation.

An important aspect of the IT Schrödinger equation is nonunitarity. The norm of the wave function is not conserved. Thus, we consider the normalized state vector

$$|\psi(t)\rangle \equiv \frac{1}{\sqrt{\langle \Psi(t) | \Psi(t) \rangle}} |\Psi(t)\rangle. \quad (91)$$

The equation of motion for this normalized state vector is

$$-\frac{d}{dt}|\psi(t)\rangle = [H(t) - \langle H(t) \rangle]|\psi(t)\rangle, \quad (92)$$

where we defined the expectation value of the Hamiltonian,

$$\langle H(t) \rangle \equiv \langle \psi(t) | H(t) | \psi(t) \rangle. \quad (93)$$

The above equation is not linear but norm conserving, which makes the asymptotic expansion easy. In terms of the dimensionless time $s = t/\tau$, the norm-conserving IT Schrödinger equation is written as

$$-\frac{d}{ds}|\tilde{\psi}(s)\rangle = \tau[\tilde{H}(s) - \langle \tilde{H}(s) \rangle]|\tilde{\psi}(s)\rangle. \quad (94)$$

2. Asymptotic expansion of the excitation probability

To prove the conjecture by Stella *et al.*,²⁰ we derive the asymptotic expansion of the excitation probability. The following theorem provides us with the IT version of the adiabatic theorem.

Theorem 4.2: *Under the same hypothesis as in Theorem 2.1, the state vector following the norm-conserving IT Schrödinger equation (94) has the asymptotic form in the limit of large τ as*

$$|\tilde{\psi}(s)\rangle = \sum_j c_j(s) |j(s)\rangle, \quad (95)$$

$$c_0(s) \approx 1 + O(\tau^{-2}), \quad (96)$$

$$c_{j \neq 0}(s) \approx \frac{A_j(s)}{\tau} + O(\tau^{-2}). \quad (97)$$

Proof: Norm-conserving IT Schrödinger equation (94) is rewritten as the equation of motion for $c_j(s)$ as

$$\frac{dc_j}{ds} = \sum_{k \neq j} \frac{c_k(s)}{\varepsilon_j(s) - \varepsilon_k(s)} \langle j(s) | \frac{d\tilde{H}(s)}{ds} | k(s) \rangle - \tau c_j(s) \left[\varepsilon_j(s) - \sum_l \varepsilon_l(s) |c_l(s)|^2 \right]. \quad (98)$$

To remove the second term on the right-hand side, we define

$$\tilde{c}_j(s) \equiv \exp\left(\tau \int_0^s d\tilde{s} \left[\varepsilon_j(\tilde{s}) - \sum_l \varepsilon_l(\tilde{s}) |c_l(\tilde{s})|^2 \right]\right) c_j(s) \quad (99)$$

and obtain the equation of motion for $\tilde{c}_j(s)$ as

$$\frac{d\tilde{c}_j}{ds} = \sum_{k \neq j} \tilde{c}_k(s) \frac{e^{\tau(\phi_j(s) - \phi_k(s))}}{\varepsilon_j(s) - \varepsilon_k(s)} \langle j(s) | \frac{d\tilde{H}(s)}{ds} | k(s) \rangle, \quad (100)$$

where we defined $\phi_j(s) \equiv \int_0^s ds' \varepsilon_j(s')$ for convenience.

Integration of this equation yields the integral equation for $\tilde{c}_j(s)$. It is useful to introduce the following quantity:

$$\delta(s) \equiv \int_0^s d\tilde{s} \sum_{l \neq 0} [\varepsilon_l(\tilde{s}) - \varepsilon_0(\tilde{s})] |c_l(\tilde{s})|^2. \quad (101)$$

Since the norm of the wave function is conserved, $\sum_l |c_l(s)|^2 = 1$ and therefore

$$\sum_l \varepsilon_l(s) |c_l(s)|^2 = \varepsilon_0(s) + \sum_{l \neq 0} [\varepsilon_l(s) - \varepsilon_0(s)] |c_l(s)|^2. \quad (102)$$

Thus, the definition of $\tilde{c}_j(s)$ is written as

$$\tilde{c}_j(s) = e^{-\tau\delta(s)} e^{\tau[\phi_j(s) - \phi_0(s)]} c_j(s). \quad (103)$$

Finally we obtain the integral equation for $c_j(s)$:

$$c_0(s) = e^{\tau\delta(s)} + e^{\tau\delta(s)} \int_0^s d\tilde{s} e^{-\tau\delta(\tilde{s})} \sum_{l \neq 0} c_l(\tilde{s}) \frac{\langle 0(\tilde{s}) | \frac{d\tilde{H}}{ds} | l(\tilde{s}) \rangle}{\varepsilon_0(\tilde{s}) - \varepsilon_l(\tilde{s})}, \quad (104)$$

$$c_{j \neq 0}(s) = e^{\tau \delta(s)} e^{-\tau[\phi_j(s) - \phi_0(s)]} \int_0^s d\tilde{s} e^{-\tau \delta(\tilde{s})} e^{\tau[\phi_j(\tilde{s}) - \phi_0(\tilde{s})]} \sum_{k \neq j} c_k(\tilde{s}) \frac{\langle j(\tilde{s}) | \frac{d\tilde{H}}{d\tilde{s}} | k(\tilde{s}) \rangle}{\varepsilon_j(\tilde{s}) - \varepsilon_k(\tilde{s})}, \quad (105)$$

where we used the initial conditions $c_0(0)=1$ and $c_{j \neq 0}=0$.

The next step is the asymptotic expansion of these integral equations for large τ . It is expected that $c_0(s)=1$ and $c_{j \neq 0}(s)=0$ for $\tau \rightarrow \infty$ because of the following argument: Since coefficient $c_0(s)$ is less than unity, $\delta(s)$ should be $\mathcal{O}(\tau^{-1})$ at most and $e^{\tau \delta(s)} = \mathcal{O}(1)$. The second factor on the right-hand side of (105) is small exponentially with τ because $\phi_j(s) - \phi_0(s)$ is positive and an increasing function of s . Thus, $c_{j \neq 0}(s) \rightarrow 0$ and then $c_0(s) \rightarrow 1$ owing to the norm conservation law.

Therefore we estimate the next term of order τ^{-1} under the assumption that $c_0(s) \gg c_{j \neq 0}(s)$. Since $\delta(s)$ is proportional to the square of $c_{j \neq 0}(s)$, we have $e^{\tau \delta(s)} \approx 1$. Thus, the $e^{\pm \tau \delta(s)}$ factors can be ignored in the τ^{-1} term estimation of (105). Consequently, evaluation of the integral equations yields

$$c_{j \neq 0}(s) \approx e^{-\tau[\phi_j(s) - \phi_0(s)]} \int_0^s d\tilde{s} e^{\tau[\phi_j(\tilde{s}) - \phi_0(\tilde{s})]} \frac{\langle j(\tilde{s}) | \frac{d\tilde{H}}{d\tilde{s}} | 0(\tilde{s}) \rangle}{\Delta_j(\tilde{s})} + \mathcal{O}(\tau^{-2}). \quad (106)$$

The excitation amplitude is estimated by integration by parts as

$$c_{j \neq 0}(s) \approx \frac{1}{\tau} [A_j(s) - e^{-\tau(\phi_j(s) - \phi_0(s))} A_j(0)] + \mathcal{O}(\tau^{-2}), \quad (107)$$

where $A_j(s)$ is defined by (12). The second term in the square brackets is vanishingly small, which is a different point from the RT dynamics. From the above expression, we find $\delta(s) = \mathcal{O}(\tau^{-2})$, that is, $e^{\tau \delta(s)} \approx 1 + \mathcal{O}(\tau^{-1})$. Therefore, we obtain (96) and (97), which is consistent with the assumption $c_0(s) \gg c_{j \neq 0}(s)$. \square

Remark: The excitation probability at the end of a QA process is proportional to τ^{-2} in the large τ limit:

$$|\langle j(1) | \tilde{\psi}(1) \rangle|^2 \approx \frac{1}{\tau^2} |A_j(1)|^2 + \mathcal{O}(\tau^{-3}). \quad (108)$$

Its difference from the upper bound for RT dynamics (64) is only in the absence of $A_j(0)$. In the IT dynamics, this term decreases exponentially because of the factor $e^{-\tau(\phi_j(s) - \phi_0(s))}$. This result proves the conjecture proposed by Stella *et al.*,²⁰ that is,

$$\epsilon_{\text{IT}}(\tau) \leq \epsilon_{\text{RT}}(\tau), \quad (109)$$

$$\epsilon_{\text{IT}}(\tau) \approx \epsilon_{\text{RT}}(\tau) \quad (\tau \rightarrow \infty). \quad (110)$$

Strictly speaking, the right-hand sides in the above equations denote the upper bound for the error rate for RT-QA, not the error rate itself. In some systems, for example, the two-level system, the error rate oscillates because $A_j(0)$ and $A_j(1)$ may cancel in (11) and becomes smaller than that of IT-QA at some τ . However, QA for ordinary optimization problems has different energy levels at initial and final times, and thus such a cancellation seldom occurs.

3. Numerical verification

We demonstrate a numerical verification of the above results by simulations of the IT and RT Schrödinger equations. For this purpose, we consider the following annealing schedules (Fig. 7):

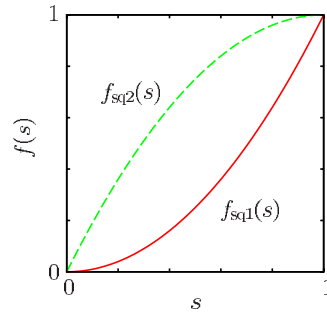


FIG. 7. (Color online) The annealing schedules defined in (111). $f_{sq1}(s)$ and $f_{sq2}(s)$ have a vanishing slope at the initial time $s=0$ and the final time $s=1$, respectively.

$$f_{sq1}(s) = s^2, \quad f_{sq2}(s) = s(2-s). \quad (111)$$

The former has a zero slope at the initial time $s=0$ and the latter at $s=1$. Thus, the $A_j(0)$ and $A_j(1)$ terms vanish with $f_{sq1}(s)$ and $f_{sq2}(s)$, respectively. Since the error rate for IT-QA depends only on $A_j(1)$, IT-QA with $f_{sq2}(s)$ should show the τ^{-4} error rate, while RT-QA with $f_{sq2}(s)$ exhibits the τ^{-2} law. On the other hand, RT-QA and IT-QA with $f_{sq1}(s)$ should have the same error rate for large τ . Figure 8 shows the residual energy with two annealing schedules for the spin-glass model presented in Sec. IV C 2, which explicitly supports our results.

V. CONVERGENCE CONDITION OF QA: QUANTUM MONTE CARLO EVOLUTION

So far, we have discussed QA with the Schrödinger dynamics. When we solve the Schrödinger equation on the classical computer, the computation time and memory increase exponentially with the system size. Therefore, some approximations are necessary to simulate QA processes for large-size problems. In most numerical studies, stochastic methods are used. In this section, we investigate two types of quantum Monte Carlo methods and prove their convergence theorems, following Ref. 43.

A. Inhomogeneous Markov chain

Since we prove the convergence of stochastic processes, it is useful to recall various definitions and theorems for inhomogeneous Markov processes.⁵ We denote the space of discrete states by \mathcal{S} and assume that the size of \mathcal{S} is finite. A Monte Carlo step is characterized by the *transition probability* from state $x (\in \mathcal{S})$ to state $y (\in \mathcal{S})$ at time step t :

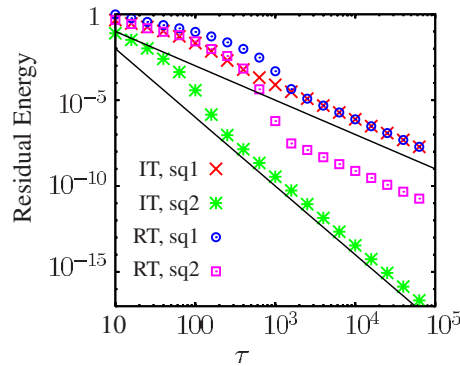


FIG. 8. (Color online) The annealing-time dependence of the residual energy for IT- and RT-QA with annealing schedules $f_{sq1}(s)$ and $f_{sq2}(s)$. The system is the spin-glass model presented in Sec. IV C 2. The solid lines stand for functions proportional to τ^{-2} and τ^{-4} . The parameters are $h=0.1$ and $\Gamma=1$.

$$G(y,x;t) = \begin{cases} P(y,x)A(y,x;t) & (x \neq y) \\ 1 - \sum_{z \in \mathcal{S}} P(z,x)A(z,x;t) & (x = y), \end{cases} \quad (112)$$

where $P(y,x)$ and $A(y,x;t)$ are called the *generation probability* and the *acceptance probability*, respectively. The former is the probability to generate the next candidate state y from the present state x . We assume that this probability does not depend on time and satisfies the following conditions:

$$\forall x, y \in \mathcal{S}: P(y,x) = P(x,y) \geq 0, \quad (113)$$

$$\forall x \in \mathcal{S}: P(x,x) = 0, \quad (114)$$

$$\forall x \in \mathcal{S}: \sum_{y \in \mathcal{S}} P(y,x) = 1, \quad (115)$$

$$\forall x, y \in \mathcal{S}, \quad \exists n > 0, \quad \exists z_1, \dots, z_{n-1} \in \mathcal{S}: \prod_{k=0}^{n-1} P(z_{k+1}, z_k) > 0, \quad z_0 = x, \quad z_n = y. \quad (116)$$

The last condition represents irreducibility of \mathcal{S} , that is, any state in \mathcal{S} can be reached from any other state in \mathcal{S} .

We define \mathcal{S}_x as the neighborhood of x , i.e., the set of states that can be reached by a single step from x :

$$\mathcal{S}_x = \{y | y \in \mathcal{S}, P(y,x) > 0\}. \quad (117)$$

The acceptance probability $A(y,x;t)$ is the probability to accept the candidate y generated from state x . The matrix $G(t)$, whose (y,x) component is given by (112), $[G(t)]_{y,x} = G(y,x;t)$, is called the *transition matrix*.

Let \mathcal{P} denote the set of probability distributions on \mathcal{S} . We regard a probability distribution p ($\in \mathcal{P}$) as the column vector with the component $[p]_x = p(x)$. The probability distribution at time t , started from an initial distribution p_0 ($\in \mathcal{P}$) at time t_0 , is written as

$$p(t, t_0) = G^{t-t_0} p_0 \equiv G(t-1)G(t-2) \cdots G(t_0) p_0. \quad (118)$$

A Markov chain is called *inhomogeneous* when the transition probability depends on time. In the following sections, we will prove that inhomogeneous Markov chains associated with QA are ergodic under appropriate conditions. There are two kinds of ergodicity, weak and strong. *Weak ergodicity* means that the probability distribution becomes independent of the initial conditions after a sufficiently long time:

$$\forall t_0 \geq 0: \lim_{t \rightarrow \infty} \sup \{ \|p(t, t_0) - p'(t, t_0)\| | p_0, p'_0 \in \mathcal{P} \} = 0, \quad (119)$$

where $p(t, t_0)$ and $p'(t, t_0)$ are the probability distributions with different initial distributions p_0 and p'_0 . The norm is defined by

$$\|p\| = \sum_{x \in \mathcal{S}} |p(x)|. \quad (120)$$

Strong ergodicity is the property that the probability distribution converges to a unique distribution irrespective of the initial state:

$$\exists r \in \mathcal{P}, \quad \forall t_0 \geq 0: \lim_{t \rightarrow \infty} \sup \{ \|p(t, t_0) - r\| | p_0 \in \mathcal{P} \} = 0. \quad (121)$$

The following two theorems provide conditions for weak and strong ergodicities of an inhomogeneous Markov chain.⁵ For proofs see Appendix B.

Theorem 5.1 (condition for weak ergodicity): *An inhomogeneous Markov chain is weakly ergodic if and only if there exists a strictly increasing sequence of positive numbers $\{t_i\}$, ($i = 0, 1, 2, \dots$), such that*

$$\sum_{i=0}^{\infty} [1 - \alpha(G^{t_{i+1}, t_i})] \rightarrow \infty, \quad (122)$$

where $\alpha(G^{t_{i+1}, t_i})$ is the coefficient of ergodicity defined by

$$\alpha(G^{t_{i+1}, t_i}) = 1 - \min \left\{ \sum_{z \in \mathcal{S}} \min\{G(z, x), G(z, y)\} \mid x, y \in \mathcal{S} \right\}, \quad (123)$$

with the notation $G(z, x) = [G^{t_{i+1}, t_i}]_{z, x}$.

The coefficient of ergodicity measures the variety of the transition probability. If $G(z, x)$ is independent of a state x , $\alpha(G)$ is equal to zero.

Theorem 5.2 (condition for strong ergodicity): *An inhomogeneous Markov chain is strongly ergodic if the following three conditions hold:*

- (1) *The Markov chain is weakly ergodic.*
- (2) *For all t there exists a stationary state $p_t \in \mathcal{P}$ such that $p_t = G(t)p_t$.*
- (3) *p_t satisfies*

$$\sum_{t=0}^{\infty} \|p_t - p_{t+1}\| < \infty. \quad (124)$$

Moreover, if $p = \lim_{t \rightarrow \infty} p_t$, then p is equal to the probability distribution r in (121).

We note that the existence of the limit is guaranteed by (124). This inequality implies that the probability distribution $p_t(x)$ is a Cauchy sequence:

$$\forall \varepsilon > 0, \quad \exists t_0 > 0, \quad \forall t, t' > t_0: |p_t(x) - p_{t'}(x)| < \varepsilon. \quad (125)$$

B. Path-integral Monte Carlo method

Let us first discuss convergence conditions for the implementation of QA by the path-integral Monte Carlo (PIMC) method.^{24,25} The basic idea of PIMC is to apply the Monte Carlo method to the classical system obtained from the original quantum system by the path-integral formula. We first consider the example of ground-state search of the Ising spin system whose quantum fluctuations are introduced by adding a transverse field. The total Hamiltonian is defined in (20). Although we only treat the two-body interaction for simplicity in this section, the existence of arbitrarily many-body interactions between the z components of the Pauli matrix and longitudinal random magnetic field $-\sum J_i \sigma_i^z$ in addition to the above Hamiltonian would not change the following argument.

In the path-integral method, the d -dimensional TFIM is mapped to a $(d+1)$ -dimensional classical Ising system so that the quantum system can be simulated on the classical computer. In numerical simulations, the Suzuki–Trotter formula^{23,24} is usually employed to express the partition function of the resulting classical system,

$$Z(t) \approx \sum_{\{\sigma_i^{(k)}\}} \exp\left(\frac{\beta}{M} \sum_{k=1}^M \sum_{\langle ij \rangle} J_{ij} \sigma_i^{(k)} \sigma_j^{(k)} + \gamma(t) \sum_{k=1}^M \sum_{i=0}^N \sigma_i^{(k)} \sigma_i^{(k+1)}\right), \quad (126)$$

where M is the length along the extra dimension (Trotter number) and $\sigma_i^{(k)}$ ($= \pm 1$) denotes a classical Ising spin at site i on the k th Trotter slice. The nearest-neighbor interaction between adjacent Trotter slices,

$$\gamma(t) = \frac{1}{2} \log\left(\coth \frac{\beta \Gamma(t)}{M}\right), \quad (127)$$

is ferromagnetic. Approximation (126) becomes exact in the limit $M \rightarrow \infty$ for a fixed $\beta = 1/k_B T$. The magnitude of interaction (127) increases with time t and tends to infinity as $t \rightarrow \infty$, reflecting the decrease in $\Gamma(t)$. We fix M and β to arbitrarily large values, which corresponds to the actual situation in numerical simulations. Therefore the theorem presented below does not directly guarantee the convergence of the system to the true ground state, which is realized only after taking the limits $M \rightarrow \infty$ and $\beta \rightarrow \infty$. We will rather show that the system converges to the thermal equilibrium represented by the right-hand side of (126), which can be chosen arbitrarily close to the true ground state by taking M and β large enough.

With the above example of TFIM in mind, it will be convenient to treat a more general expression than (126),

$$Z(t) = \sum_{x \in \mathcal{S}} \exp\left(-\frac{F_0(x)}{T_0} - \frac{F_1(x)}{T_1(t)}\right). \quad (128)$$

Here $F_0(x)$ is the cost function whose global minimum is the desired solution of the combinatorial optimization problem. The temperature T_0 is chosen to be sufficiently small. The term $F_1(x)$ derives from the kinetic energy, which is the transverse field in the TFIM. Quantum fluctuations are tuned by the extra temperature factor $T_1(t)$, which decreases with time. The first term $-F_0(x)/T_0$ corresponds to the interaction term in the exponent of (126), and the second term $-F_1(x)/T_1(t)$ generalizes the transverse-field term in (126).

For partition function (128), we define the acceptance probability of PIMC as

$$A(y, x; t) = g\left(\frac{q(y; t)}{q(x; t)}\right), \quad (129)$$

$$q(x; t) = \frac{1}{Z(t)} \exp\left(-\frac{F_0(x)}{T_0} - \frac{F_1(x)}{T_1(t)}\right). \quad (130)$$

This $q(x; t)$ is the equilibrium Boltzmann factor at a given fixed $T_1(t)$. Function $g(u)$ is the *acceptance function*, a monotone increasing function satisfying $0 \leq g(u) \leq 1$ and $g(1/u) = g(u)/u$ for $u \geq 0$. For instance, for the heat bath and the Metropolis methods, we have

$$g(u) = \frac{u}{1+u}, \quad (131)$$

$$g(u) = \min\{1, u\}, \quad (132)$$

respectively. The conditions mentioned above for $g(u)$ guarantee that $q(x; t)$ satisfies the detailed balance condition $G(y, x; t)q(x; t) = G(x, y; t)q(y; t)$. Thus, $q(x; t)$ is the stationary distribution of the homogeneous Markov chain defined by the transition matrix $G(t)$ with a fixed t . In other words, $q(x; t)$ is the right eigenvector of $G(t)$ with eigenvalue 1.

1. Convergence theorem for PIMC-QA

We first define a few quantities. The set of local maximum states of F_1 is written as \mathcal{S}_m ,

$$\mathcal{S}_m = \{x | x \in \mathcal{S}, \forall y \in \mathcal{S}_x, F_1(y) \leq F_1(x)\}. \quad (133)$$

We denote by $d(y, x)$ the minimum number of steps necessary to make a transition from x to y . Using this notation we define the minimum number of maximum steps needed to reach any other state from an arbitrary state in the set $\mathcal{S} \setminus \mathcal{S}_m$,

$$R = \min\{\max\{d(y, x) | y \in \mathcal{S}\} | x \in \mathcal{S} \setminus \mathcal{S}_m\}. \quad (134)$$

Also, L_0 and L_1 stand for the maximum changes in $F_0(x)$ and $F_1(x)$, respectively, in a single step,

$$L_0 = \max\{|F_0(x) - F_0(y)| | P(y, x) > 0, x, y \in \mathcal{S}\}, \quad (135)$$

$$L_1 = \max\{|F_1(x) - F_1(y)| | P(y, x) > 0, x, y \in \mathcal{S}\}. \quad (136)$$

Our main results are summarized in the following theorem and corollary.

Theorem 5.3 [strong ergodicity of system (128)]: *The inhomogeneous Markov chain generated by (129) and (130) is strongly ergodic and converges to the equilibrium state corresponding to the first term of the right-hand side of (130), $\exp(-F_0(x)/T_0)$, if*

$$T_1(t) \geq \frac{RL_1}{\log(t+2)}. \quad (137)$$

Application of this theorem to the PIMC implementation of QA represented by (126) immediately yields the following corollary.

Corollary 5.4 (strong ergodicity of QA-PIMC for TFIM): *The inhomogeneous Markov chain generated by the Boltzmann factor on the right-hand side of (126) is strongly ergodic and converges to the equilibrium state corresponding to the first term on the right-hand side of (126) if*

$$\Gamma(t) \geq \frac{M}{\beta} \tanh^{-1} \frac{1}{(t+2)^{2/RL_1}}. \quad (138)$$

Remark: For sufficiently large t , the above inequality reduces to

$$\Gamma(t) \geq \frac{M}{\beta} (t+2)^{-2/RL_1}. \quad (139)$$

This result implies that a power decay of the transverse field is sufficient to guarantee the convergence of QA of TFIM by the PIMC. Notice that RL_1 is of $\mathcal{O}(N)$. Thus (139) is qualitatively similar to (21).

To prove strong ergodicity it is necessary to prove weak ergodicity first. The following lemma is useful for this purpose.

Lemma 5.5 (lower bound on the transition probability): *The elements of the transition matrix defined by (112), (129), and (130) have the following lower bound:*

$$P(y, x) > 0 \Rightarrow \forall t > 0: G(y, x; t) \geq w g(1) \exp\left(-\frac{L_0}{T_0} - \frac{L_1}{T_1(t)}\right) \quad (140)$$

and

$$\exists t_1 > 0, \quad \forall x \in \mathcal{S} \setminus \mathcal{S}_m, \quad \forall t \geq t_1: G(x, x; t) \geq w g(1) \exp\left(-\frac{L_0}{T_0} - \frac{L_1}{T_1(t)}\right). \quad (141)$$

Here, w stands for the minimum nonvanishing value of $P(y, x)$,

$$w = \min\{P(y,x) | P(y,x) > 0, x, y \in \mathcal{S}\}. \quad (142)$$

Proof of Lemma 5.5: The first part of Lemma 5.5 is proved straightforwardly. Equation (140) follows directly from the definition of the transition probability and the property of the acceptance function g . When $q(y;t)/q(x;t) < 1$, we have

$$G(y,x;t) \geq wg \left(\frac{q(x;t)}{q(y;t)} \right) \frac{q(y;t)}{q(x;t)} \geq wg(1) \exp \left(-\frac{L_0}{T_0} - \frac{L_1}{T_1(t)} \right). \quad (143)$$

On the other hand, if $q(y;t)/q(x;t) \geq 1$,

$$G(y,x;t) \geq wg(1) \geq wg(1) \exp \left(-\frac{L_0}{T_0} - \frac{L_1}{T_1(t)} \right), \quad (144)$$

where we used the fact that both L_0 and L_1 are positive.

Next, we prove (141). Since x is not a member of \mathcal{S}_m , there exists a state $y \in \mathcal{S}_x$ such that $F_1(y) - F_1(x) > 0$. For such a state y ,

$$\lim_{t \rightarrow \infty} g \left(\exp \left(-\frac{F_0(y) - F_0(x)}{T_0} - \frac{F_1(y) - F_1(x)}{T_1(t)} \right) \right) = 0 \quad (145)$$

because $T_1(t)$ tends to zero as $t \rightarrow \infty$ and $0 \leq g(u) \leq u$. Thus, for all $\varepsilon > 0$, there exists $t_1 > 0$ such that

$$\forall t > t_1 : g \left(\exp \left(-\frac{F_0(y) - F_0(x)}{T_0} - \frac{F_1(y) - F_1(x)}{T_1(t)} \right) \right) < \varepsilon. \quad (146)$$

We therefore have

$$\begin{aligned} \sum_{z \in \mathcal{S}} P(z,x)A(z,x;t) &= P(y,x)A(y,x;t) + \sum_{z \in \mathcal{S} \setminus \{y\}} P(z,x)A(z,x;t) < P(y,x)\varepsilon + \sum_{z \in \mathcal{S} \setminus \{y\}} P(z,x) \\ &= 1 - (1 - \varepsilon)P(y,x), \end{aligned} \quad (147)$$

and consequently,

$$G(x,x;t) > (1 - \varepsilon)P(y,x) > 0. \quad (148)$$

Since the right-hand side of (141) can be arbitrarily small for sufficiently large t , we obtain the second part of Lemma 5.5. \square

Proof of weak ergodicity implied in Theorem 5.3: Let us introduce the following quantity:

$$x^* = \arg \min \{ \max \{ d(y,x) | y \in \mathcal{S} \} | x \in \mathcal{S} \setminus \mathcal{S}_m \}. \quad (149)$$

Comparison with the definition of R in (134) shows that the state x^* is reachable by at most R transitions from any state.

Now, consider the transition probability from an arbitrary state x to x^* . From the definitions of R and x^* , there exists at least one transition route within R steps:

$$x \equiv x_0 \neq x_1 \neq x_2 \neq \cdots \neq x_l = x_{l+1} = \cdots = x_R \equiv x^*.$$

Then Lemma 5.5 yields that, for sufficiently large t , the transition probability at each time step has the following lower bound:

$$G(x_{i+1}, x_i; t - R + i) \geq wg(1) \exp \left(-\frac{L_0}{T_0} - \frac{L_1}{T_1(t - R + i)} \right). \quad (150)$$

Thus, by taking the product of (150) from $i=0$ to $i=R-1$, we have

$$\begin{aligned}
 G^{t,t-R}(x^*,x) &\geq G(x^*,x_{R-1};t-1)G(x_{R-1},x_{R-2};t-2)\cdots G(x_1,x;t-R) \\
 &\geq \prod_{i=0}^{R-1} wg(1)\exp\left(-\frac{L_0}{T_0}-\frac{L_1}{T_1(t-R+i)}\right) \geq w^R g(1)^R \exp\left(-\frac{RL_0}{T_0}-\frac{RL_1}{T_1(t-1)}\right),
 \end{aligned}
 \tag{151}$$

where we have used monotonicity of $T_1(t)$. Consequently, it is possible to find an integer $k_0 \geq 0$ such that, for all $k > k_0$, the coefficient of ergodicity satisfies

$$1 - \alpha(G^{kR,kR-R}) \geq w^R g(1)^R \exp\left(-\frac{RL_0}{T_0}-\frac{RL_1}{T_1(kR-1)}\right), \tag{152}$$

where we eliminate the sum over z in (123) by replacing it with a single term for $z=x^*$. We now substitute annealing schedule (137). Then weak ergodicity is immediately proved from Theorem 5.1 because we obtain

$$\sum_{k=1}^{\infty} (1 - \alpha(G^{kR,kR-R})) \geq w^R g(1)^R \exp\left(-\frac{RL_0}{T_0}\right) \sum_{k=k_0}^{\infty} \frac{1}{kR+1} \rightarrow \infty. \tag{153}$$

□

Proof of Theorem 5.3: To prove strong ergodicity, we refer to Theorem 5.2. Condition (1) has already been proved. As has been mentioned, Boltzmann factor (130) satisfies $q(t)=G(t)q(t)$, which is condition (2). Thus the proof will be complete if we prove condition (3) by setting $p_t = q(t)$. For this purpose, we first prove that $q(x;t)$ is monotonic for large t :

$$\forall t \geq 0, \quad \forall x \in \mathcal{S}_1^{\min}: q(x;t+1) \geq q(x;t), \tag{154}$$

$$\exists t_1 > 0, \quad \forall t \geq t_1, \quad \forall x \in \mathcal{S} \setminus \mathcal{S}_1^{\min}: q(x;t+1) \leq q(x;t), \tag{155}$$

where \mathcal{S}_1^{\min} denotes the set of global minimum states of F_1 .

To prove this monotonicity, we use the following notations for simplicity:

$$A(x) = \exp\left(-\frac{F_0(x)}{T_0}\right), \quad B = \sum_{x \in \mathcal{S}_1^{\min}} A(x), \tag{156}$$

$$\Delta(x) = F_1(x) - F_1^{\min}. \tag{157}$$

If $x \in \mathcal{S}_1^{\min}$, the Boltzmann distribution can be rewritten as

$$q(x;t) = \frac{A(x)}{B + \sum_{y \in \mathcal{S} \setminus \mathcal{S}_1^{\min}} \exp\left(-\frac{\Delta(y)}{T_1(t)}\right)A(y)}. \tag{158}$$

Since $\Delta(y) > 0$ by definition, the denominator decreases with time. Thus, we obtain (154).

To prove (155), we consider the derivative of $q(x;t)$ with respect to $T_1(t)$,

$$\frac{\partial q(x;t)}{\partial T_1(t)} = \frac{A(x) \left[B\Delta(x) + \sum_{y \in \mathcal{S}_1^{\min}} (F_1(x) - F_1(y)) \exp\left(-\frac{\Delta(y)}{T_1(t)}\right) A(y) \right]}{T_1(t)^2 \exp\left(\frac{\Delta(x)}{T_1(t)}\right) \left[B + \sum_{y \in \mathcal{S}_1^{\min}} \exp\left(-\frac{\Delta(y)}{T_1(t)}\right) A(y) \right]^2}. \quad (159)$$

Only $F_1(x) - F_1(y)$ in the numerator has the possibility of being negative. However, the first term $B\Delta(x)$ is larger than the second one for sufficiently large t because $\exp(-\Delta(y)/T_1(t))$ tends to zero as $T_1(t) \rightarrow \infty$. Thus there exists $t_1 > 0$ such that $\partial q(x;t)/\partial T(t) > 0$ for all $t > t_1$. Since $T_1(t)$ is a decreasing function of t , we have (155).

Consequently, for all $t > t_1$, we have

$$\begin{aligned} \|q(t+1) - q(t)\| &= \sum_{x \in \mathcal{S}_1^{\min}} [q(x;t+1) - q(x;t)] - \sum_{x \notin \mathcal{S}_1^{\min}} [q(x;t+1) - q(x;t)] \\ &= 2 \sum_{x \in \mathcal{S}_1^{\min}} [q(x;t+1) - q(x;t)], \end{aligned} \quad (160)$$

where we used $\|q(t)\| = \sum_{x \in \mathcal{S}_1^{\min}} q(x;t) + \sum_{x \notin \mathcal{S}_1^{\min}} q(x;t) = 1$. We then obtain

$$\sum_{t=t_1}^{\infty} \|q(t+1) - q(t)\| = 2 \sum_{x \in \mathcal{S}_1^{\min}} [q(x;\infty) - q(x;t_1)] \leq 2\|q(x;\infty)\| = 2. \quad (161)$$

Therefore $q(t)$ satisfies condition (3):

$$\begin{aligned} \sum_{t=0}^{\infty} \|q(t+1) - q(t)\| &= \sum_{t=0}^{t_1-1} \|q(t+1) - q(t)\| + \sum_{t=t_1}^{\infty} \|q(t+1) - q(t)\| \leq \sum_{t=0}^{t_1-1} [\|q(t+1)\| + \|q(t)\|] + 2 \\ &= 2t_1 + 2 < \infty, \end{aligned} \quad (162)$$

which completes the proof of strong ergodicity.

2. Generalized transition probability

In Theorem 5.3, the acceptance probability is defined by the conventional Boltzmann form, (129) and (130). However, we have the freedom to choose any transition (acceptance) probability as long as it is useful to achieve our objective since our goal is not to find finite-temperature equilibrium states but to identify the optimal state. There have been attempts to accelerate the annealing schedule in SA by modifying the transition probability. In particular, Nishimori and Inoue³⁴ proved weak ergodicity of the inhomogeneous Markov chain for classical SA using the probability of Tsallis and Stariolo.⁴⁴ There the property of weak ergodicity was shown to hold under the annealing schedule of temperature inversely proportional to a power of time steps. This annealing rate is much faster than the log-inverse law for the conventional Boltzmann factor.

A similar generalization is possible for QA-PIMC by using the following modified acceptance probability:

$$A(y,x;t) = g(u(y,x;t)), \quad (163)$$

$$u(y,x;t) = e^{-[F_0(y)-F_0(x)]/T_0} \left[1 + (q-1) \frac{F_1(y) - F_1(x)}{T_1(t)} \right]^{1/(1-q)}, \quad (164)$$

where q is a real number. In the limit $q \rightarrow 1$, this acceptance probability reduces to the Boltzmann form. Similarly to the discussions leading to Theorem 5.3, we can prove that the inhomogeneous Markov chain with this acceptance probability is weakly ergodic if

$$T_1(t) \geq \frac{b}{(t+2)^c}, \quad 0 < c \leq \frac{q-1}{R}, \quad (165)$$

where b is a positive constant. We have to restrict ourselves to the case $q > 1$ for a technical reason as was the case previously.³⁴ We do not reproduce the proof here because it is quite straightforward to generalize the discussions for Theorem 5.3 in combination with the argument of Ref. 34. Result (165) applied to the TFIM is that, if the annealing schedule asymptotically satisfies

$$\Gamma(t) \geq \frac{M}{\beta} \exp\left(-\frac{2(t+2)^c}{b}\right), \quad (166)$$

the inhomogeneous Markov chain is weakly ergodic. Notice that this annealing schedule is faster than the power law of (139). We have been unable to prove strong ergodicity because we could not identify the stationary distribution for a fixed $T_1(t)$ in the present case.

3. Continuous systems

In the above analyses we treated systems with discrete degrees of freedom. Theorem 5.3 does not apply directly to a continuous system. Nevertheless, by discretization of the continuous space we obtain the following result.

Let us consider a system of N distinguishable particles in a continuous space of finite volume with the Hamiltonian

$$H = \frac{1}{2m(t)} \sum_{i=1}^N p_i^2 + V(\{r_i\}). \quad (167)$$

The mass $m(t)$ controls the magnitude of quantum fluctuations. The goal is to find the minimum of the potential term, which is achieved by a gradual increase in $m(t)$ to infinity according to the prescription of QA. After discretization of the continuous space (which is necessary anyway in any computer simulation with finite precision) and an application of the Suzuki–Trotter formula, the equilibrium partition function acquires the following expression in the representation to diagonalize spatial coordinates:

$$Z(t) \approx \text{Tr} \exp\left(-\frac{\beta}{M} \sum_{k=1}^M V(\{r_i^{(k)}\}) - \frac{Mm(t)}{2\beta} \sum_{i=1}^N \sum_{k=1}^M |r_i^{(k+1)} - r_i^{(k)}|^2\right), \quad (168)$$

with the unit $\hbar=1$. Theorem 5.3 is applicable to this system under the identification of $T_1(t)$ with $m(t)^{-1}$. We therefore conclude that a logarithmic increase in the mass suffices to guarantee strong ergodicity of the potential-minimization problem under spatial discretization.

The coefficient corresponding to the numerator of the right-hand side of (137) is estimated as

$$RL_1 \approx M^2NL^2/\beta, \quad (169)$$

where L denotes the maximum value of $|r_i^{(k+1)} - r_i^{(k)}|$. To obtain this coefficient, let us consider two extremes. One is that any state is reachable at one step. By definition, $R=1$ and $L_1 \approx M^2NL^2/\beta$, which yields (169). The other case is that only one particle can move to the nearest-neighbor point at one time step. With a ($\ll L$) denoting the lattice spacing, we have

$$L_1 \approx \frac{M}{2\beta} [L^2 - (L-a)^2] \approx \frac{MLa}{\beta}. \quad (170)$$

Since the number of steps to reach any configuration is estimated as $R \approx NML/a$, we again obtain (169).

C. Green's function Monte Carlo method

The PIMC simulates only the equilibrium behavior at finite temperature because its starting point is the equilibrium partition function. Moreover, it follows an artificial time evolution of Monte Carlo dynamics, not the natural Schrödinger dynamics. An alternative approach to improve these points is Green's function Monte Carlo (GFMC) method.^{25,45-47} The basic idea is to solve the IT Schrödinger equation by stochastic processes. In the present section we derive sufficient conditions for strong ergodicity in GFMC.

The evolution of states by the IT Schrödinger equation starting from an initial state $|\psi_0\rangle$ is expressed as

$$|\psi(t)\rangle = T \exp\left(-\int_0^t dt' H(t')\right) |\psi_0\rangle, \quad (171)$$

where T is the time-ordering operator. The right-hand side can be decomposed into a product of small-time evolutions,

$$|\psi(t)\rangle = \lim_{n \rightarrow \infty} \hat{G}_0(t_{n-1}) \hat{G}_0(t_{n-2}) \cdots \hat{G}_0(t_1) \hat{G}_0(t_0) |\psi_0\rangle, \quad (172)$$

where $t_k = k\Delta t$, $\Delta t = t/n$, and $\hat{G}_0(t) = 1 - \Delta t H(t)$. In the GFMC, one approximates the right-hand side of this equation by a product with large but finite n and replaces $\hat{G}_0(t)$ with $\hat{G}_1(t) = 1 - \Delta t(H(t) - E_T)$, where E_T is called the reference energy to be taken approximately close to the final ground-state energy. This subtraction of the reference energy simply adjusts the standard of energy and changes nothing physically. However, practically, this term is important to keep the matrix elements positive and to accelerate convergence to the ground state as will be explained shortly.

To realize the process of (172) by a stochastic method, we rewrite this equation in a recursive form,

$$\psi_{k+1}(y) = \sum_x \hat{G}_1(y, x; t_k) \psi_k(x), \quad (173)$$

where $\psi_k(x) = \langle x | \psi_k \rangle$ and $|x\rangle$ denotes a basis state. The matrix element of Green's function is given by

$$\hat{G}_1(y, x; t) = \langle y | 1 - \Delta t [H(t) - E_T] | x \rangle. \quad (174)$$

Equation (173) looks similar to a Markov process but is significantly different in several ways. An important difference is that Green's function is not normalized, $\sum_y \hat{G}_1(y, x; t) \neq 1$. In order to avoid this problem, one decomposes Green's function into a normalized probability G_1 and a weight w :

$$\hat{G}_1(y, x; t) = G_1(y, x; t) w(x; t), \quad (175)$$

where

$$G_1(y, x; t) \equiv \frac{\hat{G}_1(y, x; t)}{\sum_y \hat{G}_1(y, x; t)}, \quad w(x; t) \equiv \frac{\hat{G}_1(y, x; t)}{G_1(y, x; t)}. \quad (176)$$

Thus, using (173), the wave function at time t is written as

$$\begin{aligned} \psi_n(y) = & \sum_{\{x_k\}} \delta_{y, x_n} w(x_{n-1}; t_{n-1}) w(x_{n-2}; t_{n-2}) \cdots w(x_0; t_0) G_1(x_n, x_{n-1}; t_{n-1}) G_1(x_{n-1}, x_{n-2}; t_{n-2}) \\ & \cdots G_1(x_1, x_0; t_0) \psi_0(x_0). \end{aligned} \quad (177)$$

The algorithm of GFMC is based on this formula and is defined by a weighted random walk in the following sense. One first prepares an arbitrary initial wave function $\psi_0(x_0)$, all elements of which are non-negative. A random walker is generated, which sits initially ($t=t_0$) at the position x_0 with a probability proportional to $\psi_0(x_0)$. Then the walker moves to a new position x_1 following the transition probability $G_1(x_1, x_0; t_0)$. Thus this probability should be chosen non-negative by choosing parameters appropriately as described later. Simultaneously, the weight of this walker is updated by the rule $W_1 = w(x_0; t_0)W_0$ with $W_0=1$. This stochastic process is repeated to $t=t_{n-1}$. One actually prepares M independent walkers and let those walkers follow the above process. Then, according to (177), the wave function $\psi_n(y)$ is approximated by the distribution of walkers at the final step weighted by W_n ,

$$\psi_n(y) = \lim_{M \rightarrow \infty} \frac{1}{M} \sum_{i=1}^M W_n^{(i)} \delta_{y, x_n^{(i)}}, \quad (178)$$

where i is the index of a walker.

As noted above, $G_1(y, x; t)$ should be non-negative, which is achieved by choosing sufficiently small Δt (i.e., sufficiently large n) and selecting E_T within the instantaneous spectrum of the Hamiltonian $H(t)$. In particular, when E_T is close to the instantaneous ground-state energy of $H(t)$ for large t (i.e., the final target energy), $\hat{G}_1(x, x; t)$ is close to unity whereas other matrix components of $\hat{G}_1(t)$ are small. Thus, by choosing E_T this way, one can accelerate convergence of GFMC to the optimal state in the last steps of the process.

If we apply this general framework to the TFIM with the σ^z -diagonal basis, the matrix elements of Green's function are immediately calculated as

$$\hat{G}_1(y, x; t) = \begin{cases} 1 - \Delta t[E_0(x) - E_T] & (x = y) \\ \Delta t\Gamma(t) & (x \text{ and } y \text{ differ by a single-spin flip}) \\ 0 & (\text{otherwise}), \end{cases} \quad (179)$$

where $E_0(x) = \langle x | (-\sum_{ij} J_{ij} \sigma_i^z \sigma_j^z) | x \rangle$. One should choose Δt and E_T such that $1 - \Delta t(E_0(x) - E_T) \geq 0$ for all x . Since $w(x, t) = \sum_y \hat{G}_1(y, x; t)$, the weight is given by

$$w(x; t) = 1 - \Delta t[E_0(x) - E_T] + N\Delta t\Gamma(t). \quad (180)$$

One can decompose this transition probability into the generation probability and the acceptance probability as in (112):

$$P(y, x) = \begin{cases} \frac{1}{N} & (\text{single-spin flip}) \\ 0 & (\text{otherwise}), \end{cases} \quad (181)$$

$$A(y, x; t) = \frac{N\Delta t\Gamma(t)}{1 - \Delta t[E_0(x) - E_T] + N\Delta t\Gamma(t)}. \quad (182)$$

We shall analyze the convergence properties of stochastic processes under these probabilities for TFIM.

1. Convergence theorem for GFMC-QA

Similarly to the QA by PIMC, it is necessary to reduce the strength of quantum fluctuations slowly enough in order to find the ground state in the GFMC. The following theorem provides a sufficient condition in this regard.

Theorem 5.6 (strong ergodicity of QA-GFMC): *The inhomogeneous Markov process of the random walker for the QA-GFMC of TFIM, (112), (181), and (182), is strongly ergodic if*

$$\Gamma(t) \geq \frac{b}{(t+1)^c}, \quad 0 < c \leq \frac{1}{N}. \quad (183)$$

The lower bound of the transition probability given in the following lemma will be used in the proof of Theorem 5.6.

Lemma 5.7: *The transition probability of random walk in the GFMC defined by (112), (181), and (182) has the lower bound*

$$P(y,x) > 0 \Rightarrow \forall t > 0: G_1(y,x;t) \geq \frac{\Delta t \Gamma(t)}{1 - \Delta t(E_{\min} - E_T) + N \Delta t \Gamma(t)}, \quad (184)$$

$$\exists t_1 > 0, \quad \forall t > t_1: G_1(x,x;t) \geq \frac{\Delta t \Gamma(t)}{1 - \Delta t(E_{\min} - E_T) + N \Delta t \Gamma(t)}, \quad (185)$$

where E_{\min} is the minimum value of $E_0(x)$,

$$E_{\min} = \min\{E_0(x) | x \in \mathcal{S}\}. \quad (186)$$

Proof of Lemma 5.7: The first part of Lemma 5.7 is trivial because the transition probability is an increasing function with respect to $E_0(x)$ when $P(y,x) > 0$ as seen in (182). Next, we prove the second part of Lemma 5.7. According to (179) and (180), $G_1(x,x;t)$ is written as

$$G_1(x,x;t) = 1 - \frac{N \Delta t \Gamma(t)}{1 - \Delta t[E_0(x) - E_T] + N \Delta t \Gamma(t)}. \quad (187)$$

Since the transverse field $\Gamma(t)$ decreases to zero with time, the second term on the right-hand side tends to zero as $t \rightarrow \infty$. Thus, there exists $t_1 > 0$ such that $G_1(x,x;t) > 1 - \varepsilon$ for $\forall \varepsilon > 0$ and $\forall t > t_1$. On the other hand, the right-hand side of (185) converges to zero as $t \rightarrow \infty$. We therefore have (185). \square

Proof of Theorem 5.6: We show that condition (183) is sufficient to satisfy the three conditions of Theorem 5.2.

- (1) From Lemma 5.7, we obtain a bound on the coefficient of ergodicity for sufficiently large k as

$$1 - \alpha(G_1^{kN, kN-N}) \geq \left[\frac{\Delta t \Gamma(kN-1)}{1 - \Delta t(E_{\min} - E_T) + N \Delta t \Gamma(kN-1)} \right]^N \quad (188)$$

in the same manner as we derived (152), where we used $R=N$. Substituting annealing schedule (183), we can prove weak ergodicity from Theorem 5.1 because

$$\sum_{k=1}^{\infty} [1 - \alpha(G_1^{kN, kN-N})] \geq \sum_{k=k_0}^{\infty} \frac{b'^N}{(kN)^{cN}}, \quad (189)$$

which diverges when $0 < c \leq 1/N$.

- (2) The stationary distribution of the instantaneous transition probability $G_1(y,x;t)$ is

$$q(x;t) \equiv \frac{w(x;t)}{\sum_{x \in \mathcal{S}} w(x;t)} = \frac{1}{2^N} - \frac{\Delta t E_0(x)}{2^N [1 + \Delta t E_T + N \Delta t \Gamma(t)]}, \quad (190)$$

which is derived as follows. The transition probability defined by (112), (181), and (182) is rewritten in terms of weight (180) as

$$G_1(y, x; t) = \begin{cases} 1 - \frac{N\Delta t\Gamma(t)}{w(x; t)} & (x = y) \\ \frac{\Delta t\Gamma(t)}{w(x; t)} & (x \in \mathcal{S}_y; \text{ single-spin flip}) \\ 0 & (\text{otherwise}). \end{cases} \tag{191}$$

Thus, we have

$$\begin{aligned} \sum_{x \in \mathcal{S}} G_1(y, x; t)q(x; t) &= \left[1 - \frac{N\Delta t\Gamma(t)}{w(y; t)} \right] \frac{w(y; t)}{A} + \sum_{x \in \mathcal{S}_y} \frac{\Delta t\Gamma(t)}{w(x; t)} \frac{w(x; t)}{A} \\ &= q(y; t) - \frac{N\Delta t\Gamma(t)}{A} + \frac{\Delta t\Gamma(t)}{A} \sum_{x \in \mathcal{S}_y} 1, \end{aligned} \tag{192}$$

where A denotes the normalization factor,

$$\sum_{x \in \mathcal{S}} w(x; t) = \text{Tr} \left[1 - \Delta t \left(- \sum_{\langle ij \rangle} J_{ij} \sigma_i^z \sigma_j^z - E_T \right) + N\Delta t\Gamma(t) \right] = 2^N [1 + \Delta t E_T + N\Delta t\Gamma(t)], \tag{193}$$

where we used $\text{Tr} \sum J_{ij} \sigma_i^z \sigma_j^z = 0$. Since the volume of \mathcal{S}_y is N , (192) indicates that $q(x; t)$ is the stationary distribution of $G_1(y, x; t)$. The right-hand side of (190) is easily derived from the above equation.

- (3) Since the transverse field $\Gamma(t)$ decreases monotonically with t , the above stationary distribution $q(x; t)$ is an increasing function of t if $E_0(x) < 0$ and is decreasing if $E_0 \geq 0$. Consequently, using the same procedure as in (160), we have

$$\|q(t+1) - q(t)\| = 2 \sum_{E_0(x) < 0} [q(x; t+1) - q(x; t)], \tag{194}$$

and thus

$$\sum_{t=0}^{\infty} \|q(t+1) - q(t)\| = 2 \sum_{E_0(x) < 0} [q(x; \infty) - q(x; 0)] \leq 2. \tag{195}$$

Therefore the sum $\sum_{t=0}^{\infty} \|q(t+1) - q(t)\|$ is finite, which completes the proof of condition (3). \square

Remark: Theorem 5.6 asserts convergence of the distribution of random walkers to equilibrium distribution (190) with $\Gamma(t) \rightarrow 0$. This implies that the final distribution is not delta peaked at the ground state with minimum $E_0(x)$ but is a relatively mild function of this energy. The optimality of the solution is achieved after one takes the weight factor $w(x; t)$ into account: The repeated multiplication of weight factors as in (177), in conjunction with the relatively mild distribution coming from the product of G_1 as mentioned above, leads to the asymptotically delta-peaked wave function $\psi_n(y)$ because $w(x; t)$ is larger for smaller $E_0(x)$ as seen in (180).

2. Alternative choice of Green’s function

So far we have used Green’s function defined in (174), which is linear in the transverse field, allowing single-spin flips only. It may be useful to consider another type of Green’s function which accommodates multispin flips. Let us try the following form of Green’s function:

$$\hat{G}_2(t) = \exp\left(\Delta t\Gamma(t) \sum_i \sigma_i^x\right) \exp\left(\Delta t \sum_{ij} J_{ij} \sigma_i^z \sigma_j^z\right), \tag{196}$$

which is equal to $\hat{G}_0(t)$ to the order Δt . The matrix element of $\hat{G}_2(t)$ in the σ^z -diagonal basis is

$$\hat{G}_2(y, x; t) = \cosh^N(\Delta t \Gamma(t)) \tanh^\delta(\Delta t \Gamma(t)) e^{-\Delta t E_0(x)}, \quad (197)$$

where δ is the number of spins in different states in x and y . According to the scheme of GFMC, we decompose $\hat{G}_2(y, x; t)$ into the normalized transition probability and the weight:

$$G_2(y, x; t) = \left[\frac{\cosh(\Delta t \Gamma(t))}{e^{\Delta t \Gamma(t)}} \right]^N \tanh^\delta(\Delta t \Gamma(t)), \quad (198)$$

$$w_2(x; t) = e^{\Delta t N \Gamma(t)} e^{-\Delta t E_0(x)}. \quad (199)$$

It is remarkable that the transition probability G_2 is independent of $E_0(x)$, although it depends on x through δ . Thus, the stationary distribution of random walk is uniform. This property is lost if one interchanges the order of the two factors in (196).

The property of strong ergodicity can be shown to hold in this case as well.

Theorem 5.8 (strong ergodicity of QA-GFMC 2): *The inhomogeneous Markov chain generated by (198) is strongly ergodic if*

$$\Gamma(t) \geq -\frac{1}{2\Delta t} \log(1 - 2b(t+1)^{-1/N}). \quad (200)$$

Remark: For sufficiently large t , the above annealing schedule is reduced to

$$\Gamma(t) \geq \frac{b}{\Delta t(t+1)^{1/N}}. \quad (201)$$

Since the proof is quite similar to the previous cases, we just outline the idea of the proof. The transition probability $G_2(y, x; t)$ becomes smallest when $\delta=N$. Consequently, the coefficient of ergodicity is estimated as

$$1 - \alpha(G_2^{t+1, t}) \geq \left[\frac{1 - e^{-2\Delta t \Gamma(t)}}{2} \right]^N.$$

We note that R is equal to 1 in the present case because any state is reachable from an arbitrary state in a single step. From Theorem 5.1, the condition

$$\left[\frac{1 - e^{-2\Delta t \Gamma(t)}}{2} \right]^N \geq \frac{b'}{t+1} \quad (202)$$

is sufficient for weak ergodicity. From this, one obtains (200). Since the stationary distribution of $G_2(y, x; t)$ is uniform as mentioned above, strong ergodicity readily follows from Theorem 5.2.

Similarly to the case of PIMC, we can discuss the convergence condition of QA-GFMC in systems with continuous degrees of freedom. The resulting sufficient condition is a logarithmic increase in the mass as will be shown now. The operator \hat{G}_2 generated by Hamiltonian (167) is written as

$$\hat{G}_2(t) = \exp\left(-\frac{\Delta t}{2m(t)} \sum_{i=1}^N p_i^2\right) e^{-\Delta t V(\{r_i\})}. \quad (203)$$

Thus, Green's function is calculated in a discretized space as

$$\hat{G}_2(y, x; t) \propto \exp\left(-\frac{m(t)}{2\Delta t} \sum_{i=1}^N |r'_i - r_i|^2 - \Delta t V(\{r_i\})\right), \quad (204)$$

where x and y represent $\{r_i\}$ and $\{r'_i\}$, respectively. Summation over y , i.e., integration over $\{r'_i\}$, yields the weight $w(x; t)$, from which the transition probability is obtained:

$$w(x;t) \propto e^{-\Delta t V(r_i)}, \quad (205)$$

$$G_2(y,x;t) \propto \exp\left(-\frac{m(t)}{2\Delta t} \sum_{i=1}^N |r'_i - r_i|^2\right). \quad (206)$$

The lower bound for the transition probability depends exponentially on the mass: $G_2(y,x;t) \geq e^{-Cm(t)}$. Since $1 - \alpha(G_2^{t+1,t})$ has the same lower bound, the sufficient condition for weak ergodicity is $e^{-Cm(t)} \geq (t+1)^{-1}$, which is rewritten as

$$m(t) \leq C^{-1} \log(t+1). \quad (207)$$

Constant C is proportional to $NL^2/\Delta t$, where L denotes the maximum value of $|r' - r|$. The derivation of C is similar to (169) because $G_2(t)$ allows any transition to arbitrary states at one time step.

VI. SUMMARY AND PERSPECTIVE

In this paper we have studied the mathematical foundation of QA, in particular, the convergence conditions and the reduction in residual errors. In Sec. II, we have seen that the adiabaticity condition of the quantum system representing QA leads to the convergence condition, i.e., the condition for the system to reach the solution of the classical optimization problem as $t \rightarrow \infty$ following the RT Schrödinger equation. The result shows the asymptotic power decrease in the transverse field as the condition for convergence. This rate in decrease of the control parameter is faster than the logarithmic rate of temperature decrease for convergence of SA. It nevertheless does not mean the qualitative reduction in computational complexity from classical SA to QA. Our method deals with a very generic system that represents most of the interesting problems including worst instances of difficult problems, for which drastic reduction in computational complexity is hard to expect.

Section III reviews the quantum-mechanical derivation of the convergence condition of SA using the classical-quantum mapping without an extra dimension in the quantum system. The adiabaticity condition for the quantum system has been shown to be equivalent to the quasiequilibrium condition for the classical system at finite temperature, reproducing the well-known convergence condition of SA. The adiabaticity condition thus leads to the convergence condition of both QA and SA. Since the studies of QAE often exploit the adiabaticity condition to derive the computational complexity of a given problem, the adiabaticity may be seen as a versatile tool traversing QA, SA, and QAE.

Section IV is for the reduction in residual errors after finite-time quantum evolution of RT and IT Schrödinger equations. This is a different point of view from the usual context of QAE, where the issue is to reduce the evolution time (computational complexity) with the residual error fixed to a given small value. It has been shown that the residual error can become significantly smaller by the ingenious choice of the time dependence of coefficients in the quantum Hamiltonian. This idea allows us to reduce the residual error for any given QAE-based algorithm without compromising the computational complexity apart from a possibly moderate numerical factor.

In Sec. V we have derived the convergence condition of QA implemented by quantum Monte Carlo simulations of path-integral and Green's function methods. These approaches bear important practical significance because only stochastic methods allow us to treat practical large-size problems on the classical computer. A highly nontrivial result in this section is that the convergence condition for the stochastic methods is essentially the same power-law decrease in the transverse-field term as in the Schrödinger dynamics of Sec. II. This is surprising since the Monte Carlo (stochastic) dynamics is completely different from the Schrödinger dynamics. Something deep may lie behind this coincidence and it should be an interesting target of future studies.

The results presented and/or reviewed in this paper serve as the mathematical foundation of QA. We have also stressed the similarity/equivalence of QA and QAE. Even the classical SA can be viewed from the same framework of quantum adiabaticity as long as the convergence condi-

tions are concerned. Since the studies of very generic properties of QA seem to have been almost completed, fruitful future developments would lie in the investigations of problems specific to each case of optimization task by analytical and numerical methods.

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APPENDIX A: HOPF'S INEQUALITY

In this appendix, we prove inequality (22). Although Hopf³² originally proved this inequality for positive linear integral operators, we concentrate on a square matrix for simplicity.

Let M be a strictly positive $m \times m$ matrix. The strict positivity means that all the elements of M are positive, namely, $M_{ij} > 0$ for all i, j , which will be denoted by $M > 0$. Similarly, $M \geq 0$ means that $M_{ij} \geq 0$ for all i, j . We use the same notation for a vector, that is, $\mathbf{v} > 0$ means that all the elements v_i are positive.

The product of the matrix M and an m element column vector \mathbf{v} is denoted as usual by $M\mathbf{v}$ and its i th element is

$$(M\mathbf{v})_i = \sum_{j=1}^m M_{ij}v_j. \quad (\text{A1})$$

The strict positivity for M is equivalent to

$$M\mathbf{v} > 0 \quad \text{if } \mathbf{v} \geq 0, \quad \mathbf{v} \neq \mathbf{0}, \quad (\text{A2})$$

where $\mathbf{0}$ denotes the zero vector. Of course, if $\mathbf{v} = \mathbf{0}$, then $M\mathbf{v} = \mathbf{0}$.

Any real-valued vector \mathbf{v} and any strictly positive vector $\mathbf{p} > 0$ satisfy

$$\min_i \frac{v_i}{p_i} \leq \min_i \frac{(M\mathbf{v})_i}{(M\mathbf{p})_i} \leq \max_i \frac{(M\mathbf{v})_i}{(M\mathbf{p})_i} \leq \max_i \frac{v_i}{p_i}, \quad (\text{A3})$$

because

$$(M\mathbf{v})_i - \left(\min_i \frac{v_i}{p_i} \right) (M\mathbf{p})_i = \sum_{j=1}^m M_{ij} \left[v_j - \left(\min_i \frac{v_i}{p_i} \right) p_j \right] \geq 0, \quad (\text{A4})$$

$$\left(\max_i \frac{v_i}{p_i} \right) (M\mathbf{p})_i - (M\mathbf{v})_i = \sum_{j=1}^m M_{ij} \left[\left(\max_i \frac{v_i}{p_i} \right) p_j - v_j \right] \geq 0. \quad (\text{A5})$$

The above inequality implies that the difference between the maximum and minimum of $(M\mathbf{v})_i / (M\mathbf{p})_i$ is smaller than that of v_i / p_i . Following Ref. 32 we use the notation

$$\text{osc} \frac{v_i}{p_i} \equiv \max_i \frac{v_i}{p_i} - \min_i \frac{v_i}{p_i}, \quad (\text{A6})$$

which is called the oscillation. For a complex-valued vector, we define

$$\text{osc} v_i = \sup_{|\eta|=1} \text{osc} \text{Re}(\eta v_i). \quad (\text{A7})$$

It is easy to derive, for any complex c ,

$$\operatorname{osc}_i(cv_i) = |c| \operatorname{osc}_i v_i. \quad (\text{A8})$$

We can also easily prove that, if $\operatorname{osc}_i v_i = 0$, v_i does not depend on i .

We suppose that the simple ratio of matrix elements is bounded,

$$\frac{M_{ik}}{M_{jk}} \leq \kappa \quad \text{for all } i, j, k. \quad (\text{A9})$$

This assumption is rewritten by the product form as

$$\frac{(M\mathbf{v})_i}{(M\mathbf{v})_j} \leq \kappa, \quad \mathbf{v} \geq 0, \quad \mathbf{v} \neq 0, \quad (\text{A10})$$

for all i, j and such \mathbf{v} . The following theorem states that inequality (A3) is sharpened under additional assumption (A10).

Theorem A.1: *If M satisfies conditions (A2) and (A10) for any $\mathbf{p} > 0$ and any complex-valued \mathbf{v} ,*

$$\operatorname{osc}_i \frac{(M\mathbf{v})_i}{(M\mathbf{p})_i} \leq \frac{\kappa - 1}{\kappa + 1} \operatorname{osc}_i \frac{v_i}{p_i}. \quad (\text{A11})$$

Proof. We consider a real-valued vector \mathbf{v} at first. For fixed i, j and fixed $\mathbf{p} > 0$, we define X_k by

$$\frac{(M\mathbf{v})_i}{(M\mathbf{p})_i} - \frac{(M\mathbf{v})_j}{(M\mathbf{p})_j} = \sum_{k=1}^m X_k v_k. \quad (\text{A12})$$

We do not have to know the exact form of $X_k = X_k(i, j, \mathbf{p})$. When $\mathbf{v} = a\mathbf{p}$, the left-hand side of the above equation vanishes, which implies $\sum_k X_k p_k = 0$. Thus, we have

$$\frac{(M\mathbf{v})_i}{(M\mathbf{p})_i} - \frac{(M\mathbf{v})_j}{(M\mathbf{p})_j} = \sum_{k=1}^m X_k (v_k - ap_k). \quad (\text{A13})$$

Now we choose

$$a = \min_i \frac{v_i}{p_i}, \quad b = \max_i \frac{v_i}{p_i}. \quad (\text{A14})$$

Since $v_k - ap_k = (b - a)p_k - (bp_k - v_k)$, $v_k - ap_k$ takes its minimum 0 at $v_k = ap_k$ and its maximum $(b - a)p_k$ at $v_k = bp_k$. Therefore, the right-hand side of (A13) with \mathbf{p} given attains its maximum for

$$\mathbf{v} = a\mathbf{p}^- - b\mathbf{p}^+ = a\mathbf{p} + (b - a)\mathbf{p}^+, \quad (\text{A15})$$

where we defined

$$p_i^- = \begin{cases} p_i & (X_i \leq 0) \\ 0 & (X_i > 0), \end{cases} \quad p_i^+ = \begin{cases} 0 & (X_i \leq 0) \\ p_i & (X_i > 0). \end{cases} \quad (\text{A16})$$

Consequently, we have

$$\frac{(M\mathbf{v})_i}{(M\mathbf{p})_i} - \frac{(M\mathbf{v})_j}{(M\mathbf{p})_j} \leq \left[\frac{(M\mathbf{p}^+)_i}{(M\mathbf{p})_i} - \frac{(M\mathbf{p}^+)_j}{(M\mathbf{p})_j} \right] (b - a). \quad (\text{A17})$$

Since, by assumptions, $M > 0$ and $\mathbf{p} > 0$, we have

$$M\mathbf{p}^- \geq 0, \quad M\mathbf{p}^+ \geq 0, \quad M\mathbf{p} = M\mathbf{p}^- + M\mathbf{p}^+ > 0. \quad (\text{A18})$$

Moreover, $M\mathbf{p}^- > 0$ if $\mathbf{p}^- \neq 0$ and $M\mathbf{p}^+ > 0$ if $\mathbf{p}^+ \neq 0$. In either case, namely, $\mathbf{p}^- = 0$ or $\mathbf{p}^+ = 0$, the expression in the square brackets of (A17) vanishes because \mathbf{p}^+ is equal to either \mathbf{p} or 0. Thus, we may assume that both $M\mathbf{p}^- > 0$ and $M\mathbf{p}^+ > 0$. Therefore the expression in inequality (A17) is rewritten as

$$\frac{(M\mathbf{p}^+)_i}{(M\mathbf{p})_i} - \frac{(M\mathbf{p}^+)_j}{(M\mathbf{p})_j} \leq \frac{1}{1+t} - \frac{1}{1+t'}, \quad t \equiv \frac{(M\mathbf{p}^-)_i}{(M\mathbf{p}^+)_i}, \quad t' \equiv \frac{(M\mathbf{p}^-)_j}{(M\mathbf{p}^+)_j}. \quad (\text{A19})$$

Since, from assumption (A10), t and t' are bounded from κ^{-1} to κ , we find $t' \leq \kappa^2 t$, which yields

$$\frac{(M\mathbf{p}^+)_i}{(M\mathbf{p})_i} - \frac{(M\mathbf{p}^+)_j}{(M\mathbf{p})_j} \leq \frac{1}{1+t} - \frac{1}{1+\kappa^2 t}. \quad (\text{A20})$$

For $t > 0$, the right-hand side of the above inequality takes its maximum value $(\kappa-1)/(\kappa+1)$ at $t = \kappa^{-1}$. Finally, we obtain

$$\frac{(M\mathbf{v})_i}{(M\mathbf{p})_i} - \frac{(M\mathbf{v})_j}{(M\mathbf{p})_j} \leq \frac{\kappa-1}{\kappa+1} \text{osc}_i \frac{v_i}{p_i} \quad (\text{A21})$$

for any i, j . Hence it holds for the sup of the left-hand side, which yields (A11).

For a complex-valued vector \mathbf{v} , we replace v_i by $\text{Re}(\eta v_i)$. Since $M \text{Re}(\eta \mathbf{v}) = \text{Re}(\eta M\mathbf{v})$, the same argument for the real vector case yields

$$\text{osc}_i \text{Re} \left(\eta \frac{(M\mathbf{v})_i}{(M\mathbf{p})_i} \right) \leq \frac{\kappa-1}{\kappa+1} \text{osc}_i \text{Re} \left(\eta \frac{v_i}{p_i} \right). \quad (\text{A22})$$

Taking the sup with respect to η , $|\eta|=1$, on both sides, we obtain (A11).

We apply this theorem to the eigenvalue problem,

$$M\mathbf{v} = \lambda \mathbf{v}. \quad (\text{A23})$$

The Perron–Frobenius theorem states that a non-negative square matrix, $M \geq 0$, has a real eigenvalue λ_0 satisfying $|\lambda| \leq \lambda_0$ for any other eigenvalue λ . This result is sharpened for a strictly positive matrix, $M > 0$, as the following theorems.

Theorem A.2: Under hypotheses (A2) and (A10), eigenvalue equation (A23) has a positive solution $\lambda = \lambda_0 > 0$ and $\mathbf{v} = \mathbf{q} > 0$. Moreover, for any vector \mathbf{p} ($\mathbf{p} \geq 0$, $\mathbf{p} \neq 0$), the sequence

$$\mathbf{q}_n = \frac{M^n \mathbf{p}}{(M^n \mathbf{p})_k} \quad (\text{A24})$$

with k fixed converges toward such \mathbf{q} .

Theorem A.3: Under the same hypotheses, (A23) has no other non-negative solutions than $\lambda = \lambda_0$ and $\mathbf{v} = c\mathbf{q}$. For $\lambda = \lambda_0$, (A23) has no other solutions than $\mathbf{v} = c\mathbf{q}$.

Theorem A.4: Under the same hypotheses, any (complex) eigenvalue $\lambda \neq \lambda_0$ of (A23) satisfies

$$|\lambda| \leq \frac{\kappa-1}{\kappa+1} \lambda_0. \quad (\text{A25})$$

Remark: We note that the factor $(\kappa-1)/(\kappa+1)$ is the best possible if there is no further condition. For example,

$$M = \begin{pmatrix} \kappa & 1 \\ 1 & \kappa \end{pmatrix}, \quad \kappa > 1, \quad (\text{A26})$$

has eigenvalues $\lambda_0 = \kappa+1$ and $\lambda = \kappa-1$.

Proof of Theorem A.2: Let us consider two vectors \mathbf{p} and $\bar{\mathbf{p}}$ which are non-negative and unequal to 0 and define

$$\mathbf{p}_{n+1} = M\mathbf{p}_n, \quad \bar{\mathbf{p}}_{n+1} = M\bar{\mathbf{p}}_n, \quad \mathbf{p}_0 = \mathbf{p}, \quad \bar{\mathbf{p}}_0 = \bar{\mathbf{p}}. \tag{A27}$$

From hypothesis (A2), both \mathbf{p}_n and $\bar{\mathbf{p}}_n$ are strictly positive for $n > 0$. We find by repeated applications of Theorem A.1 that, for $n > 1$,

$$\text{osc}_i \frac{\bar{p}_{n,i}}{p_{n,i}} \leq \left(\frac{\kappa - 1}{\kappa + 1} \right)^{n-1} \text{osc}_i \frac{\bar{p}_{1,i}}{p_{1,i}}, \tag{A28}$$

where we used the notation $p_{n,i} = (\mathbf{p}_n)_i$. Consequently, there exists a finite constant $\lambda > 0$, such that

$$\frac{\bar{p}_{n,i}}{p_{n,i}} \rightarrow \lambda \quad (n \rightarrow \infty) \tag{A29}$$

for every i . We normalize the vectors \mathbf{p}_n and $\bar{\mathbf{p}}_n$ as

$$\mathbf{q}_n = \frac{\mathbf{p}_n}{p_{n,k}}, \quad \bar{\mathbf{q}}_n = \frac{\bar{\mathbf{p}}_n}{\bar{p}_{n,k}}, \tag{A30}$$

with k fixed. Hypothesis (A10) implies that

$$\kappa^{-1} \leq q_{n,i} \leq \kappa, \quad \kappa^{-1} \leq \bar{q}_{n,i} \leq \kappa. \tag{A31}$$

Thus, we find that

$$|\bar{q}_{n,i} - q_{n,i}| = q_{n,i} \frac{p_{n,k}}{\bar{p}_{n,k}} \left| \frac{\bar{p}_{n,i}}{p_{n,i}} - \frac{\bar{p}_{n,k}}{p_{n,k}} \right| \leq \kappa \frac{p_{n,k}}{\bar{p}_{n,k}} \text{osc}_i \frac{\bar{p}_{n,i}}{p_{n,i}}. \tag{A32}$$

Now we specialize to the case that $\bar{\mathbf{p}} = M\mathbf{p} = \mathbf{p}_1$, namely,

$$\bar{\mathbf{p}}_n = M\mathbf{p}_n = \mathbf{p}_{n+1}, \quad \bar{\mathbf{q}}_n = \mathbf{q}_{n+1}. \tag{A33}$$

Using (A28) and (A29), we estimate (A32) for $q_{n+1,i} - q_{n,i}$, which implies that the sequence \mathbf{q}_n converges to a limit vector \mathbf{q} . Because of (A31), we have $\mathbf{q} > 0$. Now (A29) reads

$$\frac{p_{n+1,i}}{p_{n,i}} = \frac{(M\mathbf{p}_n)_i}{(\mathbf{p}_n)_i} = \frac{(M\mathbf{q}_n)_i}{(\mathbf{q}_n)_i} \rightarrow \lambda_0. \tag{A34}$$

Consequently, $M\mathbf{q} = \lambda_0\mathbf{q}$. For any other initial vector $\bar{\mathbf{p}}$, the sequence $\bar{\mathbf{q}}_n$ converges to the same limit as \mathbf{q}_n because of (A28), (A29), and (A32). Theorem A.2 is thereby proved. \square

Proof of Theorem A.3: We assume that $\mathbf{v} \geq 0$ and $\mathbf{v} \neq 0$ is a solution of eigenvalue equation (A23). Since hypothesis (A2) implies $M\mathbf{v} > 0$, we have $\lambda > 0$ and $\mathbf{v} > 0$. We use this \mathbf{v} as an initial vector \mathbf{p} in Theorem A.2 and apply the last part of this theorem to

$$\frac{M^n \mathbf{v}}{(M^n \mathbf{v})_k} = \frac{\lambda^n \mathbf{v}}{\lambda^n v_k} = \frac{\mathbf{v}}{v_k}. \tag{A35}$$

Hence, the limit \mathbf{q} is equal to \mathbf{v}/v_k , that is, $\mathbf{v} = c\mathbf{q}$ and $\lambda = \lambda_0$. Therefore the first part of Theorem A.3 is proved.

Next, we take $\lambda_0 > 0$ and $\mathbf{q} > 0$ from Theorem A.2 and consider a solution of $M\mathbf{v} = \lambda\mathbf{v}$. The application of Theorem A.1 to \mathbf{q} and \mathbf{v} yields

$$\frac{|\lambda|}{\lambda_0} \operatorname{osc}_i \frac{v_i}{q_i} = \operatorname{osc}_i \frac{\lambda v_i}{\lambda_0 q_i} = \operatorname{osc}_i \frac{(M\mathbf{v})_i}{(M\mathbf{q})_i} \leq \frac{\kappa-1}{\kappa+1} \operatorname{osc}_i \frac{v_i}{q_i}, \quad (\text{A36})$$

where we used (A8). If $\lambda = \lambda_0$, the above inequality implies that $\operatorname{osc}_i v_i/q_i = 0$ or $\mathbf{v} = c\mathbf{q}$, which provides the second part of Theorem A.3.

Proof of Theorem A.4: We consider (A36). If $\lambda \neq \lambda_0$ and $\mathbf{v} \neq 0$, \mathbf{v} cannot be equal to $c\mathbf{q}$. Therefore $\operatorname{osc}_i v_i/q_i > 0$, and then (A36) yields (A25). \square

APPENDIX B: CONDITIONS FOR ERGODICITY

In this appendix, we prove Theorems 5.1 and 5.2 which provide conditions for weak and strong ergodicities of an inhomogeneous Markov chain.⁵

1. Coefficient of ergodicity

Let us recall the definition of the coefficient of ergodicity,

$$\alpha(G) = 1 - \min_{x,y \in \mathcal{S}} \left\{ \sum_{z \in \mathcal{S}} \min\{G(z,x), G(z,y)\} \right\}. \quad (\text{B1})$$

First, we prove that this coefficient is rewritten as

$$\alpha(G) = \frac{1}{2} \max_{x,y \in \mathcal{S}} \left\{ \sum_{z \in \mathcal{S}} |G(z,x) - G(z,y)| \right\}. \quad (\text{B2})$$

Proof of (B2): For fixed $x, y \in \mathcal{S}$, we define two subsets of \mathcal{S} by

$$\mathcal{S}_G^+ = \{z \in \mathcal{S} | G(z,x) - G(z,y) > 0\},$$

$$\mathcal{S}_G^- = \{z \in \mathcal{S} | G(z,x) - G(z,y) \leq 0\}. \quad (\text{B3})$$

Since the transition matrix satisfies $\sum_{y \in \mathcal{S}} G(y,x) = 1$, we have

$$\sum_{z \in \mathcal{S}_G^+} [G(z,x) - G(z,y)] = \left[1 - \sum_{z \in \mathcal{S}_G^-} G(z,x) \right] - \left[1 - \sum_{z \in \mathcal{S}_G^-} G(z,y) \right] = - \sum_{z \in \mathcal{S}_G^-} [G(z,x) - G(z,y)]. \quad (\text{B4})$$

Thus, we find

$$\begin{aligned} \frac{1}{2} \sum_{z \in \mathcal{S}} |G(z,x) - G(z,y)| &= \sum_{z \in \mathcal{S}_G^+} [G(z,x) - G(z,y)] = \sum_{z \in \mathcal{S}} \max\{0, G(z,x) - G(z,y)\} \\ &= \sum_{z \in \mathcal{S}} [G(z,x) - \min\{G(z,x), G(z,y)\}] = 1 - \sum_{z \in \mathcal{S}} \min\{G(z,x), G(z,y)\} \end{aligned} \quad (\text{B5})$$

for any x, y . Hence taking the maximum with respect to x, y on both sides, we obtain (B2). \square

To derive the conditions for weak and strong ergodicities, the following lemmas are useful.

Lemma B.1: Let G be a transition matrix. Then the coefficient of ergodicity satisfies

$$0 \leq \alpha(G) \leq 1. \quad (\text{B6})$$

Lemma B.2: Let G and H be transition matrices on \mathcal{S} . Then the coefficient of ergodicity satisfies

$$\alpha(GH) \leq \alpha(G)\alpha(H). \quad (\text{B7})$$

Lemma B.3: Let G be a transition matrix and H be a square matrix on \mathcal{S} such that

$$\sum_{z \in \mathcal{S}} H(z, x) = 0 \quad (\text{B8})$$

for any $x \in \mathcal{S}$. Then we have

$$\|GH\| \leq \alpha(G)\|H\|, \quad (\text{B9})$$

where the norm of a square matrix defined by

$$\|A\| \equiv \max_{x \in \mathcal{S}} \left\{ \sum_{z \in \mathcal{S}} |A(z, x)| \right\}. \quad (\text{B10})$$

Proof of Lemma B.1: The definition of $\alpha(G)$ implies $\alpha(G) \leq 1$ because $G(y, x) \geq 0$. From (B2), $\alpha(G) \geq 0$ is straightforward.

Proof of Lemma B.2: Let us consider a transition matrix G , a column vector a such that $\sum_{z \in \mathcal{S}} a(z) = 0$, and their product $b = Ga$. We note that the vector b satisfies $\sum_{z \in \mathcal{S}} b(z) = 0$ because

$$\sum_{z \in \mathcal{S}} b(z) = \sum_{z \in \mathcal{S}} \sum_{y \in \mathcal{S}} G(z, y) a(y) = \sum_{y \in \mathcal{S}} a(y) \left[\sum_{z \in \mathcal{S}} G(z, y) \right] = \sum_{y \in \mathcal{S}} a(y) = 0. \quad (\text{B11})$$

We define subsets of \mathcal{S} by

$$\mathcal{S}_a^+ = \{z \in \mathcal{S} | a(z) > 0\}, \quad \mathcal{S}_a^- = \{z \in \mathcal{S} | a(z) \leq 0\},$$

$$\mathcal{S}_b^+ = \{z \in \mathcal{S} | b(z) > 0\}, \quad \mathcal{S}_b^- = \{z \in \mathcal{S} | b(z) \leq 0\}. \quad (\text{B12})$$

Since $\sum_{z \in \mathcal{S}} a(z) = \sum_{z \in \mathcal{S}} b(z) = 0$, we find

$$\sum_{z \in \mathcal{S}} |a(z)| = \sum_{z \in \mathcal{S}_a^+} a(z) - \sum_{z \in \mathcal{S}_a^-} a(z) = 2 \sum_{z \in \mathcal{S}_a^+} a(z) = -2 \sum_{z \in \mathcal{S}_a^-} a(z), \quad (\text{B13})$$

$$\sum_{z \in \mathcal{S}} |b(z)| = 2 \sum_{z \in \mathcal{S}_b^+} b(z) = -2 \sum_{z \in \mathcal{S}_b^-} b(z). \quad (\text{B14})$$

Therefore, we obtain

$$\begin{aligned} \sum_{z \in \mathcal{S}} |b(z)| &= 2 \sum_{z \in \mathcal{S}_b^+} \sum_{u \in \mathcal{S}} G(z, u) a(u) = 2 \sum_{u \in \mathcal{S}_a^+} \left[\sum_{z \in \mathcal{S}_b^+} G(z, u) \right] a(u) + 2 \sum_{u \in \mathcal{S}_a^-} \left[\sum_{z \in \mathcal{S}_b^+} G(z, u) \right] a(u) \\ &\leq 2 \max_{v \in \mathcal{S}} \left\{ \sum_{z \in \mathcal{S}_b^+} G(z, v) \right\} \sum_{u \in \mathcal{S}_a^+} a(u) + 2 \min_{w \in \mathcal{S}} \left\{ \sum_{z \in \mathcal{S}_b^+} G(z, w) \right\} \sum_{u \in \mathcal{S}_a^-} a(u) = \max_{v, w \in \mathcal{S}} \left\{ \sum_{z \in \mathcal{S}_b^+} [G(z, v) \right. \\ &\quad \left. - G(z, w)] \right\} \sum_{u \in \mathcal{S}} |a(u)| \leq \max_{v, w \in \mathcal{S}} \left\{ \sum_{z \in \mathcal{S}} \max\{0, G(z, v) - G(z, w)\} \right\} \sum_{u \in \mathcal{S}} |a(u)| \\ &= \frac{1}{2} \max_{v, w \in \mathcal{S}} \left\{ \sum_{z \in \mathcal{S}} |G(z, v) - G(z, w)| \right\} \sum_{u \in \mathcal{S}} |a(u)| = \alpha(G) \sum_{u \in \mathcal{S}} |a(u)|, \end{aligned} \quad (\text{B15})$$

where we used (B5) and (B2).

Next, we consider transition matrices G , H , and $F = GH$. We take $a(z) = H(z, x) - H(z, y)$, and then (B15) is rewritten as

$$\sum_{z \in \mathcal{S}} |F(z,x) - F(z,y)| \leq \alpha(G) \sum_{u \in \mathcal{S}} |H(u,x) - H(u,y)| \quad (\text{B16})$$

for any x, y . Hence this inequality holds for the maximum of both sides with respect to x, y , which yields Lemma B.2.

Proof of Lemma B.3: Let us consider $F=GH$. We can take $a(z)=H(z,x)$ in (B15) because of the assumption $\sum_{y \in \mathcal{S}} H(y,x)=0$. Thus we have

$$\sum_{z \in \mathcal{S}} |F(z,x)| \leq \alpha(G) \sum_{u \in \mathcal{S}} |H(u,x)| \quad (\text{B17})$$

for any x . Hence this inequality holds for the maximum of both sides with respect to x , which provides Lemma B.3. \square

2. Conditions for weak ergodicity

The following theorem provides the reason why $\alpha(G)$ is called the coefficient of ergodicity.

Theorem B.4: *An inhomogeneous Markov chain is weakly ergodic if and only if the transition matrix satisfies*

$$\lim_{t \rightarrow \infty} \alpha(G^{t,s}) = 0 \quad (\text{B18})$$

for any $s > 0$.

Proof: We assume that the inhomogeneous Markov chain generated by $G(t)$ is weakly ergodic. For fixed $x, y \in \mathcal{S}$, we define probability distributions by

$$p_x(z) = \begin{cases} 1 & (z=x) \\ 0 & (\text{otherwise}), \end{cases} \quad p_y(z) = \begin{cases} 1 & (z=y) \\ 0 & (\text{otherwise}). \end{cases} \quad (\text{B19})$$

Since $p_x(t,s;z) = \sum_{u \in \mathcal{S}} G^{t,s}(z,u)p_x(u) = G^{t,s}(z,x)$ and $p_y(t,s;z) = G^{t,s}(z,y)$, we have

$$\sum_{z \in \mathcal{S}} |G^{t,s}(z,x) - G^{t,s}(z,y)| = \sum_{z \in \mathcal{S}} |p_x(t,s;z) - p_y(t,s;z)| \leq \sup\{\|p(t,s) - p'(t,s)\| \mid p_0, p'_0 \in \mathcal{P}\}. \quad (\text{B20})$$

Taking the maximum with respect to x, y on the left-hand side, we obtain

$$2\alpha(G^{t,s}) \leq \sup\{\|p(t,s) - p'(t,s)\| \mid p_0, p'_0 \in \mathcal{P}\}. \quad (\text{B21})$$

Therefore the definition of weak ergodicity (119) yields (B18).

We assume (B18). For fixed $p_0, q_0 \in \mathcal{P}$, we define the transition probabilities by

$$H = (p_0, q_0, \dots, q_0), \quad (\text{B22})$$

$$F = G^{t,s}H = (p(t,s), q(t,s), \dots, q(t,s)), \quad (\text{B23})$$

where $p(t,s) = G^{t,s}p_0$ and $q(t,s) = G^{t,s}q_0$. From (B2), the coefficient of ergodicity for F is rewritten as

$$\alpha(F) = \frac{1}{2} \sum_{z \in \mathcal{S}} |p(t,s;z) - q(t,s;z)| = \frac{1}{2} \|p(t,s) - q(t,s)\|. \quad (\text{B24})$$

Thus Lemmas B.1 and B.2 yield

$$\|p(t,s) - q(t,s)\| \leq 2\alpha(G^{t,s})\alpha(H) \leq 2\alpha(G^{t,s}). \quad (\text{B25})$$

Taking the sup with respect to $p_0, q_0 \in \mathcal{S}$ and the limit $t \rightarrow \infty$, we obtain

$$\limsup_{t \rightarrow \infty} \{ \|p(t,s) - q(t,s)\|_{p_0, q_0 \in \mathcal{P}} \} \leq 2 \lim_{t \rightarrow \infty} \alpha(G^{t,s}) = 0 \tag{B26}$$

for any $s > 0$. Therefore the inhomogeneous Markov chain generated by $G(t)$ is weakly ergodic.

Next, we prove Theorem 5.1. For this purpose, the following lemma is useful.

Lemma B.5: *Let $a_0, a_1, \dots, a_n, \dots$ be a sequence such that $0 \leq a_i < 1$ for any i .*

$$\sum_{i=0}^{\infty} a_i = \infty \Rightarrow \prod_{i=n}^{\infty} (1 - a_i) = 0. \tag{B27}$$

Proof. Since $0 \leq 1 - a_i \leq e^{-a_i}$, we have

$$0 \leq \prod_{i=n}^m (1 - a_i) \leq \prod_{i=n}^m e^{-a_i} \leq \exp\left(-\sum_{i=n}^m a_i\right). \tag{B28}$$

In the limit $m \rightarrow \infty$, the right-hand side converges to zero because of the assumption $\sum_{i=0}^{\infty} a_i = \infty$. Therefore we obtain (B27).

Proof of Theorem 5.1: We assume that the inhomogeneous Markov chain generated by $G(t)$ is weakly ergodic. Theorem B.4 yields

$$\lim_{t \rightarrow \infty} [1 - \alpha(G^{t,s})] = 1 \tag{B29}$$

for any $s > 0$. Thus, there exists t_1 such that $1 - \alpha(G^{t_1, t_0}) > 1/2$ with $t_0 = s$. Similarly, there exists t_{n+1} such that $1 - \alpha(G^{t_{n+1}, t_n}) > 1/2$ for any $t_n > 0$. Therefore,

$$\sum_{i=0}^n [1 - \alpha(G^{t_{i+1}, t_i})] > \frac{1}{2}(n + 1). \tag{B30}$$

Taking the limit $n \rightarrow \infty$, we obtain (122).

We assume (122). Lemma B.5 yields

$$\prod_{i=n}^{\infty} \{1 - [1 - \alpha(G^{t_{i+1}, t_i})]\} = \prod_{i=n}^{\infty} \alpha(G^{t_{i+1}, t_i}) = 0. \tag{B31}$$

For fixed s and t such that $t > s \geq 0$, we define n and m by $t_{n-1} \leq s < t_n$ and $t_m < t \leq t_{m+1}$. Thus, from Lemma B.2, we obtain

$$\alpha(G^{t,s}) \leq \alpha(G^{t,t_m}) \alpha(G^{t_m, t_{m-1}}) \cdots \alpha(G^{t_{n+1}, t_n}) \alpha(G^{t_n, s}) = \alpha(G^{t,t_m}) \left[\prod_{i=n}^m \alpha(G^{t_{i+1}, t_i}) \right] \alpha(G^{t_n, s}). \tag{B32}$$

In the limit $t \rightarrow \infty$, m goes to infinity and then the right-hand side converges to zero because of (B31). Thus we have

$$\lim_{t \rightarrow \infty} \alpha(G^{t,s}) = 0 \tag{B33}$$

for any s . Therefore, from Theorem B.4, the inhomogeneous Markov chain generated by $G(t)$ is weakly ergodic. □

3. Conditions for strong ergodicity

The goal of this section is to give the proof of Theorem 5.2. Before that, we prove the following theorem, which also provides the sufficient condition for strong ergodicity.

Theorem B.6: *An inhomogeneous Markov chain generated by $G(t)$ is strongly ergodic if there*

exists the transition matrix H on \mathcal{S} such that $H(z,x)=H(z,y)$ for any $x,y,z \in \mathcal{S}$ and

$$\lim_{t \rightarrow \infty} \|G^{t,s} - H\| = 0 \quad (\text{B34})$$

for any $s > 0$.

Proof: We consider $p_0 \in \mathcal{P}$ and $p(t,s)=G^{t,s}p_0$. For fixed $u \in \mathcal{S}$, we define a probability distribution r by $r(z)=H(z,u)$. We find

$$\begin{aligned} \|p(t,s) - r\| &= \sum_{z \in \mathcal{S}} \left| \sum_{x \in \mathcal{S}} G^{t,s}(z,x)p_0(x) - H(z,u) \right| = \sum_{z \in \mathcal{S}} \left| \sum_{x \in \mathcal{S}} [G^{t,s}(z,x) - H(z,u)]p_0(x) \right| \\ &\leq \sum_{z \in \mathcal{S}} \sum_{x \in \mathcal{S}} |G^{t,s}(z,x) - H(z,u)| = \sum_{z \in \mathcal{S}} \sum_{x \in \mathcal{S}} |G^{t,s}(z,x) - H(z,x)| \leq \sum_{x \in \mathcal{S}} \|G^{t,s} - H\| \\ &= |\mathcal{S}| \|G^{t,s} - H\|. \end{aligned} \quad (\text{B35})$$

Taking the sup with respect to $p_0 \in \mathcal{P}$ and using assumption (B34), we obtain

$$\limsup_{t \rightarrow \infty} \{ \|p(t,s) - r\| | p_0 \in \mathcal{P} \} = 0. \quad (\text{B36})$$

Therefore, the inhomogeneous Markov chain generated by $G(t)$ is strongly ergodic. \square

Proof of Theorem 5.2: We assume that the three conditions in Theorem 5.2 hold. Since condition (3) is rewritten as

$$\sum_{x \in \mathcal{S}} \sum_{t=0}^{\infty} |p_t(x) - p_{t+1}(x)| = \sum_{t=0}^{\infty} \|p_t - p_{t+1}\| < \infty, \quad (\text{B37})$$

we have

$$\sum_{t=0}^{\infty} |p_t(x) - p_{t+1}(x)| < \infty \quad (\text{B38})$$

for any $x \in \mathcal{S}$. Thus, the stationary state p_t converges to $p = \lim_{t \rightarrow \infty} p_t$. Now, let us define transition matrices H and $H(t)$ by $H(z,x)=p(z)$ and $H(z,x;t)=p_t(z)$, respectively. For $t > u > s \geq 0$,

$$\|G^{t,s} - H\| \leq \|G^{t,u}G^{u,s} - G^{t,u}H(u)\| + \|G^{t,u}H(u) - H(t-1)\| + \|H(t-1) - H\|. \quad (\text{B39})$$

Thus, we evaluate each term on the right-hand side and show that (B34) holds.

First term. Lemma B.3 yields that

$$\|G^{t,u}G^{u,s} - G^{t,u}H(u)\| \leq \alpha(G^{t,u}) \|G^{u,s} - H(u)\| \leq 2\alpha(G^{t,u}), \quad (\text{B40})$$

where we used $\|G^{u,s} - H(u)\| \leq 2$. Since the Markov chain is weakly ergodic [condition (1)], Theorem B.4 implies that

$$\forall \varepsilon > 0, \quad \exists t_1 > 0, \quad \forall t > t_1: \|G^{t,u}G^{u,s} - G^{t,u}H(u)\| < \frac{\varepsilon}{3}. \quad (\text{B41})$$

Second term. Since $p_t = G(t)p_t$ [condition (2)], we find

$$H(u) = G(u)H(u) = G^{u+1,u}H(u) \quad (\text{B42})$$

and then

$$G^{t,u}H(u) = G^{t,u+1}H(u) = G^{t,u+1}[H(u) - H(u+1)] + G^{t,u+1}H(u+1). \quad (\text{B43})$$

The last term on the right-hand side of the above equation is similarly rewritten as

$$G^{t,u+1}H(u+1) = G^{t,u+2}[H(u+1) - H(u+2)] + G^{t,u+2}H(u+2). \tag{B44}$$

We recursively apply these relations and obtain

$$G^{t,u}H(u) = \sum_{v=u}^{t-2} G^{t,v+1}[H(v) - H(v+1)] + G^{t,t-1}H(t-1) = \sum_{v=u}^{t-2} G^{t,v+1}[H(v) - H(v+1)] + H(t-1). \tag{B45}$$

Thus the second term in (B39) is rewritten as

$$\|G^{t,u}H(u) - H(t-1)\| = \left\| \sum_{v=u}^{t-2} G^{t,v+1}[H(v) - H(v+1)] \right\| \leq \sum_{v=u}^{t-2} \|G^{t,v+1}[H(v) - H(v+1)]\|. \tag{B46}$$

Lemmas B.1 and B.3 yield that

$$\|G^{t,v+1}[H(v) - H(v+1)]\| \leq \|H(v) - H(v+1)\| = \|p_v - p_{v+1}\|, \tag{B47}$$

where we used the definition of $H(t)$. Thus we obtain

$$\|G^{t,u}H(u) - H(t-1)\| \leq \sum_{v=u}^{t-2} \|p_v - p_{v+1}\|. \tag{B48}$$

Since $\sum_{t=0}^{\infty} \|p_t - p_{t+1}\| < \infty$ [condition (3)], for all $\varepsilon > 0$, there exists $t_2 > 0$ such that

$$\forall t > \forall u \geq t_2: \sum_{v=u}^{t-2} \|p_v - p_{v+1}\| < \frac{\varepsilon}{3}. \tag{B49}$$

Therefore

$$\forall \varepsilon > 0, \quad \exists t_2 > 0, \quad \forall t > \forall u \geq t_2: \|G^{t,u}H(u) - H(t-1)\| < \frac{\varepsilon}{3}. \tag{B50}$$

Third term. From the definitions of H and $H(t)$, they clearly satisfy

$$\lim_{t \rightarrow \infty} \|H(t) - H\| = 0, \tag{B51}$$

which implies that

$$\forall \varepsilon > 0, \quad \exists t_3 > 0, \quad \forall t > t_3: \|H(t-1) - H\| < \frac{\varepsilon}{3}. \tag{B52}$$

Consequently, substitution of (B41), (B50), and (B52) into (B39) yields that

$$\|G^{t,s} - H\| < \frac{\varepsilon}{3} + \frac{\varepsilon}{3} + \frac{\varepsilon}{3} < \varepsilon \tag{B53}$$

for all $t > \max\{t_1, t_2, t_3\}$. Since ε is arbitrarily small, (B34) holds for any $s > 0$ and then the given Markov chain is strongly ergodic from Theorem B.6, which completes the proof of the first part of Theorem 5.2.

Next, we assume $p = \lim_{t \rightarrow \infty} p_t$. For any distribution q_0 , we have $Hq_0 = p$ because

$$\sum_{x \in \mathcal{S}} H(z, x)q_0(x) = p(z) \sum_{x \in \mathcal{S}} q_0(x) = p(z). \tag{B54}$$

Thus, we obtain

$$\|q(t, t_0) - p\| = \|(G^{t-t_0} - H)q_0\| \leq \|G^{t-t_0} - H\|. \quad (\text{B55})$$

Hence it holds for the sup with respect to $q_0 \in \mathcal{P}$, which yields (121) in the limit of $t \rightarrow \infty$. Theorem 5.2 is thereby proved. \square

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