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Comparative Study of the Performance of Quantum Annealing and Simulated Annealing

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Abstract

Relations of simulated annealing and quantum annealing are studied by a mapping from the transition matrix of classical Markovian dynamics of the Ising model to a quantum Hamiltonian and vice versa. It is shown that these two operators, the transition matrix and the Hamiltonian, share the eigenvalue spectrum. Thus, if simulated annealing with slow temperature change does not encounter a difficulty caused by an exponentially long relaxation time at a first-order phase transition, the same is true for the corresponding process of quantum annealing in the adiabatic limit. One of the important differences between the classical-to-quantum mapping and the converse quantum-to-classical mapping is that the Markovian dynamics of a short-range Ising model is mapped to a short-range quantum system, but the converse mapping from a short-range quantum system to a classical one results in long-range interactions. This leads to a difference in efficiencies that simulated annealing can be efficiently simulated by quantum annealing but the converse is not necessarily true. We conclude that quantum annealing is easier to implement and is more flexible than simulated annealing. We also point out that the present mapping can be extended to accommodate explicit time dependence of temperature, which is used to justify the quantum-mechanical analysis of simulated annealing by Somma, Batista, and Ortiz. Additionally, an alternative method to solve the non-equilibrium dynamics of the one-dimensional Ising model is provided through the classical-to-quantum mapping.

I. INTRODUCTION

Quantum annealing has been developed as a generic method to solve combinatorial optimization problems using quantum-mechanical fluctuations [1–5]. It is closely related with adiabatic quantum computation [6], which can be regarded as a restricted version of quantum annealing where the time evolution follows the adiabatic condition. Quantum annealing is to be contrasted with simulated annealing, in which classical thermal fluctuations assist the system to explore the phase space toward the optimal solution [7]. A large number of comparative studies of quantum annealing and simulated annealing have been reported from theoretical, numerical, and experimental perspectives, which generally show superiority of quantum annealing over simulated annealing, at least quantitatively [1–4, 8]. An early experimental study of a disordered magnet also revealed faster relaxations toward equilibrium through a quantum path than by a real thermal annealing path [9]. Recent studies concerning the D-Wave machine show mixed results [10–24], and further careful investigations are necessary before firm conclusions are drawn.

The present paper concerns a theoretical analysis to compare quantum annealing and simulated annealing from a very different viewpoint than the above-mentioned studies. Relations between quantum and classical systems have been known for years through the path-integral formulation of quantum mechanics [25] as well as by the Suzuki-Trotter decomposition of the Boltzmann factor of a quantum system [26]. A relatively new development is a mapping of classical Markovian dynamics to a quantum system, and vice versa, in the same spatial dimension [27, 28]. This method was originally proposed in the context of the Rokhsar-Kivelson point of quantum dimer Hamiltonians. Somma *et al.* applied this idea to the analysis of simulated annealing [29] and rederived the result of Geman and Geman [30] for the temperature-annealing schedule through the adiabatic theorem of quantum mechanics. See [31] for a related development. We also refer the reader to a zero-temperature quantum Monte Carlo method employed in [32] for a different type of quantum-to-classical mapping suitable for classical stochastic studies of quantum systems.

Although the work of Somma *et al.* is quite interesting since it uses quantum mechanics to study a purely classical problem, it nevertheless includes a few points that need further scrutiny. First, only the equivalence between the equilibrium state of a classical system and the ground state of a quantum system has been emphasized. However, wider spectra of the

transition matrix and the quantum Hamiltonian should be taken into account to study the detailed behavior of the energy gap/relaxation time at a quantum/classical phase transition. Second, the converse mapping from quantum to classical systems needs to be discussed to complete a comparative study of quantum annealing and simulated annealing, in particular to determine whether or not quantum annealing can perform a wider class problems than simulated annealing does. Third, a relation needs to be established between the classical Markovian dynamics with time-dependent temperature and the time-dependent Schrödinger equation, if we want to know what happens when the temperature changes relatively quickly or when quantum annealing is applied beyond the limit of adiabatic evolution.

The goal of the present paper is to shed new light on the possibilities and limitations of quantum annealing in comparison with simulated annealing and to solve the above-mentioned problems.

This paper is organized as follows. We first review a few basic aspects of Markovian dynamics of the classical Ising model in Sec. II to fix the notation. Then, in Sec. III, we establish a mapping of classical Markovian dynamics to a quantum Hamiltonian. A few examples are given for the one-dimensional case. The converse mapping from quantum to classical systems is given in Sec. IV. Similarities and differences between the classical-to-quantum and quantum-to-classical mappings are discussed. A more general case of explicitly time-dependent temperature is analyzed and the work of Somma *et al.* is discussed in Sec. V. Summary and conclusion are given in the final section.

II. MARKOVIAN DYNAMICS OF THE CLASSICAL ISING MODEL

We briefly summarize the Markovian dynamics of the Ising model to fix the notation. The temperature T, or its inverse β, is assumed to be time-independent until otherwise stated at a later section. The master equation representing the Markovian dynamics is written as

$$\frac{dP_\sigma(t)}{dt} = \sum_{\sigma'} W_{\sigma\sigma'} P_{\sigma'}(t) = \sum_{\sigma'(\neq\sigma)} \Big(W_{\sigma\sigma'} P_{\sigma'}(t) - W_{\sigma'\sigma} P_\sigma(t) \Big), \tag{1}$$

where σ is a set of N Ising spins, $\{\sigma_1, \sigma_2, \cdots, \sigma_N\}$, and $P_\sigma(t)$ is the probability that the system is in the state σ at time t. The Hamiltonian of the Ising model will be denoted as $H_0(\sigma)$. In the context of simulated annealing and quantum annealing, the goal is to find the ground state of $H_0(\sigma)$. The transition probability from σ' to σ is denoted as $W_{\sigma\sigma'}$,

non-vanishing off-diagonal ($\sigma \neq \sigma'$) elements of which satisfy the detailed balance condition,

$$W_{\sigma\sigma'} P^{(0)}_{\sigma'} = W_{\sigma'\sigma} P^{(0)}_{\sigma} \quad \Big(P^{(0)}_{\sigma} = \frac{e^{-\beta H_0(\sigma)}}{Z},\ Z = \sum_{\sigma} e^{-\beta H_0(\sigma)} \Big). \tag{2}$$

We write $\hat{W}$ for the $2^N \times 2^N$ matrix with elements $(\hat{W})_{\sigma\sigma'} = W_{\sigma\sigma'}$. All matrices and vectors will be represented in the σ-basis. The non-vanishing off-diagonal element of $\hat{W}$ can be expressed as

$$W_{\sigma\sigma'} = w_{\sigma\sigma'} e^{-\frac{1}{2}\beta(H_0(\sigma) - H_0(\sigma'))}, \tag{3}$$

where $w_{\sigma\sigma'}$ is symmetric, $w_{\sigma\sigma'} = w_{\sigma'\sigma}$, according to the detailed balance condition (2).

The quantity $w_{\sigma\sigma'}$ can be chosen arbitrarily as long as the resulting $W_{\sigma\sigma'}$ can be regarded as a conditional probability. For example, the Metropolis update rule has

$$w_{\sigma\sigma'} = \min\left(e^{-\frac{1}{2}\beta(H_0(\sigma') - H_0(\sigma))}, e^{\frac{1}{2}\beta(H_0(\sigma') - H_0(\sigma))} \right), \tag{4}$$

and the heat-bath method is realized by

$$w_{\sigma\sigma'} = \frac{1}{e^{-\frac{1}{2}\beta(H_0(\sigma') - H_0(\sigma))} + e^{\frac{1}{2}\beta(H_0(\sigma') - H_0(\sigma))}}. \tag{5}$$

The eigenvalues of the transition matrix $\hat{W}$ are negative semi-definite. The largest eigenvalue is 0 and corresponds to thermal equilibrium. If we denote the eigenvalues as $\lambda_0 = 0 > \lambda_1 > \lambda_2 > \cdots$, a general solution to the master equation (1) is written as

$$P_{\sigma}(t) = \sum_{n=0} a_n e^{-|\lambda_n| t} \psi^{(R,n)}_{\sigma}. \tag{6}$$

Here, $\psi^{(R,n)}_{\sigma}$ is the σ component of the nth right eigenvector $\hat{\psi}^{(R,n)}$ of $\hat{W}$,

$$\hat{W}\hat{\psi}^{(R,n)} = \lambda_n \hat{\psi}^{(R,n)}. \tag{7}$$

In particular, the right eigenvector corresponding to $\lambda_0 = 0$ is

$$\psi^{(R,0)}_{\sigma} = P^{(0)}_{\sigma}. \tag{8}$$

III. QUANTUM HAMILTONIAN DERIVED FROM CLASSICAL DYNAMICS

We now derive a quantum Hamiltonian $\hat{H}$ from the classical transition matrix $\hat{W}$. The original idea comes from Castelnovo *et al.* [28], but we proceed with carefully keeping in mind the correspondence between quantum annealing and simulated annealing.

A. Construction of quantum Hamiltonian

Let us denote by $\hat{H}_0$ the diagonal matrix with $H_0(\sigma)$ as its diagonal elements, $(\hat{H})_{\sigma\sigma} = H_0(\sigma)$. A quantum Hamiltonian is then defined from $\hat{W}$ as

$$\hat{H} = -e^{\frac{1}{2}\beta\hat{H}_0}\hat{W}e^{-\frac{1}{2}\beta\hat{H}_0}. \tag{9}$$

It is straightforward to verify that $\hat{H}$ is real and symmetric, *i.e.* Hermitian, using the detailed balance condition (2). We can therefore regard $\hat{H}$ as the Hamiltonian of a quantum system. The eigenvalue spectrum of $\hat{W}$,

$$\hat{W}\hat{\psi}^{(R,n)} = \lambda_n\hat{\psi}^{(R,n)}, \tag{10}$$

is shared with $\hat{H}$:

$$\hat{H}\hat{\phi}^{(n)} = -e^{\frac{1}{2}\beta\hat{H}_0}\hat{W}\hat{\psi}^{(R,n)} = -\lambda_n\hat{\phi}^{(n)}, \tag{11}$$

where

$$\hat{\phi}^{(n)} = e^{\frac{1}{2}\beta\hat{H}_0}\hat{\psi}^{(R,n)}. \tag{12}$$

Equations (10)-(12) show one-to-one correpondence between the eigenvalues and eigenvectors of $\hat{H}$ and $\hat{W}$, which establishes a classical-to-quantum mapping in the same spatial dimension.

The classical Ising model $\hat{H}_0$ has the relaxation time toward equilibrium as $\tau = 1/|\lambda_1|$ according to Eq. (6). If $\hat{H}_0$ has a phase transition at a temperature T_c, the relaxation time diverges at T_c as a function of the system size N. If the transition is of second order, τ diverges polynomially $\tau \propto N^a$ $(a > 0)$, and the divergence is exponential $\tau \propto e^{bN}$ $(b > 0)$ at a first-order transition. Correspondingly, the quantum system $\hat{H}$ has a quantum phase transition at the system parameter determined by the correspondence (9). The energy gap $\Delta = |\lambda_1|$ between the ground state (whose energy is $\lambda_0 = 0$) and the first excited state closes polynomially $\Delta \propto N^{-a}$ at a second-order transition and exponentially $\Delta \propto e^{-bN}$ at a first-order transition.

It should be kept in mind that these discussions apply to the case of time-independent temperature for the classical dynamics and stationary states for the quantum system. This means that, in the context of simulated annealing, the system is supposed to evolve in quasi-equilibrium, *i.e.* the temperature changes very slowly such that the system stays very close

to thermal equilibrium. The corresponding quantum system is driven adiabatically, and the system is kept infinitesimally close to the instantaneous stationary state. The case with strong time dependence of temperature in simulated annealing and non-adiabatic evolution in quantum annealing will be analyzed in Sec. V.

The normalized ground-state wave function of $\hat{H}$ is written as

$$\hat{\phi}^{(0)} = \frac{e^{-\frac{1}{2}\beta\hat{H}_0}}{\sqrt{Z}} \sum_{\sigma} |\sigma\rangle, \tag{13}$$

according to Eqs. (8) and (12). If we write $\langle\hat{Q}\rangle_0$ for the expectation value of a matrix $\hat{Q}$ diagonal in the σ-basis by the ground-state wave function (13), this expectation value is equal to the thermal expectation value of the corresponding classical system,

$$\langle\hat{Q}\rangle_0 = \frac{1}{Z}\sum_{\sigma}\langle\sigma|\hat{Q}|\sigma\rangle e^{-\beta H_0(\sigma)}. \tag{14}$$

B. Explicit formulas for the quantum Hamiltonian

We next derive the explicit form of $\hat{H}$. Non-vanishing off-diagonal elements are

$$(\hat{H})_{\sigma\sigma'} = H_{\sigma\sigma'} = -e^{\frac{1}{2}\beta H_0(\sigma)} W_{\sigma\sigma'} e^{-\frac{1}{2}\beta H_0(\sigma')} = -w_{\sigma\sigma'} \ (< 0). \tag{15}$$

Diagonal elements are

$$H_{\sigma\sigma} = -W_{\sigma\sigma} = \sum_{\sigma'(\neq\sigma)} W_{\sigma'\sigma} = \sum_{\sigma'(\neq\sigma)} w_{\sigma'\sigma} e^{-\frac{1}{2}\beta(H_0(\sigma')-H_0(\sigma))}, \tag{16}$$

where the condition of probability conservation, $\sum_{\sigma'} W_{\sigma'\sigma} = 0$, has been used. These equations lead to the following form of $\hat{H}$, using $w_{\sigma\sigma'} = w_{\sigma'\sigma}$,

$$\hat{H} = \frac{1}{2}\sum_{\sigma\sigma'} w_{\sigma\sigma'}\left(e^{-\frac{1}{2}\beta(H_0(\sigma')-H_0(\sigma))}|\sigma\rangle\langle\sigma| + e^{\frac{1}{2}\beta(H_0(\sigma')-H_0(\sigma))}|\sigma'\rangle\langle\sigma'| - |\sigma'\rangle\langle\sigma| - |\sigma\rangle\langle\sigma'|\right) \tag{17}$$

$$= \sum_{\sigma}\sum_{\sigma'} w_{\sigma\sigma'}\left(e^{-\frac{1}{2}\beta(H_0(\sigma')-H_0(\sigma))}|\sigma\rangle\langle\sigma| - |\sigma'\rangle\langle\sigma|\right). \tag{18}$$

The second term of this last expression represents a transverse-field term if σ' is different from σ only by a single-spin flip because the transverse-field operator σ_i^x flips a single spin at site i. The first term is then a diagonal interaction of a usual classical Ising model with interaction range comparable to that of the original classical Ising model because the quantity in the exponent, $H_0(\sigma') - H_0(\sigma)$, includes only local interactions if σ' and σ are

different at a single site. Examples will be given below. It has hence been shown that Markovian dynamics of a classical Ising model with short-range interactions is equivalent to the stationary-state quantum mechanics of a transverse-field Ising model with comparable interaction range. It is concluded that simulated annealing under quasi-static condition can be exactly mapped to quantum annealing under adiabatic condition. In other words, if a given combinatorial optimization problem expressed in terms of a short-range Ising model can be solved efficiently by simulated annealing in the sense that no problematic first-order phase transition occurs in the process, the same is always possible by quantum annealing. In this sense, the efficiency of quantum annealing is at least comparable to that of simulated annealing.

C. One-dimensional Ising model

As a concrete example, let us discuss the simple case of the one-dimensional Ising model with nearest-neighbor interactions under a periodic boundary condition. The dynamics is supposed to proceed under single-spin flip processes. Since σ' is different from σ only at a site, which is chosen as site j,

$$H_0(\sigma') - H_0(\sigma) = 2J\sigma_j(\sigma_{j-1} + \sigma_{j+1}) = -2H_j, \tag{19}$$

where the final equality defines H_j.

First, for the heat-bath dynamics with Eq. (5), the diagonal and off-diagonal coefficients in Eq. (18) are

$$w_{\sigma\sigma'} e^{-\frac{1}{2}\beta(H_0(\sigma')-H_0(\sigma))} = \frac{e^{\beta H_j}}{e^{\beta H_j} + e^{-\beta H_j}}, \quad w_{\sigma\sigma'} = \frac{1}{e^{\beta H_j} + e^{-\beta H_j}}. \tag{20}$$

It is relatively straightforward to evaluate these expressions using Eq. (19) to find the following formula of the quantum Hamiltonian,

$$\hat{H} = \frac{N}{2} - \frac{1}{2}\tanh 2K \sum_{j=1}^{N} \sigma_j^z \sigma_{j+1}^z - \frac{1}{2\cosh 2K} \sum_{j=1}^{N} \left(\cosh^2 K - \sinh^2 K\, \sigma_{j-1}^z \sigma_{j+1}^z \right) \sigma_j^x, \tag{21}$$

where $K = \beta J$, and σ_j has been replaced by the Pauli matrix σ_j^z. Equation (21) is a one-dimensional transverse-field Ising model with nearest-neighbor interactions. In the high-temperature limit $K = 0$, Eq. (21) reduces to a non-interacting transverse-field Hamiltonian,

$$\hat{H} = \frac{N}{2} - \frac{1}{2} \sum_{j=1}^{N} \sigma_j^x, \tag{22}$$

whose ground state is completely disordered in the σ^z-basis. This is exactly the initial state of quantum annealing. In the opposite limit $K \to \infty$,

$$\hat{H} = \frac{N}{2} - \frac{1}{2}\sum_{j=1}^{N} \sigma_j^z \sigma_{j+1}^z - \frac{1}{4}\sum_{j=1}^{N} \left(1 - \sigma_{j-1}^z \sigma_{j+1}^z\right)\sigma_j^x. \tag{23}$$

The state with all σ_j^z having eigenvalue 1 is an eigenstate of this Hamiltonian. The Perron-Frobenius theorem assures that this is the unique ground state. Thus, the quasi-static simulated annealing from high temperature to zero temperature has been mapped to the behavior of the quantum system starting from the disordered state and ending up in the ordered state after an adiabatic evolution.

The usual transverse-field Ising model with the Hamiltonian

$$\hat{H} = -J\sum_{j} \sigma_j^z \sigma_{j+1}^z - \Gamma \sum_{j} \sigma_j^x \tag{24}$$

has a phase transition at $\Gamma/J = 1$. In contrast, the present model (21) with the additional term involving $\sigma_{j-1}^z \sigma_{j+1}^z$ in front of σ_j^x has no phase transition between the two limiting cases of Eqs. (22) and (23) because the original classical Ising model has no finite-temperature transition. We thus conclude that the additional term in Eq. (21) having $\sigma_{j-1}^z \sigma_{j+1}^z$ drives the system away from the quantum critical point, thus realizing a smooth (non-singular) process in the course of quantum annealing. In Eq. (21), the coefficient of the transverse-field term is small ($\cosh^2 K - \sinh^2 K = 1$) when the local spin alignment is ferromagnetic $\sigma_{j-1}^z \sigma_{j+1}^z = 1$ and is large ($\cosh^2 K + \sinh^2 K > 1$) when the spin alignment is different from the target state $\sigma_{j-1}^z \sigma_{j+1}^z = -1$. This means that the local, adaptive change of the coefficient of transverse field is effective to avoid problematic quantum phase transitions in quantum annealing. Although this lesson has been extracted from the simple one-dimensional Ising model, it may be worth considering to implement a similar process of adaptive change of the coefficient of the quantum driving term in more complicated cases when one encounters difficulties in quantum annealing.

Another comment concerns the exact solution of the quantum system (21). This Hamiltonian can be diagonalized by the Jordan-Wigner transformation as will be discussed in the next section. This serves as an additional route to the complete solution of the dynamics of the one-dimensional classical Ising model pioneered by Glauber [33].

The Metropolis method with Eq. (4) can be analyzed in the same manner. The resulting

quantum Hamiltonian is

$$\hat{H} = \frac{N}{4}(3+e^{-4K}) \\ -\frac{1}{4}(1-e^{-4K})\sum_{j=1}^{N}\left(2\sigma_j^z\sigma_{j+1}^z+\sigma_{j-1}^z\sigma_{j+1}^z\right)-\frac{1}{2}(1+e^{-2K})\sum_{j=1}^{N}\left(1-\tanh K\,\sigma_{j-1}^z\sigma_{j+1}^z\right)\sigma_j^x. \tag{25}$$

We again find that the coefficient of the transverse-field term is adaptively changed according to the alignment of the local spins, $\sigma_{j-1}^z\sigma_{j+1}^z$. Notice that the diagonal interaction term now involves next-nearest-neighbor interactions. It is of course still of short-range, but this example shows that the range generally changes slightly.

It is also possible to implement random interactions,

$$H_0(\sigma) = -\sum_{j=1}^{N} J_j\sigma_{j-1}\sigma_j. \tag{26}$$

The final expression of the Hamiltonian for the heat-bath update rule is then

$$\hat{H} = \frac{N}{2} - \frac{1}{2}\sum_j \frac{c_j s_j}{c_j^2c_{j+1}^2-s_j^2s_{j+1}^2}\sigma_{j-1}^z\sigma_j^z - \frac{1}{2}\sum_j \frac{c_{j+1}s_{j+1}}{c_j^2c_{j+1}^2-s_j^2s_{j+1}^2}\sigma_j^z\sigma_{j+1}^z \tag{27}$$

$$-\frac{1}{2}\sum_j\left(\frac{c_jc_{j+1}}{c_j^2c_{j+1}^2-s_j^2s_{j+1}^2}-\frac{s_js_{j+1}}{c_j^2c_{j+1}^2-s_j^2s_{j+1}^2}\sigma_{j-1}^z\sigma_{j+1}^z\right)\sigma_j^x, \tag{28}$$

where $c_j = \cosh\beta J_j$ and $s_j = \sinh\beta J_j$. This Hamiltonian can be reduced to a quadratic form of Fermion by the Jordan-Wigner transformation. It is not possible to completely diagonalize the quadratic form using Fourier transformation due to the lack of translational invariance. The quadratic expression nevertheless would give us a tool to analyze the classical dynamics of the one-dimensional disordered Ising model by numerical diagonalization of large systems.

D. Non-equilibrium dynamics of the one-dimensional Ising model

The quantum Hamiltonian of Eq. (21) representing the heat-bath dynamics of the one-dimensional Ising model can be solved exactly by an application of the Jordan-Wigner transformation. Before it is applied, we transform the Hamiltonian to a more customary form by performing $\pi/2$ rotations about the y-axis so that $x \to z$ and $z \to -x$. Following this transformation, local fields are along the z-direction, coupling to σ_j^z, two-body interactions are proportional to $\sigma_{j-1}^x\sigma_j^x$, and the three-body terms are $\propto \sigma_{j-1}^x\sigma_j^z\sigma_{j+1}^x$.

We introduce new operators

$$a_j = \frac{\sigma_j^x - i\sigma_j^y}{2} \prod_{\ell=1}^{j-1} (-\sigma_\ell^z) \quad \text{and} \quad a_j^\dagger = \frac{\sigma_j^x + i\sigma_j^y}{2} \prod_{\ell=1}^{j-1} (-\sigma_\ell^z)\,, \tag{29}$$

which can be verified to obey the Fermionic anti-commutation relations: $\{a_j, a_k^\dagger\} = \delta_{jk}$ and $\{a_j, a_k\} = \{a_j^\dagger, a_k^\dagger\} = 0$. With this substitution, the Hamiltonian (21) may be rewritten as

$$\hat{H} = C + J_1 \sum_{j=1}^{N} \big(a_j - a_j^\dagger\big)\big(a_{j+1} + a_{j+1}^\dagger\big) + J_2 \sum_{j=1}^{N} \big(a_{j-1} - a_{j-1}^\dagger\big)\big(a_{j+1} + a_{j+1}^\dagger\big) - \Gamma \sum_{j=1}^{N} \big(a_j^\dagger a_j - a_j a_j^\dagger\big), \tag{30}$$

with $C = N/2$, $J_1 = (\tanh 2K)/2$, $J_2 = \sinh^2 K/(2\cosh 2K)$, and $\Gamma = \cosh^2 K/(2\cosh 2K)$. Interestingly, because Fermionic annihilation and creation operators (29) carry a chain product $\prod_\ell(-\sigma_\ell^z)$, the three-body terms of the form $\sigma_{j-1}^x \sigma_j^z \sigma_{j+1}^x$ become quadratic after the transformation. For the Metropolis dynamics, the quantum Hamiltonian Eq. (25) contains also terms $\propto \sigma_{j-1}^x \sigma_{j+1}^x$ giving rise to quartic terms. The exact analytical solution is possible only for the heat-bath update rule.

Because of the way the boundary terms $\sigma_N^x \sigma_1^x$, $\sigma_N^x \sigma_1^z \sigma_2^x$, and $\sigma_{N-1}^x \sigma_N^z \sigma_1^x$ are treated in applying the transformation (29), boundary conditions require special treatments. For states with even number of Fermions, anti-periodic boundary conditions ($a_{N+k} \equiv -a_k$) should be used in Eq. (30); periodic boundary conditions ($a_{N+k} \equiv a_k$) will be used for states with odd number of Fermions.

Diagonalization of Eq. (30) is performed using a variant of the Bogolyubov transformation. The quadratic form Eq. (30) can be written in a matrix form as

$$\begin{pmatrix} \mathbf{a}^\dagger & \mathbf{a} \end{pmatrix} \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ -\mathbf{B} & -\mathbf{A} \end{pmatrix} \begin{pmatrix} \mathbf{a} \\ \mathbf{a}^\dagger \end{pmatrix}, \tag{31}$$

where the only non-zero elements of matrices $\mathbf{A}$ and $\mathbf{B}$ are

$$A_{j,j} = -\Gamma, \quad A_{j,j\pm1} = -\tfrac{1}{2} J_1, \quad A_{j,j\pm2} = -\tfrac{1}{2} J_2, \tag{32}$$

$$B_{j,j\pm1} = \mp\tfrac{1}{2} J_1, \quad B_{j,j\pm2} = \mp\tfrac{1}{2} J_2. \tag{33}$$

Here we assume that matrix indices are periodic (e.g. $B_{1,-1} \equiv B_{1,N-1}$). Matrix (31) can be diagonalized in terms of new quasiparticles with annihilation/creation operators γ_j, $\gamma_j^\dagger$ connected to a_j, $a_j^\dagger$ via a linear transformation

$$\begin{pmatrix} \mathbf{a} \\ \mathbf{a}^\dagger \end{pmatrix} = \begin{pmatrix} \mathbf{U} & \mathbf{V} \\ \mathbf{V} & \mathbf{U} \end{pmatrix} \begin{pmatrix} \boldsymbol{\gamma} \\ \boldsymbol{\gamma}^\dagger \end{pmatrix}, \tag{34}$$

so that

$$\hat{H} = \begin{pmatrix} \boldsymbol{\gamma}^\dagger & \boldsymbol{\gamma} \end{pmatrix} \begin{pmatrix} \boldsymbol{\epsilon} & \mathbf{0} \\ \mathbf{0} & -\boldsymbol{\epsilon} \end{pmatrix} \begin{pmatrix} \boldsymbol{\gamma} \\ \boldsymbol{\gamma}^\dagger \end{pmatrix} \equiv \sum_\alpha \epsilon_\alpha \left(\gamma_\alpha^\dagger \gamma_\alpha - \gamma_\alpha \gamma_\alpha^\dagger \right) \tag{35}$$

Lastly, we perform another transformation

$$\begin{pmatrix} \mathbf{F} \\ \mathbf{G} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbf{1} & \mathbf{1} \\ -\mathbf{1} & \mathbf{1} \end{pmatrix} \begin{pmatrix} \mathbf{U} \\ \mathbf{V} \end{pmatrix} \tag{36}$$

to obtain a particularly compact formulation. Single-particle energies corresponding to diagonal elements of $\boldsymbol{\epsilon}$ satisfy the eigenvalue equation,

$$\begin{aligned} \Gamma f_j + J_1 f_{j+1} + J_2 f_{j+2} &= \epsilon g_j \\ \Gamma g_j + J_1 g_{j-1} + J_2 g_{j-2} &= \epsilon f_j, \end{aligned} \tag{37}$$

where f_j and g_j are, respectively, columns of $\mathbf{F}$ and $\mathbf{G}$. Solutions to Eq. (37) can be sought in the form $f_j = f e^{ipj}, g_j = g e^{ipj}$, where p is the momentum: $p = \pi(2k+1)/N$ for a sector with even number of Fermions and $p = 2\pi k/N$ for the odd sector ($k = 0, 1, \ldots, N-1$). From the vanishing condition of the determinant for the system above, we obtain

$$\epsilon_p^2 = \left| \Gamma + J_1 e^{ip} + J_2 \mathrm{e}^{2ip} \right|^2 = \frac{1}{4} \left(1 + \tanh 2K \cdot \cos p \right)^2 . \tag{38}$$

No single-particle states with positive energies are occupied in the ground state. The ground-state energy is $E_0 = C - \sum_p \epsilon_p$ which is trivially verified to be zero as should be expected. Energies of excited states can be written as

$$E_{p_1, \ldots, p_\nu} = 2\epsilon_{p_1} + 2\epsilon_{p_2} + \cdots + 2\epsilon_{p_\nu}, \tag{39}$$

corresponding to ν excitations with momenta $p_1, \ldots, p_\nu$ chosen from the appropriate set, depending on the parity of ν. This additive form is in general agreement with the original analysis by Glauber who used a different technique to find the spectrum [33]. In the more general case of random interactions, nearest-neighbor and next-nearest-neighbor couplings become site-dependent. Single-particle energies are easily obtained numerically by diagonalizing a sparse matrix.

From Eqs. (38) and (39) we see that the gap remains finite in the thermodynamic limit $\Delta = E_{\min} = 1 - \tanh 2K > 0$ at non-zero temperature, consistent with a lack of phase transition for the classical model.

IV. QUANTUM HAMILTONIAN TO CLASSICAL DYNAMICS

The next step is to find a converse mapping from a quantum Hamiltonian to classical dynamics, again following Castelnovo *et al* [28].

Suppose we are given a quantum Hamiltonian $\hat{H}$, whose ground-state energy is chosen to be 0 by a shift of the energy standard, $\hat{H}\hat{\phi}^{(0)} = 0$. In order to derive the Markovian dynamics of a classical Ising model from the quantum Hamiltonian $\hat{H}$, we assume that this $\hat{H}$ is represented in the basis to diagonalize $\{\sigma_i^z\}_i$ and also that off-diagonal elements are negative semi-definite, $H_{\sigma\sigma'} \leq 0$ $(\sigma \neq \sigma')$. Then, according to the Perron-Frobenius theorem applied to $\hat{H}' = -\hat{H}$, the eigenvector $\hat{\phi}^{(0)}$ of $\hat{H}'$ for the largest eigenvalue is not degenerate and all its elements can be chosen to be positive. This allows us to take the logarithm of each element to define the classical Ising model,

$$H_0(\sigma) = -2 \log \phi_\sigma^{(0)}. \tag{40}$$

This definition is motivated by the opposite mapping (13) up to a constant. Then, the matrix defined by

$$\hat{W} = -e^{-\frac{1}{2}\hat{H}_0} \hat{H} e^{\frac{1}{2}\hat{H}_0} \tag{41}$$

satisfies the following conditions required for a transition matrix of classical dynamics,

$$W_{\sigma\sigma'} \geq 0 \quad (\sigma \neq \sigma') \tag{42}$$

$$(1, 1, 1, \cdots, 1)\hat{W} = 0 \tag{43}$$

$$\hat{W} e^{-\beta \hat{H}_0} \sum_\sigma |\sigma\rangle = 0 \tag{44}$$

$$W_{\sigma\sigma'} e^{-H_0(\sigma')} = W_{\sigma'\sigma} e^{-H_0(\sigma)}. \tag{45}$$

Equation (42) follows from $H_{\sigma\sigma'} \leq 0$. Equation (43) for the conservation of probability comes from

$$\sum_\sigma W_{\sigma\sigma'} = -\sum_\sigma e^{-\frac{1}{2}H_0(\sigma)} H_{\sigma\sigma'} e^{\frac{1}{2}H_0(\sigma')} = -\sum_\sigma \phi_\sigma^{(0)} H_{\sigma\sigma'} e^{\frac{1}{2}H_0(\sigma')} = 0, \tag{46}$$

where we have used $\hat{H}\hat{\phi}^{(0)} = 0$. Equation (44) for equilibrium is due to $\hat{H}\hat{\phi}^{(0)} = 0$. Finally, Eq. (45) can be derived from Eq. (41).

A quantum-to-classical mapping has thus been established. An important difference from the opposite classical-to-quantum mapping is the range of interactions in the resulting

classical Hamiltonian. To accommodate the values of $\phi_\sigma^{(0)}$ for all spin configurations of $\sigma = (\sigma_1, \cdots, \sigma_N)$, the Hamiltonian $H_0(\sigma)$ of Eq. (40) should be expressed as a linear combination of all possible products and sums of spin variables,

$$H_0(\sigma) = J^{(0)} + \sum_i J_i^{(1)} \sigma_i + \sum_{i,j} J_{ij}^{(2)} \sigma_i \sigma_j + \sum_{ijk} J_{ijk}^{(3)} \sigma_i \sigma_j \sigma_k + \cdots + J^{(N)} \sigma_1 \sigma_2 \cdots \sigma_N. \quad (47)$$

By relating this expression with $\phi_\sigma^{(0)}$ following Eq. (40) and assigning all possible values of σ to Eq. (40), we obtain a set of linear equations for the 2^N coefficients $J^{(0)}, \{J_i^{(1)}\}_i, \cdots, J^{(N)}$. Its solution generally has non-vanishing values of all those coefficients. This means that the Hamiltonian H_0 has very complicated multibody long-range interactions as given in Eq. (47) even if the original quantum Hamiltonian $\hat{H}$ has only short-range interactions. Although the eigenvalues and eigenstates are shared by the quantum $\hat{H}$ and the classical $\hat{W}$, an implementation of the classical dynamics in simulated annealing is actually inefficient due to the complicated interactions. This is in marked contrast with the opposite classical-to-quantum mapping, where short-range interactions are mapped to short-range interactions.

Another point to notice is the constraint of negative semi-definiteness of the off-diagonal elements, $H_{\sigma\sigma'} \leq 0$. This is necessary for $w_{\sigma\sigma'}$ to be positive as required for a transition matrix. This condition excludes, for example, the interesting case of an antiferromagnetic fluctuation term $\propto (\sum_i \sigma_i^x)^2$ with a positive coefficient in addition to the usual transverse-field term with a negative coefficient in $\hat{H}$, which has been shown to be effective to remove problematic first-order quantum phase transitions [34, 35].

It is possible to devise a quantum-to-classical mapping without the above-mentioned negative semi-definiteness of off-diagonal elements [28]. However, in such a case, it is necessary to choose the eigenstates of $\hat{H}$ as the basis of matrix representation to carry through the mapping, which makes it difficult to interpret the resulting classical Hamiltonian as an Ising model.

V. TIME-DEPENDENT TEMPERATURE

If the temperature has explicit dependence on time as is the case in most simulated annealing applications, the transition matrix also has time dependence. This section is devoted to classical-to-quantum correspondence in such a case

A. Classical to quantum mapping

The master equation with time-dependent transition matrix is written as

$$\frac{d\hat{P}(t)}{dt} = \hat{W}(t)\hat{P}(t), \tag{48}$$

where $\hat{P}(t)$ is a vector with element $(\hat{P}(t))_\sigma = P_\sigma(t)$. The corresponding quantum system is constructed as

$$\hat{H}(t) = -e^{\frac{1}{2}\beta(t)\hat{H}_0}\hat{W}(t)e^{-\frac{1}{2}\beta(t)\hat{H}_0}. \tag{49}$$

If we introduce a wave function as

$$\hat{\phi}(t) = e^{\frac{1}{2}\beta(t)\hat{H}_0}\hat{P}(t), \tag{50}$$

the master equation (48) is rewritten as

$$-\frac{d\hat{\phi}(t)}{dt} = \left(\hat{H}(t) - \frac{1}{2}\dot{\beta}(t)\hat{H}_0\right)\hat{\phi}(t). \tag{51}$$

This is regarded as an imaginary-time Schrödinger equation: If we rewrite the time as $t \to it$ in the time-derivative on the left-hand side, the usual form of the Schrödinger equation results,

$$i\frac{d\hat{\phi}(t)}{dt} = \left(\hat{H}(t) - \frac{1}{2}\dot{\beta}(t)\hat{H}_0\right)\hat{\phi}(t). \tag{52}$$

Equations (51) and (52) show that an additional term proportional to the time derivative of the inverse temperature is to be appended to the quantum Hamiltonian to accommodate explicit time dependence of temperature in the classical-to-quantum mapping.

B. Convergence condition of simulated annealing

Somma *et al.* [29] discussed the convergence condition that the temperature as a function of time, $T(t)$, should satisfy in simulated annealing for the system to reach the ground state. They used the classical-to-quantum mapping without explicit time dependence of temperature as developed in Sec. III, though in a slightly different form as will be discussed below. Then they applied the adiabatic theorem to the quantum system $\hat{H}$ and derived a result that is essentially equal to that of Geman and Geman [30], $\beta(t) \propto \log t/pN$, where p is an $\mathcal{O}(1)$ constant. We discuss here a few problems in their analysis and show that their result turns out to be justifiable by appropriately amending their argument.

First, the adiabatic theorem of quantum mechanics is derived from the time-dependent Schrödinger equation, but they did not discuss explicitly the relation between the original classical master equation, which governs simulated annealing, and the Schrödinger equation. Our result in Eq. (51) indicates that the master equation is written as an imaginary-time Schrödinger equation, not the usual real-time Schrödinger equation. It has, nevertheless, been shown [8] that the adiabatic theorem holds in the same form also for the imaginary-time Schrödinger equation, which validates their analysis.

The second point concerns the additional term, $-\frac{1}{2}\dot{\beta}(t)\hat{H}_0$. Somma *et al.* did not take this term into account. However, according to their result, $\beta(t) \propto \log t/(pN)$, the additional is inversely proportional to the system size and thus can be neglected in the limit of large system size. This serves as an *a posteriori* justification of their analysis using only the $\hat{H}$ term.

The final comment is on the choice of the symmetric part of the transition matrix, $w_{\sigma\sigma'}$, which they chose as $w_{\sigma\sigma'} = e^{-pN}$, where $p \approx \max_j |H_j|$. This is allowed as it does not violate the conditions that the transition matrix should satisfy. However, this choice of $w_{\sigma\sigma'}$ is different from the commonly-used heat-bath and Metropolis methods, which have explicit dependence on σ and σ'. This latter dependence is reflected in the dependence on $\sigma^z_{j-1}\sigma^z_{j+1}$ of the transverse-field term in Eqs. (21) and (25). Although it may happen that the final conclusion of Somma *et al.*, $\beta(t) \propto \log t/(pN)$, does not depend upon the specific choice of the transition matrix, it is an interesting problem to complete their analysis for more common types of $w_{\sigma\sigma'}$.

VI. SUMMARY AND CONCLUSION

We have analyzed the framework of classical-quantum correspondence of Castelnovo *et al.* and have applied it to simulated annealing of the classical Ising model to study its relation with quantum annealing using the transverse-field Ising model. It has been shown that the eigenvalue spectrum is shared by the transition matrix of the classical dynamics and the corresponding quantum Hamiltonian. It then follows that the existence or absence of a phase transition and its order are shared by the classical and quantum systems. An important consequence is that simulated annealing of the classical Ising model and quantum annealing by the corresponding transverse-field Ising model have the same degree of efficiency

as long as both are run very slowly in the change of relevant parameters, that is, in quasi-equilibrium classically and adiabatically in the quantum case. Thus, simulated annealing and quantum annealing can be regarded as equivalent if the transition matrix and the quantum Hamiltonian are chosen to satisfy the key relation of Eq. (9). The classical-to-quantum mapping has also been shown to provide an alternative solution to the non-equilibrium dynamics of the one-dimensional Ising model.

The classical and quantum approaches, nevertheless, have an important difference in the range of interactions in the Hamiltonians. The classical-to-quantum mapping yields short-range interactions for the quantum Hamiltonian if the range is short in the classical case, but the converse is not true. The classical Hamiltonian generated from a quantum system has in general very complicated many-body long-range interactions. The range of interactions affects the efficiency in implementation of annealing, and we may conclude that quantum annealing has a wider range of practical usefulness. This conclusion is reinforced by the restriction of the sign of matrix elements of quantum Hamiltonian that can be mapped to classical dynamics.

System parameters such as the temperature are changed relatively rapidly in practical applications of simulated annealing and quantum annealing. We have formulated a classical-to-quantum mapping to cover such a case. The Markovian dynamics has been shown to be mapped to an imaginary-time Schrödinger dynamics with an additional term proportional to the time-derivative of the inverse temperature. This formulation would serve as a tool to analyze the performance of rapid processes.

An overall conclusion is that simulated annealing and quantum annealing share common aspects in their essential part in spite of the complete difference of classical and quantum processes. Quantum annealing, nevertheless, covers a wider range of efficient implementation.

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