Residual Energies after Slow Quantum Annealing

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Features of the residual energy after the quantum annealing are investigated. The quantum annealing method exploits quantum fluctuations to search the ground state of classical disordered Hamiltonian. If the quantum fluctuation is reduced sufficiently slowly and linearly by the time, the residual energy after the quantum annealing falls as the inverse square of the annealing time. We show this feature of the residual energy by numerical calculations for small-sized systems and derive it on the basis of the quantum adiabatic theorem.

Combinatorial optimization problems have presented a variety of challenges in vast area of sciences. Since the number of combination usually explodes exponentially with the number of elements, they becomes unsolvable for large elements by means of checking all of the combinations. In particular, no algorithm suitable for conventional computers has been discovered to solve the non-deterministic polynomial-time (NP) problem in a time of the polynomial order of elements. The quantum annealing method has been proposed for such an intractable problem\(^1\).

The combinatorial optimization problem is often represented in terms of a classical Hamiltonian, such as a random Ising model. What we do for the problem is to find the ground state of the classical Hamiltonian. In the quantum annealing method, a quantum Hamiltonian is introduced for a classical problem. Namely quantum fluctuations are exploited to search the solution. The principle of the quantum annealing method provides us a novel algorithm for quantum computation\(^2\),\(^3\). In fact, fundamental experiments of quantum computation have been carried out\(^4\). Another importance of this method lies in implementation by conventional classical computers. The thermal (simulated) annealing is an well-known method for classical computers\(^5\). It has been shown experimentally that the quantum annealing surpasses the thermal annealing\(^6\). Hence the algorithm of quantum annealing in classical computers is expected to reduce the complexity of the problem. However it has been in question whether the exponential scaling law of the complexity regarding the problem size is replaced by the power law in the quantum algorithm. It is a great issue whether this algorithm can transform NP problems to polynomial-time solvable problems.

In this letter, we investigate the asymptotic behavior of the residual energy for long annealing time. The residual energy is defined by the energy difference between the solution by means of an algorithm and the true one. If the scaling law of the asymptotic behavior with respect to the process time is unveiled, it becomes clear how efficiently the method leads us to the true solution. For instance, the residual energy after the thermal annealing decreases with the annealing (process) time as \(\Delta E \sim 1/(\ln \tau)^\zeta\) with \(1 \leq \zeta \leq 2\),\(^6\),\(^9\) and thus extraordinarily long time is needed to obtain a closely approximate solution. The logarithmic scaling law of the residual energy reminds us of the exponential law of the complexity. For the quantum annealing method, an earlier work has estimated that the residual energy falls as \(\Delta E \sim 1/(\ln \tau)^\zeta\) with \(\zeta \sim 6\).\(^6\) However no one has confirmed numerically this scaling law of the residual energy after the quantum annealing.

We examine the scaling law numerically in the present work. The result shows that the residual energy obeys power law, \(\Delta E \sim 1/\tau^\zeta\) with \(\zeta \sim 2\) in the long \(\tau\) limit, in contrast to the earlier prediction. This asymptotic behavior is derived from the adiabatic theorem of the quantum mechanics.

Let us consider a time-dependent Hamiltonian \(H(t)\) which consists of the classical Hamiltonian \(H_0\) and the tunneling Hamiltonian \(H_T\). The classical Hamiltonian denotes the energy function representing a combinatorial optimization problem, while the tunneling Hamiltonian is responsible for quantum effects. Detailed forms of these Hamiltonians are written later. We assume the time dependence of the Hamiltonian as follows. The tunneling term dominates the Hamiltonian at the initial time, and it vanishes at the final time. The Hamiltonian changes continuously in between the initial and final times. There is no symmetry at any time which brings about degenerate ground states of the Hamiltonian. The quantum state vector stands for a solution of the combinatorial optimization problem in the quantum annealing method. The evolution of the state vector denoted by \(|\Psi(t)\rangle\) with the time \(t\) is determined by the Schrödinger equation,

\[
i \frac{d}{dt} |\Psi(t)\rangle = H(t)|\Psi(t)\rangle. \tag{1}\]

We assume that the initial state is adjusted to the ground state of the initial Hamiltonian. It follows that the approximate solution is obtained as the state vector after an evolution with the time when the Hamiltonian coin-
cides with the classical Hamiltonian. This is the process of the quantum annealing method.

The validity of the quantum annealing method originates in the adiabatic evolution of quantum mechanical states. The state evolving from the eigen state of the Hamiltonian almost retains being the eigen state. This dynamical process goes on when the change in the Hamiltonian with the time is sufficiently slow and the associated state is non-degenerate at any time. Hence the state starting from the ground state of the initial Hamiltonian arrives at an approximate ground state of the Hamiltonian at the final time. In the quantum annealing method, the final Hamiltonian is set to the classical Hamiltonian. Thus the state vector at the final time becomes an approximate ground state of the classical Hamiltonian, namely the solution of the combinatorial optimization problem.

Although we have imposed assumptions on the time dependence of the Hamiltonian, there are some degrees of freedom on that. We settle it as follows. First we denote an annealing time by \( \tau \) and consider the time period \([0, \tau]\). Taking into account the assumptions in the above, it is favored that the Hamiltonian at the initial time is identical to the tunneling Hamiltonian. This is because it is usually easy to make the exact ground eigen state of the tunneling Hamiltonian as will be seen later. Moreover it is natural to let the Hamiltonian depend on the time linearly, since the adiabatic theorem is proven for a Hamiltonian linear in the time. There is no strict insurance that the adiabatic theorem works correctly for the Hamiltonian with other time dependences. Thus we employ the following form of the Hamiltonian,

\[
H_\tau(t) = \frac{t}{\tau} H_0 + \left( 1 - \frac{t}{\tau} \right) H_T. \tag{2}
\]

Since the derivative of this Hamiltonian by the time is proportional to \(1/\tau\), the change of Hamiltonian involved by the time advance is infinitely slow in the infinite limit of \( \tau \). Using this Hamiltonian, the adiabatic theorem ensures that the final state converges to the ground eigen state of \( H_0 \) in infinite limit of \( \tau \).

We note here that the Hamiltonian \( H_\tau \) is artificial. Although we are interested in the classical Hamiltonian \( H_0 \), the Hamiltonian does not include the contribution from \( H_0 \) initially. We emphasize here that the important thing is not how the intermediate state is but how the final state is after the evolution. Hence it does not matter that the Hamiltonian at the initial time differs entirely from \( H_0 \).

For the sake of implementation of the quantum annealing, we consider two simple models as pilot cases. The first is a single-particle problem of the tight-binding model. Let us consider a one-dimensional lattice. We assume that there is one energy eigen-state at each site and the states in different sites are orthogonal each other.

The classical Hamiltonian is given by

\[
H_0 = \sum_{i=1}^{N} V_i |i\rangle \langle i|, \tag{3}
\]

where \(|i\rangle\) denotes the single-particle state of the site \(i\). \( N \) denotes the number of sites. \( V_i \) indicates the energy of the state at the site \(i\). We assume \( V_i \)'s are randomly distributed between 0 and 1. The tunneling Hamiltonian of the present system is brought by hopping between nearest neighbor sites. It is written as

\[
H_T = -\alpha \sum_{i=1}^{N-1} (|i\rangle \langle i+1| + |i+1\rangle \langle i|). \tag{4}
\]

A positive parameter \( \alpha \) denotes the strength of tunneling. The ground state of \( H_T \) as the initial state is given by \(|\Psi_0\rangle = 1/\sqrt{N} \sum_{i=1}^{N} |i\rangle\).

The next model is the random Ising spin model. The classical Hamiltonian is written as

\[
H_0 = - \sum_{<i,j>} J_{ij} S_i^z S_j^z - h \sum_i S_i^z, \tag{5}
\]

FIG. 1: Results on the tight-binding model. Calculations were performed for the system with twenty sites, \( N = 20 \). Figure (a) shows the potential energy of each site. Figure (b) shows the annealing time dependence of residual energies. Results for several tunneling energies are plotted. A straight line, \( \Delta E \propto 1/\tau^2 \), is shown for comparison. Note that both axes are logarithmic. For large \( \tau \), the residual energy obeys the power law for the annealing time. The exponent is estimated to be approximately two.
The tunneling Hamiltonian is introduced by the transverse field. The residual energy is defined by the energy difference between the energy expectation value with respect to the ground state becomes doubly degenerate.

The residual energy is written as

$$ H_T = -\alpha \sum_i S^z_i, $$

where $S^z_i$ is the z component of the spin operator at the site $i$. All spins are fully polarized along the $x$ axis in the ground state of $H_T$. It follows from this that the initial state is written as $|\Psi_0\rangle = \prod_i |\frac{1}{\sqrt{2}}(|\uparrow_i\rangle + |\downarrow_i\rangle)\rangle$, where $|\uparrow_i\rangle$ and $|\downarrow_i\rangle$ are the eigen states of $S^z_i$ with the eigen values $\frac{1}{2}$ and $-\frac{1}{2}$ respectively.

For each model we solved the Schrödinger equation numerically using the Runge-Kutta algorithm of fourth order and obtained the time dependence of the state vector. The residual energy is defined by the energy difference between the energy expectation value with respect to the final state and the ground eigen energy of the classical Hamiltonian,

$$ \Delta E = \langle \Psi(\tau)|H_0|\Psi(\tau)\rangle - E_0, $$

where $E_0$ denotes the ground eigen energy of $H_0$. In our calculation, $E_0$ is known because the system is small enough.

We show results on the tight-binding model represented by eqs. 5 and 6 in Fig.1. The potential energy at each site is randomly generated and is shown in Fig.1(a). Calculations were performed for several tunneling energies. Large value of $\alpha$ gives rise to the large energy gap at the initial time. Since the adiabatic theorem works better for larger energy gap, large $\alpha$ is preferable to lower the residual energy. However large $\alpha$ yields large derivative by the time of the Hamiltonian. Since large derivative disturbs the adiabatic evolution, large $\alpha$ is not preferable. Therefore there is an optimum $\alpha$. In the present case, it seems around $\alpha = 0.6$.

It is seen in Fig.1(b) that the logarithm of residual energy decreases almost linearly with increasing the logarithm of annealing time for long annealing time. Therefore the residual energy roughly obeys the power law with respect to the annealing time,

$$ \Delta E \propto \frac{1}{\tau^\zeta}. $$

By comparison with the line $\Delta E \propto \tau^{-2}$ drawn in the same figure, the exponent is estimated as $\zeta \sim 2$.

Results on the random Ising model given by eqs. 5 and 6 are shown in Fig.1. The system consists of nine spins in the two-dimensional square lattice with nearest neighbor interactions. The values of coupling constants are indicated by the inset in the figure. Similar to the case in Fig.1(b), the residual energy is smallest at a certain optimum $\alpha$ for a fixed $\tau$. It is clearly seen that the logarithm of residual energy is linear in $\ln\tau$ for long $\tau$. Hence the power law of the residual energy, eq.(8) holds also in the present case. Furthermore we can estimate $\zeta \sim 2$ by comparison with the straight line of $\Delta E \propto 1/\tau^2$ in the figure. This result is the same as that of the tight-binding model.

From results of numerical calculations, we naturally infer that the power law with the exponent $\zeta \sim 2$ is the universal feature in the quantum annealing method. In fact, one can derive from the adiabatic theorem that this is true. According to a rigorous theory on the adiabatic theorem, the probability to find out the excited states of $H_0$ in the final state is given by

$$ \sum_{n\neq 0}|\langle n|\Psi(\tau)\rangle|^2 \approx O\left(\frac{1}{(\epsilon\tau)^2}\right) $$

where $|n\rangle$ denotes the eigen state of $H_0$ and $n = 0$ indicates the ground state in particular. $\epsilon$ has the dimension of energy and defined by $\epsilon = \varepsilon_{\text{min}}/\epsilon^*$ where $\varepsilon_{\text{min}}$ is the minimum of energy gap above the instantaneous ground state of $H_T(t)$ and $\epsilon^*$ is the maximum of matrix element of $H_T - H_0$ among instantaneous ground state and the lowest excited state of $H_T(t)$. The value of $\epsilon^*$ is of the order of the energy unit. Equation (10) holds for $\epsilon\tau \gg 1$. Formulas for each eigen state are derived, that is, $|\langle n|\Psi(\tau)\rangle|^2 \sim O(1/(\epsilon\tau)^2)$ for $n \neq 0$ and $|\langle 0|\Psi(\tau)\rangle|^2 \sim 1 - O(1/(\epsilon\tau)^2)$. Hence, arranging the
eq. (7), we obtain that the residual energy is of the order of \( 1/(\epsilon \tau)^2 \).

\[
\Delta E = \sum_{n \neq 0} E_n |\langle n | \Psi(\tau) \rangle|^2 - E_0 \left( 1 - |\langle 0 | \Psi(\tau) \rangle|^2 \right) \\
\sim O\left( \frac{1}{(\epsilon \tau)^2} \right), \tag{11}
\]

where \( E_n \) is the eigen energy of \( \mathcal{H}_0 \). Thus it is shown that the term proportional to \( 1/\tau^2 \) dominates the residual energy in the infinite limit of \( \tau \).

We note that eq. (11) may contain higher order terms of \( 1/(\epsilon \tau) \) than \( 1/(\epsilon \tau)^2 \). We attribute fluctuations around the line of \( \Delta E \sim 1/\tau^2 \) in Fig. 1b to these additional terms.

The existence of the energy gap above the instantaneous ground state of \( \mathcal{H}_\tau(t) \) is crucial for the quantum annealing method. The argument on the basis of the eq. (11) is incorrect when the ground state is degenerate at a time during the evolution. This is obvious because of \( \epsilon = 0 \). However the Hamiltonian of disordered systems does not usually possess any symmetry which brings about degenerate ground state.

We assume that the instantaneous energy gap is always finite. The value of \( \epsilon_{\text{min}} \) depends on the problem. For problems with small \( \epsilon_{\text{min}} \), a large \( \tau \) is required in order to validate the power law of the residual energy. In other words, the quantum annealing method is more efficient for problems with larger \( \epsilon_{\text{min}} \).

For \( \epsilon \tau \sim 1 \), the adiabatic theorem does not work. Instead the Landau-Zener theory should account for the transition between two states with close energies. Consider that the energy levels of instantaneous ground and first excited states come close together at a time. The excitation energy is locally minimized at this time. According to the Landau-Zener theory, the transition probability from the ground state to the first excited state is given by \( p \sim \exp(-c \epsilon \tau) \), where \( c \) is a constant of the order of unity. If such a possible transition occurs just once, the residual energy is proportional to \( \exp(-c \epsilon \tau) \). However it is not obvious whether this exponential behavior is true for large systems, since the transition events may take place many times.

Santoro et al. have predicted the logarithmic scaling law of the residual energy on the basis of the Landau-Zener theory. We remark that our result of power law is valid for \( \tau \gg 1/\epsilon \) where the quantum adiabatic theorem is guaranteed. Since the Landau-Zener theory is intended for \( \tau \sim 1/\epsilon \), these two scaling laws may not conflict with each other. Nevertheless it should be noted that the definition of the residual energy in ref. [8] is given by the expectation value of the excitation energy among the quantum annealing process. It is natural that the residual energy is defined by the energy expectation value of the final state measured from the true ground energy, eq. (7). Furthermore no one has confirmed numerically the scaling behavior for \( \tau \sim 1/\epsilon \). In order to unveil the feature in this regime, numerical calculations for huge sized systems are desired.

We remark on the implementation of the quantum annealing for combinatorial optimization problems with large elements. In order to carry out the quantum annealing, we must compute the real-time dynamics according to the Schrödinger equation. Methods of numerical calculation for the real-time quantum dynamics have not been developed enough except for cases of one-dimensional models. Construction of a general method is a big issue. One possibility exists in the quantum Monte-Carlo method. Even though direct computations of the real-time dynamics are impossible in the quantum Monte-Carlo method, one can regard an evolution by Monte-Carlo step as a fictitious-time evolution. Some of earlier works have reported that the quantum annealing with the quantum Monte-Carlo is more efficient than the thermal annealing. However it is not clear that the adiabatic theorem works in the Monte-Carlo evolution, the residual energy may show annealing time dependence different from real-time quantum annealing. A rigorous theory on the residual energy after the Monte-Carlo evolution is left as a future work.

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