Rigorous convergence condition for adiabatic and diabatic quantum annealing

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Abstract. We derive a generic bound on the rate of decrease of transverse field for adiabatic and diabatic quantum annealing to converge to the ground state of a generic Ising model when quantum annealing is formulated as an infinite-time process. Our theorem is based on a rigorous upper bound on the excitation probability in the infinite-time limit and is a mathematically rigorous counterpart of a previously known result derived only from the leading-order term of the asymptotic expansion of adiabatic condition. Since only the excitation probability in the infinite-time limit is analyzed, the system can be excited in the intermediate time region, and thus diabatic processes are allowed. Since our theorem gives a sufficient condition of convergence for a generic transverse-field Ising model, any specific problem may allow a better, faster, control of the coefficient.

1. Introduction

Quantum annealing is an active field of research for combinatorial optimization, sampling, and quantum simulation [1 2 3]. There nevertheless exist only a very limited number of studies on mathematical conditions for convergence to the correct solution, the ground state of an Ising model, for generic or specific problems. One of such studies is the contribution by Morita and Nishimori [4 5], where a sufficient condition is discussed for the amplitude of transverse field to satisfy in the long-time limit for a generic problem. The result is a power-law (polynomial) decrease of the amplitude as a function of time, which is faster than the corresponding rate of temperature decrease in classical simulated annealing [6].

The approach of Morita and Nishimori builds on an approximate version of the “adiabatic theorem”, which takes into account only the leading-order term of the asymptotic expansion of excitation probability and ignores higher order contributions. The goal of the present paper is to fix this insufficiency and derive a mathematically rigorous condition for convergence in the infinite-time limit based on the rigorous adiabatic theorem by Jansen, Ruskai, and Seiler [7]. As a by-product, we point out
that the condition of convergence in the infinite-time limit can be satisfied without imposing a strict adiabatic condition for the whole process of annealing. This means that the ground state of the final Ising model can be reached even when the system follows a diabatic process in the intermediate time region as long as the rigorous bound we derive for the field strength is satisfied in the long-time limit. This aspect allows for a wide range of functional forms of the field strength except in the long-time limit.

We formulate the problem and present our result with its proof in the next section. The final section concludes the paper with discussions.

2. Convergence condition

2.1. Formulation

Let us consider the following time-dependent Hamiltonian,

\[ H(t) = H_{\text{Ising}} + H_{\text{TF}}(t), \]

where \( H_{\text{Ising}} \) is an arbitrary Ising Hamiltonian with general many-body interactions,

\[ H_{\text{Ising}} = - \sum_{i=1}^{N} J_i \sigma_i^z - \sum_{i,j} J_{ij} \sigma_i^x \sigma_j^z - \sum_{i,j,k} J_{ijk} \sigma_i^x \sigma_j^y \sigma_k^z - \cdots, \]

and \( H_{\text{TF}}(t) \) stands for a transverse-field term with time-dependent coefficient,

\[ H_{\text{TF}}(t) = -\Gamma(t) \sum_{i=1}^{N} \sigma_i^x, \]

where \( N \) is the total number of spins and \( \sigma_i^x \) and \( \sigma_i^z \) denote the \( x \) and \( z \) components of the Pauli matrix at site \( i \), respectively. The coefficients \( \{ J_i, J_{ij}, J_{ijk} \} \) in the Ising Hamiltonian are supposed to be scaled such that \( H_{\text{Ising}} \) is of \( \mathcal{O}(N) \). Time \( t \) is supposed to run from 0 to infinity. The coefficient will run from its large initial value \( \Gamma(0) \) to zero as \( t \to \infty \). Our goal is to derive a sufficient condition for the function \( \Gamma(t) \) to satisfy in order for the system to reach the ground state of the generic Ising model of equation (2) within a given precision in the infinite time limit \( t \to \infty \). Notice that we do not discuss computational complexity of quantum annealing for the generic problem \( \text{II} \) with \( \text{II} \), i.e., the amount of (finite but large) time to reach the solution as a function of the problem size \( N \), which is already known to be NP hard \( \text{II} \).

2.2. Adiabatic theorem

Our theory relies on the adiabatic theorem proved by Jansen, Ruskai, and Seiler \( \text{II} \). Suppose that the Hamiltonian \( H(t) \) depends on \( t \) through a dimensionless time scaled

\( \dagger \) This condition is not essential and can indeed be relaxed to an arbitrary polynomial of \( N \) since leading order terms in the following discussion are of exponential order and thus polynomial factors are inessential.
by finite computation time $\tau$, $s = t/\tau$,

$$\tilde{H}(s) \equiv H(t),$$

where $s$ runs from 0 to 1 and thus $t$ runs from 0 to $\tau$. The Schrödinger equation reads

$$i \frac{1}{\tau} \frac{\partial}{\partial s} |\psi_\tau(s)\rangle = \tilde{H}(s) |\psi_\tau(s)\rangle. \quad (5)$$

The reduced Planck constant $\hbar$ is set to 1 for simplicity. We assume that $\tilde{H}(s)$ is twice differentiable by $s$ and the instantaneous ground state of $\tilde{H}(s)$ is non-degenerate. This latter condition is automatically satisfied by the transverse-field Ising model according to the Perron-Frobenius theorem [9].

Jansen et al [7] proved the following inequality,

$$\|P_\tau(s) - P(s)\| \leq \left|\frac{d\tilde{H}(0)}{ds}\right| + \left|\frac{d\tilde{H}(s)}{ds}\right| + \frac{1}{\tau} \int_0^s ds \left( \frac{\left|\frac{d^2\tilde{H}(s)}{ds^2}\right|}{\Delta(s)^2} + \frac{7}{\Delta(s)^3} \right), \quad (6)$$

where $\|\cdots\|$ denotes the operator norm. Here $\Delta(s)$ stands for the instantaneous energy gap between the ground state and the first excite state, $\Delta(s) = \epsilon_1(s) - \epsilon_0(s)$, where $\epsilon_0(s)$ and $\epsilon_1(s)$ are instantaneous ground-state and first-excited-state energies of $\tilde{H}(s)$,

$$\tilde{H}(s) \langle j(s) \rangle = \epsilon_j(s) |j(s)\rangle \quad (j = 0, 1, \cdots). \quad (7)$$

On the left-hand side of equation (6) appear projectors onto the current running state $|\psi_\tau(s)\rangle$ and the instantaneous ground state $|0(s)\rangle$, respectively,

$$P_\tau(s) = |\psi_\tau(s)\rangle \langle \psi_\tau(s)|, \quad P(s) = |0(s)\rangle \langle 0(s)|. \quad (8)$$

It is easy to verify that the left-hand side of equation (6) is the probability of excitation,

$$\|P_\tau(s) - P(s)\| = \sqrt{\sum_{j=1}^\infty |c_j(t)|^2}, \quad (9)$$

where $c_j(s)$ is the coefficient of expansion of $|\psi_\tau(s)\rangle$ in terms of $|j(s)\rangle$,

$$|\psi_\tau(s)\rangle = \sum_{j=0}^\infty c_j(s) |j(s)\rangle. \quad (10)$$

Thus it is required to keep $\|P_\tau(s) - P(s)\|$ small if we demand that the system stays close to the instantaneous ground state at any $s$.

It is straightforward to rewrite equation (6) in terms of $t$, in place of $s$, as

$$\|P_\tau(t) - P(t)\| \leq \left|\frac{dH(0)}{\Delta(0)^2}\right| + \left|\frac{dH(t)}{\Delta(t)^2}\right| + \int_0^t dt' \left( \frac{\left|\frac{d^2H(t')}{dt'^2}\right|}{\Delta(t')^2} + \frac{7}{\Delta(t')^3} \right). \quad (11)$$
One can verify that the derivation process of equation (6) remains valid if we replace \( s \) by \( t = s \tau \) to reach equation (11) without using \( \tau \).

A commonly-used form of adiabatic condition

\[
\tau \gg \frac{| \langle 1(s) | \frac{d}{ds} | 0(s) \rangle |}{\Delta(s)^2}
\]  

(12)

corresponds to reducing the value of only the second term of the right-hand side of equation (6). We use full equation (11), one of rigorous versions of adiabatic theorem [2], to derive a sufficient condition for convergence of quantum annealing in the limit \( t \to \infty \).

We are interested in suppressing the final probability of excitation, which is evaluated by taking the limit \( t \to \infty \) on both sides of equation (11).

\[
P_{\text{excited}} \leq \lim_{t \to \infty} \| P_\tau(t) - P(t) \|. 
\]

(14)

This is a weaker condition than requiring adiabaticity in the whole range of annealing process by imposing the adiabatic condition (11) for all \( 0 < t < \infty \). In other words, we allow for a diabatic process at finite \( t \).

2.3. Evaluation of integrand

The first, and rather trivial, step is to rescale time by a factor, \( t \to \epsilon^{-1} t \). Then, all terms on the right-hand side of equation (13) become multiplied by \( \epsilon \).

\[
P_{\text{excited}} \leq \epsilon \left[ \frac{\| dH(0) \|}{\Delta(0)^2} + \lim_{t \to \infty} \frac{\| dH(t) \|}{\Delta(t)^2} + \int_0^\infty d\tilde{t} \left( \frac{\| d^2H(\tilde{t}) \|}{\Delta(\tilde{t})^2} + \frac{7 \| dH(\tilde{t}) \|}{\Delta(\tilde{t})^3} \right) \right]. 
\]

(15)

By choosing a sufficiently small value for \( \epsilon \), we observe that the task is now to find a condition to keep finite the quantities in the outer brackets on the right-hand side of equation (15).

We thus evaluate the derivatives of the Hamiltonian. Since \( H(t) \) depends on \( t \) only through \( \Gamma(t) \), we can easily obtain the following bounds,

\[
\left\| \frac{dH(t)}{dt} \right\| = | \Gamma'(t) | \left\| \sum_{i=1}^N \sigma_i ^x \right\| \leq N | \Gamma'(t) |. 
\]

(16)

Similarly,

\[
\left\| \frac{d^2H(t)}{dt^2} \right\| \leq N | \Gamma''(t) |. 
\]

(17)
The non-trivial part is to estimate a lower bound on the energy gap $\Delta(t)$, but this problem has already been solved for generic $H(t)$ in references [10, 4, 5] as

$$\Delta(t) \geq A \Gamma(t)^N,$$

where $A$ is independent of $t$ but depends on $N$ asymptotically ($N \gg 1$) as

$$A = a \sqrt{N} e^{-bN}$$

with an asymptotically-$N$-independent constants $a(>0)$ and $b$. This latter $b$ can be positive or negative depending on the problem. Deferring evaluation of the second term on the right-hand side of (15), we find that replacement of denominators and numerators of two terms in the integrand of equation (15) by equations (16), (17), (18), and (19) leads to their asymptotic upper bounds as

$$\frac{\left\| \frac{d^2H(t)}{dt^2} \right\|}{\Delta(t)^2} \lesssim \frac{e^{2bN} |\Gamma''(t)|}{a^2 \Gamma(t)^{2N}},$$

$$\frac{\left\| \frac{dH(t)}{dt} \right\|^2}{\Delta(t)^3} \lesssim \frac{\sqrt{N} e^{3bN} (\Gamma'(t))^2}{a^3 \Gamma(t)^{3N}},$$

respectively. Those upper bounds are to decrease faster than $t^{-1}$ as $t$ tends to infinity for the integral to converge in equation (15).

### 2.4. Condition on the coefficient

To understand what functional form is allowed for $\Gamma(t)$ under the above-derived condition, we express $\Gamma(t)$ for sufficiently large $t$ without losing generality as

$$\Gamma(t) = t^{-g(t)}$$

with a twice-differentiable function $g(t)$, which should be strictly positive $g(t) > 0$ because $\Gamma(t)$ is expected to tend toward 0 as $t \to \infty$. We prove the following theorem.

**Theorem 1.** Excitation probability in the infinite-time limit $P_{\text{excited}}$ can be made arbitrarily small for a large but fixed system size $N$ if the function $g(t)$ in equation (22) satisfies the following conditions for sufficiently large $t$,

$$0 < g(t) < \frac{1}{3N - 2},$$

$$|g'(t)| \leq \frac{c}{t \log t},$$

$$|g''(t)| \leq \frac{c' t^{1-(2N-1)/(3N-2)}}{\log t},$$

with positive constants $c$ and $c'$. 

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§ References [4, 5] stated that $b$ is positive, but a careful scrutiny of equation (13) of [4] or equation (28) of [5] reveals that $b$ can be positive or negative through the problem-dependent parameters $E_+, E_{\text{min}}$ and $\Gamma_0$. 
Proof. We first discuss equation (21). Insertion of equation (22) to the right-hand side of equation (21) shows that the following expression should approach 0 as \( t \to \infty \) for the term of second integrand of equation (15) to converge,

\[
\frac{t(\Gamma'(t))^2}{\Gamma(t)^{2N}} = t^{(3N-2)g(t)-1} (g(t) + g'(t)t \log t)^2
\]

for fixed \( N \). Strict positiveness of \( g(t) \) implies that the first term of the expansion of square on the right-hand side of equation (26)

\[
t^{(3N-2)g(t)-1}g(t)^2
\]

approaches 0 if and only if

\[
0 < g(t) < \frac{1}{3N - 2}
\]

for \( t \gg 1 \). If we demand that \( g(t) \) is monotonic, the above equation means that \( g(t) \) converges to a constant or is a constant.

Convergence to zero of another term of the expansion

\[
(g'(t) \log t)^2 t^{(3N-2)g(t)+1}
\]

as \( t \to \infty \) requires that

\[
|g'(t)| \leq \frac{c}{t \log t},
\]

with a constant \( c \), given that \((3N - 2)g(t) + 1 < 2\). The last piece of the expansion

\[
2g(t)g'(t)(\log t) t^{(3N-2)g(t)}
\]

leads to the same condition as above.

We next evaluate the right-hand side of equation (20),

\[
\frac{t\Gamma''(t)}{\Gamma(t)^{2N}} = t^{(2N-1)g(t)-1} \left( (g'(t)t \log t + g(t))^2 - (t^2g''(t) \log t + 2tg'(t) - g(t)) \right).
\]

Terms involving only \( g(t) \) and \( g'(t) \) automatically converge to 0 under the already-derived conditions (23) and (24). The term with \( g''(t) \) yields an additional condition

\[
|g''(t)| \leq \frac{c' t^{-\frac{(2N-1)/(3N-2)}}}{\log t},
\]

where \( c' \) is a positive constant.

It is straightforward to see that the second term in the outer parentheses on the right-hand side of equation (15) converges to zero under the conditions (23) and (24). This way, the quantity in the outer brackets on the right-hand side of (15) remains finite, and thus the right-hand side can be made arbitrarily small for fixed \( N \) by choosing \( \epsilon \) to be an arbitrarily small constant multiplied by a quantity of \( O(N^{-1/2}e^{-3bN}) \).

Example. As a simple example, one may choose a constant function,

\[
g(t) = \frac{1}{4N}.
\]
2.5. Bounded coefficient

It is often the case that one considers the following form of the Schrödinger dynamics:

\[
\frac{id\psi(t)}{dt} = s(t)H_{\text{Ising}} - (1 - s(t)) \sum_i \sigma_i^x, \tag{35}
\]

with a monotonically increasing function \(0 \leq s(t) \leq 1\), instead of equation (1) with equation (3). We show that it is possible to rewrite the theory developed in previous sections to this case if we choose \(t\) to run from 0 to \(\infty\).

Equation (35) can be rewritten as

\[
\frac{i}{s(t)} \frac{d\psi(t)}{dt} = H_{\text{Ising}} - \frac{1 - s(t)}{s(t)} \sum_i \sigma_i^x. \tag{36}
\]

Let us define

\[
\tilde{t} := \int_0^t s(t) dt, \tag{37}
\]

which is a monotonic function of \(t\). Utilizing \(\tilde{t}\), equation (36) can be rewritten as

\[
\frac{i}{s(t)} \frac{d\psi(t)}{dt} = H_{\text{Ising}} - \frac{1 - s(t)}{s(t)} \sum_i \sigma_i^x. \tag{38}
\]

With a function, \(\Gamma(\tilde{t}) := (1 - s(t))/s(t)\), equation (38) becomes

\[
\frac{i}{\tilde{t}} \frac{d\psi(t)}{dt} = H_{\text{Ising}} - \Gamma(\tilde{t}) \sum_i \sigma_i^x. \tag{39}
\]

Application of the argument in previous sections to (39) shows that, for convergence as \(\tilde{t} \to \infty\), it is sufficient that \(\Gamma(\tilde{t})\) behaves as

\[
\Gamma(\tilde{t}) = \frac{1 - s(t)}{s(t)} \propto \tilde{t}^{-\tilde{g}(\tilde{t})}, \tag{40}
\]

with \(\tilde{g}(\tilde{t})\) satisfying equations (23) to (25). Solving (40) for \(s(t)\), one obtains

\[
s(t) = \frac{1}{1 + \tilde{t}^{-\tilde{g}(\tilde{t})}} \approx 1 - \tilde{t}^{-\tilde{g}(\tilde{t})} (\tilde{t} \gg 1). \tag{41}
\]

We remark that in some cases \(\tilde{t}\) can be approximated by \(t\) when \(t\) is large. For example, if we choose \(s(t) = \tanh t\),

\[
\tilde{t} = \log \cosh t \approx t \ (t \gg 1). \tag{42}
\]

\| Notice that \(t\) in the formulation of equation (35) is often supposed to run within a finite interval \(0 \leq t \leq \tau\). Our theory does not apply to this case of finite-time development.

\[\square\] Not to be confused with the running variable in the integral in equation (15).
3. Conclusion

We have studied a sufficient condition for quantum annealing to converge to the ground state of a generic Ising model in the infinite-time limit for a given finite system size. This is a mathematically rigorous version of a previous result [1, 5], in which an approximate adiabatic condition was used. The result shows that convergence is achieved if the coefficient of the transverse-field term decreases with a power law of time or slower. This is qualitatively similar to the previous result in references [4, 5] but is different in rigorous quantification. In particular, constraints on derivatives of the coefficient did not exist before.

Our result is a sufficient condition for a generic Ising model: For any problem represented by equations (1), (2), and (3), the system will become close to the ground state of the Ising model in the infinite-time limit if the conditions in Theorem 1 are satisfied. We are unable to predict what happens if the conditions are not satisfied. It may happen that a faster decrease of $\Gamma(t)$ than we have derived here results in convergence to the ground state for a given specific problem, or it may also be the case for other examples that the system ends up in an excited state even if one spends an infinite amount of time when the conditions in Theorem 1 are not met.

Our conclusion is to be contrasted with the corresponding result for classical simulated annealing [6]. In a classical problem, the external parameter, temperature, is to be decreased as an inverse-logarithmic function of time in the limit of large computation time, which is much slower than the power law in the present quantum case. However, we should be careful not to conclude that quantum annealing is more efficient than simulated annealing since in both cases one is supposed to spend an infinitely long time to reach the solution.

We discussed the behavior of the coefficient of the transverse-field term in the infinite-time limit. No constraint is imposed on the behavior of the coefficient in the intermediate time region. Related to this fact is that we do not impose adiabaticity in the intermediate time region. This means that the system can evolve diabatically to finally reach the ground state under the present condition. We applied the adiabatic theorem only in the infinite-time limit.

It is important to remember that our goal is not to discuss computational complexity of quantum annealing. Indeed, we have discussed a very generic Ising model, which is known to be NP hard [8]. This aspect is reflected to the requirement on the parameter $\epsilon$, which dictates the rate of time development, that it should be chosen to have exponential dependence on the system size, $O(N^{-1/2}e^{-3bN})$.

We hope that developments along the line of the present work will lead to further non-trivial results to lay a firm theoretical foundation of quantum annealing.
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