Theorem on the existence of a nonzero energy gap in adiabatic quantum computation

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Adiabatic quantum computation, based on the adiabatic theorem, is a promising alternative to conventional quantum computation. The validity of an adiabatic algorithm depends on the existence of a nonzero energy gap between the ground and excited states. However, it is difficult to ascertain the exact value of the energy gap. In this paper, we put forward a theorem on the existence of nonzero energy gap for the Hamiltonians used in adiabatic quantum computation. It can help to effectively identify a large class of the Hamiltonians without energy-level crossing between the ground and excited states.

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Adiabatic quantum computation [1] offers a promising alternative to the conventional quantum computation [2, 3]. It is polynomially equivalent to the circuit model in computational power [4–6], and may be more physically realistic and implementable than the circuit model due to its inherent robustness against some types of errors [7–9]. A number of adiabatic quantum algorithms have been proposed for solving various problems [1, 4, 10–20], and several schemes have been experimentally demonstrated [2, 3]. Development of adiabatic quantum computation continues to be of great interest.

An adiabatic quantum algorithm is performed by a quantum system with a time-dependent Hamiltonian, which may be generally expressed as

\[ H(s) = (1 - s)H_i + sH_p, \]

where \( s = \frac{t}{T}, \) for \( t \in [0, T], \) is a time-dependent parameter, \( H_i \) is the initial Hamiltonian whose ground state is easy to prepare, and \( H_p \) is the problem Hamiltonian whose ground state encodes the solution to a problem. In the practical applications, \( H_p \) is usually taken as a diagonal matrix in the computational basis,

\[ H_p = \sum_z f_z |z\rangle \langle z|, \]

where \( f_z \) are real numbers, and \( z \in \{0, 1\}^n \) in the \( n \)-bit instance. The time-dependent Hamiltonian interpolates smoothly from the initial Hamiltonian to the problem Hamiltonian. The adiabatic theorem indicates that the final state of the quantum system, starting from the ground state of the initial Hamiltonian, is close to the ground state of the problem Hamiltonian if the time-dependent Hamiltonian varies sufficiently slowly. With an appropriate measurement on the system, solutions of the problem are yielded with high probability.

Adiabatic quantum computation is based on the adiabatic evolution. The “slowness” required by the adiabatic theorem is usually encoded in the adiabatic condition, \( \left( \frac{\Delta \varepsilon_n(s)}{T(\Delta \varepsilon_m(s))^2} \right) \ll 1, \) where \( \Delta \varepsilon_n(s) = \varepsilon_n(s) - \varepsilon_0(s), \) \( m \neq 0, \) is the energy gap between the ground state \( |\psi_0(s)\rangle \) and the \( m \)th excited state \( |\psi_m(s)\rangle \) of \( H(s) \). It shows that the energy gap \( \Delta \varepsilon_m(s) \) plays an important role in adiabatic quantum computation. The validity of an adiabatic algorithm, i.e., the existence of a finite runtime \( T \), completely depends on the existence of a nonzero gap, while the efficiency of the algorithm, i.e., the scaling of the runtime, depends on the value of the nonzero gap. An adiabatic quantum algorithm works only if a nonzero energy gap always exists during the evolution (see Fig. 1), i.e., \( \Delta \varepsilon_m(s) > 0 \) for \( s \in [0, 1] \) [28]. The quantum system would fail to keep at the instantaneous ground state of \( H(s) \) if the energy-level crossing between the ground and excited states happens during the evolution time (see Fig. 2). However, it is quite difficult to ascertain the exact value of the energy gap for the Hamiltonians used in adiabatic quantum computation. Due
to the difficulty, researchers have to resort to numerical simulations to evaluate the runtime of the adiabatic algorithm. For example, 3925 instances were calculated to simulate the adiabatic algorithm for solving the 3-SAT problem in Ref. [3]. 9200 instances were calculated to simulate the adiabatic algorithm for finding cliques in a random graph in Ref. [11], and 500 instances were calculated to simulate the adiabatic algorithm for factorizing integers in Ref. [12]. Yet, the approach to illustrate the validity of an adiabatic algorithm by numerical simulation is restricted by the numbers of instances as well as by the size of the problem, i.e., the number of the qubits needed, which has been no more than 20 in all these examples. So far, there has not been an effective approach to identify what kinds of \( H(s) \) are always with a nonzero energy gap.

In this paper, we address the validity issue of the adiabatic algorithm. We present a sufficient condition for identifying a large class of the Hamiltonians without energy-level crossing between the ground and excited states of the time-dependent Hamiltonian \( H(t) \) satisfies in the computational basis:

\[
|\psi_0\rangle = \begin{pmatrix} r_1 e^{i\alpha_1} \\ r_2 e^{i\alpha_2} \\ \vdots \\ r_d e^{i\alpha_d} \end{pmatrix} \equiv U \begin{pmatrix} r_1 \\ r_2 \\ \vdots \\ r_d \end{pmatrix},
\]

where all \( r_i \) are positive numbers satisfying \( \sum r_i^2 = 1 \), and

\[
U = \text{diag}(e^{i\alpha_1}, e^{i\alpha_2}, \ldots, e^{i\alpha_d})
\]

is a diagonal unitary matrix, and

1. all the nondiagonal elements of \( U^\dagger H_i U \) are nonpositive, then the energy gap between the ground and excited states of \( H(s) \) is nonzero for \( s \in [0, 1] \).

The theorem indicates that a nonzero energy gap between the ground and excited states of the time-dependent Hamiltonian \( H(s) \) is guaranteed if the initial Hamiltonian \( H_0 \) is properly chosen such that the two conditions are fulfilled. Despite the fact that these conditions restrict the choice of Hamiltonians, there is actually a large class of Hamiltonians that satisfy the conditions. For example, all the Hamiltonians for adiabatic algorithms in the previous works, to our knowledge, belong to this class.

We now prove the theorem in three steps. First, we establish an auxiliary function,

\[
F(s) \equiv [(1 - s)c_1 + sc_2] I - U^\dagger H(s) U, \quad s \in [0, 1),
\]

where \( c_1 \) is a positive number but larger than the largest eigenvalue of \( H_i \), and \( c_2 \) is a positive number but larger than the largest eigenvalue of \( H_p \). By substituting \( H(s) = (1 - s)H_i + sH_p \) into Eq. (3) and using the relation \([H_p, U] = 0\), \( F(s) \) can be recast as

\[
F(s) = (1 - s)(c_1 I - U^\dagger H_i U) + s(c_2 I - H_p).
\]

By definition, \( H_p \) is diagonal in the computational basis, and the nondiagonal elements of \( U^\dagger H_i U \) are nonpositive. Besides, it is a general property of a Hermitian matrix that the diagonal elements of it are not larger than its largest eigenvalue. Hence, \( c_1 I - U^\dagger H_i U, c_2 I - H_p \), and \( F(s) \) are all non-negative matrices. Hereafter, a matrix \( A \) is said to be non-negative if each \((A)_{ij} \geq 0\), and it is denoted by \( A \geq 0 \). Similarly, \( A > 0 \) means that \( A \) is a positive matrix, i.e., each element of it is positive, and \( A \geq B \) \( (A > B) \) means that \( A_{ij} \geq B_{ij} \) \( (A_{ij} > B_{ij}) \) for all the elements.

Second, we show that there exists a positive integer \( N_0 \) such that \( F^{N_0}(s) > 0 \). Since both \( c_1 I - U^\dagger H_i U \) and \( c_2 I - H_p \) are non-negative, there is

\[
F(s) \geq (1 - s)(c_1 I - U^\dagger H_i U) \geq 0.
\]

From Eq. (5), we have

\[
F^N(s) \geq (1 - s)^N(c_1 I - U^\dagger H_i U)^N,
\]

where \( N \) is an arbitrary positive integer. To derive Eq. (6) from Eq. (5), one may consider two non-negative matrices \( A \) and \( B \) with \( A \geq B \). Simple calculations show \( A^2 = [B + (A - B)]^2 = B^2 + B(A - B) + (A - B)B + (A - B)^2 \). Since \( B(A - B), (A - B)B, \) and \( (A - B)^2 \) are all non-negative matrices, one immediately has \( A^2 \geq B^2 \). Similarly, one may obtain \( A^N \geq B^N \) for arbitrary integers \( N \), i.e., Eq. (6).

To show the existence of \( N_0 \), we need to consider the limit of \( (c_1 I - U^\dagger H_i U)^N/(c_1 - \varepsilon_0)^N \) for \( N \rightarrow \infty \), where \( \varepsilon_0 \) is the ground-state energy of \( H_i \). By using the conditions in the theorem, we have

\[
\lim_{N \rightarrow \infty} \frac{1}{(c_1 - \varepsilon_0)^N} (c_1 I - U^\dagger H_i U)^N
= \lim_{N \rightarrow \infty} \sum_m \left(\frac{c_1 - \varepsilon_m}{c_1 - \varepsilon_0}\right)^N U^\dagger |\psi_m\rangle \langle \psi_m| U
= U^\dagger |\psi_0\rangle \langle r| U = |r\rangle \langle r| > 0,
\]

where \( \varepsilon_m \) and \( |\psi_m\rangle \) denote the eigenvalues and eigenstates of \( H_i \), respectively. Here, we have used \( |r\rangle \) to denote the column matrix \((r_1, r_2, \ldots, r_d)^T\). Equation (7) implies that there exists a sufficiently large number \( N_0 \) such that \( (c_1 I - U^\dagger H_i U)^{N_0} \) is positive, i.e.,

\[
(c_1 I - U^\dagger H_i U)^{N_0} > 0.
\]
Equations (5), (6), and (8) show that there exists a positive integer $N_0$ such that

$$F^{N_0}(s) > 0.$$  

(9)

Third, we demonstrate that the energy gap between the ground and excited states of $H(s)$ is nonzero for $s \in [0, 1]$, with the aid of the above properties of $F(s)$. Note that we have shown $F^{N_0}(s) > 0$. According to the Perron-Frobenius theorem that the eigenvector associated with the largest eigenvalue of a positive matrix is unique, $F$ has a unique eigenvector to its smallest eigenvalue when $F$ is nonnegative. That is, the initial Hamiltonians in Refs. [1, 12, 16, 17, 20] are nonpositive numbers. Equation (10) is reduced to the Hamiltonian in Ref. [12] if $a_0 = 0$ and $a_{ij} = -\frac{1}{2}M_{ij}$, the Hamiltonian in Ref. [15] if $a_0 = 0$ and $a_{ij} = -2|f_{ij}|$, and the Hamiltonian in Ref. [19] if $a_0 = \Omega \sum_{i<j} \Phi_{ij}$ and $a_{ij} = -\Omega \omega_{ij}$, where $M_{ij}$, $n_{ij}$, and $f_{ij}$ are real numbers, and $\Omega > 0$. Due to the symmetry of the quantum systems, these Hamiltonians are block diagonal, and therefore the evolutions of the systems are constrained in each subspace identified by their Hamming weight $k$. In the $k$th subspace, the ground state of $H_i$ is

$$\left|\psi_0\right> = \left(\begin{array}{c} n \\ k \end{array}\right)^{-1/2} \sum_{h(z) = k} |z\rangle,$$  

(14)

where $h(z)$ denotes the Hamming weight of $z$. Comparing Eq. (14) with the general expression for $|\psi_0\rangle$ in the theorem, we have $U = I$, $r_i = \left(\begin{array}{c} n \\ k \end{array}\right)^{-1/2}$, and hence $U^\dagger H_i U = H_i$. In this case, all $r_i$ are positive and all the non-diagonal elements of $U^\dagger H_i U$ are nonpositive. That is, these initial Hamiltonians satisfy the conditions of our theorem, and therefore they are valid to be used for adiabatic computation.

Case 2. This case includes the Hamiltonians used in Refs. [11, 13, 15, 19], which involve two-qubit interactions. The Hamiltonian in [11] reads

$$H_i = -\frac{1}{2} \sum_{i<j} (\sigma_x^i \otimes \sigma_x^j + \sigma_y^i \otimes \sigma_y^j),$$  

(12)

and the Hamiltonians in Refs. [13, 15, 19] can be generally expressed as

$$H_i = a_0 I + \sum_{i<j} a_{ij} (\sigma_x^i \otimes \sigma_x^j + \sigma_y^i \otimes \sigma_y^j + \sigma_z^i \otimes \sigma_z^j),$$  

(13)

where $a_0$ is a real number, and $a_{ij}$ are nonpositive numbers. Equation (13) is reduced to the Hamiltonian in Ref. [13] if $a_0 = 0$ and $a_{ij} = -\frac{1}{2}M_{ij}$, the Hamiltonian in Ref. [15] if $a_0 = 0$ and $a_{ij} = -2|f_{ij}|$, and the Hamiltonian in Ref. [19] if $a_0 = \Omega \sum_{i<j} \Phi_{ij}$ and $a_{ij} = -\Omega \omega_{ij}$, where $M_{ij}$, $n_{ij}$, and $f_{ij}$ are real numbers, and $\Omega > 0$. Due to the symmetry of the quantum systems, these Hamiltonians are block diagonal, and therefore the evolutions of the systems are constrained in each subspace identified by their Hamming weight $k$. In the $k$th subspace, the ground state of $H_i$ is

$$\left|\psi_0\right> = \left(\begin{array}{c} n \\ k \end{array}\right)^{-1/2} \sum_{h(z) = k} |z\rangle,$$  

(14)

Comparing Eq. (14) with the general expression for $|\psi_0\rangle$ in the theorem, we have $U = I$, $r_i = \left(\begin{array}{c} n \\ k \end{array}\right)^{-1/2}$, and hence $U^\dagger H_i U = H_i$. In this case, all $r_i$ are positive and all the non-diagonal elements of $U^\dagger H_i U$ are nonpositive. That is, these initial Hamiltonians satisfy the conditions of our theorem, and therefore they are valid to be used for adiabatic computation.

Case 3. This case includes the Hamiltonians used in Refs. [4, 10, 18], which involve many-body interactions. They can be expressed as

$$H_i = I - |\psi_0\rangle \langle \psi_0|,$$  

(15)

where $|\psi_0\rangle = \frac{1}{\sqrt{d}} \sum_{i=1}^d |i\rangle$, and $d$ denotes the dimensions of the quantum system. $|\psi_0\rangle$ is the unique ground state of the Hamiltonian. Clearly, the initial Hamiltonian defined by Eq. (14) satisfies the conditions of our theorem too.

Case 4. The Hamiltonian used in Ref. [14] reads

$$H_i = g(\sigma_x^1 + \sigma_x^2 + \cdots + \sigma_x^n),$$  

(16)

where $g$ is a positive number. It describes an $n$-qubit system, in which all the qubits interact with the same magnetic field with strength $g$. The ground state is

$$|\psi_0\rangle = \left(\begin{array}{c} 0 \cdots 1 \\ \sqrt{2} \end{array}\right)^n.$$  

(17)

Comparing Eq. (17) with the general expression for $|\psi_0\rangle$ in the theorem, we have $|\psi_0\rangle = U(\left|0\right> + \left|1\right>)^\otimes n$. 


with \( U = \sigma_z^1 \otimes \sigma_z^2 \otimes \cdots \otimes \sigma_z^n \), and hence \( U^\dagger H_i U = -g(\sigma_z^1 + \sigma_z^2 + \cdots + \sigma_z^n) \). In this case, all \( r_i \) are positive and all the nondiagonal elements of \( U^\dagger H_i U \) are nonpositive. It satisfies the conditions of our theorem, and therefore the initial Hamiltonian defined by Eq. (16) is valid to be used for adiabatic computation. Note that the Hamiltonian defined by Eq. (10) can also be considered as an instance of Case 1 up to a unitary transformation.

So far, we have checked the Hamiltonians from previous work on adiabatic quantum computation and found that they obey the conditions of our theorem.

After having shown that all the Hamiltonians used in the previous works belong to the class identified by our theorem, we now give an example to illustrate that if the conditions of the theorem are not met, the energy-level crossing between the ground and excited states may happen. Let \( H_1 = -2\sigma_x \otimes I + I \otimes \sigma_x + I \otimes \sigma_x - 2\sigma_x \otimes \sigma_x \), and \( H_p = \text{diag}(0, 2, 6, 8) \). For this example, \( |\psi_i\rangle = \frac{\sqrt{1 + 2\sqrt{2}}}{4}(\sqrt{2} - 1, 1, \sqrt{2} - 1, 1)^T \). Comparing it with the general expression in the theorem, we have \( r_i > 0, U = I \), and hence \( U^\dagger H_i U = H_i \). It follows that the Hamiltonian fulfills the first condition in the theorem but does not meet the second one. In this case, the Hamiltonian may not be valid for adiabatic quantum computation. Indeed, numerical simulation shows that the energy-level crossing between the ground and excited states occurs during the evolution time (see Fig. 3).

![Fig. 3. Numerical simulation of energy levels for the illustrative example.](image)

Our theorem provides a simple approach to examine the existence of a nonzero energy gap for the Hamiltonian used in the adiabatic quantum algorithm. It may be helpful in choosing alternative Hamiltonians for an adiabatic algorithm. As shown above, all the initial states in the previous papers are an equal-weight superposition of computational bases. However, the theorem shows that it is not necessary for the coefficients \( r_i \) to be equal. The theorem only requires that \( r_i \) are positive and the nondiagonal elements of \( U^\dagger H_i U \) are nonpositive, which can sufficiently guarantee the validity of the Hamiltonian being with a nonzero energy gap. This gives a reference scheme for constructing initial Hamiltonians. Indeed, in some instances, the solutions to problems may be more likely to be found in some certain region of state space rather than another. Thus, one may like to input a nonuniform prior distribution into the adiabatic algorithm by following the requirement of the theorem. Besides, it is also interesting to note that the existence of a nonzero energy gap is independent of the elements of \( H_p \) in the computational basis as long as \( H_i \) fulfills the conditions in the theorem. In passing, we would like to point out that although the statement of the theorem is based on the expression \( H(s) = (1 - s)H_i + sH_p \) with \( s = t/T \), the theorem is also valid for the general interpolation scheme, \( H(t) = a(t)H_i + b(t)H_p \), as long as \( a(t) \) and \( b(t) \) are monotonic functions satisfying \( a(0) = 1, b(0) = 0, a(T) = 0, \) and \( b(T) = 1 \).

Our discussions have focused on the validity issue of the Hamiltonian used in the adiabatic algorithm, i.e., the existence of a finite runtime \( T \), which is determined by a nonzero energy gap. A Hamiltonian being without level crossing is only a necessary condition for the adiabatic quantum computation. It should be noted that the gap between two noncrossing levels may still be exponentially small or even worse [31, 32]. Another fundamental issue is the efficiency of the adiabatic algorithm, i.e., the scaling of the runtime, which depends on the value of the nonzero gap. The efficiency or the computational complexity of the adiabatic computation is described by the scaling of the inverse square of minimum energy gap, which is related to the problem size [1, 22]. However, it is quite difficult to theoretically analyze the changing trend of the energy gap for a general Hamiltonian since the dimensions of the time-dependent Hamiltonian increase exponentially with the problem size. We do not attempt to resolve the efficiency issue in this paper.

In conclusion, we put forward a theorem on the existence of a nonzero energy gap for the Hamiltonians in adiabatic quantum computation. It can help to effectively identify a large class of the Hamiltonians with a nonzero energy gap. We have used the theorem to examine the validity of the Hamiltonians in previous papers, and it shows that all the Hamiltonians, examined by us, belong to this class.

[1] E. Farhi, J. Goldstone, S. Gutmann, and M. Siper, arXiv:quant-ph/0001106; E. Farhi, J. Goldstone, S. Gutmann, J. Lapan, A. Lundgren, and D. Preda, Science 292, 472 (2001).
[2] D. Deutsch, Proc. R. Soc. A 425, 73 (1989).
[3] D. P. DiVincenzo, Fort. Phys. 48, 771 (2000).
[4] W. van Dam, M. Mosca, and U. Vazirani, Proceedings of the 42nd Symposium on Foundations of Computer Science (IEEE Computer Society Press, Los Alamitos, 2001), pp. 279–287.
[5] D. Aharonov, W. van Dam, J. Kempe, Z. Landau, S. Lloyd, and O. Regev, SIAM J. Comput. 37, 166 (2007).
[6] A. Mizel, D. A. Lidar, and M. Mitchell, Phys. Rev. Lett. 99, 070502 (2007).
[7] A. M. Childs, E. Farhi, and J. Preskill, Phys. Rev. A 65, 012322 (2001).
[8] J. Roland and N. J. Cerf, Phys. Rev. A 71, 032330 (2005).
[9] J. Aberg, D. Kult, and E. Sjöqvist, Phys. Rev. A 71, 060312 (2005).
[10] J. Roland and N. J. Cerf, Phys. Rev. A 65, 042308 (2002).
[11] A. M. Childs, E. Farhi, J. Goldstone, and S. Gutmann, Quantum Inf. Comput. 2, 181 (2002).
[12] T. Hogg, Phys. Rev. A 67, 022314 (2003).
[13] R. Schützhold and G. Schaller, Phys. Rev. A 74, 060304 (2006).
[14] X. Peng, Z. Liao, N. Xu, G. Qin, X. Zhou, D. Suter, and J. Du, Phys. Rev. Lett. 101, 220405 (2008).
[15] G. Schaller and R. Schützhold, Quantum Inf. Comput. 10, 0109 (2010).
[16] N. G. Dickson and M. H. S. Amin, Phys. Rev. Lett. 106, 050502 (2011).
[17] F. Gaitan and L. Clark, Phys. Rev. Lett. 108, 010501 (2012).
[18] S. Garnerone, P. Zanardi, and D. A. Lidar, Phys. Rev. Lett. 108, 230506 (2012).
[19] M. Hofmann and G. Schaller, Phys. Rev. A 89, 032308 (2014).
[20] F. Gaitan and L. Clark, Phys. Rev. A 89, 022342 (2014).
[21] M. Steffen, W. van Dam, T. Hogg, G. Breyla, and I. L. Chuang, Phys. Rev. Lett. 90, 067903 (2003).
[22] R. Harris et al., Phys. Rev. B 82, 024511 (2010).
[23] M. W. Johnson et al., Nature (London) 473, 194 (2011).
[24] Z. Bian, F. Chudak, W. G. Macready, L. Clark, and F. Gaitan, Phys. Rev. Lett. 111, 130505 (2013).
[25] M. Born and V. Fock, Z. Phys. 51, 165 (1928).
[26] D. Bohm, Quantum Theory (Prentice-Hall, New York, 1951).
[27] A. Messiah, Quantum Mechanics (North-Holland, Amsterdam, 1962).
[28] A level crossing at the end of the runtime does not affect the validity of the algorithm, since each ground state of $H_p$ encodes a solution to the problem.
[29] C. D. Meyer, Matrix Analysis and Applied Linear Algebra (Society for Industrial and Applied Mathematics, Philadelphia, 2000).
[30] The authors in Refs. [13, 15, 19] also considered another type of Hamiltonian, expressed as $H_i = a_0 I + \sum_{i<j} a_{ij} (\sigma_i^x \otimes \sigma_j^x + \sigma_i^y \otimes \sigma_j^y )$. Since they did not give an expression of the initial state, we do not examine the existence of the nonzero energy gap for this type of Hamiltonian here.
[31] E. Farhi, J. Goldstone, S. Gutmann, and D. Nagaj, Int. J. Quantum Inf. 6, 503 (2008).
[32] It is also worth noting that the annealing schedule provided by R. D. Somma, D. Nagaj, and M. Kieferova, Phys. Rev. Lett. 109, 050501 (2012), for solving the glued-trees problem, is still efficient even though the minimum energy gap of the Hamiltonian is exponentially small in the problem size.