Quantum algorithm for obtaining the eigenstates of a physical system

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Abstract

We propose a quantum algorithm for solving the following problem: given the Hamiltonian of a physical system and one of its eigenvalues, how to obtain the corresponding eigenstate? The algorithm is based on the resonance phenomena. For a probe qubit coupled to a quantum system, the system exhibits a resonance dynamics when the frequency of the probe qubit matches a transition frequency in the system. Therefore the system can be guided to evolve to the eigenstate with known eigenvalue by inducing resonance between the probe qubit and a designed transition in the system. This algorithm can also be used to obtain the energy spectrum of a physical system and can achieve even a quadratic speedup over the phase estimation algorithm.

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Introduction.—Obtaining the eigenstates and energy spectrum of a physical system is of fundamental importance in quantum physics and quantum chemistry. In principle, the task can be achieved by solving the Schrödinger equation of the system. In most cases, however, the Schrödinger equations can not be solved exactly, and numerical approaches such as full diagonalization or Monte Carlo methods are not efficient in terms of the size of the system on a classical computer. The quantum phase estimation algorithm (PEA) \[^{1}\] has been proposed for solving the following problem efficiently: given an unitary operator \(U\), and one of its eigenstate \(|\Psi\rangle\), how to estimate the phase factor \(\theta\) of the corresponding eigenvalue \(e^{i\theta}\) of \(U\)? And later the PEA is applied for solving the Schrödinger equation of a system on a quantum compute to obtain the energy eigenvalues and eigenstates of a physical system \[^{2, 3}\]. The success probability of the PEA is proportional to the square of the overlap of the guess state with the real eigenstate of the system. Adiabatic quantum evolution (AQE) is another quantum algorithm for preparing an eigenstate of a system \[^{4}\]. In AQE, however, one can only prepare the ground state of the system, and the scaling the runtime of the algorithm remains an open question in the case where the ground state of the system is degenerate.

In this paper, we propose a different quantum algorithm for obtaining an arbitrary eigenstate of a physical system by asking the following question: given the Hamiltonian of a system and one of its eigenvalues, how to obtain the corresponding eigenstate of the system? This algorithm is based on the resonance phenomena that for a probe qubit coupled to a physical system, the probe exhibits a dynamical response when it resonates with a transition in the system. Therefore the system can be guided to evolve to the eigenstate with known eigenvalue by inducing a resonance between the probe qubit and a transition in the system. The algorithm can even achieve a quadratic speedup over the PEA, and can also be used to obtain the energy spectrum of a system.

The algorithm.—Without loss of generality, we illustrate the algorithm by showing how to obtain the ground state of a physical system provided the ground state energy is already known. Details of the algorithm are as follows.

We construct a quantum register \(R\) of \((n + 1)\) qubits, which contains one ancilla qubit and an \(n\)-qubit quantum register that represents a physical system of dimension \(N = 2^n\). A probe qubit is coupled to \(R\) and the Hamiltonian of the entire \((n + 2)\)-qubit system is in
the form
\[ H = \frac{1}{2} \omega \sigma_z + I_2 \otimes H_R + c \sigma_x \otimes B, \]
where \( I_2 \) is the two-dimensional identity operator, \( \sigma_x \) and \( \sigma_z \) are the Pauli matrices. The first term in the above equation is the Hamiltonian of the probe qubit, the second term is the Hamiltonian of the register \( R \), and the third term describes the interaction between the probe qubit and \( R \). Here, \( \omega \) is the frequency of the probe qubit (\( \hbar = 1 \)), and \( c \) is the coupling strength between the probe qubit and \( R \), and \( c \ll \omega \). The Hamiltonian of \( R \) is in the form
\[ H_R = |0\rangle\langle 0| \otimes [\epsilon_0 (|0\rangle\langle 0|)^\otimes n] + |1\rangle\langle 1| \otimes H_S, \]
where \( H_S \) is the Hamiltonian of the system and \( \epsilon_0 \) is a parameter that is set as a reference point to the ground state energy \( E_1 \) of \( H_S \). \( B \) is an operator that acts on the register \( R \), which can be varied for different systems. The operator \( B = \sigma_x \otimes A \), and \( A \) acts on the state space of the system. The construction of operator \( A \) depends on the system and will be discussed in the following sections.

To run the algorithm, first we prepare the probe qubit in its excited state \( |1\rangle \) and the register \( R \) in a reference state \( |\Phi\rangle = |0\rangle^\otimes(n+1) \), which is an eigenstate of \( H_R \) with eigenvalue \( \epsilon_0 \), the \((n+2)\) qubits are in state \( |\Psi_0\rangle = |1\rangle|\Phi\rangle = |1\rangle|0\rangle^\otimes n \). Then evolve the entire \((n+2)\)-qubit system with the Hamiltonian \( H \) for time \( t \). After that, perform a measurement on the probe qubit in basis of \( |0\rangle \). When the probe qubit decays to its ground state \( |0\rangle \), the last \( n \) qubits of the register \( R \) evolves to the ground state of the system with large probability.

The circuit for the algorithm is shown in Fig. 1.

In basis of \( \{ |\Psi_0\rangle = |1\rangle|0\rangle^\otimes n, |\Psi_i\rangle = |0\rangle|1\rangle|\varphi_i\rangle \}, i = 1, \cdots, N \), where \( |\varphi_i\rangle \) are the eigenstates of \( H_S \) with the corresponding eigenvalues \( E_i \), the Hamiltonian \( H \) in Eq. (1) is in the form: \( H_{00} = \frac{1}{2} \omega + \epsilon_0; H_{0i} = H_{i0} = c\langle \varphi_i | A |0\rangle^\otimes n, \) and \( H_{ii} = -\frac{1}{2} \omega + E_i \), for \( i \geq 1 \); and \( H_{ij} = 0 \) for \( i, j \geq 1 \) and \( i \neq j \). The ground state \( |\varphi_1\rangle \) of \( H_S \) is encoded in the basis state \( |\Psi_1\rangle = |0\rangle|1\rangle|\varphi_1\rangle \). With the initial state being set as \( |\Psi_0\rangle \), the Schrödinger equation \( i \frac{d}{dt} |\Psi\rangle = H |\Psi\rangle \) describes the evolution of the entire \((n+2)\)-qubit system from \( |\Psi_0\rangle \) to states \( |\Psi_i\rangle = |0\rangle|1\rangle|\varphi_i\rangle \) through \( N \) independent channels.

When the parameter \( \epsilon_0 \) satisfies the condition \( E_1 - \epsilon_0 = \omega \), which means the transition frequency between the reference state and the state \( |\Psi_1\rangle \) matches the frequency of the probe qubit, we have \( H_{00} = H_{11} = \frac{1}{2} \omega + \epsilon_0 \), and the system evolves from the initial state \( |\Psi_0\rangle \) to the state \( |\Psi_1\rangle = |0\rangle|1\rangle|\varphi_1\rangle \) reaches maximal probability at time \( t \sim 1/ (c|\langle \varphi_1 | A |0\rangle^\otimes n|) \),
provides that the energy gap between the ground state and the first excited state of the system is finite. Then the last \( n \) qubits of the register \( R \) evolves to the ground state \( |\varphi_1\rangle \) of the system with high probability. The evolution time \( t \) is the runtime of the algorithm, and will be discussed in the next section.

**Efficiency of the algorithm.** The efficiency of the algorithm depends on the runtime \( t \) and the probability of the system being evolved to state \( |\Psi_1\rangle \) which encodes the ground state of the physical system, \( P = |\langle \Psi_1 | U(t) | \Psi_0 \rangle |^2 \). In general, we can not solve the Schrödinger equation exactly to obtain \( P(t) \) of the algorithm, but we can estimate the runtime \( t \) by considering some special cases.

In the algorithm, when the frequency of the probe qubit matches the transition frequency between the reference state \( |\Phi\rangle \) and the eigenstate \( 1 \rangle |\varphi_j\rangle \) of \( H_R \), the probability of the \((n+2)\)qubit system being transferred from the initial state \( |\Psi_0\rangle \) to the state \( |\Psi_1\rangle \) reaches maximum at certain time \( t \). There is also a probability for the system being transferred to other states \( |\Psi_j\rangle \), \( j = 2, \ldots, N \). By applying the first-order perturbation theory, this probability can be formulated as \[3\]

\[
\sin^2 \left( \frac{\Omega_{0j}}{2} t \right) \frac{Q_{0j}^2}{Q_{0j}^2 + (E_j - \epsilon_0 - \omega)^2}, \quad j = 2, \ldots, N
\]

where \( Q_{0j} = 2c |\langle \varphi_j | A | 0 \rangle|^n \), and \( \Omega_{0j} = \sqrt{Q_{0j}^2 + (E_j - \epsilon_0 - \omega)^2} \). From the above equation one can see that as the transition frequency between the reference state and the state \( 1 \rangle |\varphi_j\rangle \) becomes closer to the frequency of the probe qubit, the probability of the system being evolved to state \( |\varphi_j\rangle \) is higher. Based on this analysis, the runtime of the algorithm must be in between of the two assumed special cases of the system: all the excited states \( |\varphi_j\rangle \), \( j = 2, \ldots, N \) are degenerate at the lowest or the highest possible energy levels of the system. By assuming that the ground state of the system is non-degenerate and the excited states are \((N-1)\)-fold degenerate, we can calculate \( P(t) \) by exactly solving the Schrödinger equation.

In the algorithm, the state \( A|0\rangle^\otimes n \) can be expanded by the complete set of the eigenstates of the system \( \{ |\varphi_i\rangle, i = 1, 2, \ldots, N \} \) as \( A|0\rangle^\otimes n = \sum_{i=1}^{N} d_i |\varphi_i\rangle \), where \( d_i = \langle \varphi_i | A | 0 \rangle^\otimes n \) and \( \sum_{i=1}^{N} |d_i|^2 = 1 \). Suppose the excited states of the system are \((N-1)\)-fold degenerate with eigenvalue \( E' + \frac{1}{2} \), let \( |\Psi_2\rangle = |0\rangle|1\rangle \frac{1}{\sqrt{N-1}} \sum_{i=2}^{N} |\varphi_i\rangle \) and \( d_1 = d \), the Hamiltonian matrix of \( H \) in basis \( \{ |\Psi_0\rangle = |1\rangle|0\rangle|0\rangle^\otimes n, |\Psi_1\rangle = |0\rangle|1\rangle|\varphi_1\rangle, |\Psi_2\rangle = |0\rangle|1\rangle \frac{1}{\sqrt{N-1}} \sum_{i=2}^{N} |\varphi_i\rangle \} \) can be written
as

\[
H = \begin{pmatrix}
\frac{1}{2}\omega + \varepsilon_0 & cd & c\sqrt{1-|d|^2} \\
 cd & \frac{1}{2}\omega + \varepsilon_0 & 0 \\
c\sqrt{1-|d|^2} & 0 & E'
\end{pmatrix}.
\] (4)

Let \( |\Psi(t)\rangle = c_0(t) |\Psi_0\rangle + c_1(t) |\Psi_1\rangle + c_2(t) |\Psi_2\rangle \), the Schrödinger equation with the above Hamiltonian can be solved exactly and

\[
c_1(t) = 4 cd \sum_x \frac{(iE' + x)e^{xt}}{12ix^2 - 8 (E' + 1)x + 4ic^2 - 4iE' - i},
\] (5)

where \( x \) satisfies the equation

\[
4x^3 + 4i (E' + 1)x^2 + (4c^2 - 4E' - 1)x + i(4c^2d^2E' - 2c^2d^2 + 2c^2 - E') = 0.
\] (6)

The probability of the system being evolved from the initial state \( |\Psi_0\rangle \) to the state \( |\Psi_1\rangle \) is \( P(t) = |c_1(t)|^2 \). It depends on the evolution time \( t \), the coupling coefficient \( c \), the overlap of the state \( A|0\rangle^\otimes n \) with the ground state of the system, \( d = \langle \varphi_1 | A|0\rangle^\otimes n \), and the eigenvalue \( E' + \frac{1}{2} \) of the state \( |\Psi_2\rangle \) and therefore can be expressed as \( P(c, d, E', t) \). It reaches its maximal value as the runtime \( t \sim \frac{1}{cd} \). The runtime of the algorithm can be reduced if one can construct an unitary operator \( A \) such that \( A|0\rangle^\otimes n \) is close to the ground state \( |\varphi_1\rangle \) of the system. Operator \( A \) can be constructed in some simple way to satisfy this condition in practice, e.g., in an application of our algorithm for obtaining eigenstates and energy spectrum of water molecule through nuclear magnetic resonance, we set \( A = H_d^\otimes n \), where \( H_d \) is the Hadamard matrices. The construction of operator \( A \) can be achieved using some state preparation techniques [6–9].

The coupling coefficient \( c \) is related to the parameter \( d \), here we set \( c = d^\alpha \). In the following, we suppose the ground state energy of the system \( E_1 = 1 \). By setting \( \omega = 1 \) and \( \varepsilon_0 = 0 \), we study the variation of the success probability of the algorithm \( P(E', d, \alpha, t) \) with respect to the parameters \( E', d, \alpha \) and \( t \).

In Fig. 2, we set \( d = 0.01 \) and plot the variation of \( P \) with respect to \( t \) and \( E' \) by setting \( \alpha = 1 \) in Fig. 2(a) and \( \alpha = 0 \) in Fig. 2(b), respectively. From the figures we can see that as \( E' \) increases, \( P \) becomes a periodic function with respect to the evolution time \( t \). And \( P \) reaches unity quickly at small \( E' \) in the case \( \alpha = 1 \) while at large \( E' \) in the case \( \alpha = 0 \).
TABLE I. Results for variation of the exponent $\alpha$ vs. $d$ while keeping $P = 0.99$ as $E' = 20$. The runtime $t$ of the algorithm is shown and compared with $1/d^2$, the efficiency of the phase estimation algorithm.

| $d$   | 0.01 | 0.02 | 0.05 | 0.1  | 0.2  | 0.4  |
|-------|------|------|------|------|------|------|
| $\alpha$ | 0.7  | 0.6  | 0.5  | 0.35 | 0.2  | 0    |
| $t$   | 3925 | 815  | 140  | 35   | 11   | 4    |
| $1/d^2$ | 10000 | 2500 | 400  | 100  | 25   | 7    |

In Fig. 3, by setting $d = 0.01$, we show the variation of $P$ versus $E'$ at $t = \frac{\pi}{2c^d} = \frac{\pi}{2d(1+\alpha)}$ for $\alpha = 0, 0.5, \text{and} 1$, respectively. From the figure we can see that as the exponent $\alpha$ increases, $P$ reaches unity quickly, and only at large $E'$, the success probability $P$ can be close to unity for small exponent $\alpha$.

In Fig. 4, by setting $d = 0.01$ and $E' = 5$, we show the variation of $P$ versus the evolution time $t$ for $\alpha = 0, 0.5, \text{and} 1$, respectively. We can see that $P$ increases as $\alpha$ increases, $P$ is a periodic function of $t$ and the period decreases as $\alpha$ increases. And $P$ can be finitely large even in the case $\alpha = 0$.

The runtime of the algorithm scales as $t \sim 1/(c\langle \varphi_1|A|0\rangle^{\otimes n})$, we can make a guess on $t$ to run the algorithm. And from Fig. 4, we can see that there is a large probability for the success probability of the algorithm $P$ to be finitely large with a guessed runtime $t$.

It is important to study the scaling of the exponent $\alpha$ with respect to $d$ since the runtime of the algorithm is determined by $1/d^{(1+\alpha)}$. In Table I, we show the results for the variation of the exponent $\alpha$ vs. $d$ while keeping $P = 0.99$ as $E' = 20$. From the Table we can see that as $d$ increases, the exponent $\alpha$ decreases even to zero at $d = 0.4$. This means that the runtime of the algorithm scales as $1/d$, while in PEA, the success probability of the algorithm scales as $d^2$, which means the algorithm has to be executed for $1/d^2$ times to obtain the eigenstates. There is a quadratic speedup of our algorithm over the PEA in this case. If we lower the success probability to $P = 0.94$, $\alpha$ can decrease to zero even at $d = 0.1$, and the evolution time is reduced to 15.

Fig. 5 shows the variation of the exponent $\alpha$ vs. $d$ for $E' = 2, 5, 10, 20$, respectively, while keeping $P = 0.9$. We can see that as $E'$ increases, $\alpha$ decreases quickly and even reaches zero.
at large $d$. This indicates that the runtime of the algorithm can scale as $1/d$ while keeping a very high success probability $P = 0.9$.

The time evolution operator $U(t) = \exp(-iHt)$ of the algorithm can be implemented efficiently through the Trotter formula \[10\] on a quantum computer:

$$U(t) = \left[ e^{-i\left(\frac{1}{2}\omega_\sigma_z + H_R\right)t/M} e^{-i{\sigma_x} \otimes B} t/M \right]^M + O\left(\frac{1}{M}\right),$$

where $M$ is a large number.

Obtaining the energy spectrum of the system.—In this algorithm, when the transition frequency between the reference state and an eigenstate of the system matches the frequency of the probe qubit, it contributes the most to the decay of the probe qubit. By performing measurements on the probe qubit in basis of $|0\rangle$ to obtain its decay probability, a peak in the decay rate of the probe qubit will be observed. Therefore by varying the frequency of the probe qubit or the eigenvalue of reference state $\varepsilon_0$, and run the algorithm, we can locate the transition frequencies between the reference state and the eigenstates of the system \[11\]. Therefore obtain the energy spectrum of the system. The detailed procedure is as follows.

First, we estimate the range of the energy spectrum of the system and set $[\omega_{\text{ini}}, \omega_{\text{fin}}]$ as the range of transition frequency between the reference state and the eigenstates of the system. The frequency range is then discretized into $q$ intervals, where each interval has a width of $\Delta \omega = (\omega_{\text{fin}} - \omega_{\text{ini}})/q$. The frequency points are set as $\omega_k = \omega_{\text{ini}} + k\Delta \omega$ ($k = 0, \ldots, q$), and form a frequency set. We set the frequency of the probe qubit to be $\omega_k$, and let the entire system evolve with the Hamiltonian $H$ for time $t$. Then read out the state of the probe qubit by performing a measurement on the probe qubit in basis $|0\rangle$. Repeat the whole procedure many times to obtain the decay probability of the probe qubit. Then set the probe qubit in another frequency and repeat the above procedure until run over all the frequency points in the frequency set.

An application of our algorithm for obtaining eigenstates and the energy spectrum of water molecule have been implemented experimentally through nuclear magnetic resonance.

Discussion.—For the Schrödinger equation $H_S|\psi\rangle = E|\psi\rangle$ of the system, an eigenvalue of $H_S$ can be obtained if its corresponding eigenstate is known, and vice versa. Various methods based on a guess state of the system have been developed to obtain the eigenstates of the system including PEA. Here, we proposed a quantum algorithm for obtaining the eigenstates of a system while the corresponding eigenvalue is known. The algorithm is based on a physical phenomena that when a probe qubit is coupled to a quantum system, the transition in the system that resonates with the qubit contributes the most to the dynamics
of the probe qubit.

In the PEA for obtaining eigenstates and eigenenergies of a system, the success probability of obtaining the $k$-th eigenstate $|\varphi_k\rangle$ of the system is $|d_k|^2$, where $d_k$ is the overlap of the guess state with $|\varphi_k\rangle$. And the number of times the algorithm has to be run to obtain the eigenstate $|\varphi_k\rangle$ and its corresponding eigenenergy is proportional to $1/|d_k|^2$. In our algorithm, the overlap of the state $A|0\rangle^\otimes n$ with the eigenstate of the $i$-th energy level of the system is $d_i = \langle \varphi_i | A | 0 \rangle^\otimes n$. The runtime of the algorithm $1/|d_i| \leq t \leq 1/|d_i|^2$, the lower limit of the runtime of the algorithm is consistent with the quantum speed limit for a system moving from an initial state to a final state \[12\].

In this algorithm, all the eigenstates of the system are “labeled” by their eigenenergies, and an eigenstate of interest is obtained by searching its “label” through inducing resonance with the probe qubit. The probability of the system being evolved to the target state is amplified by introducing a resonance between the probe qubit and a transition between the reference state and the target state of the system. This is equivalent to applying a quantum transformation on the system to achieve a quantum speedup in searching the target state. In general, it can be viewed as an amplitude amplification technique \[13\]. This explains why the lower bound of the runtime of the algorithm is $1/|d_i|$, which is the efficiency of the Grover’s algorithm for the search problem \[14\]. And because of this property of the algorithm, for a given eigenvalue of the system, all the corresponding eigenstates can be obtained, even for degenerate eigenstates, in which case the adiabatic quantum evolution algorithm cannot prepare all the eigenstates.

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FIG. 1. Quantum circuit for obtaining the eigenstates of a physical system. $U(\tau)$ is a time evolution operator driven by a Hamiltonian given in Eq. (1). The first line represents a probe qubit, the second line is an ancilla qubit and the last $n$ qubits represent the quantum system.
FIG. 2. (Color online) The probability of the entire \((n + 2)\)-qubit system being evolved from the state \(|\Psi_0\rangle\) to the state \(|\Psi_1\rangle\) vs. the evolution time \(t\) and \(E'\). In (a) the parameter \(\alpha = 1\); and in (b) \(\alpha = 0\).
FIG. 3. (Color online) The variation of $P$ vs. $E'$ at $t = \frac{\pi}{2} \frac{1}{d^{\frac{1}{\alpha}}}$, for $\alpha = 0, 0.5, 1$ respectively by setting $d = 0.01$. The black solid line shows the results for $\alpha = 0$; the red dashed line shows the results for $\alpha = 0.5$; and the blue dotted line shows the results for $\alpha = 1$, respectively.
FIG. 4. (Color online) The variation of $P$ vs. the evolution time $t$ for $\alpha = 0, 0.5, 1$ respectively, by setting $d = 0.1$ and $E' = 5$. The black solid line shows the results for $\alpha = 0$; the red dashed line shows the results for $\alpha = 0.5$; and the blue dotted line shows the results for $\alpha = 1$, respectively.
FIG. 5. (Color online) The variation of the exponent \( \alpha \) vs. \( d \) for \( E' = 2, 5, 10, 20 \), respectively, while keeping \( P = 0.9 \). The black filled square shows the results for \( E' = 2 \); the red filled circle shows the results for \( E' = 5 \); the blue filled triangle shows the results for \( E' = 10 \); and the cyan filled star shows the results for \( E' = 20 \), respectively.