Quantum algorithm for obtaining the eigenstates of a physical system

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We propose a quantum algorithm for solving the following problem: given the Hamiltonian of a physical system and one of its eigenvalues, how do we obtain the corresponding eigenstate? The algorithm is based on the resonance phenomenon. For a probe qubit coupled to a quantum system, the system exhibits 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 a known eigenvalue by inducing the 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 quadratic speedup over the phase estimation algorithm.

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I. 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 cannot 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] was proposed for solving the following problem efficiently: given an unitary operator U and one of its eigenstates $|\Psi\rangle$, how do we estimate the phase factor θ of the corresponding eigenvalue $e^{i\theta}$ of U? Later, the PEA was applied for solving the Schrödinger equation of a system on a quantum computer to obtain the energy eigenvalues and eigenstates of a system [2,3]. 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 scaling the run time of the algorithm remains an open question in the case where the ground state is degenerate. In Ref. [5], a quantum algorithm was proposed for preparing ground states of quantum systems in time $\sqrt{N}$, where N is the size of the system. The algorithm can also be applied for preparing arbitrary eigenstates of a quantum system.

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 do we obtain the corresponding eigenstate of the system? This algorithm is based on the resonance phenomenon 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 a known eigenvalue by inducing a resonance between the probe qubit and a transition in the system. The algorithm can also be used to obtain the energy spectrum of a system. It can achieve a quadratic speedup over the PEA in obtaining the eigenstates and the corresponding eigenvalues of a physical system, even for degenerate eigenstates. Compared with the algorithm in Ref. [5], our algorithm requires fewer resources, and the implementation of our algorithm is easier. In the algorithm in Ref. [5], one has to know the absolute value of the eigenenergy of a desired eigenstate to prepare the momentum state on the auxiliary qubits. While our algorithm works even when one does not know the exact eigenvalue of the desired eigenstate. A detailed comparison of our algorithm with the algorithm in Ref. [5] is presented in Sec. IV.

II. 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

$$H = -\tfrac{1}{2}\omega\sigma_z \otimes I_2^{\otimes(n+1)} + I_2 \otimes H_R + c\sigma_x \otimes B, \qquad (1)$$

where I_2 is the two-dimensional identity operator and σ_x and σ_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, ω is the frequency of the probe qubit ($\hbar = 1$), c is the coupling strength between the probe qubit and R, and $c \ll \omega$. The Hamiltonian of R is in the form

$$H_R = |0\rangle\langle 0| \otimes [\varepsilon_0(|0\rangle\langle 0|)^{\otimes n}] + |1\rangle\langle 1| \otimes H_S, \qquad (2)$$

where H_S is the Hamiltonian of the system and ε_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.

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 ε_0; the $(n+2)$ qubits are in state $|\Psi_0\rangle = |1\rangle|\Phi\rangle = |1\rangle|0\rangle|0\rangle^{\otimes n}$. Then we evolve the entire $(n+2)$-qubit system with the Hamiltonian H for time t. After that, we perform a measurement on the

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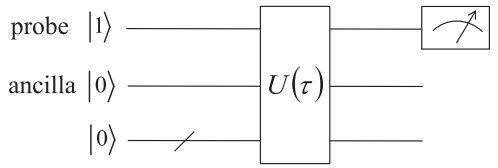

FIG. 1. Quantum circuit for obtaining the eigenstates of a physical system. $U(\tau)$ is a time evolution operator driven by a Hamiltonian given in Eq. (1). The first line represents a probe qubit, the second line is an ancilla qubit, and the last n qubits represent the quantum system.

probe qubit in the basis of $|0\rangle$. When the probe qubit decays to its ground state $|0\rangle$, the last n qubits of the register R evolve to the ground state of the system with large probability. The circuit for the algorithm is shown in Fig. 1.

In the basis of $\{|\Psi_0\rangle = |1\rangle|0\rangle|0\rangle^{\otimes n}, |\Psi_i\rangle = |0\rangle|1\rangle|\varphi_i\rangle, i = 1,\ldots,N\}$, 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 $H_{00} = \frac{1}{2}\omega + \varepsilon_0$; $H_{i0} = H_{0i}^* = c\langle\varphi_i|A|0\rangle^{\otimes n}$ and $H_{ii} = -\frac{1}{2}\omega + E_i$ for $i \geqslant 1$, and $H_{ij} = 0$ for $i,j \geqslant 1$ 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 ε_0 satisfies the condition $E_1 - \varepsilon_0 = \omega$, which means the transition frequency between the reference state and the state $|\Psi_1\rangle$ matches the frequency of the probe qubit, we have $H_{00} = H_{11} = \frac{1}{2}\omega + \varepsilon_0$, and the system evolves from the initial state $|\Psi_0\rangle$ to the state $|\Psi_1\rangle = |0\rangle|1\rangle|\varphi_1\rangle$ and reaches maximal probability at time $t \sim 1/(c|\langle\varphi_1|A|0\rangle^{\otimes n}|)$, provided that the energy gap between the ground state and the first excited state of the system $E_2 - E_1 \gg c$. Then the last n qubits of the register R evolve to the ground state $|\varphi_1\rangle$ of the system with high probability.

III. EFFICIENCY OF THE ALGORITHM

The efficiency of the algorithm depends on the run time 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 cannot solve the Schrödinger equation exactly to obtain $P(t)$ of the algorithm, but we can estimate the run time 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 $|1\rangle|\varphi_1\rangle$ 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 a 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 [6]

$$\sin^2\left(\frac{\Omega_{0j}\tau}{2}\right)\frac{Q_{0j}^2}{Q_{0j}^2 + (E_j - \varepsilon_0 - \omega)^2}, \quad j = 2,\ldots,N, \quad (3)$$

where $Q_{0j} = 2c|\langle\varphi_j|A|0\rangle^{\otimes n}|$ and $\Omega_{0j} = \sqrt{Q_{0j}^2 + (E_j - \varepsilon_0 - \omega)^2}$. From the above equation one can see that as the transition frequency between the reference state and the state $|1\rangle|\varphi_j\rangle$ gets closer to the frequency of the probe qubit, the probability of the system being evolved to the state $|\varphi_j\rangle$ is higher. Based on this analysis, the run time of the algorithm must be in between 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 nondegenerate 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 $E' + \frac{1}{2}$, and 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 the 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

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

Let $|\Psi(t)\rangle = c_0(t)|\Psi_0\rangle + c_1(t)|\Psi_1\rangle + c_2(t)|\Psi_2\rangle$, and suppose the ground-state energy of the system $E_1 = 1$. By setting $\omega = 1$ and $\varepsilon_0 = 0$, the Schrödinger equation with the above Hamiltonian can be solved exactly, and

$$c_1(t) = 4cd\sum_x \frac{(E'-x)e^{-ixt}}{-12x^2 + 8(E'+1)x + 4c^2 - 4E' - 1}, \quad (5)$$

where x are the eigenvalues of the Hamiltonian matrix in Eq. (4) with $\omega = 1$ and $\varepsilon_0 = 0$.

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 run time $t \sim \frac{1}{cd}$. The run time of the algorithm can be reduced if one can construct an operator A such that $A|0\rangle^{\otimes n}$ is close to the ground state $|\varphi_1\rangle$ of the system. The construction of operator A can be achieved using some state preparation techniques [7–10].

The coupling coefficient c is related to the parameter d; here, we set $c = d^\alpha$. In the following, with $E_1 = 1$, $\omega = 1$, 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, α, and t.

We set $d = 0.01$ and plot the variation of P with respect to t and E' by setting $\alpha = 1$ and $\alpha = 0$ in Figs. 2 and 3, respectively. From Figs. 2 and 3 we can see that as E' increases, P becomes a periodic function with respect to the evolution time t. P reaches unity quickly at small E' in the case with $\alpha = 1$ and at large E' in the case with $\alpha = 0$.

In Fig. 4, by setting $d = 0.01$, we show the variation of P versus E' at $t = \frac{\pi}{2}\frac{1}{cd} = \frac{\pi}{2}\frac{1}{d^{(1+\alpha)}}$ for $\alpha = 0$, 0.5, and 1. From Fig. 4 we can see that as the exponent α increases, P reaches

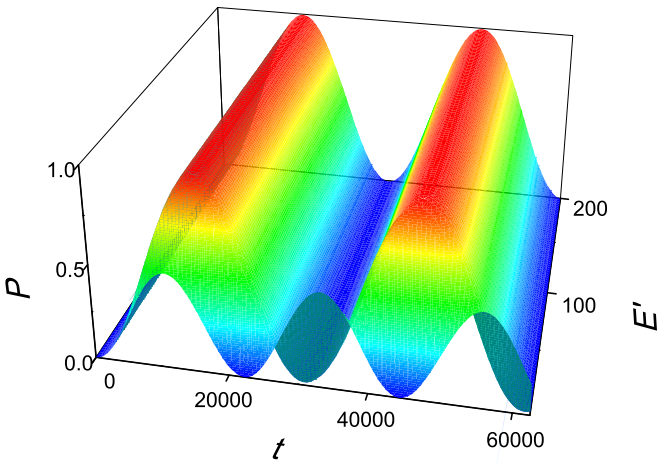

FIG. 2. The probability of the entire $(n+2)$-qubit system being evolved from the state $|\Psi_0\rangle$ to the state $|\Psi_1\rangle$ vs the evolution time t and E'. The parameter $\alpha = 1$. Atomic units are used.

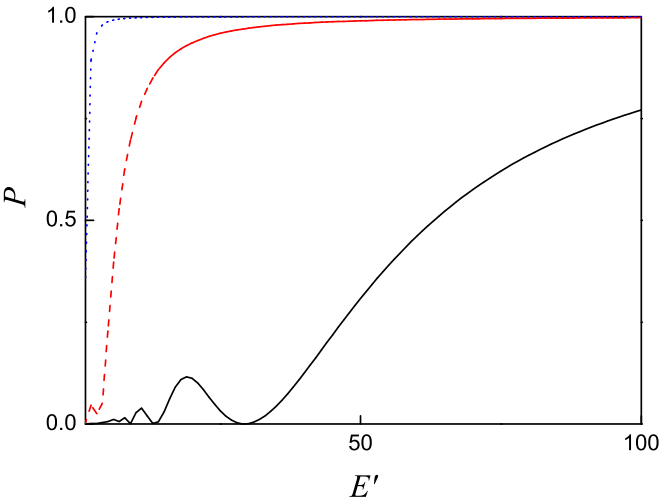

FIG. 4. The variation of P vs E' at $t = \frac{\pi}{2}\frac{1}{d^{1+\alpha}}$ for $\alpha = 0, 0.5, 1$ while setting $d = 0.01$. The black solid line shows the results for $\alpha = 0$; the red dashed line shows the results for $\alpha = 0.5$, and the blue dotted line shows the results for $\alpha = 1$. Atomic units are used.

unity quickly, and only at large E' can the success probability P be close to unity for a small exponent α.

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

The run time of the algorithm scales as $t \sim 1/(c|\langle\varphi_1|A|0\rangle^{\otimes n}|)$, and we can make a guess on t to run the algorithm. From Fig. 5, we can see that there is a large probability for the success probability of the algorithm P to be finitely large with a guessed run time t.

It is important to study the scaling of the exponent α with respect to d since the run time of the algorithm is determined by $1/d^{(1+\alpha)}$. In Table I, we show the results for the variation of the exponent α vs d while keeping $P = 0.99$ when $E' = 20$. From Table I we can see that as d increases, the exponent α decreases even to zero at $d = 0.4$. This means that the run time 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 $1/d^2$ 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 $P = 0.94$, α can decrease to zero even at $d = 0.1$, and the evolution time is reduced to 15.

Figure 6 shows the variation of the exponent α vs d for $E' = 2, 5, 10, 20$ while keeping $P = 0.9$. We can see that as E' increases, α decreases quickly and even reaches zero at large d. This indicates that the run time of the algorithm can scale as $1/d$ while keeping a very high success probability $P = 0.9$.

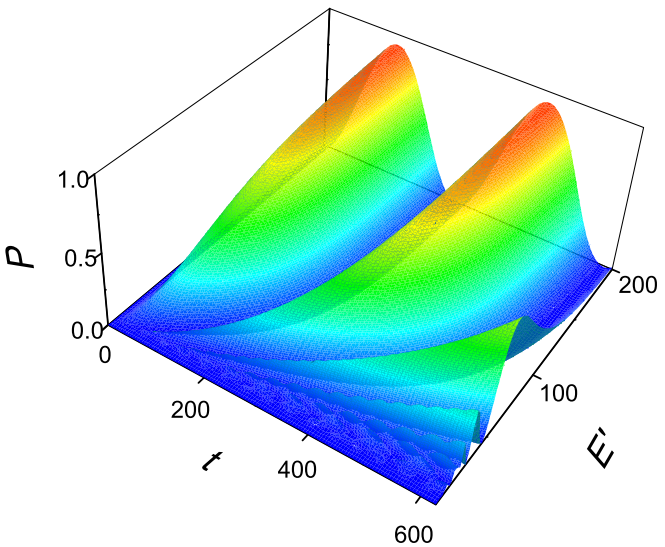

FIG. 3. The same as in Fig. 2, except $\alpha = 0$. Atomic units are used.

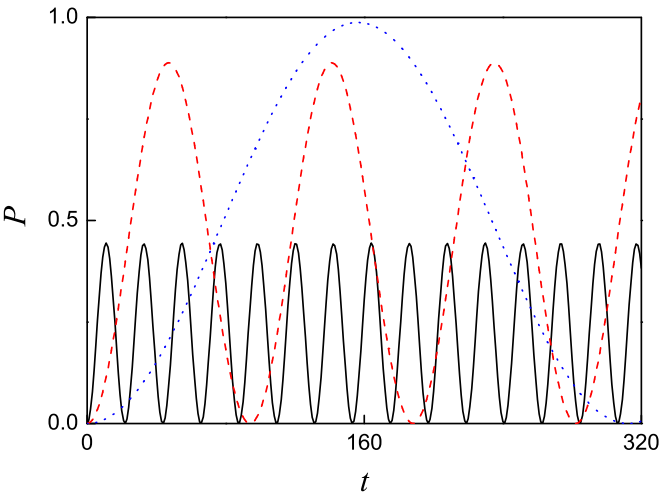

FIG. 5. The variation of P vs the evolution time t for $\alpha = 0, 0.5, 1$ while setting $d = 0.1$ and $E' = 5$. The black solid line shows the results for $\alpha = 0$; the red dashed line shows the results for $\alpha = 0.5$, and the blue dotted line shows the results for $\alpha = 1$. Atomic units are used.

TABLE I. Results for variation of the exponent α vs d while keeping $P = 0.99$ when $E' = 20$. The run time 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
α	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

The time evolution operator $U(t) = \exp(-iHt)$ of the algorithm can be implemented efficiently through the Trotter formula [11] on a quantum computer.

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 the 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 ε_0 and running the algorithm, we can locate the transition frequencies between the reference state and the eigenstates of the system. Therefore this algorithm can also be used to obtain the energy spectrum of the system. The procedures are the same as in Ref. [12].

IV. 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. Here, we proposed a quantum algorithm for obtaining the eigenstates of a system when the corresponding eigenvalue is known.

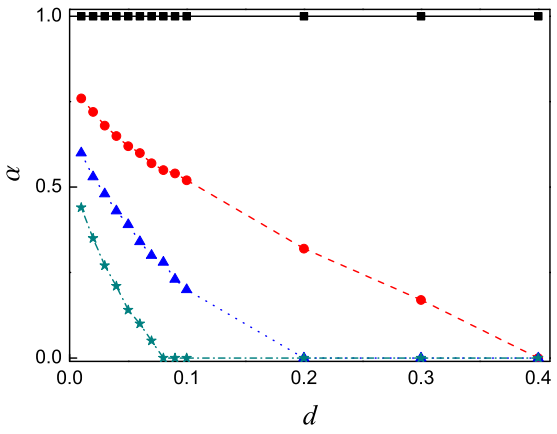

FIG. 6. The variation of the exponent α vs d for $E' = 2,5,10,20$ (atomic units are used) while keeping $P = 0.9$. The black squares show the results for $E' = 2$, the red circles show the results for $E' = 5$, the blue triangles show the results for $E' = 10$, and the cyan stars show the results for $E' = 20$.

In the following we compare our algorithm with the PEA, the algorithm we proposed in Ref. [12], and the algorithm in Ref. [5].

In the PEA, the success probability for obtaining the kth eigenstate $|\varphi_k\rangle$ of the system is d_k^2, where $d_k = |\langle\varphi_k|\psi_s\rangle|$ is the overlap of the eigenstate $|\varphi_k\rangle$ with the guess state $|\psi_s\rangle$ of the system. Therefore, the run time of the PEA for obtaining the eigenstate $|\varphi_k\rangle$ and its corresponding eigenenergy is $\tau_0 \frac{1}{d_k^2}$, where τ_0 is the run time of the PEA each time. For the algorithm in Ref. [12], the run time of the algorithm for obtaining the eigenstate $|\varphi_k\rangle$ and its corresponding eigenenergy scales as $1/(|\langle\varphi_k|A|\varphi_i\rangle|^2 d_k^2)$.

To the algorithm in Ref. [12], we add one ancilla qubit in the present algorithm, and then we can prepare the initial input state of the register R as $|\Phi\rangle = |0\rangle^{\otimes(n+1)}$, which is set as a reference state to the physical system. With this, one can vary the eigenvalue ε_0 of the reference state while keeping the frequency of the probe qubit fixed; it is more convenient for experimental implementation. The reference state $|\Phi\rangle$ is an eigenstate of H_R; therefore the overlap of the initial state with the eigenstate of H_R is 1. The state $A|0\rangle^{\otimes n} = |\psi_s\rangle$ can be considered a guess state of the kth eigenstate of the system. The run time of the algorithm for obtaining the eigenstate $|\varphi_k\rangle$ and its corresponding eigenvalue of the system is $1/(cd_k)$. In this algorithm, we have shown that the run time of the algorithm scales as $1/d_k \leqslant t \leqslant 1/d_k^2$, which means our algorithm can achieve even quadratic speedup over the phase estimation algorithm and the algorithm in Ref. [12].

We now compare our algorithm with the algorithm in Ref. [5]. In this algorithm, a procedure contains the inverse phase estimation algorithm, and Grover's algorithm is proposed and acts as a filter to suppress the amplitude of the eigenstates outside of the bandwidth and amplify the amplitude of the desired eigenstates. Compared with this algorithm, our algorithm has following advantages: our algorithm requires fewer resources than the algorithm in Ref. [5]. In Ref. [5] one has to prepare on the auxiliary qubits a momentum state which is associated with the eigenvalue of an eigenstate of the system. One has to prepare the absolute value of the phase factor and therefore requires more qubits than our algorithm, which requires $(n + 2)$ qubits in total. The implementation of our algorithm is simpler and easier than the algorithm in Ref. [5]. The algorithm in Ref. [5] contains procedures of PEA and Grover's algorithm; the PEA contains a number of controlled unitary operations and has to be implemented a number of times, and Grover's algorithm has to be run the square root of N times. However, in our algorithm, one only has to implement the unitary operator by applying Trotter's formula and performing single-qubit measurements on the probe qubit. In the algorithm in Ref. [5], one has to know the absolute value of the eigenenergy of a desired eigenstate to prepare the momentum state on the auxiliary qubits. In our algorithm, the algorithm works even when one does not know the exact eigenenergy of the desired eigenstate. One can make a guess about the range of the eigenenergy of the system, then locate the eigenenergy and find out the corresponding eigenstate. This approach is described in the last paragraph of Sec. III.

Preparing a guess state as input to an algorithm is equivalent to measuring the guess state with the eigenstates of the

system and then taking the measurement result as input to the algorithm. The success probability of the input state being in the kth eigenstate of the system is $|\langle\varphi_k|\psi_s\rangle|^2$. In our present algorithm, by introducing a reference state, the overlap is always 1. Therefore in our algorithm we can obtain quadratic speedup over the phase estimation algorithm and the algorithm in Ref. [12]. The unitary evolution of the algorithm can provide quantum speedup.

In this algorithm, all eigenstates of the system are "labeled" by their eigenenergies, and an eigenstate of interest is obtained by searching its label by 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 designed transition between the reference state and the target state of the system. In general, it can be viewed as an amplitude amplification technique [5,13]. This is equivalent to applying a quantum transformation to the system to achieve a quantum speedup in searching the target state. This explains why the lower bound of the run time of the algorithm is $1/d_k$, which is the efficiency of Grover's search algorithm [13,14]. 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. Grover's algorithm cannot be used directly to find the eigenstates of a physical system since the eigenstates are unknown and the Hamiltonian matrix of the system in general is not diagonal. In our algorithm, by designing the algorithm based on the resonance phenomena, the system can be evolved to the desired eigenstate and can achieve quadratic speedup over the phase estimation algorithm.

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