Quantum computational method of finding the ground-state energy and expectation values

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We propose a quantum computational way of obtaining a ground-state energy and expectation values of observables of interacting Hamiltonians. It is based on the combination of the adiabatic quantum evolution to project a ground state of a noninteracting Hamiltonian onto a ground state of an interacting Hamiltonian and the phase estimation algorithm to retrieve the ground-state energy. The expectation value of an observable for the ground state is obtained with the help of the Hellmann-Feynman theorem. As an illustration of our method, we consider a displaced harmonic oscillator, a quartic anharmonic oscillator, and a potential scattering model. The results obtained by this method are in good agreement with the known results.

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I. INTRODUCTION

Quantum simulation might be a real application of medium-scale quantum computers with 50–100 qubits [1]. As Feynman suggested, a quantum computer can simulate quantum systems better than a classical computer because it is also a quantum system [2]. Lloyd demonstrated that almost all quantum systems can be simulated on quantum computers [3]. Abrams and Lloyd presented a quantum algorithm to find eigenvalues and eigenvectors of a unitary operator based on the quantum phase estimation algorithm [4]. Although it is an efficient quantum algorithm, there is room for improvement. First, one has to prepare an input state close to unknown eigenstates. Second, it has been little explored how to obtain physical properties except the energy spectrum.

In this paper, we propose a refined quantum computational method to calculate the ground-state energy and expectation values of observables for interacting quantum systems. The main idea is as follows. Adiabatic turning on of an interaction makes the ground state of a noninteracting system evolve to the ground state of an interacting system. During the adiabatic evolution, the phase estimation algorithm extracts the phase of an evolving quantum system continuously without the collapse of a quantum state. So the ground energy of an interacting system is obtained as a function of coupling strength. With the help of the Hellmann-Feynman theorem [5], the expectation value of an observable for the ground state of an interacting system is obtained. As a test of our method, we simulate on classical computers three quantum systems: A displaced harmonic oscillator, a quartic anharmonic oscillator [6], and a potential scattering model [7].

II. METHOD

Let us start with a brief review of Abrams and Lloyd's algorithm. Its goal is to find eigenvalues E_n and eigenstates $|E_n\rangle$ of a time-independent Schrödinger equation

$$H|E_n\rangle = E_n|E_n\rangle. \tag{1}$$

Their key idea to solve Eq. (1) is to consider its time evolution

$$e^{-iHt/\hbar}|\Psi_I\rangle = \sum_{n=0} e^{-iE_n t/\hbar} a_n |E_n\rangle, \tag{2}$$

where $|\Psi_I\rangle = \Sigma_n a_n |E_n\rangle$ is an input or trial state. The information on eigenvalues E_n in the input state is transferred to index qubits by applying the quantum phase estimation algorithm. The measurement of the index qubits gives us a good approximation to E_n with probability $|a_n|^2$, and makes $|\Psi_I\rangle$ collapse to $|E_n\rangle$. It is instructive to compare Eq. (2) with the quantum Monte Carlo method which uses the imaginary time $\tau = it$ to project the input state onto the ground state [8]

$$\lim_{\tau\to\infty} e^{-H\tau/\hbar}|\Psi_I\rangle \simeq e^{-E_0\tau/\hbar} a_0 |E_0\rangle. \tag{3}$$

First, in order to find the ground-state energy, both Eqs. (2) and (3) require a good input state close to $|E_0\rangle$. If the input state does not contain the information about the ground state, both will fail. Second, for each run, while Eq. (2) outputs E_n randomly, Eq. (3) produces E_0 always. Finally, Eq. (2) is a real time evolution; however, Eq. (3) is the imaginary time evolution, i.e., a diffusion process, which is implemented by classical random walks.

Our goal is to find a ground-state energy with probability 1 even if an input state contains little information on the ground state. Our method uses a real time projection onto the ground state by adiabatically turning on an interaction. Ortiz *et al.* suggested the use of the Gell-Mann–Low theorem to find the spectrum of a Hamiltonian with quantum computers [9,10]. Farhi *et al.* developed the adiabatic quantum computation [11].

We divide the Hamiltonian H into two parts: Noninteracting Hamiltonian H_0 and interaction H_1, $H = H_0 + H_1$. As usual, it is assumed that the eigenvalues W_n and eigenstates $|W_n\rangle$ of H_0 are known, $H_0|W_n\rangle = W_n|W_n\rangle$. We recast H to be time-dependent

$$H(t) = H_0 + f(t)H_1 + E_c, \tag{4}$$

where a slowly varying function $f(t)$ satisfies $f(0)=0$ and $f(T_R)=1$ with running time T_R. The role of the constant energy E_c will be explained later. As the interaction is turned on slowly, the input state $|W_0\rangle$ evolves adiabatically to $|E_0\rangle$

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$$\hat{T}e^{-i/\hbar\int_0^t H(t')dt'}|W_0\rangle \simeq e^{-i/\hbar\int_0^t E_0(t')dt'}|E_0\rangle, \tag{5}$$

where $\hat{T}$ is a time-ordering operator [13]. Notice the similarity and difference between Eqs. (2), (3), and (5). The quantum phase estimation algorithm can extract the information on E_0 from Eq. (5). Since, during the adiabatic evolution, the quantum system is in an instantaneous ground state $|E_0(t)\rangle$ of $H(t)$, one can apply frequently the phase estimation algorithm without the collapse of the quantum state to the excited states.

Since the phase $\phi=E_n t/\hbar$ is defined in $0\leq\phi<2\pi$, the phase estimation algorithm gives us only the absolute value of an energy $|E_n|$. Its sign can be determined by adding E_c. When E_0 is negative, while W_0 is positive, $E_c>E_0$ makes all the spectrum positive. Also E_c is useful for stabilizing the algorithm. If $|E_0|$ is close to zero, a long time is needed to make the phase $\phi=E_0 t/\hbar$ finite.

The expectation value of an observable $\mathcal{O}$ can be obtained with the help of the Hellmann-Feynman theorem [5]. It states that if $H(\alpha)|E_n(\alpha)\rangle=E_n(\alpha)|E_n(\alpha)\rangle$ with parameter α, then the following relation holds:

$$\frac{dE_n(\alpha)}{d\alpha}=\langle E_n(\alpha)|\frac{dH}{d\alpha}|E_n(\alpha)\rangle. \tag{6}$$

By modifying the full Hamiltonian to have a linear coupling to $\mathcal{O}$, $H(t)=H_0+f(t)(H_1+\alpha\mathcal{O})+E_c$, Eq. (6) becomes

$$\left.\frac{dE_n(\alpha)}{d\alpha}\right|_{\alpha=0}=\langle E_n|\mathcal{O}|E_n\rangle. \tag{7}$$

Therefore, the expectation value of an observable is obtained from a derivative of $E_n(\alpha)$ at $\alpha=0$. In practice, Eq. (7) is obtained from a numerical approximation $\langle E_n|\mathcal{O}|E_n\rangle=[E_n(\alpha)-E_n(-\alpha)]/2\alpha+\mathcal{O}(\alpha^2)$. This is comparable with an expectation estimation algorithm [12]. Notice that our scheme does not require the repeated measurements and the average over the individual outcomes [1].

III. APPLICATION TO QUANTUM SYSTEMS

A. Displaced harmonic oscillator

As an illustration of our method, let us consider a simple Hamiltonian,

$$H_0=\frac{p^2}{2m}+\frac{m\omega^2x^2}{2},\quad H_1=\lambda x. \tag{8}$$

For convenience, we set $\hbar=m=\omega=1$. It is well known that Eq. (8) is exactly solvable, a usual perturbation theory for it works well, and its ground state is a coherent state.

The first step to quantum simulation is to map a physical system to a qubit system. The position x in Eq. (8) is continuous, but qubits are discrete. A usual approach is to discretize x. Another way is to map the eigenstates $|n\rangle$ of H_0 to the computational basis of N qubits, $|n\rangle=|j_{N-1}\rangle\otimes|j_{N-2}\rangle\otimes\cdots|j_0\rangle$ with $n=j_{N-1}2^{N-1}+j_{N-2}2^{N-2}+\cdots+j_0 2^0$ and $j_k=0$ or 1. Then H_0 is given by a diagonal matrix,

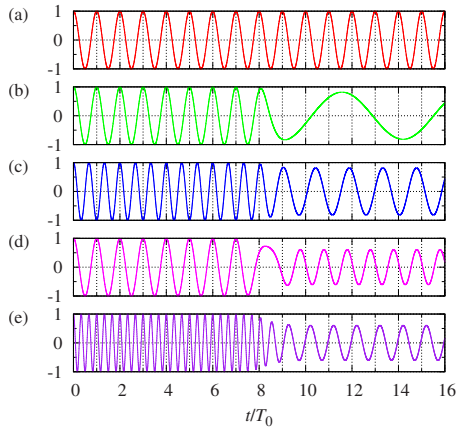

FIG. 1. (Color online) Re$\{a_0(t)\}$ as a function of t/T_0 for (a) $\lambda=0$ and $E_c=0$, (b) $\lambda=0.9$ and $E_c=0$, (c) $\lambda=0.9$ and $E_c=0.25$, (d) $\lambda=\sqrt{2}$ and $E_c=0$, and (e) $\lambda=\sqrt{2}$ and $E_c=1.0$. Here $N=4$ and $T_0=2\pi\hbar/W_0=4\pi$ with $W_0=\hbar\omega/2$.

$$H_0\approx\sum_{n=0}^{2^N-1}\left(n+\frac{1}{2}\right)|n\rangle\langle n|. \tag{9}$$

The quantum dynamics of Eq. (9) was simulated on an NMR quantum computer by Somaroo *et al.* [14]. On the other hand, H_1 is written as a tridiagonal matrix,

$$H_1\approx\frac{1}{\sqrt{2}}\sum_{n=0}^{2^N-2}(\sqrt{n}|n\rangle\langle n+1|+\sqrt{n}|n+1\rangle\langle n|). \tag{10}$$

A quantum state $|\psi(t)\rangle$ at time t can be expressed in terms of $|n\rangle$, $|\psi(t)\rangle=\Sigma_{n=0}^{2^N-1}a_n(t)|n\rangle$.

The adiabatic time evolution (5) is implemented by solving the time-dependent Schrödinger equation with the fourth-order Runge-Kutta method on a classical computer. We take $N=3-6$. We assume that the phase estimation algorithm is implemented very accurately. The adiabatic switching-on function $f(t)$ used here is given by $f(t)=\frac{1}{2}+\frac{1}{2}\tanh(20t/T_R-10)$. One may expect it would take a long time for a quantum system to evolve adiabatically. However, in the case considered here, it takes the running time $T_R=15\ T_0$ to obtain the ground-state energy with accuracy $\Delta E_0=|E_0^{\text{exact}}-E_0^{\text{num}}|\leq 10^{-6}$, where $T_0\equiv 2\pi/\omega$ is the period of the ground state of H_0, $E_0^{\text{exact}}=\frac{1}{2}\hbar\omega-\lambda^2/2m\omega^2$, and E_0^{num} is the numerical value.

Figure 1 shows how the dynamical phase of the system changes as the interaction is slowly turned on. In Fig. 1(a), $\lambda=0$, and the oscillation period is T_0. Figures 1(b) and 1(c) show how the constant energy E_c is used to change the frequency corresponding to the ground-state energy of an interacting Hamiltonian. In Fig. 1(b), $\lambda=0.9$ and $E_c=0$. So the frequency $E_0/\hbar$ becomes very low. However, in Fig. 1(c), the constant energy $E_c=1/4$ shifts the frequency so it can be easily measured. In Figs. 1(d) and 1(e), we take $\lambda=\sqrt{2}$ so the exact energy is $E_0=-1/2$. Since the phase estimation algorithm produces only the absolute value of energy, $|E_0|$, the constant energy E_c is added in Eq. (4) to decide its sign. In

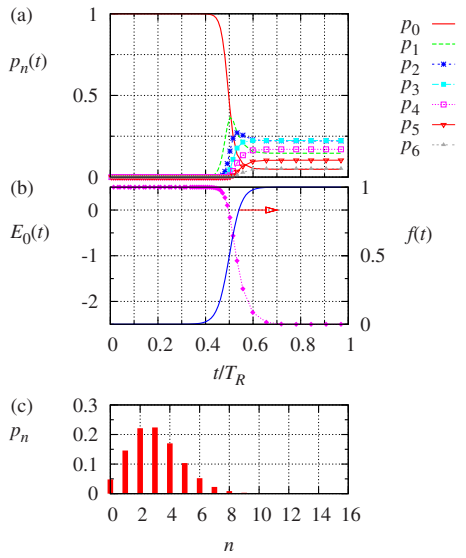

FIG. 2. (Color online) (a) Probability $p_n(t)=|a_n(t)|^2$ of qubits in the computational basis $|n\rangle$, and (b) the instantaneous ground-state energy $E_0(t)$ in the unit of $\hbar\omega$ as a function of the dimensionless time t/T_R for $\lambda=\sqrt{6}$. In (b), $f(t)$ is an adiabatically switching-on function. (c) At $t=T_R$, p_n obeys the Poisson distribution of a coherent state.

Fig. 1(d), $E_c=0$. At the end of running, the estimated energy is $E_0=1/2$. So the phase estimation algorithm fails to calculate the exact ground-state energy $E_0=-1/2$. However, in Fig. 1(e), $E_c=1$. The phase estimation algorithm gives us the energy 1/2. So we know that the exact energy is $E_0=1/2-1=-1/2$.

For any λ, the ground state of Eq. (8) is a coherent state. As shown in Fig. 2, the probability that qubits are in the number state $|n\rangle$ follows a Poisson distribution. So the ground state obtained by the quantum simulation might be called a *pseudocoherent state* because it is defined on the truncated Hilbert space. It is a collective state of N qubits.

The coherent state is also characterized by the minimum uncertainties in x and p. Its mean square deviation of x, $\Delta x^2=\langle x^2\rangle-\langle x\rangle^2$, is 1/2 for any λ. The ground state of Eq. (8) is displaced from the origin to $x=-\lambda$. So $\langle x\rangle=-\lambda$. With the help of the Hellmann-Feynman theorem, we calculate $\langle x^2\rangle$ for $\lambda=0$ and $\lambda=1$. To this end, the final Hamiltonian is modified as $H(t)=H_0+f(t)(\lambda x+\alpha x^2)+E_c$. Figure 3 shows the ground-state energy $E_0(\alpha)$ as a function of α. The derivative of $E_0(\alpha)$ at $\alpha=0$ gives us the expectation value of x, $\langle x^2\rangle = dE_0(\alpha)/d\alpha|_{\alpha=0}$. As illustrated in Fig. 3, we have $\langle x^2\rangle=0.02/0.04=1/2$ for $\lambda=0$. Thus $\Delta x^2=1/2$. For $\lambda=1$, $\langle x^2\rangle=0.03/0.02=3/2$. Again we have $\Delta x^2=3/2-1=1/2$.

B. Quartic anharmonic oscillator

Let us consider an anharmonic oscillator, whose Hamiltonian is given by

$$H_0=\frac{p^2}{2m}+\frac{m\omega^2x^2}{2},\quad H_1=\lambda x^4, \tag{11}$$

where $\lambda>0$ is the coupling constant. In their seminal paper [6], Bender and Wu showed that the Rayleigh-Schrödinger

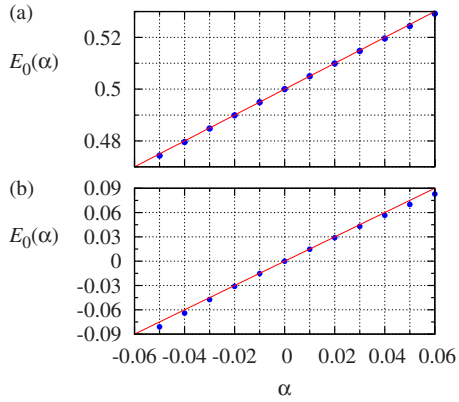

FIG. 3. (Color online) Ground state energy $E_0(\alpha)$ in the unit of $\hbar\omega$ as a function of α for (a) $\lambda=0$ and (b) $\lambda=1$. The points are numerical results. The line in (a) is the plot of $f(\alpha)=\frac{1}{2}(\alpha+1)$. In (b), the line is the plot of $g(\alpha)=\frac{3}{2}\alpha$.

perturbation theory for Eq. (11) becomes divergent for any λ. Various nonperturbative methods have been applied to this simple model.

One can write $H_1=(\lambda/4)(a^\dagger+a)^4=3\lambda/4+(\lambda/4)V$, where

$$\begin{aligned}V_{mn}=&\sqrt{(n\pm1)(n\pm2)(n\pm3)(n+2\pm2)}\,\delta_{m,n\pm4}\\&+2(2n+1\pm2)\sqrt{(n\pm1)(n+1\pm1)}\,\delta_{m,n\pm2}\\&+6n(n+1)\,\delta_{m,n}.\end{aligned} \tag{12}$$

The matrix of Eq. (12) is denser than Eq. (10). So more qubits are used in Eq. (12) in order to get the accurate energy.

Figure 4 shows the ground-state energy $E_0(\lambda)$ and $\Delta x^2(\lambda)$ as a function of λ. For $\lambda=2.0$ and time step $\Delta t=5.0\times10^{-5}$, we obtain $E_0=0.951\,568\,472\,125$, which is comparable to the best known results $E_0=0.951\,568\,472\,722$ [15]. For the calculation of Δx^2, we obtain $E_0(\lambda,\alpha)$ of $H_0+\lambda H_1+\alpha x^2$ for $\alpha=\pm0.001$. Thus we have $\langle x^2\rangle\approx[E_0(\lambda,\alpha)-E_0(\lambda,-\alpha)]/2\alpha$.

C. Potential scattering model

Finally, we consider spinless electrons with a contact potential with Hamiltonian

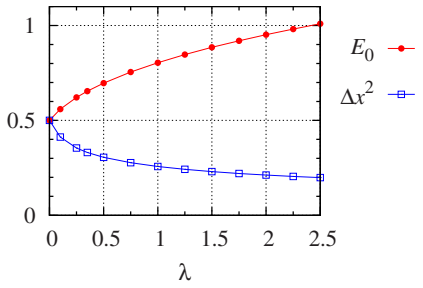

FIG. 4. (Color online) For a quartic anharmonic oscillator, (a) $E_0(\lambda)$ in the unit of $\hbar\omega$ and (b) Δx^2 as a function of λ. Here $N=6$ and $T_R=15\ T_0$.

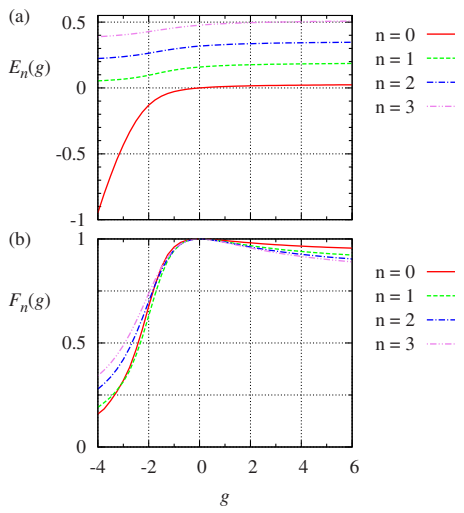

FIG. 5. (Color online) (a) Energy levels E_n (in arbitrary units) and fidelity F_n as a function of g. Here $N=6$ and $\Delta=10/64$.

$$H_0 = \sum_{n=1}^{2^N} \epsilon_n c_n^\dagger c_n, \quad H_1 = \frac{g}{2^N} \sum_{n,m} c_n^\dagger c_m, \tag{13}$$

where $\epsilon_n=(n-1)\Delta$ with level spacing Δ, $c_n^\dagger$ is a creation operator, and g is the coupling constant. Although this model is very simple and exactly solvable, it contains rich physics [7]. The naive perturbation theory breaks down no matter small g is. For an attractive potential, i.e., $g<0$, the lowest eigenstate of Eq. (13) becomes a bound state. Also it exhibits the Anderson orthogonality catastrophe [16] which states that the ground state of H_0+H_1 becomes orthogonal to the ground state of H_0 in the thermodynamic limit.

We map the single-particle energy level of H_0 to a computational basis, $|n\rangle=c_n^\dagger c_n|\text{vac}\rangle$, where $|\text{vac}\rangle$ is a vacuum state. In Eq. (13), H_0 can be written as a diagonal matrix, $(H_0)_{mn}=\epsilon_n\delta_{mn}$, whereas H_1 are given by $(H_1)_{mn}=g/2^N$, which is more dense than Eqs. (10) and (12).

As g is turned on adiabatically, the initial state $|n\rangle$ evolves to the final state $|E_n(g)\rangle$. We use the notation $|E_n(0)\rangle=|\epsilon_n\rangle=|n\rangle$. Figure 5(a) illustrates the single-particle levels $E_n(g)$. One can see that there is one bound state with negative energy $E_0(g)<0$ for $g<0$, but otherwise it is positive. Figure 5(b) shows the fidelity $F_n(g)=|\langle E_n(g)|n\rangle|^2$ as a function of g. Surprisingly, it is also calculated with the help of the Hellmann-Feynman theorem. One can rewrite $F_n(g)=\langle E_n(g)|\mathcal{O}|E_n(g)\rangle$ with $\mathcal{O}=|n\rangle\langle n|$. As shown in Fig. 5(b), the fidelity decreases more rapidly for $g<0$ than for $g>0$. One can see that even single-particle levels for $g=0$ and $g<0$ become orthogonal. It is interesting that the fidelity between the interacting and noninteracting many-body ground states can be obtained from all the information of single-particle levels [17].

IV. CONCLUSIONS

In conclusion, we have proposed a method to find the ground-state energy by adiabatically turning on an interaction. The expectation values of an observable have been obtained by switching on a modified interaction which contains an observable and by applying the Hellmann-Feynman theorem. Our method has been successfully tested by solving three quantum systems. We expect that our method could be applied to the simulation of more interesting quantum systems.

Finally, let us discuss the limits of our method. Our method is based on the combination of adiabatic quantum computation and the phase estimation algorithm. So, the computational resources needed to implement our method are approximately equal to the sum of those involved in adiabatic quantum computation and the phase estimation algorithm. The running time of the adiabatic evolution increases if the gap between the energy levels decreases. However, it is expected that the quantum Zeno effect [18] might release this limitation. A quantum state after applying a quantum phase estimation algorithm is approximately given by $|\Psi(t)\rangle \approx a_0|E_0\rangle_S|\omega_0\rangle_I+a_1|E_1\rangle_S|\omega_1\rangle_I$, where $|a_1|^2=1-\epsilon$ and $|a_1|^2=\epsilon$ for small ϵ and subscripts S and I refer to the system and the index qubits, respectively. The measurement on the index qubits gives us $|\Psi(t)\rangle=|E_0\rangle_S|\omega_0\rangle_I$ with high probability. The frequent applications of a quantum phase estimation algorithm and measurement on the index qubits could accelerate an adiabatic evolution. This will be investigated in a future study.

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