Quantum Computational Method of Finding the Ground State Energy and Expectation Values

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We propose a new 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 non-interacting 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 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 new 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 an interaction makes the ground state of a non-interacting 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

\[
H|E_n\rangle = E_n|E_n\rangle .
\]  

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

\[
e^{-iHt}\Psi_I = \sum_{n=0} e^{-iE_n t \hbar} a_n |E_n\rangle,
\]

where \( \Psi_I = \sum_n a_n |E_n\rangle \) 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 \( \Psi_I \) collapse to \( |E_n\rangle \). It is instructive to compare (2) with the quantum Monte Carlo method which uses the imaginary time \( \tau = it \) to project the input state onto the ground state [8].

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

First, in order to find the ground state energy, both (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 (2) outputs \( E_n \) randomly, (3) produces \( E_0 \) always. Finally, (2) is a real time evolution, however, (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: non-interacting 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, \(H_0|W_n\rangle = W_n|W_n\rangle\).

The adiabatic time evolution \(5\) is implemented by
\[
\hat{T} e^{-\frac{i}{\hbar} \int_0^t H(t') dt'} |W_0\rangle \simeq e^{-\frac{i}{\hbar} \int_0^t E_0(t') dt'} |E_0\rangle, \tag{5}
\]
where \(\hat{T}\) is a time-ordering operator \[12\]. Notice the similarity and difference between \[13\], \[14\], and \[15\]. The quantum phase estimation algorithm can extract the information on \(E_0\) from \(E_0\) for it works well, and its ground state is a coherent state.

The adiabatic time evolution \(5\) is exact only if \(E_0\) is close to zero, a long time needs to make the phase \(\hat{\Phi} = E_0 t /\hbar\) finite.

The expectation value of an observable \(O\) can be obtained with the help of the Hellmann-Feynman theorem \[9\]. It states that if \(H(\alpha)|E_0(\alpha)\rangle = E_0(\alpha)|E_0(\alpha)\rangle\) with parameter \(\alpha\), then the following relation holds
\[
\frac{dE_0(\alpha)}{d\alpha} = \langle E_0(\alpha)|\frac{dH}{d\alpha}|E_0(\alpha)\rangle. \tag{6}
\]

By modifying the full Hamiltonian to have a linear coupling to \(O\), \(H(t) = H_0 + f(t)(H_1 + \alpha O) + E_c\), \(\ref{5}\) becomes
\[
\frac{dE_0(\alpha)}{d\alpha}_{\alpha=0} = \langle E_n|O|E_n\rangle. \tag{7}
\]

Therefore, the expectation value of an observable is obtained from a derivative of \(E_0(\alpha)\) at \(\alpha = 0\). In practice, \(\ref{5}\) is obtained from a numerical approximation \(\langle E_0|O|E_0\rangle \approx |E_0 + (\frac{E_0 - E_0(-\alpha)}{2\alpha}) + O(\alpha^2)|\), 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,
\[
H_0 = \frac{\beta^2}{2m} + \frac{m\omega^2 x^2}{2}, \quad H_1 = \lambda x. \tag{8}
\]
For convenience, we set \(h = m = \omega = 1\). It is well known that \(\ref{8}\) 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 \(\ref{8}\) 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, \(|n\rangle = |j_{N-1} \rangle \otimes |j_{N-2} \rangle \otimes \ldots |j_0 \rangle\) with \(n = j_{N-1} 2^{N-1} + j_{N-2} 2^{N-2} + \ldots + j_0 2^0\) and \(j_k = 0\) or 1. Then \(H_0\) is given by a diagonal matrix,
\[
H_0 \approx \sum_{n=0}^{2^N-1} (n + \frac{1}{2}) |n\rangle\langle n|, \tag{9}
\]

The quantum dynamics of \(\ref{9}\) was simulated on an NMR quantum computer by Somaroo et al. \[14\]. On the other hand, \(H_1\) is written as a tridiagonal matrix,
\[
H_1 \approx \frac{1}{\sqrt{2}} \sum_{n=0}^{2^N-2} \left( \sqrt{n} |n+1\rangle\langle n| + \sqrt{n+1} |n\rangle\langle n+1| \right). \tag{10}
\]

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

The adiabatic time evolution \(\ref{5}\) is implemented by solving the time-dependent Schrödinger equation with the forth-order Runge-Kutta method on a classical computer. We take \(N = 3 \times 6\). 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 \(T_0 = 2\pi /\omega\) is the period of the ground state of \(H_0\), \(E_0^{\text{exact}} = \frac{1}{2} h \omega - \frac{1}{2m} c^2\), and \(E_0^{\text{num}}\) is the numerical value.

Fig. 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 \(T_0\). Figs. 1 (b) and (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 \(E_0/h\) become 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 (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 (a) to decide its sign. In 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 (c), $E_c = 1$. 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 $\lambda$, the ground state of $\Box$ 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 pseudo-coherent 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 $\lambda$. The ground state of $\Box$ 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 $H(t) = H_0 + f(t)(\lambda x + \alpha x^2) + E_c$. Fig. 3 shows the ground state energy $E_0(\alpha)$ as a function of $\alpha$. The derivative of $E_0(\alpha)$ at $\alpha = 0$ gives us the expectation value of $x$, $\langle x^2 \rangle = \frac{dE_0(\alpha)}{d\alpha} |_{\alpha=0}$. 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 $\Delta x^2 = 3/2 - 1 = 1/2$. 

FIG. 1: (color online). Re $\{\langle a(t) \rangle\}$ 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 $W_0 = \hbar\omega/2$.

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 $t/T_0$ for $\lambda = \sqrt{6}$. In (b), $f(t)$ is an adiabatically switching-on function. (c) At $t = T_0$, $p_n$ obeys the Poisson distribution of a coherent state.

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

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

\[ H_0 = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}, \quad H_1 = \lambda x^4, \quad (11) \]

where \( \lambda > 0 \) is the coupling constant. In their seminal paper [2], Bender and Wu showed that the Rayleigh-Schrödinger perturbation theory for (11) becomes divergent for any \( \lambda \). Various non-perturbative methods have been applied to this simple model.

One can write \( H_1 = \frac{1}{4}(a^\dagger a)^4 + \frac{3\lambda}{2} + \frac{\lambda}{2} V \), where

\[
V_{mn} = \sqrt{(n+1)(n+2)(n+3)(n+2+2)} \delta_{m,n+4} + 2(2n+1+2)\sqrt{(n+1)(n+1+1)} \delta_{m,n+2} + 6n(n+1) \delta_{m,n} . \quad (12)
\]

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

![Graph showing ground state energy](image)

**FIG. 4:** (color online). For a quartic anharmonic oscillator, (a) \( E_0(\lambda) \) in the unit of \( \hbar \omega \) and (b) \( \Delta x^2 \) as a function of \( \lambda \). Here \( N = 6 \) and \( T_R = 15 T_0 \).

Fig. 4 shows the ground state energy \( E_0(\lambda) \) and \( \Delta x^2(\lambda) \) as a function of \( \lambda \). For \( \lambda = 2.0 \) and time step \( \Delta t = 5.0 \times 10^{-5} \), we obtain \( E_0 = 0.951\,568\,472\,125 \), which is comparable to the best known results \( E_0 = 0.951\,568\,472\,722 \) [13]. For the calculation of \( \Delta x^2 \), we obtain \( E_0(\lambda, \alpha) \) of \( H_0 + \lambda H_1 + \alpha x^4 \) for \( \alpha = \pm 0.001 \). 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

\[ H_0 = \sum_{n=1}^{2^N} \epsilon_n c_n^\dagger c_n, \quad H_1 = \frac{g}{2N} \sum_{n,m} c_n^\dagger c_m , \quad (13) \]

where \( \epsilon_n = (n-1)\Delta \) with level spacing \( \Delta \), \( c_n^\dagger \) is a creation operator, and \( g \) 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 (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 (13), \( H_0 \) can be written as a diagonal matrix, \( (H_0)_{mm} = \epsilon_n \delta_{mn} \). Whereas \( H_1 \) are given by \( (H_1)_{mn} = g/2^N \), which is more dense than (10) and (12).

![Graph showing fidelity](image)

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

As \( g \) is turned on adiabatically, the initial state \( | n \rangle \) evolves to the final state \( | E_n(g) \rangle \). We use the notation \( | E_n(0) \rangle = | \epsilon_n \rangle = | n \rangle \). Fig. 5 (a) illustrates the single-particle levels \( E_n(g) \). One see that there is one bound state with negative energy \( E_0(g) < 0 \) for \( g < 0 \), but otherwise it is positive. Fig. 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 Hellman-Feynman theorem. One can rewrite \( F_n(g) = | \langle E_n(g) | O | E_n(g) \rangle | \) with \( O = | n \rangle \langle n | \). As shown in Fig. 5 (b), the fidelity decrease 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 non-interacting many-body ground states can be obtained from all the information of single-particle levels [17].
IV. CONCLUSIONS

In conclusion, we have proposed a new method to find the ground state energy by adiabatically turning on an interaction. The expectation values of an observable has 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 is 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 \(\epsilon\) 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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