Improving approximate vacuum prepared by the adiabatic quantum computation

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Abstract

According to the quantum adiabatic theorem, we can in principle obtain a true vacuum of a quantum system starting from a trivial vacuum of a simple Hamiltonian. In actual adiabatic digital quantum simulation with finite time length and non-infinitesimal time steps, we can only obtain an approximate vacuum that is supposed to be a superposition of a true vacuum and excited states. We propose a procedure to improve the approximate vacuum.

Keywords: approximate vacuum, adiabatic quantum computation, digital simulation

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1 Introduction

Recently, quantum computers have been developed for studying several systems\cite{1}. The D-wave is the quantum annealing machine suitable for solving optimization problems\cite{2}. It will be one of the most important subjects for quantum computers to find the lowest energy or the lowest energy state of a quantum system. Some quantum systems have been analyzed by digital quantum simulators of universal type. The (1+1)-dimensional Schwinger model\cite{3} is one of the most famous quantum field theory that has been analyzed by digital quantum simulators\cite{5,6}. One of the bench mark of the analysis is to evaluate vacuum expectation values of physical quantities. It has been observed that certain vacuum expectation value varies in time under a constant Hamiltonian\cite{5}. This means that the approximate vacuum prepared by the adiabatic quantum computation is not a true vacuum but a superposition of a true vacuum and exited states. Time average of the vacuum expectation value slightly differs from the exact value that is known for the case the number of qubits is small\cite{5,7}. Therefore, it is desirable to reduce the affects of the exited states.

The purpose of this paper is to propose a procedure to improve an approximate vacuum reducing affects of excited states. For a one-qubit system based on the (1+1)-dimensional Schwinger model, we show a concrete digital quantum simulation result. We improve an approximate vacuum and a vacuum expectation value of a physical quantity does not varies in time. We also propose a procedure to improve an approximate vacuum for the two-qubits case. Our procedure can be applied successively and approximate precision can in principle be improved gradually. Our procedure can be generalized to an $n$-qubits system.

2 One-qubit system

We consider a one-qubit system described by the simple Hamiltonian

$$\hat{H} = -JH, \quad J > 0,$$

where $H$ is the Hadamard gate $H = \frac{1}{2}(Z + X)$. This Hamiltonian corresponds to the (1+1)-dimensional Schwinger model with a special value of a coupling constant formulated on a spatial lattice composed of only two sites. We construct an approximate vacuum of $\hat{H}$ starting from the trivial vacuum of the initial Hamiltonian $\hat{H} = -JZ$ by the adiabatic quantum computation. We use the following slowly time varying Hamiltonian

$$\hat{H}(s) = (1 - s)\hat{H}_0 + s\hat{H}, \quad 0 \leq s \leq 1,$$

where $s = \frac{t}{T}$ and $T$ is a sufficiently long time length for the adiabatic quantum computation. For $0 \leq t \leq T$ we use $\hat{H}(s)$ and for $t \geq T$ we fix $\hat{H}(s)$ as $\hat{H} = -JH$. According to the adiabatic theorem, we can obtain the true vacuum of $\hat{H}$ at $t = T$, if $T$ is sufficiently large, $\hat{H}(s)$ changes very slowly with respect to $s$, and the vacuum is not degenerate for $\hat{H}(s), 0 \leq s \leq 1$. Fig.1 shows a time variation of the expectation value of $Z$ by the instantaneous vacuum. In the time region $t \geq T$, a periodic oscillation is observed. To the worse, the center of the oscillation slightly differs from $\frac{1}{\sqrt{2}}$ that is the exact vacuum expectation value of $Z$. Therefore, we cannot obtain the exact value $\frac{1}{\sqrt{2}}$ by the time average over a period. The cause of the oscillation is that the approximate vacuum $|\psi\rangle$ is a superposition of the true vacuum $|E_0\rangle$ and the exited state $|E_1\rangle$,

$$|\psi\rangle = \alpha|E_0\rangle + \beta|E_1\rangle, \quad |\alpha|^2 + |\beta|^2 = 1,$$

where $H|E_0\rangle = 1$ and $H|E_1\rangle = -1$. We propose a procedure to reduce the value $|\beta|$ and improve the approximate vacuum. We prepare one ancilla bit, and put the state $|0\rangle|\psi\rangle$ into the quantum circuit in Fig.2. By this quantum circuit the quantum state $|0\rangle|\psi\rangle$ transforms as

$$|0\rangle|\psi\rangle \rightarrow \alpha|0\rangle|E_0\rangle + \beta|1\rangle|E_1\rangle.$$ 

We measure the first qubit by the basis $\{|0\rangle, |1\rangle\}$. If we obtain $|0\rangle$, which occurs with the probability $|\alpha|^2$, we measure $Z$ for the second qubit. If we obtain $|1\rangle$, which occurs with the small probability $|\beta|^2$,
we discard the state. Repeating this measurement many times we can obtain \( \langle E_0 | Z | E_0 \rangle \) with a sufficient precision. Fig.3 shows our simulation result, where at the time \( t = T \), the quantum circuit in Fig.2 is inserted. In Fig.3 we do not adopt the discard procedure for the case \( |1\rangle \). We simulate the value \( |\alpha|^2 \langle E_0 | Z | E_0 \rangle + |\beta|^2 \langle E_1 | Z | E_1 \rangle \), which in our result is 0.706760. The expectation value \( \langle E_0 | Z | E_0 \rangle \) can be obtained by multiplying this value by \( \frac{1}{|\alpha|^2 - |\beta|^2} \) in this case. Our result is \( 2|\alpha|^2 - 1 = 0.999242 \) and we have \( 0.706760 \times \frac{1}{0.999242} = 0.707296 \), which is our approximation value to the exact value \( \frac{1}{\sqrt{2}} \).

3 Two-qubits system and generalization

We propose a procedure to improve an approximate vacuum obtained by the adiabatic quantum computation for a two-qubit system. We consider the following approximate vacuum

\[ |\psi\rangle = \alpha |E_0\rangle + \beta |E_1\rangle + \gamma |E_2\rangle + \delta |E_3\rangle, \tag{5} \]

where \( |E_0\rangle \) is the true vacuum and \( |E_i\rangle, i = 1, 2, 3 \) is the \( i \)-th exited state. Our ideal goal is to perform the following transformation

\[ |00\rangle|\psi\rangle \rightarrow \alpha |00\rangle|E_0\rangle + \beta |01\rangle|E_1\rangle + \gamma |10\rangle|E_2\rangle + \delta |11\rangle|E_3\rangle. \tag{6} \]

After this transformation, measuring the first two qubits, if we obtain \( |00\rangle \) we have the true vacuum \( |E_0\rangle \).

For the system Hamiltonian \( \hat{H} \), we set \( \hat{U}(\theta) = e^{-i\frac{\theta}{2}\hat{H}} \). We put \( |00\rangle|\psi\rangle \) into the quantum circuit in Fig.4. We will have the following transformation

\[
|00\rangle|\psi\rangle \rightarrow \frac{1}{4} |00\rangle(1 + ie^{-i\frac{1}{2}E_0\theta} + (ie^{-i\frac{1}{2}E_0\theta})^2 + (ie^{-i\frac{1}{2}E_0\theta})^3)|E_0\rangle \\
+ (1 + ie^{-i\frac{1}{2}E_1\theta} + (ie^{-i\frac{1}{2}E_1\theta})^2 + (ie^{-i\frac{1}{2}E_1\theta})^3)|E_1\rangle \\
+ (1 + ie^{-i\frac{1}{2}E_2\theta} + (ie^{-i\frac{1}{2}E_2\theta})^2 + (ie^{-i\frac{1}{2}E_2\theta})^3)|E_2\rangle \\
+ (1 + ie^{-i\frac{1}{2}E_3\theta} + (ie^{-i\frac{1}{2}E_3\theta})^2 + (ie^{-i\frac{1}{2}E_3\theta})^3)|E_3\rangle \\
+ \frac{1}{4} |01\rangle(\cdots) + \frac{1}{4} |10\rangle(\cdots) + \frac{1}{4} |11\rangle(\cdots). \tag{7} \]

We define an approximation value of \( E_0 \) by \( E'_0 = \langle \psi | \hat{H} | \psi \rangle \), which can be estimated by a simple quantum simulation. We set the parameter \( \theta \) by \( E'_0 \theta = \pi \). Since \( E'_0 \) is close to \( E_0 \) the coefficient of \( \alpha|00\rangle|E_0\rangle \) in Eq.(7) will satisfy \( \frac{1}{4}|1 + ie^{-i\frac{1}{2}E_0\theta} + (ie^{-i\frac{1}{2}E_0\theta})^2 + (ie^{-i\frac{1}{2}E_0\theta})^3| \approx 1 \), and the coefficients of \( \beta|00\rangle|E_1\rangle, \gamma|00\rangle|E_2\rangle \) and \( \delta|00\rangle|E_3\rangle \) are expected to be small compared with 1. We measure the first two qubits. The state \( |00\rangle \) will be obtained with high probability. We discard other states \( |01\rangle, |10\rangle \) and \( |11\rangle \). Thus we have obtained an approximate vacuum more close to the true vacuum \( |E_0\rangle \). This procedure can in principle be repeated ad infinitum with improving the value \( E'_0 \).

For an \( n \)-qubits system, we prepare \( n \) ancilla qubits in the state \( |0\rangle|0\rangle\cdots|0\rangle \). Using the Hadamard gate on the ancilla qubits and acting the controlled-\( \hat{U}(\theta) \) gates between each ancilla bit and an \( n \)-qubits approximate vacuum (Fig.5), we can improve the approximate vacuum obtained by the adiabatic quantum computation.

4 Summary

We have proposed a procedure to improve an approximate vacuum obtained by the adiabatic quantum computation. We have shown a concrete quantum simulation result for a simple Hamiltonian in one-qubit system. We also have given a quantum circuit to improve an approximate vacuum for a two-qubits system. Our procedure can be easily generalized to an \( n \)-qubits system.
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Figure Captions

Fig.1 Vacuum expectation value of $Z$ by qasm-simulator of IBM. We set $J = \frac{\pi}{4}, T = 36$ and one time-step width is $\frac{1}{2T}$. We use $10^6$ shots.

Fig.2 (a) Quantum circuit that separates the true vacuum and the exited state. (b) Concrete quantum circuit of (a) consists of fundamental gates in Qiskit; $Rz(\theta) = e^{-i\frac{\theta}{2}Z}, Rx(\theta) = e^{-i\frac{\theta}{2}X}$ and $S = |0\rangle\langle 0| + i|1\rangle\langle 1|$. 

Fig.3 Vacuum expectation value of $Z$. At the time $t = T = 36$, the quantum circuit in Fig.2 is inserted. The main cause of the discontinuity at $t = T$ derives mainly from the vanishment of the cross term Re($\bar{\alpha}\beta\langle E_0|Z|E_1\rangle$).

Fig.4 Quantum circuit that approximately separates the true vacuum and the exited states.

Fig.5 Quantum circuit that approximately separates the true vacuum and the exited states for an $n$-qubits system.
Fig. 1

\[ |0\rangle \quad H \quad H \quad |\psi\rangle \quad H \]

Fig. 2  

(a)  

\[ |0\rangle \quad H \quad |\psi\rangle \quad R_z(\pi/2) \quad R_x(\pi/4) \quad Y \quad R_x(-\pi/4) \quad R_z(-\pi/2) \quad Y \]

(b)  

Fig. 3
Fig. 4

\[ |0\rangle \quad H \quad |0\rangle \quad H \]

\[ |\psi\rangle \quad \hat{U}(\theta) \quad (\hat{U}(\theta))^2 \]

Fig. 5

\[ |0\rangle \quad H \quad |0\rangle \quad H \quad |0\rangle \quad H \quad |0\rangle \quad H \]

\[ |\psi\rangle \quad \hat{U}(\theta) \quad (\hat{U}(\theta))^2 \quad (\hat{U}(\theta))^4 \quad (\hat{U}(\theta))^{2n-1} \]