Quantum adiabatic optimization for nuclear ground state

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Introduction

A class of processes known as quantum adiabatic optimization is used to solve optimization problems on a quantum computer. The foundation of this adiabatic quantum computing is the adiabatic theorem of quantum mechanics. The system can modify its configuration in accordance with gradually changing circumstances. If the system starts in a close approximation of the Hamiltonian's ground state, it will eventually reach to its appropriate eigenstate.
The quantum many-body states and operators must be converted into qubit basis states and operations using a variety of encodings and transformations to simulate the Hamiltonian H. To illustrate our approach, we have used the deuteron Hamiltonian using Jordan-Wigner transformation (JW) [1] and then used the modified Quantum Phase Estimation (QPE) algorithm to obtain its ground state energy for various basis sizes.

Encodings and Transformations

The fermionic creation and annihilation operator in JW transformation are

$$\begin{aligned}\sigma^{(+)} =&\frac{1}{2}(X - iY) = \begin{bmatrix}0 & 0\\ 1 & 0\end{bmatrix}\\ \sigma^{(-)} =&\frac{1}{2}(X + iY) = \begin{bmatrix}0 & 1\\ 0 & 0\end{bmatrix}.\end{aligned} \tag{1}$$

Here X and Y are Pauli matrices. We operate with Pauli Z on all the qubits that come before j to incorporate the parity. Deuteron Hamiltonian obtained for 2, 3 and 4 basis size using EFT potential [1] are

$$\begin{aligned}H_2 =&5.9067091I + 0.218291Z_0 - 6.125Z_1\\ &- 2.143304(X_0X_1 + Y_0Y_1),\end{aligned} \tag{2}$$

$$\begin{aligned}H_3 =&H_2 + 9.625(I - Z_2) - 3.91312(X_1X_2\\ &+ Y_1Y_2),\end{aligned} \tag{3}$$

$$\begin{aligned}H_4 =&28.657I + 0.218Z_0 - 6.125Z_1 - 9.625Z_2 -\\ &13.125Z_3 - 2.143(X_0X_1 + Y_0Y_1) - 3.913\\ &(X_1X_2 + Y_1Y_2) - 5.671(X_2X_3 + Y_2Y_3).\end{aligned} \tag{4}$$

Adiabatic time evolution

Given a time-independent Hamiltonian H, the solution of the Schrodinger equation

$$i\frac{d}{dt}\left|\psi(t)\right\rangle = H\left|\psi(t)\right\rangle, \tag{5}$$

with initial quantum state $|\psi(0)\rangle$ is given by

$$\left|\psi(t)\right\rangle = \exp(-iHt)\left|\psi(t)\right\rangle. \tag{6}$$

Eigenstate will simply acquire a phase $\exp(-iHt)$ and for other states, we can obtain the eigenstate of a system by performing adiabatic time evolution [2]. The adiabatic theorem says that in the time limit tends to be infinite, the final state obtained by the evolution will be the ground state of the system, and a QPE based quantum algorithm for the same is given in the next section.

Modified QPE

We can discover the ground state energy eigenvalues using a number of techniques, including variational quantum eigensolver (VQE) [1], quantum phase estimation (QPE), and linear combination of unitaries

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(LCU) [3]. To generate ground state energy eigenvalues that are closer to the outcomes from the precise diagonalization using conventional numerical techniques ("true value"), we need the correct ansatz (our estimated ground state energy eigen function) in all of these methods [4]. In this study, we present a technique called "Modified QPE" where we obtain the eigenstate of a system by performing adiabatic time evolution on the state register. Which converge the ansatz until it gives state fidelity approximately equal to one and leads us to a true ground state from closer approximate guesses shown in Fig. 1.
The first step of the algorithm is to choose a suitable ansatz for the state register and then apply QPE [5] for small time steps to obtain energy eigenvalues. From this we obtain a new state from the measurement results of system qubits and then compute its state fidelity with the required eigenstate. If it is not approximately one then initialize this measured state and repeat the same procedure iteratively to obtain the required eigenstate.

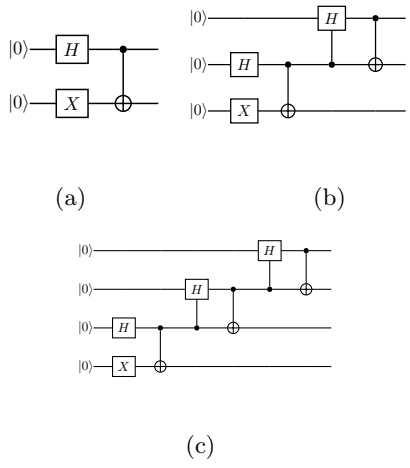

FIG. 1: Ansatz for convergence, for JW transformations with $N = 2$(a), 3(b) and 4(c) respectively

Results and Discussions

All simulations are performed on qiskit (version: 0.19.1) on the IBM platform and QASM simulator with 8192 shots. We implemented modified QPE to obtain the new eigenstate then calculated its state fidelity with the required eigenstate and computed the convergence of energy eigenvalues using QPE at each iteration steps (See Fig. 2).

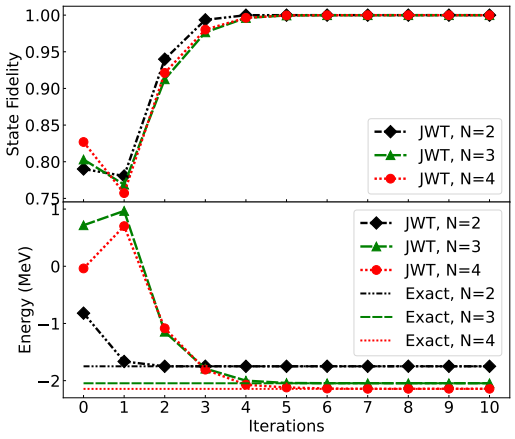

FIG. 2: State fidelity between ground state (top) and binding energy (bottom) with each iteration for 2, 3, and 4 basis size (N) using JW transformation and 2 ancilla qubits.

We have successfully used a modified Quantum Phase Estimation Algorithm to find out the convergence of a non-parameterized ansatz to an eigenstate and then obtained binding energy values for deuteron in EFT truncated at different basis sizes, using QPE. Although the method is applied to a specific problem, it can be used in general to any many-body problem.

References

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