Quantum simulation through variational approach involving linear combination of unitary operators

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Introduction

Classical computers face difficulties in simulating any quantum system due to the exponential growth in resource requirements with the increase of particles in the problem. We can overcome this difficulty through quantum computers, which have become a reality in the current Noisy Intermediate Scale Quantum Computers (NISQ) era. With the advancement of qubit technology, significant progress has been made in quantum chemistry and recently in nuclear physics [1, 2, 3]. Researchers have started to examine various quantum algorithms such as Quantum Phase estimation (QPE), Variational Quantum Eigensolver (VQE), and Linear Combination of Unitaries (LCU). Among all these, VQE is most popularly used for approximate state preparation and energy calculation which is based on the variational principle.

We have used two methods for our work. First, we have used VQE for the ground state energy calculation [1]. Second, we implement the variational approach through LCU to calculate the ground state energy. The expectation value of non-unitary operator is calculated as proposed in Ref. [2].

Expectation Value calculation

In this work, we are calculating the expectation value of the deuteron Hamiltonian in effective field (EFT) theory potential, which has been expended in terms of Pauli strings. We have used Gray code encoding as it uses fewer qubits and is more efficient [1, 2].

$$
\begin{aligned}
H_2 &= 5.9067091I - 6.34329Z_0 - 4.28661X_0 \\
H_3 &= 7.765855I - 7.984145Z_0 - 1.859145Z_1 \\
&\quad + 1.640855Z_0Z_1 - 2.143305(X_0 + X_0Z_1) \\
&\quad - 3.91312(X_1 - Z_0X_1) \\
H_4 &= 14.328I - 7.814X_0 - 3.913X_1 \\
&\quad + 3.913Z_0X_1 - 1.422Z_0 - 8.422Z_1 \\
&\quad + 3.527X_0Z_1 - 4.922Z_0Z_1
\end{aligned}
$$

VQE uses a parameterized state $|\psi(\theta)\rangle$ in which θ is parameter[1]. It exploits the variational principle to find the best value of θ for which the expectation value of operator H is minimum. The expectation value calculation for quadrupole moment of deuteron using LCU is discussed in Ref.[2]. In this work, we will implement this method for Hamiltonian as an operator to obtain expectation value and hence binding energy of deuteron.

Variational method through LCU: In this paper we are using variational principle which requires a parametrized state $|\psi(\theta)\rangle$. We realize this parameterized state through quantum circuit by operating parameterized unitary gates on the initial $|0\rangle$ in such a way that $|\psi(\theta) = U(\theta)\,|0\rangle\rangle$. We then apply this state $|\psi(\theta)\rangle$ as a quantum state to the LCU circuit, as shown in Fig. 1. To calculate the expectation value $\langle\psi|H|\psi\rangle$ we calculate the overlap of $|\psi\rangle$ with $H\,|\psi\rangle$; this is done with the help of swap test [2]. We then use a classical optimizer to produce a new set of parameters that reduces the expectation value. We call this algorithm expectation value calculator (EVC); that continues to iteratively

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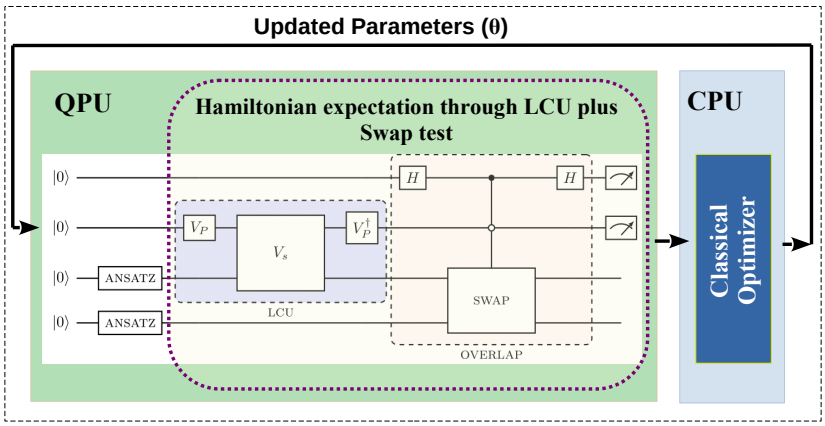

FIG. 1: **Expectation value calculator**. The quantum state prepared as ansatz is fed into the expectation value calculator circuit, which computes $\langle H \rangle$. The result is passed to the classical optimizer, run on the classical processing unit (CPU), takes the $\langle H \rangle$ and obtains a new set of parameters which are fed back to quantum processing unit (QPU).

reduce expectation value until it can no longer do so. The final obtained parameter for which expectation value is minimum will give the required ground state wave function. A general flowchart including the circuit is shown in Fig. 1.

Simulation Results

First, we have calculated ground state energy for the deuteron using EFT potential. We perform the calculation for basis size $n = 2$ and 4. We used IBM's Qiskit software to calculate with its QASM simulator. We execute the algorithm for 100000 shots. The expectation value is calculated with VQE and our variational algorithm and compared with exact results (computed on classical computer). For a large value of n, the result of exact diagonalization gets close to the experimental value of $-2.226(2)$MeV. The classical optimization has been obtained through the Constrained Optimization By Linear Approximation algorithm (COBYLA), and the final results are given in Table I.

TABLE I: Energy (in MeV) is calculated with the QASM simulator using EFT potential for $n = 2$ and 4. Exact value represent the result obtained from classical diagonalization.

Basis size n	Exact value	VQE	EVC
2	-1.74916	-1.74890	-1.77369
4	-2.14539	-2.08663	-2.10998

Conclusion

VQE results are more accurate and less prone to error due to lower circuit depth, while our proposed algorithm is highly prone to error due to larger circuit depth. It also has many multi-qubit gates, which are more prone to error, but this method can be used to calculate the expectation value of observables that are non-unitary, which is not possible in the case of VQE. The calculation of the expectation value of the non-unitary operator is in progress.

References

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