Symmetry Verification and Circuit Implementation using Qiskit

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***Abstract*— For near-term quantum computer, Quantum Error Mitigation (QEM) has recently attracted attention as a solution to reduce errors in quantum computers. In this paper, we introduce one of the QEM protocols, symmetry verification, and implement it using Qiskit. To check the performance, we use the VQE (Variational Quantum Eigensolver) to find the ground-state energy of hydrogen molecule (H_2) on two qubits.**

Keywords—Quantum computer, Quantum Error Mitigation, Symmetry Verification

I. INTRODUCTION

Quantum computers have been attracting attention since the idea was first proposed in the 1980s because they have advantages compared to classical computers such as exponentially faster calculations. However, some errors may occur during qubit control or during the operation. Quantum Error Correction (QEC) has been studied steadily since Peter Shor's 9 qubit code in 1995 to reduce errors in quantum computers [1]. Quantum computing with quantum error correction is called fault-tolerant quantum computing, and for practical fault-tolerant quantum computers require structural designs with high threshold and low overhead. Surface code is the most common architecture due to its high threshold and its advantage of being composed of near-neighbor operations [2,3].

However, to implement the logical qubits of quantum error correction codes, a large number of physical qubits are required, and the number of physical qubits actually implemented is hundreds. Therefore, there are currently technical limitations to implement quantum error correction in real quantum computers. To overcome this problem, Quantum Error Mitigation (QEM), which reduces the errors instead of correcting them, has recently attracted attention as a solution for near-term quantum computers. There are some protocols, called Zero-Noise Extrapolation (ZNE) and Probabilistic Error Cancellation (PEC), proposed by Temme et al. in 2017 [4].

X. Bonet-Monroig et al. suggest a mitigation protocol using symmetry existing in the quantum mechanical system, called Symmetry Verification (SV) [5]. In this paper, we introduce the Symmetry Verification protocol and Variational Quantum Eigensolver (VQE). We implement the symmetry verification using Qiskit, a Python library by IBM. To check the performance, we use the VQE to find the ground-state energy of a hydrogen molecule (H_2) on two qubits.

II. SYMMETRY VERIFICATION

Quantum error mitigation is attracting attention as a solution to reduce errors occurring in implementable quantum computers in the near future. In 2018, X. Bonet-Monroig et al. use the symmetry existing in the quantum mechanical system. When the errors break the symmetries of the ideal quantum state, we can identify the errors and remove them via post-selection. It is similar to a quantum error detection code.

In quantum systems, the Hamiltonian ($\hat{H}$) exists, and symmetry ($\hat{S}$) is a unitary operator that commutes with the Hamiltonian.

$$[\hat{H}, \hat{S}] = \hat{H}\hat{S} - \hat{S}\hat{H} = 0 \tag{1}$$

In this case, $\hat{H}$ may be diagonalized within the eigenspaces of $\hat{S}$, i.e. eigenstates $|\psi\rangle$ can be chosen in such a way that $\hat{S}|\psi\rangle = s|\psi\rangle$, where s is an eigenvalue of $\hat{S}$. However, in real quantum computers, noise may shift the state out of the target eigenspace. Thus, by checking whether the system remains in the target space in the middle or at the end of a calculation, we can reduce the effect of noise.

A. Ancilla Symmetry Verification

The simplest way of symmetry verification is the use of an ancilla qubit to measure Pauli symmetry $\hat{S} \in P$. We can write $\hat{S}$ in terms of its tensor factors, $\hat{S} = \bigotimes_i \hat{S}_i$, where $\hat{S}_i \in \{I, X, Y, Z\}$ and let N_s be the number of nontrivial $\hat{S}_i$. To each $\hat{S}_i$, we can perform a corresponding rotation $\hat{R}_i = \{exp\left(i\frac{\pi}{2}Y\right), exp\left(i\frac{\pi}{2}X\right), I\}$ such that $\hat{R}_i|\hat{S}_i = 1\rangle = |0\rangle$. $|\hat{S}_i = 1\rangle$ means eigenstate with an eigenvalue of 1 for $\hat{S}_i$. The circuit for verification is shown in Fig. 1(a). When the ancilla qubit reads 1, we discard this circuit run. If the quantum processors have linear connectivity, the ancilla qubit may be shuffled via SWAP gates as shown in Fig. 1(b). In both cases, the circuit depth is $O(N_s)$

B. In-line Symmetry Verification

Instead of using ancilla qubit, the symmetry $\hat{S}$ can be encrypted onto the computational degree of freedom of a qubit in the system. In the case of all-to-all connectivity, circuit depth is $O(\log N_s)$ because qubit coupling is performed in a binary tree manner. The circuit for this method is shown in Fig. 1(c). In the case of linear connectivity, the circuit depth is $O(N_s)$ as shown in Fig. 1(d)\

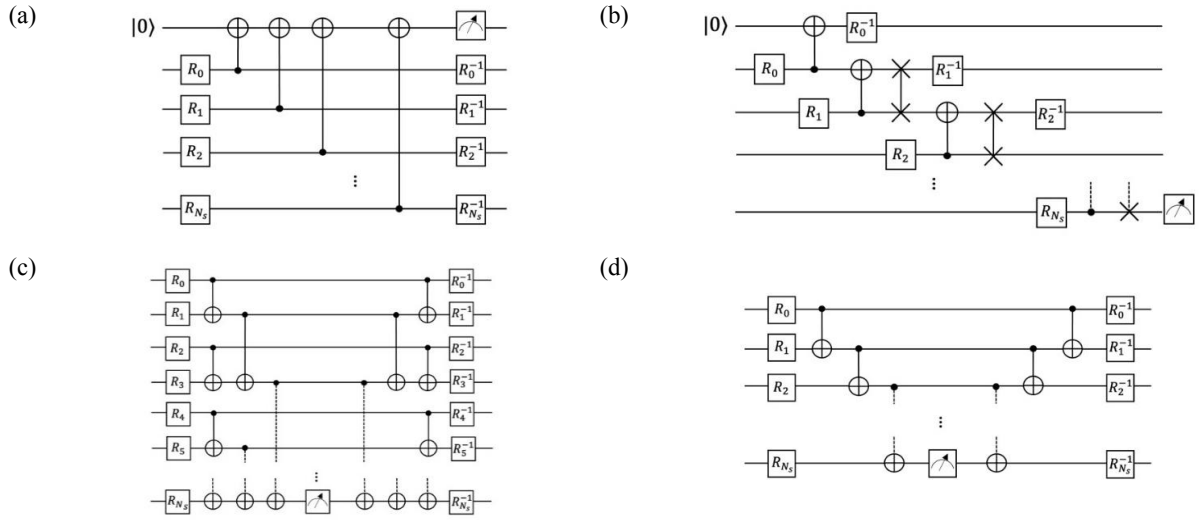

Fig. 1. Symmetry verification circuit. (a),(b) Quantum circuit for ancilla symmetry verification. (c),(d) Quantum circuit for in-line symmetry verification.

III. Variational Quantum Eigensolver

The Variational Quantum Eigensolver (VQE) was originally developed by Peruzzo et al. [6], and its theoretical framework was formalized by McClean et al. [7]. It is the most promising NISQ algorithm for quantum chemistry because it aims to compute an upper bound for the ground-state energy of a given Hamiltonian. It is also a hybrid classical-quantum algorithm in which the expectation value of the energy is computed using a quantum algorithm and minimized using a classical optimization algorithm.

According to the Rayleigh-Ritz variational principle, the ground state energy E_0 associated with a given Hamiltonian $\hat{H}$ is bounded by

$$E_0 \leq \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} \tag{2}$$

The VQE therefore aims to find a trial wavefunction $|\psi\rangle$, such that the expectation value of the Hamiltonian is minimized. We briefly introduce the process of VQE to perform this minimization task on a quantum computer [8].

A. VQE pipeline

1) Hamiltonian construction and representation : The first step of VQE is to define the system for which we want to find the ground state. There are two ways – first and second quantization. In second quantization, the Hamiltonian can be expressed in terms of fermionic operators, known as creation and anhiliation operators.

2) *Encoding of operators* : quantum computers can only measure observables expressed in a Pauli basis, $P_a \in \{I, X, Y, Z\}^{\otimes N}$ for N qubits. In the second quantization, the Hamiltonian is expressed as a linear combination of fermionic operators, so we need to transform it to the weighted sum of Pauli operators as follows :

$$\hat{H} = \sum_a w_a P_a \tag{3}$$

with w_a a weight. There are different types of transformation such as Jordan-Wigner transformation, Bravyi-Kitaev transformation.

3) *Ansatz and state preparation* : Once the Hamiltonian has been prepared that can be measured on a quantum computer, we need to define an ansatz (or ansatz wavefunction) as a parametrized quantum circuit. We can express the trial wavefunction $|\psi\rangle$ as the parametrized unitary $U(\theta)$ to an initial state (e.g. $|0\rangle$) for N qubits as

$$|\psi(\theta)\rangle = U(\theta)|0\rangle^{\otimes N} \tag{4}$$

A general method to obtain ansatz is the unitary coupled cluster (UCC), and to obtain the initial state is the Hartree-Fock method.

4) *Parameter Optimization* : Once the trial wavefunction has been prepared, the expectation value is computed. Based on the computation result and the optimization algorithm, we can compute and update the ansatz parameters iteratively until convergence.

IV. Circuit Implementation

To check the performance, we use the VQE to find the ground-state energy of hydrogen molecule (H_2) on two qubits. We follow the previous work by O'Malley, which implements the VQE on a real quantum computer and suggests the software schematic [9]. We use the Bravyi-Kitaev transformation to convert the STO-3G basis for H_2 into a qubit Hamiltonian. The Hamiltonian can be represented by only two qubits as follows :

$$\hat{H} = h_o II + h_1 IZ + h_2 ZI + h_3 XX + h_4 YY + h_5 ZZ \tag{6}$$

where h_i depends on the fixed bond length of hydrogen molecule. This parameter we use for implementation is in Table 1 of the Appendix in [9]. The Hamiltonian commutes with symmetry $\hat{S} = ZZ$, so our target subspace is $ZZ = -1$.

We follow the Unitary Coupled Cluster (UCC) ansatz, which in this case depends on a single parameter θ

$$U(\theta) = \exp(-i\theta X_0 Y_1) \tag{7}$$

so that a parameterized wave function $|\psi(\theta)\rangle$ for the ground state of a hydrogen molecule is given as

$$|\psi(\theta)\rangle = \exp(-i\theta X_0 Y_1)\,|01\rangle \tag{8}$$

where $|01\rangle$ is initial state of the Eq. (1) using the Hartree-Fock method. This parameterized wave function can be decomposed using standard methods, as shown in Fig. 2. Then VQE works by variationally optimizing θ of the ansatz in order to minimize the expectation value. To check the performance of the symmetry verification protocols, we use in-line symmetry verification.

To test symmetry verification in the presence of realistic noise, we simulate the circuit, as shown in Fig. 3 on ibmq-lima, IBMQ backend. When the measurement result is 0, we discard this circuit run because our target subspace is $ZZ = -1$. As a result, at all bond distances, we observe that the energy value of the circuit with symmetry verification (red) is closer to the exact value (green) than the unmitigated circuit (blue).

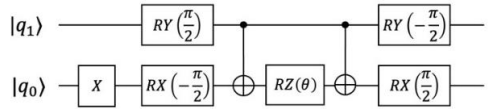

Fig. 2. Software quantum circuit diagram of the VQE except for measuring the expectation value.

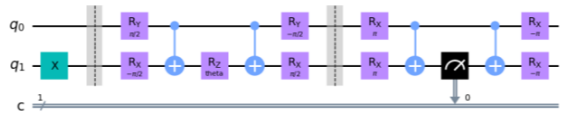

Fig. 3. Qiskit circuit diagram of the VQE with in-line symmetry verification.

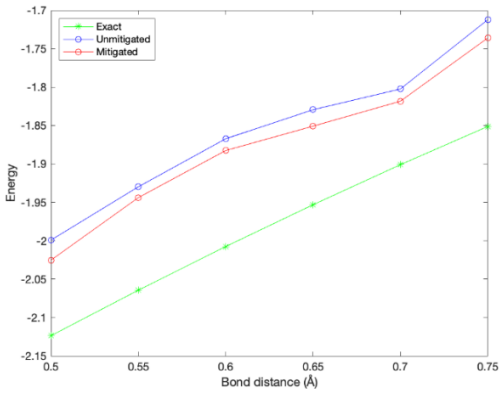

Fig. 4. Simulation Result.

V. Discussion

Quantum Error Mitigation (QEM) has recently attracted attention as a solution for near-term quantum computers. One of the QEM protocols is symmetry verification using symmetry existing in the quantum system, like quantum error detection. We implement it using Qiskit, and to check the performance, we use the Variational Quantum Eigensolver (VQE) to find the ground-state energy of a hydrogen molecule (H_2) on two qubits. As a result, at all bond distances, we observe that the energy value of the circuit with symmetry verification is better than that of the unmitigated circuit.

We expect that we can check the performance for a specific noise model, e.g., dephasing channel for future studies.

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