Implementation of Complex Unitary Coupled-Cluster Wavefunctions

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In today's quantum computers, gate errors accumulate as the circuit deepens, making it difficult to perform high-precision calculations. Therefore, it is important to realize shallower circuits in quantum calculations. In this study, we developed an efficient implementation of the complex-parameter UCC (Unitary Coupled-Cluster) circuit and found a clear improvement in accuracy compared to the conventional method.
Keywords: ab-initio calculation, quantum computing, unitary coupled-cluster method

1. Introduction

The UCC method is a representative method for quantum chemistry calculations of multi-electron systems, but its naive implementation is very deep and has accuracy problems. We have extended the real-parameter UCC circuit proposed by Yordanov et al. [1] to complex parameters with almost no change in depth, enabling more efficient calculations of a wider range of multi-electron systems.

2. Methodology

Under Jordan-Wigner transformation, implementation of fermionic excitation operators involves a series of CNOT gates as shown in Fig. 1 (from Fig. 1 of [1] with edits), which we call "CNOT ladders." The number of pairs of the ladders for the operator varies depending on the implementation method.

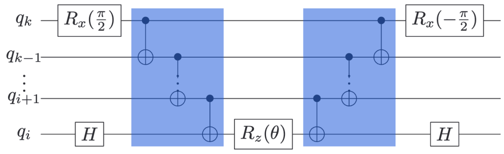

Fig. 1. CNOT ladders (blue section)

2-1. Naive Implementation

When implemented naively, the single fermionic excitation operator that excites 2 electrons results in a deep circuit with 2 pairs of CNOT ladders for a real parameter and 4 pairs for a complex parameter.

2-2. Efficient Implementation

A more efficient method has been proposed by Yordanov et al. which has only 1 pair of CNOT ladders for a real parameter θ. When extending this parameter to a complex number and representing the complex parameter in rectangular form ($\tau = \theta_1 + i\theta_2$), the number of CNOT ladder pairs doubles (Fig. 2)[2]. However, with the method we propose, the operator can be expressed almost at the same circuit depth (Fig. 3) by representing the parameter in polar form ($\tau = \theta e^{i\lambda}$).

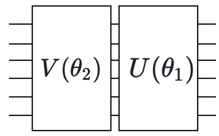

Fig. 2. Complex circuit in rectangular form

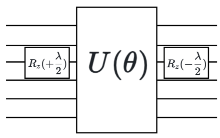

Fig. 3. Complex circuit in polar form

3. Results and Discussion

To validate the proposed method, we implemented a four-qubit single-electron excitation operator with a complex parameter using both the naive and proposed methods (Fig. 4, 5). The number of pairs of CNOT ladders in this example is 4 and 1, respectively. We set the parameters to $\theta_1 = \theta_2 = \theta = \pi/4$, $\lambda = \pi/2$ so that the theoretical values of the output are equal.

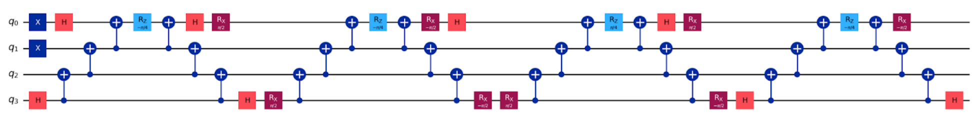

Fig. 4. The naive method

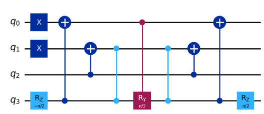

Fig. 5. The proposed method

The circuit output was sampled on a real quantum computer (IBM Osaka), and the results are shown in Fig. 6. While the exact solution only produces outputs of 0011 and 1010, the naive implementation shows noticeable incorrect values even after error mitigation, while the proposed method significantly suppresses such values.

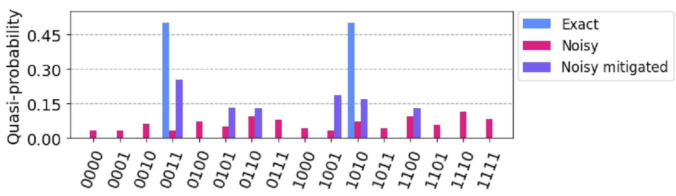

Fig. 6. Sampling results for the naive method

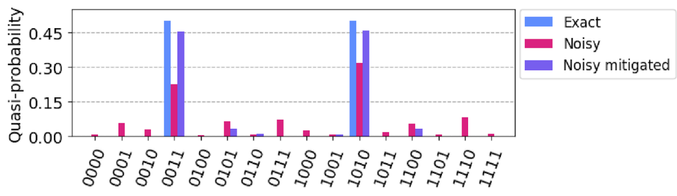

Fig. 7. Sampling results for the proposed method

References

[1] Yordan S. Yordanov, David R. M. Arvidsson-Shukur, and Crispin H. W. Barnes, Phys. Rev. A, 102, 062612 (2020)
[2] Nobuyuki Yoshioka, Takeshi Sato, Yuya O. Nakagawa, Yu-ya Ohnishi, and Wataru Mizukami, Phys. Rev. Research, 4, 013052 (2022)