Calculating Ground-State-Energy of $LiCoO_2$ by using Fragment molecular orbital-based Variational Quantum Eigensolver

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Abstract. Variational Quantum Eigensolver (VQE) is a quantum computer algorithm that calculates the ground state energy and is highly anticipated to be effective in the development of new materials, such as in the field of drug and battery development. However, current quantum computers are limited in the number of qubits they can use, which limits the application of VQE to molecules used in industry. To solve this problem, this study proposes the use of FMO/VQE. The Fragment Molecular Orbital (FMO) method divides the whole system into small fragments for processing. FMO/VQE is a method that applies the FMO method to VQE.[1] In this study, to demonstrate the effectiveness of FMO/VQE, the ground state energy of LiCoO_2, which is used as the anode material of a secondary battery, was calculated using FMO/VQE. By doing so, the number of qubits required by the conventional VQE algorithm was reduced from 24 to a maximum of 14. Nevertheless, almost the same accuracy (99.989%) as the results obtained by the classical method was obtained. This study shows that the proposed VQE algorithm can be successfully applied in the field of battery and drug discovery.

Keywords: VQE, Quantum Computing, Lithium-ion batteries

1 Introduction

The ground state of a molecule and its energy are the most stable state and lowest energy that a molecule can have. Knowing this information can be used to understand the bonds between molecules and the structure of molecules, which can be used in various fields of chemical research, such as the development of new drugs or new anode materials for secondary batteries. Currently, the ground state energy of a molecule is mostly calculated on classical computers. However, when the number of atoms in a molecule increases or the atomic number of the atoms in a molecule is large, the number of particles to be considered increases, and the interactions of each particle to be considered increase exponentially. The interactions of each particle are considered in the Hamiltonian of the molecule, and representing this molecular Hamiltonian on a computer requires a large amount of memory and computation. Therefore, calculating the ground

state energy of a molecule using a classical computer is difficult to apply to large molecules.

Quantum computers are a recently emerging field, and there is a lot of research going on. Quantum computers use different qubits than classical computers, i.e., quantum bits, which are qubits with superposition of 0 and 1 states, unlike bits that represent only 0 and 1 in classical computers. This is why, in calculating the ground state energy of a molecule, when the number of particles increases and the memory required doubles, a quantum computer can do the calculation with one more qubit. Where a classical computer would require an exponential increase in memory, a quantum computer can solve with a polynomial increase in qubits. Therefore, even large molecules that are currently incomputable can be computed by quantum computers. The quantum computer algorithm Quantum Phase Estimation (QPE) is an algorithm that calculates the eigenvalues and eigenstates of a unitary matrix on a quantum computer, which can be used to find the ground state energy of a molecule. However, QPE is known to be very accurate and requires a large number of qubits to implement. Current quantum computers are said to be at the level of noisy intermediate-scale quantum devices (NISQs). NISQ means that the quantum computer is noisy and has intermediate-scale qubits. Current quantum computers are still noisy and lack accuracy, and the number of qubits is still low, in the tens or hundreds, making it difficult to implement QPEs.

Variational Quantum Eigensolver (VQE) is an algorithm for solving eigenvalue problems using these NISQ-level quantum computers, which uses both quantum and classical computers. VQE uses variational principles to construct a parameterized trial wave function to obtain the basis of the molecular Hamiltonian. The algorithm iterates by adjusting the parameters until this basis value converges to a constant value to obtain an upper bound on the ground state energy of the molecule. In this process, the molecular Hamiltonian and the test wavefunction are replaced by quantum circuits, and the process of obtaining the expectation value is performed by a quantum computer, and the optimization process of adjusting the parameters of the test wavefunction is performed by a classical computer. Unlike QPE, VQE does not require many qubits, and the optimization that is difficult for current quantum computers is calculated by a classical computer, so there are many expectations that quantum computers can be commercialized in the NISQ era. However, current quantum computers have too many errors, their accuracy decreases significantly as the circuit depth increases, and the number of qubits available is limited, which is insufficient to calculate very large molecules. Therefore, one of the various methods to solve this problem is the Fragment Molecular Orbital method based Variational Quantum Eigensolver (FMO/VQE). FMO/VQE was first devised by Hocheol Lim, et al. as an algorithm that applies the FMO method, a quantum chemistry method, to VQE to improve the limitations of VQE due to the limitations of current quantum computers. The FMO method approximates the ground-state energy of the whole molecule by dividing the whole system into small pieces, and then finds the ground-state energy of the small pieces (monomer) and the pair of small pieces (dimer) and uses them to approximate the ground-state energy of the whole molecule. By breaking the molecule into smaller pieces, the maximum size of the system that needs to be considered in the overall calculation can be reduced, and this can be applied to VQE to reduce the number of cubits required and the depth of the quantum

circuit. Therefore, FMO/VQE is expected to be a way to utilize quantum computers in the near future.
In this paper, we use FMO/VQE to calculate the ground state energy of LiCoO2, a representative material used as an anode material for secondary batteries, and compare it with classical computer calculations. We also compare the accuracy of FMO/VQE with classical VQE to confirm the feasibility of FMO/VQE in the NISQ era.

2 Method

2.1 Lithium-ion battery

Lithium-ion batteries are one of the secondary batteries used in various industries. A lithium-ion battery consists of an anode material, a cathode material, and an electrolyte, where lithium oxide is used as the anode material. This compound has a layered structure of CoO_2^-oxide, with Li^+ ions bonded between each layer. The energy charge depends on the degree to which the lithium ions are oxidized in the oxide. Lithium is known to have a limited number of reserves in the world. Many methods have been proposed as solutions to this problem, one of which is an approach that seeks to maximize the energy charged per lithium ion. This is a critical situation, both in terms of lithium reserves and in terms of battery miniaturization. To calculate the amount of energy stored per lithium, it is essential to calculate the ground state of the molecule. However, this calculation is classically performed, and the ability to calculate larger molecules or more diverse combinations is limited. In this study, we show the results of applying the VQE algorithm to LiCoO2 molecules and demonstrate the applicability of quantum computers in the field of battery development.

2.2 A Subsection Sample

2.3 A Subsection Sample

3 Result

3.1 A Subsection Sample

Please note that the first paragraph of a section or subsection is not indented. The first paragraphs that follows a table, figure, equation etc. does not have an indent, either.

Subsequent paragraphs, however, are indented.

Sample Heading (Third Level). Only two levels of headings should be numbered. Lower level headings remain unnumbered; they are formatted as run-in headings.

Sample Heading (Forth Level). The contribution should contain no more than four levels of headings. The following Table 1 gives a summary of all heading levels.

Table 1. Table captions should be placed above the tables.

Heading level	Example	Font size and style
Title (centered)	**Lecture Notes**	14 point, bold
1st-level heading	**1 Introduction**	12 point, bold
2nd-level heading	**2.1 Printing Area**	10 point, bold
3rd-level heading	**Run-in Heading in Bold.** Text follows	10 point, bold
4th-level heading	*Lowest Level Heading.* Text follows	10 point, italic

Displayed equations are centered and set on a separate line.

$$x + y = z \tag{1}$$

Please try to avoid rasterized images for line-art diagrams and schemas. Whenever possible, use vector graphics instead (see Fig. 1).

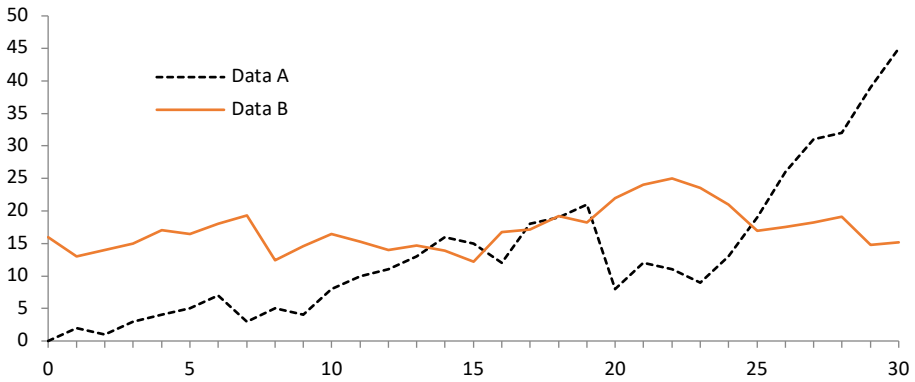

Fig. 1. A figure caption is always placed below the illustration. Short captions are centered, while long ones are justified. The macro button chooses the correct format automatically.

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