Research of Different Variant ADAPT-VQE Algorithms for NISQ Device

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***Abstract*—Quantum simulation of chemical systems is one of the most promising applications of quantum computers in the near future. Variational Quantum Eigensolvers(VQE) are the leading algorithms for molecular simulations on quantum hardware, and the performance of VQE depends on the design of Ansatz quantum circuits to obtain the ground state energy of molecules. However, the fixed Ansatz design cost is too large on NISQ devices, and this paper surveys the literature related to an Adapt VQE algorithm that dynamically generates Ansatz.**

***Keywords*: Quantum Computer, Quantum chemistry, ADAPT-VQE, Ansatz Design**

I. Introduction

Simulation of quantum chemical systems in classical computers faces an "exponential wall" of algorithmic complexity that can be avoided by using quantum computer simulations. Although quantum computers are overwhelmingly faster than conventional computers for specific tasks, current quantum computers are Noisy Intermediate Scale Quantum computer (NISQ) devices that have significant limitations on the cost of quantum algorithms, so improvements to conventional quantum algorithms are needed to reduce the required hardware cost. One of these algorithms, the VQE, is considered to be suitable for NISQ computers. However, the performance of the VQE algorithm depends heavily on the design of the Ansatz quantum circuit that generates the wave function. And the UCC Ansatz, which is considered as the "Golden Standard", still has too much cost in the face of strongly correlated systems. Therefore, this paper investigates an ADAPT VQE algorithm for dynamic generation of Ansatz

II. ADAPT-VQE Work Flow

Unlike the fixed Ansatz used in traditional VQE algorithms, the ADAPT VQE algorithm grows dynamically, so ADAPT VQE is a Problem tailored Ansatz. ADAPT VQE selectively adds operators from a predefined operator pool until a specific criterion is reached, resulting in a higher quality Ansatz with lower cost, based on the following principles Each selected operator restores the maximum relevant energy of the system. Fig 1, show the ADAPT VQE Algorithm work flow.

ADAPT-VQE focus on two points: 1. how to define the pool of operators. 2. How to define the criteria for choosing the operators to join Ansatz in each iteration.

According to the above two core points, this paper discusses three types of ADAPT-VQE.

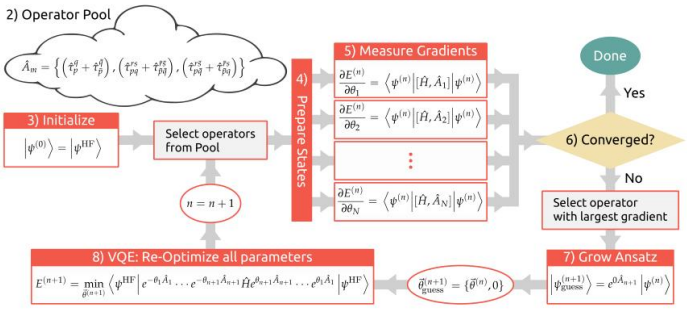

Fig1. ADAPT-VQE Flow Chart

III. Literature Review

Paper1:Fermonic-ADAPT-VQE

Since it is called the "Golden Standard" UCCSD Ansatz faces some drawbacks when applied to NISQ devices, such as the inability to accurately calculate the ground state energy of strongly correlated systems and the high cost due to the deep quantum circuit. The UCCSD Ansatz is a fixed Ansatz, which means that for the same molecule in different geometrical configurations, the Ansatz is the same but the optimized parameters are different. Thus, the idea of the ADAPT VQE algorithm was called Fermonic ADAPT VQE by subsequent researchers because of the reference to the UCCSD Ansatz in the selection of the operator pool.

Fermonic-ADAPT-VQE is able to construct different adaptive Ansatz for different geometric configurations of the same molecule, which makes this algorithm a good advantage in facing strongly correlated systems. The proposed ADAPT-VQE makes it possible to simulate strongly correlated systems using NISQ devices in the future.

In paper 1, simulations were performed for LiH, BeH2 and H6 molecules, which are increasingly complex, and a comparison with the "Golden Standard" UCCSD Ansatz. Fig 2 shows

that the UCCSD Ansatz is fixed and therefore cannot achieve chemical accuracy for BeH2 and H6 with increasing atomic spacin. In contrast, ADAPT-VQE can be used to achieve convergence accuracy with more stringent convergence conditions.

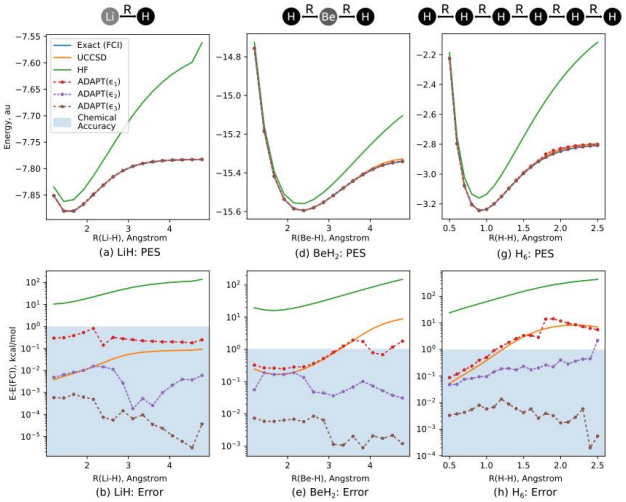

Fig 2.Dissociation curves for LiH, BeH2, and H6.

Paper2:Qubit-ADAPT-VQE

Paper 2 is based on the idea of ADAPT-VQE algorithm, but improves the composition of the operator pool and proposes Qubit-ADAPT-VQE. Qubit-ADAPT-VQE explores how many operators should be included in the operator pool to be complete, and finds more hardware efficient operators, further improving the algorithm of ADAPT-VQE The paper gives an idea of how to determine whether the operator pool is complete or not.

The paper provides a mathematical criterion for determining the completeness of the operator pool and demonstrates that the number of operators satisfying the "minimum complete operator pool" grows linearly with the number of qbits. Since the larger the operator pool, the more additional measurements required per iteration, the growth of the additional measurement cost of the "minimum complete pool" is considered moderate, suggesting that future implementations of larger chemical systems on NISQ devices are possible.

Paper3:TETRIS-ADAPT-VQE

The TETRIS-ADAPT algorithm proposed in Paper 3 follows the definition of the operator pool in the Qubit-ADAPT VQE algorithm, however, the restriction of adding only one operator in one iteration is removed. Since most of the operator pools in the qubit-ADAPT-VQE algorithm act on only some of the quantum bits, adding only one operator in each iteration will leave the unacted quantum bits idle, so this algorithm makes each quantum bit act on as many operators as possible in each iteration by gradient and acting position.

Compared with the qubit-ADAPT VQE algorithm, this algorithm generates denser but shallower Ansatz quantum lines without increasing the number of variational parameters and CNOT gates. In the small molecule regime, TETRIS-ADAPT-VQE and qubit-ADAPT-VQE have the same accuracy but shallower quantum circuit.

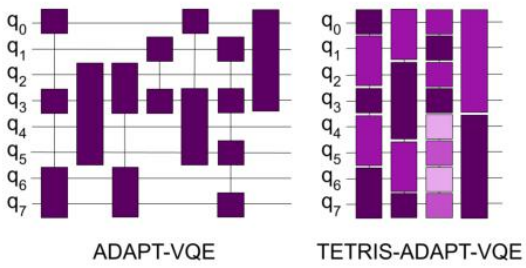

Fig 3.Schematic diagram of ansatz preparation circuits produced by ADAPT-VQE (left) and TETRIS-ADAPT-VQE (right).

IV. Conclusion

ADAPT-VQE has lower hardware cost than the traditional VQE algorithm and adapts to strongly correlated systems. Different variants of ADAPT-VQE algorithms can be classified according to the composition of the operator pool and the strategy of growing Ansatz. By comparing the three ADAPT-VQE algorithms in this study, we can know that the future direction of ADAPT-VQE development is to find more efficient operator pools and more adaptive Ansatz generation strategies.

Reference

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