A brief implementation of Variational Quantum Eigensolver

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Abstract

This article illustrates the implementation of Variational Quantum Eigensolver(VQE) on the quantum computers. Then, this article discusses about the obstacles encountered during the implementation and reviews some possible directions on applying VQE. The source codes used in this paper can be found in: https://github.com/lengentyh/VQE

1 Introduction

Calculating the ground state of a quantum system plays a crucial role in simulations for quantum systems. For example, the structure and then the thermodynamic properties can be obtained through the knowledge of the ground state properties. A long-established method is to conjecture the ground state wave function through the Rayleigh-Ritz variational principle. [1] With the use of the quantum computer, the Variational Quantum Eigensolver(VQE) algorithm may accelerate the calculation. Furthermore, by suitable modelling on the Hamiltonian, the calculating process may be regarded as a faster eigenvalue calculator. Therefore, the VQE may apply to accelerate the calculations which require eigensolvers.

2 Methods for Implementation

The quantum computaional processes are conventionally illustrated through the picture of quantum circuits and gate operations, which is suitable to be described through second quantization. In coincidence, the technique is also useful while dealing with quantum many-body problems. Before getting on the simulation of a quantum system, the system's Hamiltonian should be written in the second quantized form.

More specifically, the annihilation operator on i^{th} qubit is $\hat{Q}_i = \frac{1}{2}(\hat{x}_i - i\hat{y}_i)$. A clever reader might found $\left[\hat{Q}_i, \hat{Q}_j\right] = 0$, which doesn't satisfy the fermionic statistics. It is therefore necessary to apply a mapping on these operators to correct the statistics for

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[1] Appendices A

simulations about fermions. Such mappings can be the Jordan-Wigner transformation [2], the parity transformation or the Bravyi-Kitaev transformation [3].

2.1 The algorithm

The idea of the Variational Quantum Eigensolver is to decompose the system's Hamiltonian into tensor products of Pauli matrices. Then, its expected value can be calculated through summing the expected values of each Pauli terms with weights.[4] The reason for this decomposition is that the expected values of the Pauli terms are easier to be measured on the quantum computers. Since the eigenvalues of the Pauli matrice are ± 1, some techniques are used to simplify the calculation. The details are described in section 2.1.2.

The expected value of the system's Hamiltonian is then optimized in the parameters space on classical computers. The parameters generated from last iteration becomes the inputs of the ansatz for new iteration. By the Rayleigh-Ritz variational principle, the expected value of the system's Hamiltonian converges to the system's ground state energy with the proceeding optimization. A shematic diagram is shown in figure 1.

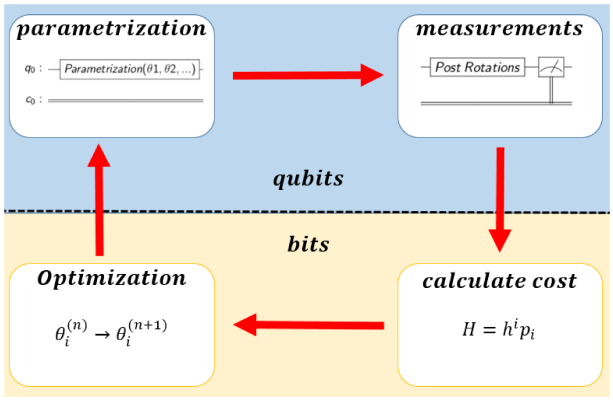


Figure 1: the cycling process for lowering the expected value

2.1.1 Hardware-efficient ansatz

As mentioned above, the ground state energy is calculated through optimizing parameters on the ansatz. A wise choice of ansatz reduces amount of iterations while its parameters space maintains the ability to cover the Hilbert space. A more rigorous choice may request the ansatzs to be interpretable in the subject. But, since the obstacles on the hardware, this request may be too expensive. Therefore, the ansatzs in the cases of this article are rather efficient on calculation than meaningful in the subject.

According to the expressibilities for the Hilbert space of the ansatzs studied by Sim et al. (2019) and the consideration of the amount of the gate operations [5],the circuit shown in figure 2 is chosen to be the building block of the ansatz for this article. The ansatz is then constructed through repeating the circuit for four times.

[2] A brief description of the Jordan-Wigner transformation can be found in Appendices B. More details can be found in Nielsen (2005), Setia and Whitfield (2018), Mcardle et al. (2020)

[3] Seeley et al. (2012), Setia and Whitfield (2018), Mcardle et al. (2020)

[4] Kandala et al. (2017)

[5] The detail reasons for this consideration is described in section 3.1

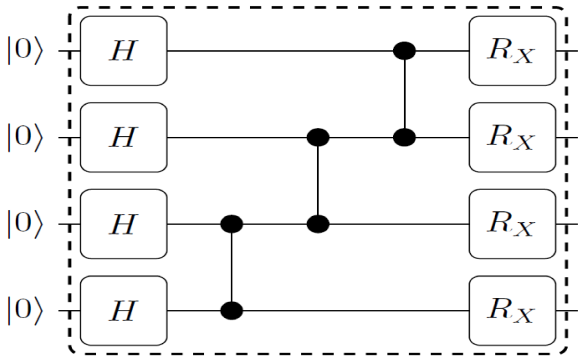


Figure 2: a layer of the hardware-efficient ansatz, Sim et al. (2019)

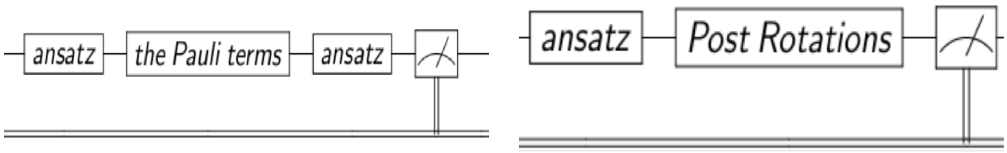
2.1.2 Measurements and Data analysis

After choosing a proper basis functions, the matrix elements of the second quantized Hamiltonian can be calculated. This matrix can be expanded through the tensor products of the Pauli matrices

$$\hat{H} = h^{ijk\cdots}\hat{P}_i \otimes \hat{P}_j \otimes \hat{P}_k ... \tag{1}$$

, where given i the $\hat{P}_i$ is a Pauli matrix or the identity matrix. The coefficients are calculated by $h^{ijk\cdots} = 2^{-\lceil \frac{N}{2} \rceil} tr(\hat{H} \cdot (\hat{P}_i \otimes \hat{P}_j \otimes \hat{P}_k ...))$, where $N \geq 2$ is the dimension of the Hamiltonian.

As we learned from the quantum mechanics, the expected value of a Hamiltonian is calculate through $\langle E \rangle = \langle \psi | \hat{H} | \psi \rangle$. Intuitively, one would use the circuit in figure 3(a) to obtain the expected value on a quantum computer. But, since the eigenvalues of



(a) the circuit that is constructed intuitively.

(b) the minimum-circuit required.

Figure 3: Two different measurements

the Pauli matrices are ± 1, only the application of an ansatz is needed. The circuit is displayed in figure 3(b). The reason for such implementation can be illustrate through a measurement of the expected value of $\hat{Z}$. Let $|\psi\rangle = \begin{pmatrix} \psi_0 \\ \psi_1 \end{pmatrix}$, the expected value is $\langle E_z \rangle = \langle \psi | \hat{Z} | \psi \rangle = \begin{pmatrix} \psi_0 \psi_1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \psi_0 \\ \psi_1 \end{pmatrix} = |\psi_0|^2 - |\psi_1|^2$. Therefore, the expected value of $\hat{Z}$ can be *"calculated"* through the measurement on the parameterized circuit only. Due

to the relation [6]

$$\hat{Z} = H\hat{X}H \tag{2}$$

the expected value of $\hat{X}$ can be calculated in a similar way but with a **post-rotation** before measuring as shown in figure 4. By using the relation $\hat{Y} = \hat{S}\hat{X}\hat{S}^{\dagger}$, where $\hat{S} = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$, the expected value of $\hat{Y}$ can be calculated in the same way. The measurements for tensor products of the Pauli matrices are straightly deduced from the above cases.

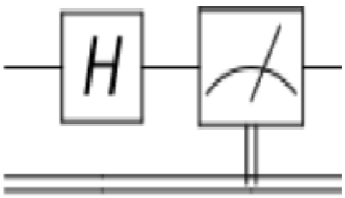


Figure 4: The post-rotation for measuring the expected value of $\hat{X}$

2.2 Implementation through Qiskit

The matrix of the Hamiltonian is chosen to be

$$\begin{bmatrix} 17.125 & -8 & 0 & -8 \\ -8 & 16.28125 & -8 & 0 \\ 0 & -8 & 16 & -8 \\ -8 & 0 & -8 & 16.28125 \end{bmatrix} \tag{3}$$

The coefficients of the Pauli terms are list in table 1.

table 1

	I	X	Y	Z
I	16.421875	-8	0	0.140625
X	0	-8	0	0
Y	0	0	0	0
Z	0.28125	0	0	0.28125

The results of the calculations are listed in table 2. The backends of the quantum circuits are chosen to be the least busy backends that is capable of transpile the circuit. The optimization use the COBYLA method in the scipy.optimize.minimize package.The exact result is calculate through the scipy.linalg package. These programs are compiled on intel(R) Core(TM) m3-7Y30 CPU @ 1.00 GHz 1.61 GHz.

[6]The H without hat is the **Hardmard matrix** $H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$, not the matrix of the Hamiltonian

table 2					
shots	max iteration	convergence	eigenvalue	relative error	time used
The exact result	-	-	0.41160781	-	0:00:00.218597
1024	1000	10^{-6}	10.4932373	2449.3290%	0:11:17.945527
1024	1000	10^{-7}	0.5538940	34.5684%	0:17:12.701684
8192	500	10^{-6}	0.4323610	5.04198%	0:15:08.988190
8192	500	10^{-5}	0.4474449	8.70661%	0:21:43.774035
8192	500	10^{-4}	0.4371071	6.19505%	0:19:42.753071
8192	250	10^{-4}	0.4986115	21.1375%	0:10:38.790930
4096	500	10^{-4}	0.4492188	9.13758%	0:14:04.983862
4096	500	10^{-5}	0.4370575	6.18299%	0:12:06.048704
4096	500	10^{-6}	0.4947128	20.1903%	0:17:00.911596

3 Disscussion

3.1 Advantages

The VQE has advantages compared to the algorithm that run only on classical computers. First, it requires less amount of operations per iteration for a parallel computation. As mentioned in section 2.1, each iteration in the VQE requires at most $4^{\log_2 N} \cdot n_{shot}$ operations,[7] while the other algorithm, such as, QR algorithm, Power iteration requires more than N^3 operations in each iteration. But, this advantage is significant only when $N \geq n_{shot}$.

On the other hand, the construction of the ansatzs with parameters on exponents may be easier on quantum computers. One can fist decompose the parameterized matrices on the exponents into Pauli terms. Then, Trotterize the product. Since the Pauli matrices are generators of the $SU(2)$ and the eigenvalues of the Pauli matrices are ± 1, one can transform an exponential operator into phase evolution using CNOT gates and Rotation gates. An example for such technique can be found in ch. 4.7.3 of Nielsen and Chuang (2011) or Barkoutsos et al. (2018).

Beside, the hybrid nature of the VQE makes it currently more plausible. Because some gate operations on quantum computers are prone to make errors, it is better to reduce the amount of operations in that kind as many as possible.[8] An example for such operations is the operations of CNOT gates between topologically far qubits. Then, there may be less operational errors occurred during the computation on quantum computers. The advantage of the hybrid algorithm compared to other algorithm that run fully on the quantum computer is that it can usually require "shorter" quantum circuit to get the result. Since it is possible to assign parts of the computation to classical computers, the calculations that require "long" quantum circuit on quantum computer can thus be avoided.

3.2 Current Obstacles

As mentioned in the previous section, the advantages of a quantum computer appears only when the scale of the matrix is extremely large. Although the same parallel computation requires less qubits in quantum computer than bits in classical computer, it still

[7] That is, the amount of Pauli terms

[8] In other words, it is better to have a "shorter circuit depth"

numerous amount of qubits to demonstrate the advantages. Otherwise, the scale of the matrix needed for showing the advantages increased and the time spent would be much longer. This obstacle becomes significant especially for computation using public quantum computers. Since each iteration is regarded as an independent job, it spent much time on queuing for an iterative process such as optimization.

Another obstacle is that the CNOT operations have good performance only when the qubits involved are topologically neighbored. Therefore, it is difficult for the ansatzs which required complex entanglements among qubits to have good performance. Especially for the ansatz that its parameters may give intuitions. The ansatzs mentioned in section 4.1 are examples. Due to this obstacle, it may be hard to see the meaning of the ansatzs that have good performance,such as the hardware-efficient ansatzs mentioned in section 2.1. And it may be difficult to choose an ansatz that can be applied to all kinds of matrices.

4 Applications

4.1 Molecules

The Self-Consistent Field(SCF) approximation, also known as the Hatree-Fock approximation, is a very important technique for computing a quantum many-body system. The idea is to construct the system's eigenstates through linear combination of the eigenstates from each individuals. Then, the equation of motion derived from the variational principle is an eigenvalue equation.[9] The procedure of a SCF calculation starts from an initial wave function and then minimizes the difference between both sides of the eigenvalue equation through iterations.

Although the SCF approximation in wave function base calculations has the exact influence from exchanging the individual wave functions, the correlations of the individual wave functions are absent in this approximation. Therefore, various of method are proposed to correctly treat the correlations with the SCF calculations. Such a treatment for computing the system's ground state wave function is varing the SCF-calculated wave function with an suitable ansatz.

In the field of computational quantum chemistry, there are two important ansatzs that are chemically interpretable. First, the ansatz of the *Configuration Interaction (CI)* is generated through

$$|\psi_{CI}\rangle = (\hat{I} + A_1^{ij}\hat{c}_i\hat{c}_j + A_2^{ijlm}\hat{c}_i^\dagger\hat{c}_j^\dagger\hat{c}_l\hat{c}_m + ...etc.)\,|\psi_{SCF}\rangle \tag{4}$$

, where the A_k in the equation are the parameters of this ansatz. Similar to the ansatz of the CI, the ansatz of the *Coupled Cluster (CC)* is generated through

$$|\psi_{CI}\rangle = e^{\hat{T}}\,|\psi_{SCF}\rangle \tag{5}$$

,where $\hat{T} = t_1^{ij}\hat{c}_i\hat{c}_j + t_2^{ijlm}\hat{c}_i^\dagger\hat{c}_j^\dagger\hat{c}_l\hat{c}_m + ...etc.$. Since the calculations are variational, these ansatz should be properly normalized. Therefore, the ansatz of CC should become $|\psi_{CI}\rangle = e^{\hat{T}-\hat{T}^\dagger}\,|\psi_{SCF}\rangle$ and is called Unitary Couple Cluster (UCC).[10] The chemical interpretation is that the actual state of the system is generated from the interaction between the SCF states (the so called "configuration").

[9] Patterson and Bailey (2007)

[10] Mcardle et al. (2020),Lee et al. (2018)

Notes that, the amount of the parameters in CI increase exponentially as more configurations are considered. So does the exponential operator in UCC. Therefore, the calculation by applying VQE may have advantages. Not only the ansatzs may be easier to prepared, but the time spent on computation may also be shorter for large enough systems.

4.2 VQSE [11]

The Variational Quantum State Eigensolver (VQSE) is an VQE-based algorithm which diagonalize the density matrix of the qubits ρ, which can be used to observe the entangled states.

The cost function of VQSE is

$$c(\theta) = tr(\hat{\rho}(\theta)\hat{H}) \tag{6}$$

, where $\hat{H}$ is a known diagonal Hamiltonian in the standard basis with non-negative eigenvalues. The cost function can be further written as $c(\theta) = \sum_k E^k \langle \mathbf{e}_k | \hat{\rho}(\theta) | \mathbf{e}_k \rangle \equiv \sum_k E^k p_k$. The eigenvectors $|\mathbf{e}_k\rangle$ are ordered such that $E_k \leq E_{k+1}$ is increasing.

Assume the density matrix is diagonalizable, and its eigenvectors are ordered such that the eigenvalues $\lambda_{k+1} \leq \lambda_k$ is decreasing. With these special ordering, the value $\sum_k E^k p_k$ is Schur concave.[12] Therefore, $\sum_k E^k p_k \geq \sum_k E^k \lambda_k$ since $\overrightarrow{\lambda}$ majorizes $\overrightarrow{p}$. That is, the cost function is minimized when the density matrix $\hat{\rho}(\theta)$ is diagonal.

Since the direct measurement would destroy the entanglements of the qubits, the VQSE is a plausible way to observe the entanglements through diagonalizing the density matrix. This technique may be useful for obtaining the ground state prepared by VQE, which can be used to calculate further physical properties.

4.3 Others

Although the VQE is to find the ground state properties, it may be possible to find the first excited states through the Discriminative VQE (DVQE). The idea is to find the lowest energy in the space that is orthogonal to the ground state. [13] The method may be generalized to find the higher excited states.

The VQE can be applied not only for science, but also for social problems. An example is the Quantum Approximate Optimization Algorithm (QAOA) algorithm, which uses VQE with a cost function that can be mapped to interesting social problems. [14]

5 Conclusion

The VQE can be regarded as a faster eigensolver, which is useful in many fields of science. With some proper models, it may has significant influence in solving societal problems. The current obstacles are lacking amount of qubits, the difficulty of finding ansatzs with good performance and the difficulty of interpreting these ansatzs. Despite the current obstacles, the VQE still may be one of the most achievable algorithm on NISQ in the near future.

[11] Cerezo et al. (2020)

[12] According to Theorem.1 in Roventa (2012)

[13] Tilly et al. (2020)

[14] Farhi et al. (2014)

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Appendices

A The Rayleigh-Ritz Variational Principle [15]

Theorem. *The expected value of an Hamiltonian $\hat{H}$ with its eigenfunctions be a complete set would satisfy:*

$$\langle\psi|\,\hat{H}\,|\psi\rangle \geq E_g \tag{7}$$

,where E_g is the ground state eigenenery of this Hamiltonian.

Proof. Since the normalized eigenfunctions of the Hamiltonian $|\phi_n\rangle$ form a complete set, let $|\psi\rangle = \sum_n c_n\,|\phi_n\rangle$. Then, $\langle\psi|\,\hat{H}\,|\psi\rangle = \sum_{i,j} c_i^* c_j E_j\,\langle\phi_i|\phi_j\rangle = \sum_j E_j|c_j|^2 \geq E_g$, where E_j are the eigenenergy corresponding to $|\phi_j\rangle$. □

B The Jordan-Wigner transformation [16]

Continue to the notations in section 2.1. Define

$$\hat{W}_i \equiv (-1)^{i-1}(\otimes_{k=1}^{i-1}\hat{Z}_k)\otimes\hat{Q}_i\otimes\hat{I}\otimes...\otimes\hat{I} \tag{8}$$

as the mapping on the annihilation operator on the i^{th} qubit. The mapping on the creation operator can be defined through similar ways. Since $\left\{\hat{X}_j,\hat{Z}_j\right\}=0$, $\left\{\hat{Y}_j,\hat{Z}_j\right\}=0$ and $\left\{\hat{Z}_j,\hat{Z}_k\right\}=0$, hence, $\left\{\hat{W}_l,\hat{W}_m\right\}=0$ for $l<m$. On the other hand,$\left\{\hat{W}_n,\hat{W}_n\right\}=0$ because $\left\{\hat{Q}_i,\hat{Q}_i\right\}=\frac{1}{4}(\left\{\hat{X}_i,\hat{X}_i\right\}-\left\{\hat{Y}_i,\hat{Y}_i\right\})=0$. Therefore, all the mapped annihilation operators $\hat{W}_i$ satisfy the fermionic statistics. But, the disadvantage of this transformation is that it applies numerous Z-gate operations on the qubits in front, which lengthens the circuit and may increase the operational error rate.

[15] Griffiths and Schroeter (2018)
[16] Nielsen (2005)