Coupled cluster singles and doubles variational quantum eigensolver ansatz for electronic structure calculations

Rongxin Xia*, Sabre Kais†
Department of Chemistry, Department of Physics and Astronomy, Birck Nanotechnology Center
Purdue University, West Lafayette, Unites States
Email: *xiar@purdue.edu, †kais@purdue.edu

Abstract—Variational quantum eigensolver (VQE) for electronic structure calculations is believed to be one major potential application of near term quantum computing. Among all proposed VQE algorithms, the unitary coupled cluster singles and doubles excitations (UCCSD) VQE ansatz has achieved high accuracy and received a lot of research interest. However, the first order trotterization UCCSD VQE has gate complexity up-bounded to $O(n^3)$ using Jordan-Wigner transformation, where $n$ is the number of qubits of the Hamiltonian. The high complexity makes UCCSD VQE difficult to be implemented on near term quantum computer. Here we introduce a new VQE ansatz based on the particle preserving exchange gate to achieve excitations. The proposed improved VQE ansatz has gate complexity up-bounded to $O(n^4)$. Numerical results of simple molecular systems such as $\text{BeH}_2$, $\text{H}_2\text{O}$, $\text{N}_2$, $\text{H}_2$, and $\text{H}_6$ using the proposed improved VQE ansatz gives very accurate results within chemical accuracy of about $10^{-3}$ Hartree.

Index Terms—VQE, UCCSD, electronic structure calculations

I. INTRODUCTION

Quantum computing has been developing rapidly in recent years as a promising new paradigm for solving many problems in science and engineering. One major potential application of quantum computing is solving quantum chemistry problems [1] such as electronic structure of molecules, which has received a lot of research interest and achieved a big success in both algorithmic development and experimental implementation. The early development of electronic structure calculations was based on the quantum phase estimation algorithm developed by Kitaev [2], Abrams and Lloyd [3] and used to find spectrum of simple molecular systems [4]–[9]. More recently, hybrid classical-quantum algorithms have been developed such as the variational quantum eigensolver (VQE) [10]–[13] and quantum machine learning techniques [14] for electronic structure calculations. Moreover, many experiments have been conducted on quantum computers to show that electronic structure calculations of simple molecules are possible on current Noisy Intermediate-Scale Quantum (NISQ) devices [15]–[17].

One of the promising quantum algorithms to perform electronic structure calculations is based on unitary coupled cluster [18] singles and doubles (UCCSD), which implements the quantum computer version of UCCSD as the VQE ansatz [10], [19], [20] to calculate the ground state from a Hartree-Fock reference state. The results from UCCSD VQE achieve high accuracy. However, the gate complexity for first order trotterization UCCSD VQE is up-bounded to $O(n^3)$ using Jordan-Wigner transformation where $n$ is the number of qubits of the Hamiltonian. This makes it difficult to implement on current NISQ devices. Here we introduce a new VQE ansatz based on the particle preserving exchange gate [20], [21] to achieve excitations, which has gate complexity up-bounded to $O(n^4)$ and has comparable accuracy compared to UCCSD VQE. By reducing the gate complexity, our proposed VQE ansatz might be more favorable for current NISQ devices.

The rest of the paper is organized as follows: The first section gives a brief introduction to the method of UCCSD VQE ansatz. Then we give a detailed description of our proposed coupled cluster singles and doubles VQE ansatz. We also show our proposed VQE is a simplified version of the first order trotterization UCCSD VQE. Finally, we give the numerical simulation results of $\text{BeH}_2$, $\text{H}_2\text{O}$, $\text{N}_2$, $\text{H}_2$, and $\text{H}_6$ using UCCSD VQE and our improved VQE.

II. UCCSD VQE

The electronic structure Hamiltonian can be written in second quantization as:

$$H = \sum_{ij} h_{ij} a_i^\dagger a_j + \sum_{ijkl} h_{ijkl} a_i^\dagger a_j^\dagger a_k a_l$$

(1)

where the one-electron integrals $h_{ij}$ and the two-electron integrals $h_{ijkl}$ can be calculated by orbital integrals. Using Jordan-Wigner transformation we can rewrite the Hamiltonian in the Pauli matrices form:

$$H = \sum_i a_i \sigma_i + \sum_{ij} b_{ij} \sigma_i \sigma_j + ...$$

(2)

where $a_i, b_{ij}$ are general coefficients and $\sigma$ are Pauli matrices $\sigma^x, \sigma^y, \sigma^z$ and $2 \times 2$ identity matrix.

In unitary coupled-clustered single-double excitations, we can calculate the ground state from the Hartree-Fock reference state by excitation operators of the form:

$$|\phi\rangle = e^{T(\bar{\sigma}) - T^\dagger(\bar{\sigma})} |\phi_{HF}\rangle$$

(3)
where \(T(\vec{\theta}) = T_1(\vec{\theta}_1) + T_2(\vec{\theta}_2)\) is the excitation operator, \(|\phi_{HF}\rangle\) is the Hartree-Fock reference state and \(\vec{\theta}\) is the set of adjustable parameters. The single excitation operator can be written as \(T_1(\vec{\theta}_1) = \sum_{i,j} \theta_{ij} a_i^\dagger a_j\) and the double excitation operator can be written as \(T_2(\vec{\theta}_2) = \sum_{i,j,k,l} \theta_{ijkl} a_i^\dagger a_j a_k^\dagger a_l\).

We can minimize \(\langle \phi | H | \phi \rangle\) to get the ground state energy by optimizing \(\vec{\theta}\).

Considering an \(n\) qubit Hamiltonian, the number of spin orbitals is \(n\) and the total excitation terms in \(T\) is \(O \left( \left( N_{occ} \right)^2 \times \left( N_{virt} \right) \right)\), where \(N_{occ}\) is the number of occupied orbitals, \(N_{virt}\) is the number of virtual orbitals. \(n = N_{occ} + N_{virt}\) is the number of qubits of the Hamiltonian or the total number of orbitals.

The first order trotterization UCCSD can be written as:

\[
e^{T(\vec{\theta})-T^\dagger(\vec{\theta})} \approx \prod_{i,j} e^{\theta_{ij} (a_i^\dagger a_j - a_j^\dagger a_i)} \times \prod_{i,j,k,l} e^{\theta_{ijkl} (a_i^\dagger a_j a_k^\dagger a_l - a_k^\dagger a_l a_i a_j)} \tag{4}
\]

To map the first order trotterization UCCSD to qubits, we should use same transformation, Jordan-Wigner transformation, as we do for the Hamiltonian to transform creation and annihilation operators into Pauli matrices. Each term in equation (2) can be implemented as a unitary gate by Jordan-Wigner transformation. Since the cost of Jordan-Wigner transformation is \(O(n)\), the gate complexity for the first order trotterization UCCSD VQE is \(O \left( \left( N_{occ} \right)^2 \times \left( N_{virt} \right) \times n \right) < O(n^5)\) using Jordan-Wigner transformation [1], [19].

UCCSD VQE has shown high accuracy in electronic structure calculations. However, one problem of the UCCSD VQE is the large complexity. The first order trotterization UCCSD VQE has up-bounded \(O(n^4)\) terms and \(O(n^5)\) gate complexity if using Jordan-Wigner transformation. Here, we propose a new coupled cluster singles and doubles VQE ansatz using the particle preserving exchange gate [20], [21]. The gate complexity of our proposed ansatz scales as \(O \left( \left( N_{occ} \right)^2 \times \left( N_{virt} \right) \right) < O(n^4)\). In the numerical simulations, we show that our proposed ansatz can achieve comparable accuracy to the UCCSD VQE.

III. THE COUPLED CLUSTER SINGLES AND DOUBLES VQE ANSATZ

The Jordan-Wigner transformation makes each qubit represent whether the corresponding spin orbital is occupied or not. When qubit \(i\) is in \(|0\rangle\), spin orbital \(i\) is not occupied and when qubit \(i\) is in \(|1\rangle\) spin orbital \(i\) is occupied. Thus we can write down a particle preserving exchange gate \(U_{ex} [20], [21]\) between two qubits as:

\[
U_{ex}(\theta) = \begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & \cos \theta & -\sin \theta & 0 \\
0 & \sin \theta & \cos \theta & 0 \\
0 & 0 & 0 & 1
\end{bmatrix}
\]

The particle preserving exchange gate \(U_{ex}\) will not change the total occupation when applied to arbitrary states. Suppose we have two qubits in \(|10\rangle\), which represents that the first spin orbital is occupied and the second spin orbital is not occupied. If we apply \(U_{ex}\) to this state we have:

\[
U_{ex}(\theta)|10\rangle = \cos \theta |10\rangle + \sin \theta |01\rangle \tag{5}
\]

which corresponds to a single excitation between one spin occupied and one virtual spin orbitals.

We can also write down a particle preserving exchange gate \(U_{ex}'\) between four qubits as in Fig. 1. Suppose we have four qubits in \(|1010\rangle\), which represents the first and the third spin orbitals are occupied while the second and the fourth orbitals are not occupied. If we apply \(U_{ex}'\) to this state we have:

\[
U_{ex}'(\theta)|1010\rangle = \cos \theta |1010\rangle + \sin \theta |0101\rangle \tag{6}
\]

which corresponds to a double excitation between two occupied and two virtual orbitals.

We can write down an operator \(U\) by \(U_{ex}\) and \(U_{ex}'\) to achieve single and double excitations from the Hartree-Fock reference state:

\[
|\Phi\rangle = U(\vec{\theta})|\phi_{HF}\rangle = \prod_{i,j} U_{ex_{i,j}}(\theta_{ij}) \prod_{i,j,k,l} U_{ex_{i,j,k,l}}(\theta_{ijkl})|\phi_{HF}\rangle \tag{7}
\]

where \(U_{ex_{i,j}}\) represents \(U_{ex}\) between qubits \(i, j\), \(U_{ex_{i,j,k,l}}\) represents \(U_{ex}'\) between qubits \(i, j, k, l\) and \(\vec{\theta}\) is the set of adjustable parameters. We can minimize \(\langle \Phi | H | \Phi \rangle\) to get the ground state energy by optimizing \(\vec{\theta}\).

\(U_{ex}(\theta)\) and \(U_{ex}'(\theta)\) can be decomposed into elementary quantum gates with gate complexity \(O(1)\) because the sizes of matrices of \(U_{ex}(\theta)\) and \(U_{ex}'(\theta)\) are \(O(1)\). One possible decomposition can be grey code [22]. \(U_{ex}(\theta)\) can be decomposed to:

\[
\begin{array}{c}
R_y(\theta) \\
\end{array}
\]

And \(U_{ex}'(\theta)\) can be decomposed as in Fig. 2. In our simulation, \(U_{ex}(\theta)\) and \(U_{ex}'(\theta)\) are implemented by Qiskit [23]. To save simulation time, \(U_{ex}(\theta)\) and \(U_{ex}'(\theta)\) are implemented as single unitary gates as the UCCSD VQE implementation in Qiskit [23].

A. Excitation list selection

One important part of the proposed VQE is to choose the excitation list, or to decide between which spin orbitals the excitation will occur. One trivial selection of the excitation list we use for our proposed coupled cluster singles and doubles VQE ansatz is to allow all possible excitations as in Algorithm 1.
Algorithm 1 Coupled cluster singles and doubles VQE for all possible excitation

1: for orbital, in occupied orbitals and orbital, in virtual orbitals do
2: Construct \( U_{ex} \) between qubit \( i \) and \( j \).
3: end for
4: for orbital, orbital, in occupied orbitals and \( j > i \) do
5: for orbital, orbital, in virtual orbitals and \( l > k \) do
6: Construct \( U'_{ex} \) between qubit \( i, j, k, l \).
7: end for
8: end for

Algorithm 2 Coupled cluster singles and doubles VQE considering spin symmetry

1: for orbital, in spin-up occupied orbitals and orbital, in spin-up virtual orbitals do
2: Construct \( U_{ex} \) between qubit \( i \) and \( j \).
3: end for
4: for orbital, in spin-down occupied orbitals and orbital, in spin-down virtual orbitals do
5: Construct \( U_{ex} \) between qubit \( k \) and \( l \).
6: end for
7: for orbital, in spin-up occupied orbitals and orbital, in spin-up virtual orbitals do
8: for orbital, in spin-down occupied orbitals and orbital, in spin-down virtual orbitals do
9: Construct \( U'_{ex} \) between qubit \( i, j, k, l \).
10: end for
11: end for
12: for orbital, orbital, in spin-up occupied orbitals and \( j > i \) do
13: for orbital, orbital, in spin-up virtual orbitals and \( l > k \) do
14: Construct \( U'_{ex} \) between qubit \( i, j, k, l \).
15: end for
16: end for
17: for orbital, orbital, in spin-down occupied orbitals and \( j > i \) do
18: for orbital, orbital, in spin-down virtual orbitals \( l > k \) do
19: Construct \( U'_{ex} \) between qubit \( i, j, k, l \).
20: end for
21: end for

In Algorithm 1, we do not consider spin symmetry. The single excitation can occur between any one occupied and one virtual spin orbitals. The double excitation can take place between any two occupied and two virtual spin orbitals. Moreover, we can add additional restrictions on the excitation list by considering the spin symmetry: the excitation can only happen between same spin orbitals. In this case, the single excitation can only happen between one occupied and one virtual spin orbitals with same spin. The double excitation must happen between one spin-up occupied orbital, one spin-up virtual orbital, one spin-down occupied orbital and one spin-down virtual orbital or must happen between two occupied and two virtual spin orbitals with same spin. We can have Algorithm 2 by adding spin symmetry restriction.

The term complexity of our ansatz for both Algorithm 1 and Algorithm 2 scales as \( O \left( \left( N^{occ} \right)^2 \times \left( N^{virt} \right)^2 \right) \). The required elementary quantum gates for \( U_{ex} \) and \( U'_{ex} \) are both \( O(n) \). Thus the gate complexity of our ansatz for both Algorithm 1 and Algorithm 2 scales as \( O \left( \left( \left( N^{occ} \right)^2 \times \left( N^{virt} \right)^2 \right) \right) < O(n^4) \).

B. Relation to UCCSD VQE ansatz

Here, we present that our proposes VQE ansatz is a simplified version of UCCSD VQE ansatz. Consider a single excitation term in first order trotterization UCCSD:

\[
e^{i\theta(a_i^\dagger a_i - a_i^\dagger a_i)}
\]

If using Jordan-Wigner transformation \( a_j = \frac{1}{2}(\sigma_j^x + i\sigma_j^y) \otimes \sigma_j^{n-j-1} \) and \( a_i^\dagger = \frac{1}{2}(\sigma_i^x - i\sigma_i^y) \otimes \sigma_i^{n-j-1} \). By setting \( j > i \) we get [20]:

\[
e^{\frac{\pi}{4} a_i^\dagger a_j^\dagger a_i a_j} = e^{\frac{\pi}{4} a_i a_j a_i^\dagger a_j^\dagger} = U_{ex,i,j}
\]

In equation (9), \( \otimes^{j-1}_{a=\ell+1} \sigma_z^a \) is for the parity. If we remove the parity term we get:

\[
e^{\frac{\pi}{4} a_i^\dagger a_j^\dagger a_i a_j} = U_{ex,i,j}
\]

Thus our particle conservation exchange gate \( U_{ex} \) for the single excitation is the single excitation term in first order trotterization UCCSD VQE without considering the parity. Also, consider a double excitation term in first order trotterization UCCSD VQE:

\[
e^{i\theta(a_i^\dagger a_i^\dagger a_i a_i)}
\]

If using Jordan-Wigner transformation for \( i > l > j > k \) we get [20]:

\[
e^{\frac{\pi}{4} a_i^\dagger a_i^\dagger a_i a_i} = e^{\frac{\pi}{4} a_i^\dagger a_i^\dagger a_i a_i}
\]

In equation (12), \( \otimes^{j-1}_{a=\ell+1} \sigma_z^a \) is for the parity. If we remove the parity term we get:

\[
e^{\frac{\pi}{4} a_i^\dagger a_i^\dagger a_i a_i} = U_{ex,k,j,l,i}(\theta)
\]
Thus our particle preserving exchange gate $U'_{ex}$ for the double excitation is the double excitation term in first order trotterization UCCSD VQE without considering the parity. Our proposed VQE is the simplified version of first order trotterization UCCSD VQE by not considering the parity. The reduced gate complexity of our VQE comes from removing the parity term in UCCSD VQE.

IV. NUMERICAL SIMULATION RESULTS

In this section, we present numerical results of BeH$_2$, H$_2$O, N$_2$, H$_4$ and H$_6$ by using our proposed VQE with the real rotation gates $U_{ex}$ and $U'_{ex}$ and UCCSD. For each numerical simulation, the orbital integrals are calculated using STO-3G minimal basis by PySCF [24] and the Hamiltonian is obtained by Jordan-Wigner transformation. In the figures in this section, Algorithm 1 refers to the Algorithm 1 allowing all possible excitation. Algorithm 2 refers to the Algorithm 2 only allowing spin symmetry excitations. UCCSD refers to UCCSD VQE described in [20] and implemented by Qiskit [23], which only allows spin symmetry excitations. The optimization is performed by the sequential least squares programming (SLSQP) algorithm [25].

For BeH$_2$ we consider first 2 spin orbitals with lowest energies are always occupied and first 2 spin orbitals with highest energies are never occupied, corresponding to 10 active spin orbitals with 4 electrons. Fig. 3(a) shows the ground state energies calculated by our VQE and UCCSD VQE. We also show the error between the VQE results and the diagonalization of the Hamiltonian as in Fig. 3(b). We can see that our VQE achieves similar and even better accuracy compared to UCCSD VQE.

For H$_2$O we consider first 4 spin orbitals with lowest energies are always occupied, corresponding to 10 active spin orbitals and 6 electrons. Fig. 4(a) shows the ground state energies calculated by our VQE and UCCSD. We also show the error between the VQE results and the diagonalization of the Hamiltonian as in Fig. 4(b). We can see that our VQE achieves similar accuracy compared to UCCSD VQE except one data point, which may be caused by optimization trapped in local minimum. Algorithm 2 and UCCSD which have same excitation list have similar accuracy indicating removing parity terms may not affect final results. Furthermore, Algorithm 1 performs better than Algorithm 2 and UCCSD VQE when the bond length is large, which indicates at large bond lengths considering all possible excitations may be better than spin symmetry excitations.

For N$_2$ we consider first 8 spin orbitals with lowest energies
The ground state energies of BeH$_2$ calculated by our proposed VQE compared with UCCSD VQE.

The errors of ground state energies of BeH$_2$ calculated by our VQE compared with UCCSD VQE.

Fig. 3. VQE results of BeH$_2$ by our proposed VQE compared with UCCSD VQE.

The ground state energies of H$_2$O calculated by our proposed VQE compared with UCCSD VQE.

The errors of ground state energies of H$_2$O calculated by our VQE compared with UCCSD VQE.

Fig. 4. VQE results of H$_2$O by our proposed VQE compared with UCCSD VQE.

The ground state energies of N$_2$ with 10 active spin orbitals and 6 active electrons calculated by our proposed VQE compared with UCCSD VQE.

The errors of ground state energies of N$_2$ 10 active spin orbitals and 6 active electrons calculated by our VQE compared with UCCSD VQE.

Fig. 5. VQE results of N$_2$ 10 active spin orbitals and 6 active electrons by our proposed VQE compared with UCCSD VQE.

are always occupied and first 2 spin orbitals with highest energies are never occupied, corresponding to 10 active spin orbitals and 6 active electrons. Fig. 5(a) shows the ground state energies calculated by our VQE and UCCSD VQE. We also show the error between the VQE results and the diagonalization of the Hamiltonian as in Fig. 5(b). For small bond lengths, our proposed VQE achieves similar accuracy compared to UCCSD. When the bond length increases, our proposed VQE performs worse at some data points which may be caused by optimization trapped in the local minimum. Same as we observed in the results of H$_2$O, Algorithm 1 performs better than Algorithm 2 and UCCSD VQE at large bond lengths. Moreover, though both considering only spin symmetry excitations, Algorithm 2 performs better than UCCSD VQE at large bond lengths.

Furthermore, we also show VQE results of N$_2$ with less spin orbitals restricted. We now have first 8 spin orbitals with lowest energies are always occupied for N$_2$, corresponding to 12 active spin orbitals and 6 electrons. Fig. 6(a) shows the ground state energies calculated by our VQE and UCCSD VQE. We also present the error between the VQE results and the diagonalization of the Hamiltonian as in Fig. 6(b). We can see that when less spin orbitals are restricted, our proposed VQE performs worse than UCCSD VQE for large bond lengths, but still achieve a comparable accuracy with UCCSD VQE.

For H$_4$ we do not have any restrictions on the spin orbitals,
(a) The ground state energies of $N_2$ 12 active spin orbitals and 6 active electrons calculated by our proposed VQE compared with UCCSD VQE.

(b) The errors of ground state energies of $N_2$ 12 active spin orbitals and 6 active electrons calculated by our VQE compared with UCCSD VQE.

Fig. 6. VQE results of $N_2$ with 12 active spin orbitals and 6 active electrons by our proposed VQE compared with UCCSD VQE.

corresponding to 8 active spin orbitals and 4 electrons. Fig. 7(a) shows the ground state energies calculated by our VQE and UCCSD VQE. We also show the error between the VQE results and the diagonalization of the Hamiltonian as in Fig. 7(b). We can see that our VQE achieves similar accuracy compared to UCCSD VQE.

For $H_6$ we do not have any restrictions on the spin orbitals, corresponding to 12 active spin orbitals and 6 active electrons. Fig. 8(a) shows the ground state energies calculated by our VQE and UCCSD. We also show the error between the VQE results and the diagonalization of the Hamiltonian as in Fig. 8(b). We can see that our VQE achieves a little worse but still similar accuracy with UCCSD VQE.

V. CONCLUSION

We have introduced a new VQE ansatz based on the particle preserving exchange gate [20], [21]. We have shown our proposed VQE has reduced gate complexity from up-bounded to $O(n^5)$ of UCCSD VQE to up-bounded to $O(n^4)$ if using Jordan-Wigner transformation. In numerical simulations of $\text{BeH}_2$, $\text{H}_2\text{O}$, $N_2$, $H_4$ and $H_6$, we have shown that our proposed VQE have achieved comparable accuracy compared to UCCSD VQE, which may indicate removing of parity terms in UCCSD VQE have little effect on results for simple molecular systems. Our numerical simulation results also indicate that allowing all possible excitations may help to achieve better results at large bond lengths. With reduced complexity and
high accuracy, our proposed VQE ansatz might provide a new promising direction to implement electronic structure calculations on NISQ devices with chemical accuracy.

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