Efficient quantum circuits for quantum computational chemistry

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The VQE (variational quantum eigensolver) is a hybrid classical-quantum algorithm that can determine the energy eigenvalues of molecules by solving the electronic structure problem. Compared to other purely quantum algorithms, the VQE requires shallower quantum circuits and is more noise tolerant, which makes it a potential application for early NISQ (noisy intermediate-scale quantum) computers. The VQE works by minimizing the expectation value of a molecular Hamiltonian with respect to a parametrized ansatz state. The majority of ansatz states, so far considered by the scientific community, like the UCCSD (unitary coupled-cluster single and double), are derived from classical algorithms, and correspond to a combination of electron (fermionic) excitations applied to an initial guess ansatz state. Therefore, constructing efficient circuits that perform the action of fermionic excitations is critical for the practical realization of the VQE. Here, we introduce the concept of a “qubit excitation”, which compared to a fermionic excitation, does not account for fermionic anti-commutation relations. We then construct circuits, optimized in terms of $CNOT$ gates, that perform such single and double qubit excitations. Finally, we modify the functionality of these circuits to account for fermionic anti-commutation relations. In this way we obtain circuits for single and double fermionic excitations that reduce the number of $CNOT$ gates used, by factors of 2 and 8, respectively, compared to circuits constructed with the standard stair-case $CNOT$ structures.

I. INTRODUCTION

It is anticipated that quantum computers will be able to simulate quantum systems more efficiently and precisely than classical computers. A promising method to perform this task on emerging NISQ (noisy intermediate-scale quantum) [1, 2] computers is the VQE (variational quantum eigensolver) algorithm [3–6]. The VQE is a variational hybrid classical-quantum algorithm that determines the eigenvalues of a Hamiltonian operator by minimizing its expectation value, with respect to a parametrized ansatz state. Hence, the VQE can be used to solve the electronic structure problem [7, 8] and determine the ground state energy eigenvalue of a molecular Hamiltonian. Compared to other purely quantum algorithms, for eigenvalue determination, like the quantum phase estimation algorithm [9, 10], the VQE requires more measurements and classical post-processing, but it is more noise tolerant and requires much shallower quantum circuits.

A major challenge in the practical realization of the VQE on NISQ computers is the construction of the ansatz state and the circuit that implements this state, which we refer to as the ansatz circuit. In the context of the molecular electronic structure problem, a VQE ansatz state models the occupancies of molecular orbitals by electrons. That’s why most ansatz states, currently considered by the scientific community, for example the UCCSD [11, 12], the $k$-upCCGSD [13] and the ADAPT-VQE [14], are adapted from classical algorithms, for example the CCSD [8], and correspond to a product of parametrized single and double electron (fermionic) excitations, applied to an initial ansatz state, often chosen to be the Hartree-Fock state. Therefore, constructing efficient quantum circuits that simulate the action of single and double fermionic excitations, is critical to the practical realization of the VQE on NISQ computers. The standard method to construct such circuits is using stair-case $CNOT$ structures [11, 15]. We describe this method briefly in Sec.II A. However, constructing circuits for fermionic excitations in this way is highly inefficient in terms of $CNOT$ gates, which are the current bottleneck of NISQ computers [1, 16, 17].

In this work we introduce a strategy to construct circuits, optimized in terms of $CNOT$ gates, that perform single and double fermionic excitations. The strategy is based on initially constructing circuits to perform excitations that does not account for the fermionic anti-commutation relations. We term these simplified excitations as “qubit excitations”. To perform such single qubit excitations we use a circuit structure that performs an exchange interaction operation [18–20]. Then we expand this circuit to construct one that performs double qubit excitations. Finally we modify these qubit excitations circuits to account for fermionic anti-commutation relations. In this way, we obtain circuits that perform fermionic excitations in a more efficient way, compared to circuits constructed with stair-case $CNOT$ structures.

The paper is organised as follows: Sec.II A describes briefly how to construct circuits for fermionic excitations using stair-case $CNOT$ structures. In Sec.II B we outline a method, which we use to implement multi-qubit-controlled rotations. Sec.III A describes how to construct circuits that perform single and double qubit excitations, and Sec.III B shows how to modify these qubit excitation circuits to perform fermionic excitations instead. We summarize our results in Sec.IV.
II. THEORETICAL BACKGROUND

Throughout this paper we assume the Jordan-Wigner encoding [7, 21] for the electronic structure problem, where the occupancy of molecular orbital \( i \) is represented by the state of qubit \( q_i \).

A. Standard method to construct circuits for fermionic excitations

In this section, we provide a brief description of what is a fermionic excitation within the context of molecular VQE simulations, and we review the standard method to construct circuits that perform these excitations. Single and double fermionic excitations are defined, respectively, by the unitaries

\[
U_{ik}^{FS}(\theta) = \exp \left[ -\theta (a_i^\dagger a_k - a_k^\dagger a_i) \right] \\
U_{ijkl}^{FD}(\theta) = \exp \left[ -\theta (a_i^\dagger a_j^\dagger a_k a_l - a_l^\dagger a_k^\dagger a_j a_i) \right],
\]

where \( a_i^\dagger \) and \( a_i \) denote fermion creation and annihilation operators that obey the anti-commutation relations

\[
\{a_i, a_j^\dagger\} = \delta_{i,j}, \quad \{a_i, a_j\} = \{a_i^\dagger, a_j^\dagger\} = 0.
\]

The angle \( \theta \) is a variational parameter, whose physical meaning can be interpreted as the duration of an interaction. Within the Jordan-Wigner encoding, \( a \) and \( a^\dagger \) can be written in terms of qubit operators as

\[
a_i = Q_i \prod_{r=0}^{i-1} Z_r = \frac{1}{2} (X_i + iY_i) \prod_{r=0}^{i-1} Z_r \\
a_i^\dagger = Q_i^\dagger \prod_{r=0}^{i-1} Z_r = \frac{1}{2} (X_i - iY_i) \prod_{r=0}^{i-1} Z_r,
\]

where

\[
Q_i = \frac{1}{2} (X_i - iY_i), \quad Q_i^\dagger = \frac{1}{2} (X_i + iY_i).
\]

are qubit creation and annihilation operators that act to change the occupancy of orbital \( i \). The product of Pauli \( Z \) operators acts as an exchange phase factor accounting for the anti-commutation relations of \( a \) and \( a^\dagger \).

Using Eq. (3), the single fermionic excitation can be re-written in terms of qubit gate operators as

\[
U_{ik}^{FS}(\theta) = \exp \left[ -\frac{\theta}{2} (X_i Y_k - Y_k X_i) \prod_{r=k+1}^{i-1} Z_r \right] = \\
\exp \left[ -\frac{i\theta}{2} X_i Y_k \prod_{r=k+1}^{i-1} Z_r \right] \exp \left[ \frac{i\theta}{2} Y_k X_i \prod_{r=k+1}^{i-1} Z_r \right]
\]

Each of the two exponentials of Pauli operators, on the second line in Eq.(5), can be implemented using a structure similar to that in Fig.1. The base of the structure, consisting of the CNOTs and the \( R_{z}(\theta) \), performs the exponential \( U = \exp \left[ -i\theta \prod_{r=k+1}^{i-1} Z_r \right] \). Individual \( Z \) Pauli operators in the exponent can be transformed to \( X \) or \( Y \) Pauli operators, by \( x \) or \( y \) basis rotations, respectively, applied to the corresponding qubits.

In a similar way, the double fermionic excitation can be re-written in terms of qubit gate operators as

\[
U_{ijkl}^{FD}(\theta) = \exp \left[ -\frac{\theta}{8} (X_i X_j Y_k X_l + Y_i X_j X_k X_l - X_i X_j Y_k Y_l - Y_i X_j X_k Y_l) \prod_{r=k+1}^{i-1} \prod_{r'=l+1}^{j-1} Z_{r} \right],
\]

which is a product of 8 exponentials of Pauli operators that can be implemented by 8 stair-case CNOT structures.

B. Constructing multi-qubit-controlled rotations

In this section, we outline a method, used in [22], to construct circuits that implement multi-qubit-controlled rotations. The method is used to construct the circuits for the qubit excitations below, and is intended to minimize the usage of CNOT gates, without using ancilla qubits.

We denote a \( R_\theta(\theta) \) rotation on a target qubit \( q_0 \), controlled by qubits \( \{q_1..q_m\} \) in the state \( |1..1\rangle \), as \( R_\theta(q_1..q_m; q_0) \). Then we can write a \( m \)-qubit controlled rotation as decomposition to two opposite half-rotations, controlled by \( (m - 1) \) qubits, as

\[
R_\theta(q_1..q_m; q_0) = CNOT(q_1; q_0)R_y\left(\frac{\theta}{2}; \{q_2..q_m\}, q_0\right) \\
\times CNOT(q_1, q_0)R_y\left(\frac{\theta}{2}; \{q_2..q_m\}, q_0\right),
\]

FIG. 1: Stair-case CNOT structure implementing the exponential \( U = \exp \left[ -i\theta X_k \prod_{r=k+1}^{i-1} Z_r \right] \). The \( Y_k \) and the \( X_i \) operators in the exponent are produced by \( x \) and \( y \) basis rotations of qubits \( q_i \) and \( q_k \), respectively, using the \( H \) and the \( R_{z}(\pm \frac{\pi}{2}) \) gates.
or equivalently, as

\[ R_y(\theta, \{q_1..q_m\}, q_0) = R_y\left(\frac{\theta}{2}, \{q_2..q_m\}, q_0\right) \text{CNOT}(q_1, q_0) \times R_y\left(-\frac{\theta}{2}, \{q_2..q_m\}, q_0\right) \text{CNOT}(q_1, q_0). \quad (8) \]

By decomposing the controlled rotations further, the overall operation is brought down to CNOTs and single-qubit rotations. Implementing directly Eq.(7) or Eq.(8) results in a circuit with \((2^{m+1} - 2)\) CNOT gates. However, for \(m > 2\), Eq.(7) and Eq.(8) can be combined alternately to cancel adjacent CNOTs (see Fig.2), and obtain a circuit with \((2^{m-1} + 2)\) CNOTs. \(R_z\) and \(R_x\) controlled rotations can be obtained by basis rotations of the control qubit. It is also useful to note that in Eq.(7) and Eq.(8) CZ (controlled-phase) gates can be used instead of CNOTs.

\[ \text{FIG. 2: Circuit for a } R_y(\theta) \text{ rotation on a target qubit } q_0, \text{ controlled by the state } |q_1q_2\rangle = |11\rangle. \text{ The first half-rotation } R_y\left(\frac{\theta}{2}, \{q_1\}, q_0\right) \text{ is implemented as in Eq.(7), and the second half-rotation } R_y\left(-\frac{\theta}{2}, \{q_1\}, q_0\right) \text{ as in Eq.(8). This allows the two middle CNOTs between qubits } q_0 \text{ and } q_1 \text{ to be cancelled.} \]

### III. RESULTS

In this section, we begin by defining the concept of a qubit excitation. Next, we construct circuits to perform single and double qubit excitations. Then we describe how to modify these circuits to perform single and double fermionic excitations instead.

#### A. Qubit excitations

We define a qubit excitation as an excitation generated by the qubit creation and annihilation operators, \(Q\) and \(Q^\dagger\), given in Eq.(4). These operators satisfy the relations

\[ \{Q_i, Q_j^\dagger\} = I, \quad \{Q_i, Q_j\} = 0 \quad \text{if } i \neq j, \]

\[ \{Q_i, Q_j\} = [Q_i^\dagger, Q_j^\dagger] = 0. \quad (9) \]

These relations correspond to neither fermions nor bosons, and some authors \([23]\) have termed them as parafermionic. Then, single and double qubit excitations are expressed, respectively, by the unitaries

\[ U_{ik}^{Q^S}(\theta) = \exp\left[ -i\frac{\theta}{2}(Q_i^\dagger Q_k - Q_k^\dagger Q_i) \right] \]

\[ U_{ijkl}^{Q^D}(\theta) = \exp\left[ -i\theta(Q_i^\dagger Q_j^\dagger Q_l Q_i - Q_k^\dagger Q_l^\dagger Q_i Q_j) \right]. \quad (10) \]

We note that qubit excitations, although termed differently, have been considered in previous works. For example, the authors of \([24]\) proposed a simplified UCCSD ansatz state, constructed by qubit excitations instead of fermionic excitations.

#### 1. Circuit for a single qubit excitation

The single qubit excitation can be re-written in terms of qubit gate operators as

\[ U_{ik}^{Q^S}(\theta) = \exp\left[ -i\frac{\theta}{2}(X_i Y_k - Y_i X_k) \right] \]

This unitary is equivalent to an exchange interaction, which can be performed by the circuit in Fig.3a. The controlled \(R_y(\theta)\) rotation in this circuit can be implemented as in Eq.(8), using CZs instead of CNOTs. In this way the circuit identity in Fig.4 can be applied to reduce the number of CNOTs by one, and obtain the explicit circuit, for single qubit excitations in Fig.3b. This circuit has optimal CNOT count and CNOT depth of 3.

\[ \text{FIG. 3: a) Circuit performing an exchange interaction operation equivalent to the single qubit excitation in Eq.(11). b) Explicit circuit, for a single qubit excitation, obtained by implementing the controlled } R_y(\theta) \text{ as in Eq.(8), and using the identity in Fig.4.} \]

#### d) A circuit identity that performs an operation equivalent to a CNOT followed by a CZ. The advantage of the circuit on d) is that it requires one CNOT as compared to two for c). We term this identity as a controlled-XZ (or ZX if reversed)
2. Circuit for double qubit excitations

The double qubit excitation can be re-written in terms of qubit gate operators as

\[
U_{ijkl}^{QD}(\theta) = \exp \left[ -i \frac{\theta}{8} (X_i Y_j X_k X_l + Y_i X_j X_k Y_l + Y_i Y_j X_k X_l - X_i X_j Y_k Y_l - X_i X_j Y_k X_l - X_i Y_j Y_k Y_l - X_i Y_j X_k Y_l) \right].
\] (12)

This is a unitary operation that continuously exchanges the \(|1100\rangle\) and \(|0011\rangle\) states, and acts trivially on all other states. To implement this operation we can use a similar circuit construction as for the single qubit excitation. However, to ensure that the operation exchanges the states \(|1100\rangle\) and \(|0011\rangle\) only if the parities of the qubit pairs \(q_0\) and \(q_1\), and \(q_2\) and \(q_3\), are even. To perform this kind of parity-controlled exchange operation we construct the circuit in Fig. (5). The first two \(CNOT\)s, between qubits \(q_0\) and \(q_1\), and qubits \(q_2\) and \(q_3\), determine and record the parity of the two pairs on qubits \(q_1\) and \(q_3\), respectively. Next, the gates in the dotted rectangle perform an exchange operation, controlled by the values of qubits \(q_1\) and \(q_3\). Finally, the last two \(CNOT\)s correct for the parity determination.

![Fig. 5: Circuit performing the double qubit excitation in Eq.(12). The explicit circuit is given in Fig.9.](image)

The controlled-\(R_y(\theta)\) rotation in Fig.5 is implemented by the circuit in Fig.8, and the circuit identity in Fig.4 is used again to reduce the number of \(CNOT\)s by one. In this way, we obtain the explicit circuit for a double qubit excitation in Fig.9. The circuit has a \(CNOT\) count of 13 and \(CNOT\) depth of 11. We note that [25, 26] suggest a similar circuit, for the same operation, which also has a \(CNOT\) count of 13, but a higher \(CNOT\) depth of 13.

B. Fermionic excitations

The expressions for fermionic excitations, in Eq.(5) and Eq.(6), differ from those for qubit excitations, in Eq.(11) and Eq.(12), only by the additional products of Pauli \(Z\) operators in their exponents, that account for the fermionic anti-commutation relations of operators \(a\) and \(a^\dagger\). In the case of the single fermionic excitation, the Pauli \(Z\) operators act to change the sign of the excitation parameter \(\theta\) if the parity of the qubit set \(\{q_{k+1}\cdots q_{i-1}\}\) is odd. Similarly, for the double fermionic excitation the sign of \(\theta\) is changed if the parity of the qubit set \(\{q_{j+1}\cdots q_{i-1}q_{i+1}\cdots q_{k-1}\}\) is odd. Hence, the fermionic excitations are expressed in terms of qubit excitations as

\[
U_{ik}^{QS}(\theta) = \begin{cases} U_{ik}^{QS}(\theta) & \text{if } \text{par}\{q_{k+1}\cdots q_{i-1}\} = 0 \\ U_{ik}^{QS}(-\theta) & \text{if } \text{par}\{q_{k+1}\cdots q_{i-1}\} = 1 \end{cases},
\] (13)

\[
U_{ijkl}^{FD}(\theta) = \begin{cases} U_{ijkl}^{QD}(\theta) & \text{if } \text{par}\{q_{j+1}\cdots q_{i-1}q_{i+1}\cdots q_{k-1}\} = 0 \\ U_{ijkl}^{QD}(-\theta) & \text{if } \text{par}\{q_{j+1}\cdots q_{i-1}q_{i+1}\cdots q_{k-1}\} = 1 \end{cases}.
\] (14)

Below, we show how to modify the circuits for single and double qubit excitations to perform fermionic excitations instead. We do this by introducing a stair-case \(CNOT\) structure, as in Fig.1, that wraps each of the controlled-\(R_y(\theta)\) rotations, in the circuits in Fig.3 and Fig.5, and changes the rotations signs depending on the parity of the corresponding qubits.

1. Circuit for single fermionic excitations

The modified circuit for single fermionic excitations, obtained from the circuit in Fig.3a, is given in Fig.6. The parity of the qubit set \(\{q_{k+1}\cdots q_{i-1}\}\) is determined by the stair-case \(CNOT\) structure and recorded on qubit \(q_{i-1}\). The two \(CZ\) gates between qubits \(q_j\) and \(q_{i-1}\) are used to change the sign of the \(R_y(\theta)\) rotation, if qubit \(q_{i-1}\) is in state \(|1\rangle\) (corresponding to odd parity). The controlled-\(R_y(\theta)\) rotation is implemented as for the single qubit excitation circuit so that the circuit identity, from Fig.4, can be applied again to reduce the number of \(CNOT\)s by one. Defining \(n = j - i + 1\) as the total number of qubits involved in the excitation, for \(n \geq 2\), the circuit in Fig.6 has \(CNOT\) count of \((2n - 1)\) and \(CNOT\) depth of \(\max[5, 2n - 3]\). For \(n = 2\), the circuit is the same as that in Fig.3b. In comparison, implementing a fermionic single excitation in the standard way, using 2 stair-case \(CNOT\) structures, results in a circuit with \(CNOT\) count and \(CNOT\) depth of \((4n - 4)\).
The modified circuit for a double fermionic excitation, obtained from the circuit in Fig. 5, is given in Fig. 7. The parity of the set of qubits \{q_{i+1}, q_{i-1}, q_i, q_k\}, is determined by a stair-case construction and recorded on qubit \(q_{i-1}\). The two CZ gates between qubits \(q_i\) and \(q_{i-1}\) are used to change the sign of the controlled \(R_y(\theta)\) rotation, if qubit \(q_{i-1}\) is in state \(|1\rangle\). The controlled \(R_y(\theta)\) is implemented again as in Fig. 8, so that the circuit identity, from Fig. 4, is applied to reduce the number of CNOTs by one. Defining \(n = i - j + k - l + 2\) as the total number of qubits participating in the excitation, the circuit in Fig. 7 has a CNOT count of \(2n + 5\) and CNOT depth of \(\max[13, 2n - 1]\) for \(n \geq 5\). For \(n = 4\) the circuit is identical to that in Fig. 5 (and Fig. 9). In comparison, implementing a fermionic double excitation in the standard way, using 8 stair-case structures, results in a circuit with a CNOT count and a CNOT depth of \((16n - 16)\).

IV. SUMMARY

In this work we defined the concept of a qubit excitation as an excitation generated by qubit creation and annihilation operators. We introduced circuits, optimized in terms of CNOT gates, to perform such single and double qubit excitations. We then demonstrated how to expand the functionality of these qubit excitation circuits to account for fermionic anti-commutation relations and perform fermionic excitations instead. To our knowledge the circuits introduced here offer the most efficient way to implement double qubit and fermionic excitations, in terms of both CNOT gate count and CNOT depth. Compared to circuits, constructed with the previously used stair-case CNOT structures, the circuits suggested here reduce the number of CNOT gates by a factor of 2 and 8, for single and double excitations, respectively. The circuits introduced in this work, present a significant optimization towards implementing VQE algorithms on NISQ computers.

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