

Electronic Supplementary Information

A Quantum Computing View on Unitary Coupled Cluster Theory

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MULTIPLICATION TABLES FOR C_{2v} AND D_{2h}

For the sake of completeness, we state the multiplication tables for the point groups C_{2v} and D_{2h} that the main text refers to here:

Table I. Multiplication table for the C_{2v} point group.

	A_1	A_2	B_1	B_2
A_1	A_1	A_2	B_1	B_2
A_2	A_2	A_1	B_2	B_1
B_1	B_1	B_2	A_1	A_2
B_2	B_2	B_1	A_2	A_1

Table II. Multiplication table for the D_{2h} point group.

	A_g	A_u	B_{1g}	B_{2g}	B_{3g}	B_{1u}	B_{2u}	B_{3u}
A_g	A_g	A_u	B_{1g}	B_{2g}	B_{3g}	B_{1u}	B_{2u}	B_{3u}
A_u	A_u	A_g	B_{1u}	B_{2u}	B_{3u}	B_{1g}	B_{2g}	B_{3g}
B_{1g}	B_{1g}	B_{1u}	A_g	B_{3g}	B_{2g}	A_u	B_{3u}	B_{2u}
B_{2g}	B_{2g}	B_{2u}	B_{3g}	A_g	B_{1g}	B_{3u}	A_u	B_{1u}
B_{3g}	B_{3g}	B_{3u}	B_{2g}	B_{1g}	A_g	B_{2u}	B_{1u}	A_u
B_{1u}	B_{1u}	B_{1g}	A_u	B_{3u}	B_{2u}	A_g	B_{3g}	B_{2g}
B_{2u}	B_{2u}	B_{2g}	B_{3u}	A_u	B_{1u}	B_{3g}	A_g	B_{1g}
B_{3u}	B_{3u}	B_{3g}	B_{2u}	B_{1u}	A_u	B_{2g}	B_{1g}	A_g

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REDUCTION OF CNOT GATE COUNT FOR UCCSD BY USING THE TABLEAU REPRESENTATION AND JORDAN-WIGNER TRANSFORMATION

The structure of single and double excitations obtained using the JW transformation is easy to compile using the tableau representation and its algebra, which will be explained in more detail in the subsequent section. Reductions of at least 50% in the number of CNOT gates can be obtained for both singles and doubles when comparing with the typical exponential map of Pauli strings that has been described in section ???. Here, a matrix consisting of mutually commuting Pauli strings is first diagonalized and then exponentiated instead of exponentiating each Pauli string individually.

When the Jordan-Wigner transformation is used to encode UCC excitations, a non-local parity operator is needed to introduce the required phase change by a string of Z operators between the excitation qubits (for single excitations) or between the occupied and between the virtual qubits (for double excitations) [1]. For this reason, the scaling of the CNOT count increases by the number of qubits (N) in addition with the $N_{\text{occ}}^2 N_{\text{virt}}^2$ bottleneck of double excitations for UCCSD, yielding an upper-bound of $O(N^5)$ number of CNOT gates. However, due to its structure, a simple compilation of UCCSD operators can be performed based on the tableau representation, which reduces the CNOT gate count significantly.

The compilation of UCCSD excitations is separated in two steps. First, the parity operator is factorised for a set of four commuting Pauli strings. Second, the remaining qubit excitations are diagonalized with Clifford gates.

Tableau representation and its algebra

We use a binary array to represent matrices consisting of Pauli strings. This array has three blocks ($[X, Z, s]$), where each row is a Pauli string. The j -th components of the i -th Pauli string are obtained from $(X_{i,j}, Z_{i,j})$ and defined as

$$(X_{i,j}, Z_{i,j}) = \begin{cases} (0, 0) & j\text{-th qubit has } \mathbb{1}^{(j)} \\ (0, 1) & j\text{-th qubit has } \hat{\sigma}_z^{(j)} \\ (1, 0) & j\text{-th qubit has } \hat{\sigma}_x^{(j)} \\ (1, 1) & j\text{-th qubit has } \hat{\sigma}_y^{(j)} \end{cases}. \quad (1)$$

In addition, the s block is a single column containing the sign of the Pauli string. For example, a matrix describing the addition of two Pauli strings $(+\hat{\sigma}_y^{(0)}\hat{\sigma}_z^{(1)}\hat{\sigma}_x^{(2)} - \hat{\sigma}_x^{(0)}\hat{\sigma}_z^{(1)}\hat{\sigma}_y^{(2)})$ can be represented with the following tableau:

$$\begin{bmatrix} +\hat{\sigma}_y^{(0)}\hat{\sigma}_z^{(1)}\hat{\sigma}_z^{(2)}\hat{\sigma}_x^{(3)} \\ -\hat{\sigma}_x^{(0)}\hat{\sigma}_z^{(1)}\hat{\sigma}_z^{(2)}\hat{\sigma}_y^{(3)} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 1 & | & 1 & 1 & 1 & 0 & | & 0 \\ 1 & 0 & 0 & 1 & | & 0 & 1 & 1 & 1 & | & 1 \end{bmatrix}. \quad (2)$$

Representation of a linear combination of Pauli strings in the tableau representation () is useful to display the correlation information between these operators in a more visual way. Then, it becomes easier to apply unitary operators from the Clifford group (C) to simplify P into either all $\hat{\sigma}_z$ or diagonal operators (Z). The Clifford group in \mathbb{C}^2 is generated by the Hadamard, phase and conditional-NOT gates (H, S and CNOT, respectively). Both H and S are one-qubit gates. For example, H(a) applies H to qubit a . The CNOT-gate (also CX) is a two qubit gate; it applies $\hat{\sigma}_x$ to qubit b to the $|1\rangle$ -part of qubit a . Furthermore, the CZ(a, b)-gate applies $\hat{\sigma}_z$ to qubit b conditioned on qubit a being in $|1\rangle$; it is equal to H(b)CX(a, b)H(b).

We can define C as a product of several Clifford gates working in an initial linear combination of Pauli strings (P_1) such that

$$P_1 = CP_2C^\dagger, \quad (3)$$

where P_2 is the updated tableau pertaining the C unitary transformation, see Table III for a summary of tableau algebra when using Clifford gates.

For example, when P_1 is the tableau from Eq. (2) $(+\hat{\sigma}_y^{(0)}\hat{\sigma}_z^{(1)}\hat{\sigma}_z^{(2)}\hat{\sigma}_x^{(3)} - \hat{\sigma}_x^{(0)}\hat{\sigma}_z^{(1)}\hat{\sigma}_z^{(2)}\hat{\sigma}_y^{(3)})$ and C equals to CX(1, 2), the following is obtained:

$$\begin{bmatrix} 1 & 0 & 0 & 1 & | & 1 & 1 & 1 & 0 & | & 0 \\ 1 & 0 & 0 & 1 & | & 0 & 1 & 1 & 1 & | & 1 \end{bmatrix} = C \begin{bmatrix} 1 & 0 & 0 & 1 & | & 1 & 0 & 1 & 0 & | & 0 \\ 1 & 0 & 0 & 1 & | & 1 & 0 & 1 & 1 & | & 1 \end{bmatrix} C^\dagger, \quad (4)$$

Table III. Tableau sign and block update when applying Clifford gates.

Gate	Sign update	Block update
H(a)	$s_i = s_i \oplus X_{i,a} \otimes Z_{i,a}$	swap($X_{i,a}, Z_{i,a}$)
S(a)	$s_i = s_i \oplus X_{i,a} \otimes (Z_{i,a} \oplus 1)$	$Z_{i,a} = X_{i,a} \oplus Z_{i,a}$
CX(a, b)	$s_i = s_i \oplus X_{i,a} \otimes Z_{i,b} \otimes (X_{i,b} \oplus Z_{i,a} \oplus 1)$	$Z_{i,a} = Z_{i,a} \oplus Z_{i,b}$ $X_{i,b} = X_{i,a} \oplus X_{i,b}$
CZ(a, b)	$s_i = s_i \oplus X_{i,a} \otimes X_{i,b} \otimes (Z_{i,a} \oplus Z_{i,b})$	$Z_{i,a} = X_{i,b} \oplus Z_{i,a}$ $Z_{i,b} = X_{i,a} \oplus Z_{i,b}$

or,

$$\begin{bmatrix} +\hat{\sigma}_y^{(0)} \hat{\sigma}_z^{(1)} \hat{\sigma}_z^{(2)} \hat{\sigma}_x^{(3)} \\ -\hat{\sigma}_x^{(0)} \hat{\sigma}_z^{(1)} \hat{\sigma}_z^{(3)} \hat{\sigma}_y^{(3)} \end{bmatrix} = \text{CX}(1, 2) \begin{bmatrix} +\hat{\sigma}_y^{(0)} \hat{\sigma}_z^{(2)} \hat{\sigma}_x^{(3)} \\ -\hat{\sigma}_x^{(0)} \hat{\sigma}_z^{(3)} \hat{\sigma}_y^{(3)} \end{bmatrix} \text{CX}(1, 2), \quad (5)$$

where $\text{CX}(a, b)^\dagger = \text{CX}(a, b)$ is used (also, in the future $\text{H}(a)^\dagger = \text{H}(a)$ and $\text{CZ}(a, b) = \text{CZ}(a, b)^\dagger$). Following up with the $\text{CZ}(2, 3)$ gate will remove the $\hat{\sigma}_z$ operators completely,

$$\begin{bmatrix} +\hat{\sigma}_y^{(0)} \hat{\sigma}_z^{(2)} \hat{\sigma}_x^{(3)} \\ -\hat{\sigma}_x^{(0)} \hat{\sigma}_z^{(3)} \hat{\sigma}_y^{(3)} \end{bmatrix} = \text{CZ}(2, 3) \begin{bmatrix} +\hat{\sigma}_y^{(0)} \hat{\sigma}_x^{(3)} \\ -\hat{\sigma}_x^{(0)} \hat{\sigma}_y^{(3)} \end{bmatrix} \text{CZ}(2, 3), \quad (6)$$

which yields the same results obtained previously for the removal of the parity operator (a continuous non-local string of $\hat{\sigma}_z$ operators obtained with the JW transformation). This is useful because $CC^\dagger = \mathbb{1}$ and several Pauli strings have the same parity operator (or similar) and large reductions of two-qubit gate counts are obtained using this compilation technique.

Tableau compilation of single excitations/de-excitations

Grouping four mutually commutative Pauli strings within the same spatial-orbitals yields a better reduction for single excitations/de-excitations than compilation of one single excitation at a time. In this subsection the spin-orbital notation is different, the occupied α spin-orbitals is i (a) and the occupied (virtual) β spin-orbital is \bar{i} (\bar{a}). Then, the first group to compile contains excitations/de-excitations within the same spin, $\hat{a}_a^\dagger \hat{a}_i - \hat{a}_i^\dagger \hat{a}_a + \hat{a}_{\bar{a}}^\dagger \hat{a}_{\bar{i}} - \hat{a}_{\bar{i}}^\dagger \hat{a}_{\bar{a}}$, and the Jordan-Wigner transformation yields,

$$\begin{aligned} \text{JW}(\hat{a}_a^\dagger \hat{a}_i + \hat{a}_a^\dagger \hat{a}_{\bar{i}} - h.c.) &= i \frac{1}{2} \bigotimes_{k=\bar{i}+1}^{a-1} \hat{\sigma}_z^{(k)} (+\hat{\sigma}_y^{(i)} \hat{\sigma}_z^{(\bar{i})} \hat{\sigma}_x^{(a)} \\ &\quad - \hat{\sigma}_x^{(i)} \hat{\sigma}_z^{(\bar{i})} \hat{\sigma}_y^{(a)} + \hat{\sigma}_y^{(\bar{i})} \hat{\sigma}_z^{(a)} \hat{\sigma}_x^{(\bar{a})} - \hat{\sigma}_x^{(\bar{i})} \hat{\sigma}_z^{(a)} \hat{\sigma}_y^{(\bar{a})}), \end{aligned} \quad (7)$$

where the spatial-orbital parity operator ($\bigotimes_{k=\bar{i}+1}^{a-1} \hat{\sigma}_z^{(k)}$) can be factorised from a tableau of pseudo-qubit-excitations. First, the parity operator is factorised using $\text{U}_{s,ss,p}$,

$$\bigotimes_{k=\bar{i}+1}^{a-1} \hat{\sigma}_z^{(k)} \begin{pmatrix} +\hat{\sigma}_y^{(i)} \hat{\sigma}_z^{(\bar{i})} \hat{\sigma}_x^{(a)} \\ +\hat{\sigma}_y^{(\bar{i})} \hat{\sigma}_z^{(a)} \hat{\sigma}_x^{(\bar{a})} \\ -\hat{\sigma}_x^{(i)} \hat{\sigma}_z^{(\bar{i})} \hat{\sigma}_y^{(a)} \\ -\hat{\sigma}_x^{(\bar{i})} \hat{\sigma}_z^{(a)} \hat{\sigma}_y^{(\bar{a})} \end{pmatrix} = \text{U}_{s,ss,p} \begin{bmatrix} +\hat{\sigma}_y^{(i)} \hat{\sigma}_z^{(\bar{i})} \hat{\sigma}_x^{(a)} \\ +\hat{\sigma}_y^{(\bar{i})} \hat{\sigma}_z^{(a)} \hat{\sigma}_x^{(\bar{a})} \\ -\hat{\sigma}_x^{(i)} \hat{\sigma}_z^{(\bar{i})} \hat{\sigma}_y^{(a)} \\ -\hat{\sigma}_x^{(\bar{i})} \hat{\sigma}_z^{(a)} \hat{\sigma}_y^{(\bar{a})} \end{bmatrix} \text{U}_{s,ss,p}^\dagger, \quad (8)$$

where $\text{U}_{s,ss,p}$ is a unitary transformation that contains $(L+1)$ two-qubit gates (L is the span of the k -index),

$$\text{U}_{s,ss,p} = \left(\bigotimes_{k=i+1}^{\bar{a}-2} \text{CX}(k, k+1) \right) \text{CZ}(a-1, a) \text{CZ}(a-1, \bar{a}). \quad (9)$$

Second, the remaining tableau (pertaining pseudo-single-qubit-excitations) is diagonalised with $U_{s,ss}$

$$\begin{bmatrix} +\hat{\sigma}_y^{(i)} \hat{\sigma}_z^{(\bar{i})} \hat{\sigma}_x^{(a)} \\ +\hat{\sigma}_y^{(\bar{i})} \hat{\sigma}_z^{(a)} \hat{\sigma}_x^{(\bar{a})} \\ -\hat{\sigma}_x^{(i)} \hat{\sigma}_z^{(\bar{i})} \hat{\sigma}_y^{(a)} \\ -\hat{\sigma}_x^{(\bar{i})} \hat{\sigma}_z^{(a)} \hat{\sigma}_y^{(\bar{a})} \end{bmatrix} = U_{s,ss} \begin{bmatrix} -\hat{\sigma}_z^{(i)} \\ -\hat{\sigma}_z^{(\bar{i})} \\ +\hat{\sigma}_z^{(a)} \\ +\hat{\sigma}_z^{(\bar{a})} \end{bmatrix} U_{s,ss}^\dagger, \quad (10)$$

where $U_{s,ss}$ is a unitary transformation that contains three two-qubit gates,

$$U_{s,ss} = CZ(\bar{i}, a)H(*)CZ(i, a)CZ(\bar{i}, \bar{a})S(*)H(*). \quad (11)$$

We used (*) to denote that the corresponding one-qubit gate is applied to all the four pertaining qubits.

The second group contains single excitations/de-excitations with different spin, $\hat{a}_a^\dagger \hat{a}_i - \hat{a}_i^\dagger \hat{a}_a + \hat{a}_a^\dagger \hat{a}_{\bar{i}} - \hat{a}_{\bar{i}}^\dagger \hat{a}_a$, and the Jordan-Wigner transformation yields,

$$JW(\hat{a}_a^\dagger \hat{a}_i + \hat{a}_a^\dagger \hat{a}_{\bar{i}} - h.c.) = i \frac{1}{2} \bigotimes_{k=\bar{i}+1}^{a-1} \hat{\sigma}_z^{(k)} (+\hat{\sigma}_y^{(i)} \hat{\sigma}_z^{(\bar{i})} \hat{\sigma}_z^{(a)} \hat{\sigma}_x^{(\bar{a})} \quad (12)$$

$$- \hat{\sigma}_x^{(i)} \hat{\sigma}_z^{(\bar{i})} \hat{\sigma}_z^{(a)} \hat{\sigma}_y^{(\bar{a})} + \hat{\sigma}_y^{(\bar{i})} \hat{\sigma}_z^{(a)} - \hat{\sigma}_x^{(\bar{i})} \hat{\sigma}_y^{(a)}), \quad (13)$$

where the same spatial-orbital parity operator ($\bigotimes_{k=\bar{i}+1}^{a-1} \hat{\sigma}_z^{(k)}$) and a second tableau of opposite spin pseudo qubit excitations are obtained. The parity operator can be factorised with the same unitary transformation ($U_{s,ss,p}$) and because $U_{s,ss,p}^\dagger U_{s,ss,p} = \mathbb{1}$ further reduction of two-qubit gates is obtained. Then, the second tableau is diagonalized with the $U_{s,os}$,

$$\begin{bmatrix} +\hat{\sigma}_y^{(i)} \hat{\sigma}_z^{(\bar{i})} \hat{\sigma}_z^{(a)} \hat{\sigma}_x^{(\bar{a})} \\ +\hat{\sigma}_y^{(\bar{i})} \hat{\sigma}_z^{(a)} \\ -\hat{\sigma}_x^{(\bar{i})} \hat{\sigma}_y^{(a)} \\ -\hat{\sigma}_x^{(i)} \hat{\sigma}_z^{(\bar{i})} \hat{\sigma}_z^{(a)} \hat{\sigma}_y^{(\bar{a})} \end{bmatrix} = U_{s,os} \begin{bmatrix} -\hat{\sigma}_z^{(i)} \\ +\hat{\sigma}_z^{(\bar{i})} \\ -\hat{\sigma}_z^{(a)} \\ +\hat{\sigma}_z^{(\bar{a})} \end{bmatrix} U_{s,os}^\dagger, \quad (14)$$

where $U_{s,os}$ is an unitary transformation that contains four two-qubit gates,

$$U_{s,os} = CZ(\bar{i}, \bar{a})CZ(a, \bar{a})H(*)CZ(i, \bar{a})CZ(\bar{i}, a)S(*)H(*). \quad (15)$$

The total number of two-qubit gates must be multiplied by two to complete the unitary transformation, application of U followed by U^\dagger . Then the total number of two-qubit gates is $2((L+1)+7) = 16+2L$, which greatly improves over the basic exponential map of individual Pauli strings that requires $32+16L$ two-qubit gates.

Tableau compilation of double excitations/de-excitations

The JW-transformation of a double excitation/de-excitation reads, [2]

$$\begin{aligned} JW(\hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i - h.c.) &= i \frac{1}{8} \bigotimes_{k=i+1}^{j-1} \hat{\sigma}_z^{(k)} \bigotimes_{c=a+1}^{b-1} \hat{\sigma}_z^{(c)} (+\hat{\sigma}_y^{(i)} \hat{\sigma}_x^{(j)} \hat{\sigma}_x^{(a)} \hat{\sigma}_x^{(b)} + \hat{\sigma}_x^{(i)} \hat{\sigma}_y^{(j)} \hat{\sigma}_x^{(a)} \hat{\sigma}_x^{(b)} \\ &- \hat{\sigma}_x^{(i)} \hat{\sigma}_x^{(j)} \hat{\sigma}_y^{(a)} \hat{\sigma}_x^{(b)} - \hat{\sigma}_x^{(i)} \hat{\sigma}_x^{(j)} \hat{\sigma}_x^{(a)} \hat{\sigma}_y^{(b)} - \hat{\sigma}_x^{(i)} \hat{\sigma}_y^{(j)} \hat{\sigma}_y^{(a)} \hat{\sigma}_y^{(b)} \\ &- \hat{\sigma}_y^{(i)} \hat{\sigma}_x^{(j)} \hat{\sigma}_y^{(a)} \hat{\sigma}_y^{(b)} + \hat{\sigma}_y^{(i)} \hat{\sigma}_y^{(j)} \hat{\sigma}_x^{(a)} \hat{\sigma}_y^{(b)} + \hat{\sigma}_y^{(i)} \hat{\sigma}_y^{(j)} \hat{\sigma}_y^{(a)} \hat{\sigma}_x^{(b)}), \end{aligned} \quad (16)$$

where the parity operator $(\bigotimes_{k=i+1}^{j-1} \hat{\sigma}_z^{(k)} \bigotimes_{c=a+1}^{b-1} \hat{\sigma}_z^{(c)})$ is factorised with $U_{d,p}$,

$$\bigotimes_{k=i+1}^{j-1} \hat{\sigma}_z^{(k)} \bigotimes_{c=a+1}^{b-1} \hat{\sigma}_z^{(c)} \begin{pmatrix} +\hat{\sigma}_y^{(i)} \hat{\sigma}_x^{(j)} \hat{\sigma}_x^{(a)} \hat{\sigma}_x^{(b)} \\ +\hat{\sigma}_x^{(i)} \hat{\sigma}_y^{(j)} \hat{\sigma}_x^{(a)} \hat{\sigma}_x^{(b)} \\ -\hat{\sigma}_x^{(i)} \hat{\sigma}_x^{(j)} \hat{\sigma}_y^{(a)} \hat{\sigma}_x^{(b)} \\ -\hat{\sigma}_x^{(i)} \hat{\sigma}_x^{(j)} \hat{\sigma}_x^{(a)} \hat{\sigma}_y^{(b)} \\ -\hat{\sigma}_x^{(i)} \hat{\sigma}_y^{(j)} \hat{\sigma}_y^{(a)} \hat{\sigma}_y^{(b)} \\ -\hat{\sigma}_x^{(i)} \hat{\sigma}_x^{(j)} \hat{\sigma}_y^{(a)} \hat{\sigma}_y^{(b)} \\ +\hat{\sigma}_y^{(i)} \hat{\sigma}_y^{(j)} \hat{\sigma}_x^{(a)} \hat{\sigma}_y^{(b)} \\ +\hat{\sigma}_y^{(i)} \hat{\sigma}_y^{(j)} \hat{\sigma}_y^{(a)} \hat{\sigma}_x^{(b)} \end{pmatrix} = U_{d,p} \begin{bmatrix} +\hat{\sigma}_y^{(i)} \hat{\sigma}_x^{(j)} \hat{\sigma}_x^{(a)} \hat{\sigma}_x^{(b)} \\ +\hat{\sigma}_x^{(i)} \hat{\sigma}_y^{(j)} \hat{\sigma}_x^{(a)} \hat{\sigma}_x^{(b)} \\ -\hat{\sigma}_x^{(i)} \hat{\sigma}_x^{(j)} \hat{\sigma}_y^{(a)} \hat{\sigma}_x^{(b)} \\ -\hat{\sigma}_x^{(i)} \hat{\sigma}_x^{(j)} \hat{\sigma}_x^{(a)} \hat{\sigma}_y^{(b)} \\ -\hat{\sigma}_x^{(i)} \hat{\sigma}_y^{(j)} \hat{\sigma}_y^{(a)} \hat{\sigma}_y^{(b)} \\ -\hat{\sigma}_x^{(i)} \hat{\sigma}_x^{(j)} \hat{\sigma}_y^{(a)} \hat{\sigma}_y^{(b)} \\ +\hat{\sigma}_y^{(i)} \hat{\sigma}_y^{(j)} \hat{\sigma}_x^{(a)} \hat{\sigma}_y^{(b)} \\ +\hat{\sigma}_y^{(i)} \hat{\sigma}_y^{(j)} \hat{\sigma}_y^{(a)} \hat{\sigma}_x^{(b)} \end{bmatrix} U_{d,p}^\dagger, \quad (17)$$

where $U_{d,p}$ is a unitary transformation built with L two-qubit gates (L is the addition of k and c spans) and $U_{d,p}$ reads,

$$U_{d,p} = \left(\bigotimes_{k=i+1}^{j-2} \text{CX}(k, k+1) \right) \text{CX}(j-1, a+1) \left(\bigotimes_{c=a+1}^{b-2} \text{CX}(c, c+1) \right) \text{CZ}(b-1, b). \quad (18)$$

The remaining Pauli strings is a double qubit excitation and is separated into two tableaux,

$$P_{d,x} = \begin{bmatrix} -\hat{\sigma}_x^{(i)} \hat{\sigma}_y^{(j)} \hat{\sigma}_y^{(a)} \hat{\sigma}_y^{(b)} \\ -\hat{\sigma}_y^{(i)} \hat{\sigma}_x^{(j)} \hat{\sigma}_y^{(a)} \hat{\sigma}_y^{(b)} \\ +\hat{\sigma}_y^{(i)} \hat{\sigma}_y^{(j)} \hat{\sigma}_x^{(a)} \hat{\sigma}_y^{(b)} \\ +\hat{\sigma}_y^{(i)} \hat{\sigma}_y^{(j)} \hat{\sigma}_y^{(a)} \hat{\sigma}_x^{(b)} \end{bmatrix} \quad (19)$$

$$P_{d,y} = \begin{bmatrix} +\hat{\sigma}_y^{(i)} \hat{\sigma}_x^{(j)} \hat{\sigma}_x^{(a)} \hat{\sigma}_x^{(b)} \\ +\hat{\sigma}_x^{(i)} \hat{\sigma}_y^{(j)} \hat{\sigma}_x^{(a)} \hat{\sigma}_x^{(b)} \\ -\hat{\sigma}_x^{(i)} \hat{\sigma}_x^{(j)} \hat{\sigma}_y^{(a)} \hat{\sigma}_x^{(b)} \\ -\hat{\sigma}_x^{(i)} \hat{\sigma}_x^{(j)} \hat{\sigma}_x^{(a)} \hat{\sigma}_y^{(b)} \end{bmatrix}. \quad (20)$$

Then, the $P_{d,y}$ tableau is diagonalized with $U_{d,y}$

$$\begin{bmatrix} +\hat{\sigma}_y^{(i)} \hat{\sigma}_x^{(j)} \hat{\sigma}_x^{(a)} \hat{\sigma}_x^{(b)} \\ +\hat{\sigma}_x^{(i)} \hat{\sigma}_y^{(j)} \hat{\sigma}_x^{(a)} \hat{\sigma}_x^{(b)} \\ -\hat{\sigma}_x^{(i)} \hat{\sigma}_x^{(j)} \hat{\sigma}_y^{(a)} \hat{\sigma}_x^{(b)} \\ -\hat{\sigma}_x^{(i)} \hat{\sigma}_x^{(j)} \hat{\sigma}_x^{(a)} \hat{\sigma}_y^{(b)} \end{bmatrix} = U_{d,y} \begin{bmatrix} -\hat{\sigma}_z^{(i)} \\ -\hat{\sigma}_z^{(j)} \\ +\hat{\sigma}_z^{(a)} \\ +\hat{\sigma}_z^{(b)} \end{bmatrix} U_{d,y}^\dagger, \quad (21)$$

where the unitary transformation reads,

$$U_{d,y} = \text{H}(\ast) \text{CZ}(i, j) \text{CZ}(i, a) \text{CZ}(i, b) \text{CZ}(j, a) \text{CZ}(j, b) \text{CZ}(a, b) \text{S}(\ast) \text{H}(\ast). \quad (22)$$

Furthermore, diagonalisation of the $P_{d,x}$ tableau is obtained with

$$\begin{bmatrix} -\hat{\sigma}_x^{(i)} \hat{\sigma}_y^{(j)} \hat{\sigma}_y^{(a)} \hat{\sigma}_y^{(b)} \\ -\hat{\sigma}_y^{(i)} \hat{\sigma}_x^{(j)} \hat{\sigma}_y^{(a)} \hat{\sigma}_y^{(b)} \\ +\hat{\sigma}_y^{(i)} \hat{\sigma}_y^{(j)} \hat{\sigma}_x^{(a)} \hat{\sigma}_y^{(b)} \\ +\hat{\sigma}_y^{(i)} \hat{\sigma}_y^{(j)} \hat{\sigma}_y^{(a)} \hat{\sigma}_x^{(b)} \end{bmatrix} = U_{d,x} \begin{bmatrix} -\hat{\sigma}_z^{(i)} \\ -\hat{\sigma}_z^{(j)} \\ +\hat{\sigma}_z^{(a)} \\ +\hat{\sigma}_z^{(b)} \end{bmatrix} U_{d,x}^\dagger, \quad (23)$$

where $U_{d,x}$ is quite similar to $U_{d,y}$,

$$U_{d,x} = \text{S}(\ast) U_{d,y}. \quad (24)$$

In conclusion, the total number of two-qubit gates needed to double excitations is $24+2L (2(L+6+6))$ which greatly improves over the basic compilation requiring $48 + 16L$ two-qubit gates. More importantly, the JW complexity due to the parity operator is reduced by 87.5% for both single and double excitations.

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