Double excitation unitary circuit

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Here, we consider a quantum circuit that performs the following unitary:

$$\hat{U}^{pq}_{rs} = e^{t^{pq}_{rs}\hat{\tau}^{pq}_{rs}}$$
$$\hat{\tau}^{pq}_{rs} = \left(a_p^\dagger a_q^\dagger a_r a_s - a_s^\dagger a_r^\dagger a_q a_p\right)$$

For the ordering, we adopt our discussion to the convention of quantum computing $(a_p^\dagger a_q^\dagger a_r a_s)$, rather than quantum chemistry $(a_p^\dagger a_q^\dagger a_s a_r)$.

Using the Jordan-Wigner (JW) transform, we have

$$p^\dagger = \frac{1}{2}\left(X_p - iY_p\right)\bigotimes_{t=p+1}^{n} Z_t \tag{1}$$

$$p = \frac{1}{2}\left(X_p + iY_p\right)\bigotimes_{t=p+1}^{n} Z_t \tag{2}$$

and therefore

$$\hat{\tau}^{pq}_{rs} = \frac{1}{16}\left(X_p - iY_p\right)\left(\bigotimes_{t=p+1}^{n} Z_t\right)\otimes\left(X_q - iY_q\right)\left(\bigotimes_{u=q+1}^{n} Z_u\right)\otimes\left(X_r + iY_r\right)\left(\bigotimes_{v=r+1}^{n} Z_v\right)\otimes\left(X_s + iY_s\right)\left(\bigotimes_{w=s+1}^{n} Z_w\right) - h.c. \tag{3}$$

In the standard UCCSD, we always assume the ordering of qubits as $p > q > r > s$. Then, the above equation can be decomposed as

$$\begin{aligned}
\hat{\tau}^{pq}_{rs} =& \frac{1}{16}\left(X_p - iY_p\right)\left(\bigotimes_{t=p+1}^{n} Z_t\right)\\
&\otimes\left(X_q - iY_q\right)\left(\bigotimes_{u=q+1}^{p-1} Z_u\right) Z_p \left(\bigotimes_{u'=p+1}^{n} Z_{u'}\right)\\
&\otimes\left(X_r + iY_r\right)\left(\bigotimes_{v=r+1}^{q-1} Z_v\right) Z_q \left(\bigotimes_{v'=q+1}^{p-1} Z_{v'}\right) Z_p \left(\bigotimes_{v''=p+1}^{n} Z_{v''}\right)\\
&\otimes\left(X_s + iY_s\right)\left(\bigotimes_{w=s+1}^{r-1} Z_w\right) Z_r \left(\bigotimes_{w'=r+1}^{q-1} Z_{w'}\right) Z_q \left(\bigotimes_{w''=q+1}^{p-1} Z_{w''}\right) Z_p \left(\bigotimes_{w'''=p+1}^{n} Z_{w'''}\right) - h.c.
\end{aligned} \tag{4}$$

Since $Z_p^2 = I$, performing the tensor products $\bigotimes_{t=p+1}^{n} Z_t$ and $\bigotimes_{v=r+1}^{q-1} Z_v$ for even times becomes the identity operation, while $\bigotimes_{u=q+1}^{p-1} Z_u$ and $\bigotimes_{w=s+1}^{r-1} Z_w$ survive. Therefore,

$$
\begin{aligned}
\hat{\tau}_{rs}^{pq} =& \frac{1}{16}\left(X_p - iY_p\right) \\
&\otimes \left(X_q - iY_q\right)\left(\bigotimes_{u=q+1}^{p-1} Z_u\right) Z_p \\
&\otimes \left(X_r + iY_r\right) Z_q \left(\bigotimes_{v'=q+1}^{p-1} Z_{v'}\right) Z_p \\
&\otimes \left(X_s + iY_s\right)\left(\bigotimes_{w=s+1}^{r-1} Z_w\right) Z_r Z_q \left(\bigotimes_{w''=q+1}^{p-1} Z_{w''}\right) Z_p - h.c. \\
=& \frac{1}{16}\left(\bigotimes_{w=s+1}^{r-1} Z_w\right)\left(\bigotimes_{w''=q+1}^{p-1} Z_{w''}\right)\left(X_p - iY_p\right)\underbrace{Z_p Z_p Z_p}_{Z_p} \otimes \left(X_q - iY_q\right)\underbrace{Z_q Z_q}_{I_q} \otimes \left(X_r + iY_r\right) Z_r \otimes \left(X_s + iY_s\right) - h.c.
\end{aligned}
\tag{5}
$$

Furthermore, since

$$(X_p - iY_p)Z_p = +(X_p - iY_p) \tag{6a}$$
$$(X_p + iY_p)Z_p = -(X_p + iY_p) \tag{6b}$$
$$Z_p(X_p - iY_p) = -(X_p - iY_p) \tag{6c}$$
$$Z_p(X_p + iY_p) = +(X_p + iY_p) \tag{6d}$$

we obtain

$$
\begin{aligned}
\hat{\tau}_{rs}^{pq} =& -\frac{1}{16}\left(\bigotimes_{w=s+1}^{r-1} Z_w\right)\left(\bigotimes_{w''=q+1}^{p-1} Z_{w''}\right) \otimes \left(X_p - iY_p\right) \otimes \left(X_q - iY_q\right) \otimes \left(X_r + iY_r\right) \otimes \left(X_s + iY_s\right) - h.c. \\
=& \frac{1}{16}\left(\bigotimes_{w=s+1}^{r-1} Z_w\right)\left(\bigotimes_{w''=q+1}^{p-1} Z_{w''}\right) \otimes \Big(- X_pX_qX_rX_s + X_rX_sY_pY_q - Y_pX_qY_rX_s - X_pY_qY_rX_s \\
& - Y_pX_qX_rY_s - X_pY_qX_rY_s + X_pX_qY_rY_s - Y_pY_qY_rY_s + iY_pX_qX_rX_s + iX_pY_qX_rX_s + iY_pY_qX_rY_s \\
& + iY_pY_qY_rX_s - iX_pX_qX_rY_s - iX_pX_qY_rX_s - iY_pX_qY_rY_s - iX_pY_qY_rY_s\Big) - h.c.
\end{aligned}
\tag{7}
$$

Because of $h.c.$, the real terms will cancel out, and we finally have (setting $w \to t,\ w'' \to u$)

$$\hat{\tau}_{rs}^{pq} = \frac{i}{8}\left(\bigotimes_{t=s+1}^{r-1} Z_t\right)\left(\bigotimes_{u=q+1}^{p-1} Z_u\right)\Big(+ Y_pX_qX_rX_s + X_pY_qX_rX_s + Y_pY_qX_rY_s + Y_pY_qY_rX_s \tag{8}$$

$$- X_pX_qX_rY_s - X_pX_qY_rX_s - Y_pX_qY_rY_s - X_pY_qY_rY_s\Big) \tag{9}$$

A. $p > r > q > s$

We can investigate the different ordering cases. Here, we assume $p > r > q > s$. Using the anti-commutation relation of the fermion operators,

$$p^\dagger q^\dagger r s = -p^\dagger r q^\dagger s \tag{10}$$

for $q \neq r$. Then,

$$
\begin{aligned}
\hat{\tau}^{pq}_{rs} &= a_p^\dagger a_q^\dagger a_r a_s - h.c. \\
&= \frac{1}{16}\left(X_p - iY_p\right)\left(\bigotimes_{t=p+1}^{n} Z_t\right) \\
&\otimes \left(X_q - iY_q\right)\left(\bigotimes_{u=q+1}^{r-1} Z_u\right) Z_r \left(\bigotimes_{u'=r+1}^{p-1} Z_{u'}\right) Z_p \left(\bigotimes_{u''=p+1}^{n} Z_{u''}\right) \\
&\otimes \left(X_r + iY_r\right)\left(\bigotimes_{v'=r+1}^{p-1} Z_{v'}\right) Z_p \left(\bigotimes_{v''=p+1}^{n} Z_{v''}\right) \\
&\otimes \left(X_s + iY_s\right)\left(\bigotimes_{w=s+1}^{q-1} Z_w\right) Z_q \left(\bigotimes_{w'=q+1}^{r-1} Z_{w'}\right) Z_r \left(\bigotimes_{w''=r+1}^{p-1} Z_{w''}\right) Z_p \left(\bigotimes_{w'''=p+1}^{n} Z_{w'''}\right) - h.c. \\
&= \frac{1}{16}\left(X_p - iY_p\right) Z_p \otimes \left(X_q - iY_q\right) Z_q \otimes Z_r \left(X_r + iY_r\right) Z_r \otimes \left(X_s + iY_s\right) \otimes \left(\bigotimes_{w=s+1}^{q-1} Z_w\right)\left(\bigotimes_{w''=r+1}^{p-1} Z_{w''}\right) - h.c. \\
&= -\frac{1}{16}\left(\bigotimes_{w=s+1}^{q-1} Z_w\right)\left(\bigotimes_{w''=r+1}^{p-1} Z_{w''}\right) \otimes \left(X_p - iY_p\right) \otimes \left(X_q - iY_q\right) \otimes \left(X_r + iY_r\right) \otimes \left(X_s + iY_s\right) - h.c. \qquad (11)
\end{aligned}
$$

This is exactly the same as Eq. (7) except that w and w'' run over $s+1 \sim q-1$ and $r+1 \sim p-1$, respectively (in Eq. (7), $w = s+1 \sim r-1$ and $w = q+1 \sim p-1$). Hence, for this ordering $p > r > q > s$,

$$
\begin{aligned}
\hat{\tau}^{pq}_{rs} = \frac{i}{8}\left(\bigotimes_{t=s+1}^{q-1} Z_t\right)\left(\bigotimes_{u=r+1}^{p-1} Z_u\right)\Big(&+ Y_pX_qX_rX_s + X_pY_qX_rX_s + Y_pY_qX_rY_s + Y_pY_qY_rX_s \qquad (12) \\
&- X_pX_qX_rY_s - X_pX_qY_rX_s - Y_pX_qY_rY_s - X_pY_qY_rY_s\Big) \qquad (13)
\end{aligned}
$$

One might work out with other cases, but one can show that the general rule is that the CNOT ladders (the Z-tensors) occur between the largest two qubits, and between the smallest two qubits.

To see this, let us re-label and sort p, q, r, s in ascending order as $i_1 < i_2 < i_3 < i_4$. Suppose the JW transformation is performed to these fermion operators. As described above, each fermion operator generates, whether creation or annihilation operators:

$$
\begin{aligned}
i_1 &\to \sigma_{i_1} Z_{i_2} Z_{i_3} Z_{i_4}\left(\bigotimes_{j_1=i_1+1}^{i_2-1} Z_{j_1}\right)\left(\bigotimes_{j_2=i_2+1}^{i_3-1} Z_{j_2}\right)\left(\bigotimes_{j_3=i_3+1}^{i_4-1} Z_{j_3}\right)\left(\bigotimes_{j_4=i_4+1}^{n} Z_{j_4}\right) \qquad (14) \\
i_2 &\to \sigma_{i_2} Z_{i_3} Z_{i_4}\left(\bigotimes_{j_2=i_2+1}^{i_3-1} Z_{j_2}\right)\left(\bigotimes_{j_3=i_3+1}^{i_4-1} Z_{j_3}\right)\left(\bigotimes_{j_4=i_4+1}^{n} Z_{j_4}\right) \qquad (15) \\
i_3 &\to \sigma_{i_3} Z_{i_4}\left(\bigotimes_{j_3=i_3+1}^{i_4-1} Z_{j_3}\right)\left(\bigotimes_{j_4=i_4+1}^{n} Z_{j_4}\right) \qquad (16) \\
i_4 &\to \sigma_{i_4}\left(\bigotimes_{j_4=i_4+1}^{n} Z_{j_4}\right) \qquad (17) \\
& \qquad (18)
\end{aligned}
$$

For convenience, we have decomposed $\bigotimes_{j=i+1}^{n} Z_j$, which is separated by the used indices. Here, $\sigma = \sigma^+$ for a creation operator or σ^- for a annihilation operator, and they are defined as

$$\sigma^+ = \frac{1}{2}\left(X - iY\right) \qquad (19)$$

$$\sigma^- = \frac{1}{2}\left(X + iY\right) \qquad (20)$$

and, from Eqs. (21), they have the following properties:

$$\sigma^+ Z = \sigma^+ \tag{21a}$$
$$\sigma^- Z = -\sigma^- \tag{21b}$$
$$Z\sigma^+ = -\sigma^+ \tag{21c}$$
$$Z\sigma^- = \sigma^- \tag{21d}$$

Now, we consider the JW transform of the whole operator $p^\dagger q^\dagger rs$. First, notice that, there is no Z-tensor below the lowest index i_1, as the JW transformation gives the I-tensor for all fermion operators in $\hat{\tau}_{rs}^{pq}$. With *even* numbers $(2k)$ of fermion operators, there is neither the Z-tensor above the highest index i_4 because of the cancellation $Z^{2k} = I$ (however, this is not the case for the odd-number fermion operators, $Z^{2k+1} = Z$).

Among the nearest-neighbor qubit-pairs for i_4, i_3, i_2, i_1 (that is, the $i_4 - i_3$ pair, $i_3 - i_2$ pair, and $i_2 - i_1$ pair), it should be obvious that generally the Z-tensor between i_2 and i_3 cancels out (two arising from the JW transformation of i_1 and i_2). On the other hand, we always have $\bigotimes_{j=i_1+1}^{i_2-1} Z_j$ and $\bigotimes_{j=i_3+1}^{i_4-1} Z_j$ (appearing once and three times, respectively).

Now, what happens to $Z_{i_2}, Z_{i_3}, Z_{i_4}$? They are simply converted to the parity (sign) when combined with σ^+ and σ^- (Eqs. (21)). Because of the anti-symmetry of fermion operators, it suffices to test only the cases where $i_4^\dagger$ comes most left, and $p > q$ and $r > s$ for $p^\dagger q^\dagger rs$. Below, we omit the Z-tensors and only consider the sign change.

$$i_4^\dagger i_3^\dagger i_2 i_1 \to \sigma_4^+ \otimes (Z_4\sigma_3^+) \otimes (Z_4 Z_3 \sigma_2^-) \otimes (Z_4 Z_3 Z_2 \sigma_1^-) = \sigma_4^+ \otimes \sigma_3^+ \otimes (-\sigma_2^-) \otimes \sigma_1^-$$
$$i_4^\dagger i_2^\dagger i_3 i_1 \to \sigma_4^+ \otimes (Z_4 Z_3\sigma_2^+) \otimes (Z_4 \sigma_3^-) \otimes (Z_4 Z_3 Z_2 \sigma_1^-) = \sigma_4^+ \otimes (-\sigma_3^-) \otimes \sigma_2^- \otimes \sigma_1^-$$
$$i_4^\dagger i_1^\dagger i_3 i_2 \to \sigma_4^+ \otimes (Z_4 Z_3 Z_2\sigma_1^+) \otimes (Z_4 \sigma_3^-) \otimes (Z_4 Z_3 \sigma_2^-) = \sigma_4^+ \otimes (-\sigma_3^-) \otimes \sigma_2^- \otimes \sigma_1^+$$

Therefore, the sign is always negative, as long as $p > q$ and $r > s$. Other strings can be always generalized from this result: for example, $i_4^\dagger i_3^\dagger i_1 i_2$ is simply the negative of $i_4^\dagger i_3^\dagger i_2 i_1$ (because the anti-commutator $[i_1, i_2]_+ = 0$). Another example is $i_3^\dagger i_1^\dagger i_4 i_2$, but this is simply the Hermitian-conjugate of $i_2^\dagger i_4^\dagger i_1 i_3 = i_4^\dagger i_2^\dagger i_3 i_1$, which is already discussed above.

B. Excitations to the same orbitals

Assume $p > q > r > s$. We consider the Jordan-Wigner transformation of the following doubles:

1. τ_{ps}^{pq}
2. τ_{rs}^{pr}
3. τ_{rs}^{ps}

Other excitations are easily transformed using these results. We first note that the number operator for the orbital p is

$$a_p^\dagger a_p = \frac{1}{2}(I_p - Z_p) \tag{22}$$

1. τ_{ps}^{pq}

$$\begin{aligned}
\hat{\tau}_{ps}^{pq} &= \left(a_p^\dagger a_q^\dagger a_p a_s - h.c.\right) \\
&= -\left(a_p^\dagger a_p a_q^\dagger a_s - h.c.\right) \\
&= -\frac{1}{8}(I_p - Z_p) \otimes (X_q - iY_q)\left(\bigotimes_{t=q+1}^{p-1} Z_t\right) Z_p \otimes (X_s + iY_s)\left(\bigotimes_{u=s+1}^{q-1} Z_u\right) Z_q \left(\bigotimes_{v=q+1}^{p-1} Z_v\right) Z_p - h.c. \\
&= -\frac{1}{8}\left(\bigotimes_{u=s+1}^{q-1} Z_u\right) \otimes (I_p - Z_p) \otimes \underbrace{(X_q - iY_q)Z_q}_{(X_q - iY_q)} \otimes (X_s + iY_s) - h.c. \\
&= -\frac{1}{8}\left(\bigotimes_{u=s+1}^{q-1} Z_u\right) \otimes (X_qX_s - Z_pX_qX_s + Y_qY_s - Z_pY_qY_s - iY_qX_s + iZ_pY_qX_s + iX_qY_s - iZ_pX_qY_s) - h.c. \\
&= i\frac{1}{4}\left(\bigotimes_{u=s+1}^{q-1} Z_u\right) \otimes (Y_qX_s - Z_pY_qX_s - X_qY_s + Z_pX_qY_s) \qquad (23)
\end{aligned}$$

2. τ_{qs}^{pq}

$$\begin{aligned}
\tau_{qs}^{pq} &= \left(a_p^\dagger a_q^\dagger a_q a_s - h.c.\right) \\
&= \left(a_p^\dagger a_s a_q^\dagger a_q - h.c.\right) \\
&= \frac{1}{8}(X_p - iY_p) \otimes (X_s + iY_s)\left(\bigotimes_{t=s+1}^{q-1} Z_t\right) Z_q \left(\bigotimes_{u=q+1}^{p-1} Z_u\right) Z_p \otimes (I_q - Z_q) \\
&= \frac{1}{8}\left(\bigotimes_{t=s+1}^{q-1} Z_t\right)\left(\bigotimes_{u=q+1}^{p-1} Z_u\right) \underbrace{(X_p - iY_p)Z_p}_{(X_p - iY_p)} \otimes (X_s + iY_s) \otimes \underbrace{Z_q(I_q - Z_q)}_{(Z_q - I_q)} \\
&= \frac{1}{8}\left(\bigotimes_{t=s+1}^{q-1} Z_t\right)\left(\bigotimes_{u=q+1}^{p-1} Z_u\right) \otimes (X_pZ_qX_s - X_pX_s + Y_pZ_qY_s - Y_pY_s + iX_pZ_qY_s - iX_pY_s - iY_pZ_qX_s + iY_pX_s) - h.c. \\
&= i\frac{1}{4}\left(\bigotimes_{t=s+1}^{q-1} Z_t\right)\left(\bigotimes_{u=q+1}^{p-1} Z_u\right) \otimes (X_pZ_qY_s - Y_pZ_qX_s - X_pY_s + Y_pX_s) \qquad (24)
\end{aligned}$$

3. τ_{rs}^{ps}

$$
\begin{aligned}
\tau_{rs}^{ps} &= \left(a_p^\dagger a_s^\dagger a_r a_s - h.c.\right) \\
&= -\left(a_p^\dagger a_r a_s^\dagger a_s - h.c.\right) \\
&= -\frac{1}{8}(X_p - iY_p)\otimes(X_r + iY_r)\left(\bigotimes_{t=r+1}^{p-1} Z_t\right) Z_p \otimes (I_s - Z_s) - h.c. \\
&= -\frac{1}{8}\left(\bigotimes_{t=r+1}^{p-1} Z_t\right)\otimes \underbrace{(X_p - iY_p)Z_p}_{(X_p - iY_p)} \otimes (X_r + iY_r)\otimes(I_s - Z_s) - h.c. \\
&= -\frac{1}{8}\left(\bigotimes_{t=r+1}^{p-1} Z_t\right)\otimes\left(X_pX_r - X_pX_rZ_s + Y_pY_r - Y_pY_rZ_s - iY_pX_r + iY_pX_rZ_s + iX_pY_r - iX_pY_rZ_s\right) - h.c. \\
&= i\frac{1}{4}\left(\bigotimes_{t=r+1}^{p-1} Z_t\right)\otimes\left(X_pY_rZ_s - Y_pX_rZ_s - X_pY_r + Y_pX_r\right)
\end{aligned} \tag{25}
$$

I. SUMMARY (GENERALIZED)

We generalize our result. Given a randomly ordered two-electron fermion operator, one only needs to do the following:

1. Rearrange the operator to $p^\dagger q^\dagger rs$ with $p > q$ and $r > s$, and $\max(p,q,r,s) = p$ in terms of qubit. This may require to use the anti-commutation relation and may change the sign.

2. Check the identity among p, q, r, s.

   (a) If $q \neq r, s$:
   Sort p, q, r, s in ascending order and relabel them as $i_1 < i_2 < i_3 < i_4$. Note that, from the step 1, $p = i_4$ is automatically assigned). Then,

$$\hat{\tau}_{rs}^{pq} = \frac{i}{8}\left(\bigotimes_{t=i_1+1}^{i_2-1} Z_t\right)\left(\bigotimes_{u=i_3+1}^{i_4-1} Z_u\right)\Big(+ Y_pX_qX_rX_s + X_pY_qX_rX_s + Y_pY_qX_rY_s + Y_pY_qY_rX_s$$
$$- X_pX_qX_rY_s - X_pX_qY_rX_s - Y_pX_qY_rY_s - X_pY_qY_rY_s\Big) \tag{26}$$

   (b) If $p = r$: (Make sure $q \neq s$ because if $q = s$, $\hat{\tau}_{rs}^{pq} = 0$)

$$\hat{\tau}_{rs}^{pq} = i\frac{1}{4}\left(\bigotimes_{u=s+1}^{q-1} Z_u\right) \otimes (Y_qX_s - Z_pY_qX_s - X_qY_s + Z_pX_qY_s) \tag{27}$$

   (c) If $q = r$:

$$\hat{\tau}_{rs}^{pq} = i\frac{1}{4}\left(\bigotimes_{t=s+1}^{q-1} Z_t\right)\left(\bigotimes_{u=q+1}^{p-1} Z_u\right) \otimes (X_pZ_qY_s - Y_pZ_qX_s - X_pY_s + Y_pX_s) \tag{28}$$

   (d) If $q = s$:

$$\hat{\tau}_{rs}^{pq} = i\frac{1}{4}\left(\bigotimes_{t=r+1}^{p-1} Z_t\right) \otimes (X_pY_rZ_s - Y_pX_rZ_s - X_pY_r + Y_pX_r) \tag{29}$$

If t_{rs}^{pq} is a parameter to be optimized and thus **can absorb the sign**, *one can ignore the sign.* This means, for methods like CCGSD, one would simply skip the step 1 above and directly use Eq. (26) by assigning i_1, i_2, i_3, i_4.

A. Example 1: $\hat{\tau}_{30}^{74}$

1. Set the operator in descending order for the creation and annihilation blocks,
$$\hat{\tau}_{30}^{74} = a_7^\dagger a_4^\dagger a_3 a_0 - h.c. \tag{30}$$
That is, we have set $p = 7, q = 4, r = 3, s = 0$.
2. Since $p \neq r$ and $q \neq r, s$, we use equation (a). Let $i_1 = 0, i_2 = 3, i_3 = 4, i_4 = 7$.
3. A quantum circuit would be

$$\begin{aligned}
\hat{\tau}_{30}^{74} = & \frac{i}{8}\left(\bigotimes_{t=0+1}^{3-1} Z_t\right)\left(\bigotimes_{u=4+1}^{7-1} Z_u\right)\Big(+ Y_7X_4X_3X_0 + X_7Y_4X_3X_0 + Y_7Y_4X_3Y_0 + Y_7Y_4Y_3X_0 \\
& - X_7X_4X_3Y_0 - X_7X_4Y_3X_0 - Y_7X_4Y_3Y_0 - X_7Y_4Y_3Y_0\Big) \\
= & \frac{i}{8}\left(Z_1Z_2\right)\left(Z_5Z_6\right)\Big(+ Y_7X_4X_3X_0 + X_7Y_4X_3X_0 + Y_7Y_4X_3Y_0 + Y_7Y_4Y_3X_0 \\
& - X_7X_4X_3Y_0 - X_7X_4Y_3X_0 - Y_7X_4Y_3Y_0 - X_7Y_4Y_3Y_0\Big) \\
= & \frac{i}{8}\Big(X_0Z_1Z_2X_3X_4Z_5Z_6Y_7 + X_0Z_1Z_2X_3Y_4Z_5Z_6X_7 + Y_0Z_1Z_2X_3Y_4Z_5Z_6Y_7 + X_0Z_1Z_2Y_3Y_4Z_5Z_6Y_7 \\
& - Y_0Z_1Z_2X_3X_4Z_5Z_6X_7 - X_0Z_1Z_2Y_3X_4Z_5Z_6X_7 - Y_0Z_1Z_2Y_3X_4Z_5Z_6Y_7 - Y_0Z_1Z_2Y_3Y_4Z_5Z_6X_7\Big)
\end{aligned} \tag{31}$$

Comparing this result with OpenFermion, we confirm our derivation is correct.

```
p=7
q=4
r=3
s=0
Epqrs=FermionOperator(str(p)+"^ "+str(q) +"^ " + str(r) + " " +str(s) + " ")
jordan_wigner(Epqrs-hermitian_conjugated(Epqrs))

0.125j [X0 Z1 Z2 X3 X4 Z5 Z6 Y7] +
0.125j [X0 Z1 Z2 X3 Y4 Z5 Z6 X7] +
-0.125j [X0 Z1 Z2 Y3 X4 Z5 Z6 X7] +
0.125j [X0 Z1 Z2 Y3 Y4 Z5 Z6 Y7] +
-0.125j [Y0 Z1 Z2 X3 X4 Z5 Z6 X7] +
0.125j [Y0 Z1 Z2 X3 Y4 Z5 Z6 Y7] +
-0.125j [Y0 Z1 Z2 Y3 X4 Z5 Z6 Y7] +
-0.125j [Y0 Z1 Z2 Y3 Y4 Z5 Z6 X7]
```

B. Example 2: $\hat{\tau}_{60}^{84}$

1. Set $p=8, q=4, r=6, s=0$.
2. Since $p \neq r$ and $r \neq r, s$, we use equation (a). Let $i_1=0, i_2=4, i_3=6, i_4=8$.
3. A quantum circuit would be

$$\hat{\tau}_{60}^{84} = \frac{i}{8}\left(\bigotimes_{t=1}^{3} Z_t\right)\left(\bigotimes_{u=7}^{7} Z_u\right)\Big(+ Y_8X_4X_6X_0 + X_8Y_4X_6X_0 + Y_8Y_4X_6Y_0 + Y_8Y_4Y_6X_0 \tag{32}$$

$$- X_8X_4X_6Y_0 - X_8X_4Y_6X_0 - Y_8X_4Y_6Y_0 - X_8Y_4Y_6Y_0\Big)$$

$$= \frac{i}{8}\Big(X_0Z_1Z_2Z_3X_4X_6Z_7Y_8 + X_0Z_1Z_2Z_3Y_4X_6Z_7X_8 + Y_0Z_1Z_2Z_3Y_4X_6Z_7Y_8 + X_0Z_1Z_2Z_3Y_4Y_6Z_7Y_8$$

$$- Y_0Z_1Z_2Z_3X_4X_6Z_7X_8 - X_0Z_1Z_2Z_3X_4Y_6Z_7X_8 - Y_0Z_1Z_2Z_3X_4Y_6Z_7Y_8 - Y_0Z_1Z_2Z_3Y_4Y_6Z_7X_8\Big) \tag{33}$$

Comparing this result with OpenFermion, we confirm our derivation is correct.

```
p=8
q=4
r=6
s=0
Epqrs=FermionOperator(str(p)+"^ "+str(q) +"^ " + str(r) + " " +str(s) + " ")
jordan_wigner(Epqrs-hermitian_conjugated(Epqrs))

0.125j [X0 Z1 Z2 Z3 X4 X6 Z7 Y8] +
-0.125j [X0 Z1 Z2 Z3 X4 Y6 Z7 X8] +
0.125j [X0 Z1 Z2 Z3 Y4 X6 Z7 X8] +
0.125j [X0 Z1 Z2 Z3 Y4 Y6 Z7 Y8] +
-0.125j [Y0 Z1 Z2 Z3 X4 X6 Z7 X8] +
-0.125j [Y0 Z1 Z2 Z3 X4 Y6 Z7 Y8] +
0.125j [Y0 Z1 Z2 Z3 Y4 X6 Z7 Y8] +
-0.125j [Y0 Z1 Z2 Z3 Y4 Y6 Z7 X8]
```

C. Example 3. $\hat{\tau}_{06}^{62}$

1. Set the operator in descending order for the creation and annihilation blocks,

$$\hat{\tau}_{06}^{62} = \left(a_6^\dagger a_2^\dagger a_0 a_6 - h.c.\right) = -\left(a_6^\dagger a_2^\dagger a_6 a_0 - h.c.\right) = -\hat{\tau}_{60}^{62} \tag{34}$$

2. Set $p = 6, q = 2, r = 6, s = 0$.
3. Since $p = r$, use equation (b),

$$\begin{aligned}
\hat{\tau}_{06}^{62} = -\hat{\tau}_{60}^{62} &= -i\frac{1}{4}\left(\bigotimes_{u=0+1}^{2-1} Z_u\right) \otimes \left(Y_2X_0 - Z_6Y_2X_0 - X_2Y_0 + Z_6X_2Y_0\right) \\
&= -i\frac{1}{4}\left(Z_1\right) \otimes \left(Y_2X_0 - Z_6Y_2X_0 - X_2Y_0 + Z_6X_2Y_0\right) \\
&= -i\frac{1}{4}\left(X_0Z_1Y_2 - X_0Z_1Y_2Z_6 - Y_0Z_1X_2 + Y_0Z_1X_2Z_6\right)
\end{aligned} \tag{35}$$

This agrees with the result from OpenFermion.

```
p=6
q=2
r=0
s=6
Epqrs=FermionOperator(str(p)+"^ "+str(q) +"^ " + str(r) + " " +str(s) + " ")
jordan_wigner(Epqrs-hermitian_conjugated(Epqrs))

-0.25j [X0 Z1 Y2] +
0.25j [X0 Z1 Y2 Z6] +
0.25j [Y0 Z1 X2] +
-0.25j [Y0 Z1 X2 Z6]
```

D. Example 4. $\hat{\tau}_{20}^{62}$

1. Set $p = 6, q = 2, r = 2, s = 0$.
2. Since $q = r$, use equation (c),

$$\begin{aligned}
\hat{\tau}_{20}^{62} &= i\frac{1}{4}\left(\bigotimes_{t=0+1}^{2-1} Z_t\right)\left(\bigotimes_{u=2+1}^{6-1} Z_u\right)\otimes\left(X_6Z_2Y_0 - Y_6Z_2X_0 - X_6Y_0 + Y_6X_0\right) \\
&= i\frac{1}{4}\left(Z_1\right)\otimes\left(Z_3Z_4Z_5\right)\otimes\left(X_6Z_2Y_0 - Y_6X_2X_0 - X_6Y_0 + Y_6X_0\right) \\
&= i\frac{1}{4}\left(Y_0Z_1Z_2Z_3Z_4Z_5X_6 - X_0Z_1X_2Z_3Z_4Z_5Y_6 - Y_0Z_1Z_3Z_4Z_5X_6 + X_0Z_1Z_3Z_4Z_5Y_6\right)
\end{aligned} \tag{36}$$

This agrees with the result from OpenFermion.

```
p=6
q=2
r=2
s=0
Epqrs=FermionOperator(str(p)+"^ "+str(q) +"^ " + str(r) + " " +str(s) + " ")
jordan_wigner(Epqrs-hermitian_conjugated(Epqrs))

-0.25j [X0 Z1 Z2 Z3 Z4 Z5 Y6] +
0.25j [X0 Z1 Z3 Z4 Z5 Y6] +
0.25j [Y0 Z1 Z2 Z3 Z4 Z5 X6] +
-0.25j [Y0 Z1 Z3 Z4 Z5 X6]
```

E. Example 5: $\hat{\tau}_{53}^{73}$

1. Set $p = 7, q = 3, r = 5, s = 3$.
2. Since $q = s$, use equation (d),

$$\begin{aligned}
\hat{\tau}_{53}^{73} &= i\frac{1}{4}\left(\bigotimes_{t=5+1}^{7-1} Z_t\right) \otimes (X_7Y_5Z_3 - Y_7X_5Z_3 - X_7Y_5 + Y_7X_5) \\
&= i\frac{1}{4}(Z_6) \otimes (X_7Y_5Z_3 - Y_7X_5Z_3 - X_7Y_5 + Y_7X_5) \\
&= i\frac{}{4}(Z_3Y_5Z_6X_7 - Z_3X_5Z_6Y_7 - Y_5Z_6X_7 + X_5Z_6Y_7)
\end{aligned} \tag{37}$$

Again, this agrees with OpenFermion,

```
p=7
q=3
r=5
s=3
Epqrs=FermionOperator(str(p)+"^ "+str(q) +"^ " + str(r) + " " +str(s) + " ")
jordan_wigner(Epqrs-hermitian_conjugated(Epqrs))

-0.25j [Z3 X5 Z6 Y7] +
0.25j [Z3 Y5 Z6 X7] +
0.25j [X5 Z6 Y7] +
-0.25j [Y5 Z6 X7]
```