CIS state preparation on quantum circuit

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0.1 Pauli rotation

$$R_x(\theta) = e^{-i\theta X/2} = \begin{bmatrix} \cos(\theta/2) & -i\sin(\theta/2) \\ -i\sin(\theta/2) & \cos(\theta/2) \end{bmatrix} \tag{1}$$

$$R_y(\theta) = e^{-i\theta Y/2} = \begin{bmatrix} \cos(\theta/2) & -\sin(\theta/2) \\ \sin(\theta/2) & \cos(\theta/2) \end{bmatrix} \tag{2}$$

$$R_z(\theta) = e^{-i\theta Z/2} = \begin{bmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{bmatrix} \tag{3}$$

1 CIS and circuit

1.1 Single-reference CI wave functions

The FCI wave function is often dominated by a single reference configuration, usually the Hartree-Fock state. It is then convenient to think of the FCI wave function as generated from this reference configuration by the application of a linear combination of spin-orbital excitation operators

$$|\mathrm{FCI}\rangle = \left(1 + \sum_{AI} \hat{X}_I^A + \sum_{A>B, I>J} \hat{X}_{IJ}^{AB}\right) |\mathrm{HF}\rangle \tag{4}$$

where, for example,

$$\hat{X}_I^A |\mathrm{HF}\rangle = C_I^A a_A^\dagger a_I |\mathrm{HF}\rangle \tag{5}$$

$$\hat{X}_{IJ}^{AB} |\mathrm{HF}\rangle = C_{IJ}^{AB} a_A^\dagger a_B^\dagger a_I a_J |\mathrm{HF}\rangle \tag{6}$$

Thus, we may characterize the determinants in the FCI expansion as single (S), double (D), triple (T), quadruple (Q), and higher excitation relative to the Hartree-Fock state.

1.2 CIS

$$|\mathrm{FCI}\rangle = \left(1 + \sum_{AI} \hat{X}_I^A\right)|\mathrm{HF}\rangle = \left(1 + \sum_{AI} C_I^A a_A^\dagger a_I\right)|\mathrm{HF}\rangle \tag{7}$$

1.3 Exact state preparation of CIS on quantum circuit

Applying $R_y(\theta) = e^{i(\theta/2)Y}$ on $|0\rangle$ gives

$$R_y(\theta)|0\rangle = \cos(\theta/2)|0\rangle + \sin(\theta/2)|1\rangle \tag{8}$$

1.3.1 Control-F_y gates

We first define two types of control rotation gates, which we call CF_y^X and CF_y^Z,

$$CF_y^X(\theta) = (1 \otimes R_y(\theta))\mathrm{CNOT}(1 \otimes R_y(-\theta)) = \begin{bmatrix} 1 & 0 \\ 0 & R_y(\theta)XR_y(-\theta) \end{bmatrix}, \tag{9}$$

where

$$R_y(\theta)XR_y(-\theta) = \begin{bmatrix} \cos(\theta/2) & -\sin(\theta/2) \\ \sin(\theta/2) & \cos(-\theta/2) \end{bmatrix} \begin{bmatrix} \sin(-\theta/2) & \cos(-\theta/2) \\ \cos(-\theta/2) & -\sin(-\theta/2) \end{bmatrix} \tag{10}$$

$$= \begin{bmatrix} -2\sin(\theta/2)\cos(\theta/2) & \cos^2(\theta/2) - \sin^2(\theta/2) \\ -\sin^2(\theta/2) + \cos^2(\theta/2) & 2\sin(\theta/2)\cos(\theta/2) \end{bmatrix} \tag{11}$$

$$= \begin{bmatrix} -\sin(\theta) & \cos(\theta) \\ \cos(\theta) & \sin(\theta) \end{bmatrix} \tag{12}$$

while

$$CF_y^Z(\theta) = (1 \otimes R_y(\theta))\mathrm{CZ}(1 \otimes R_y(-\theta)) = \begin{bmatrix} 1 & 0 \\ 0 & R_y(\theta)ZR_y(-\theta) \end{bmatrix}, \tag{13}$$

where

$$R_y(\theta)ZR_y(-\theta) = \begin{bmatrix} \cos(\theta/2) & -\sin(\theta/2) \\ \sin(\theta/2) & \cos(\theta/2) \end{bmatrix} \begin{bmatrix} \cos(-\theta/2) & -\sin(-\theta/2) \\ -\sin(-\theta/2) & -\cos(-\theta/2) \end{bmatrix} \tag{14}$$

$$= \begin{bmatrix} \cos^2(\theta/2) - \sin^2(\theta/2) & 2\sin(\theta/2)\cos(\theta/2) \\ 2\sin(\theta/2)\cos(\theta/2) & \sin^2(\theta/2) - \cos^2(\theta/2) \end{bmatrix} \tag{15}$$

$$= \begin{bmatrix} \cos(\theta) & \sin(\theta) \\ \sin(\theta) & -\cos(\theta) \end{bmatrix} \tag{16}$$

Note also that

$$F_y^Z(\theta)|0\rangle = \cos(\theta)|0\rangle + \sin(\theta)|1\rangle \tag{17}$$

$$F_y^X(\theta)|1\rangle = \cos(\theta)|0\rangle + \sin(\theta)|1\rangle \tag{18}$$

We also make use of $C^n(F_y^X)$ gate, which make use of $n-1$ ancilla qubits and $2(n-1)$ Toffoli gates.

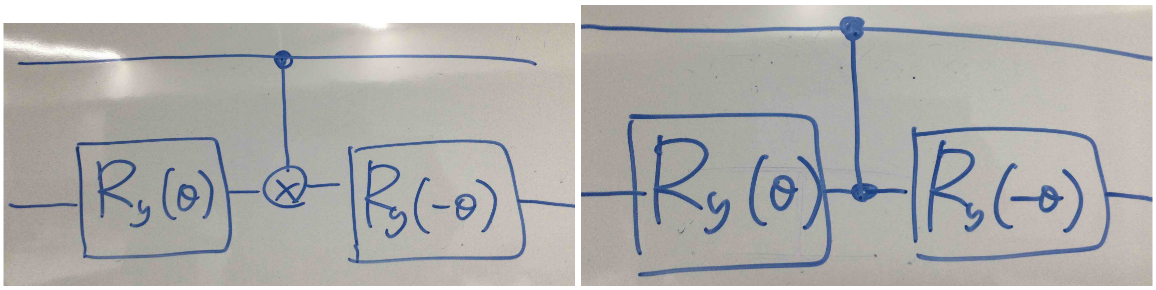

Figure 1: Diagram of CF_y^X gate (left) and CF_y^Z gate (right)

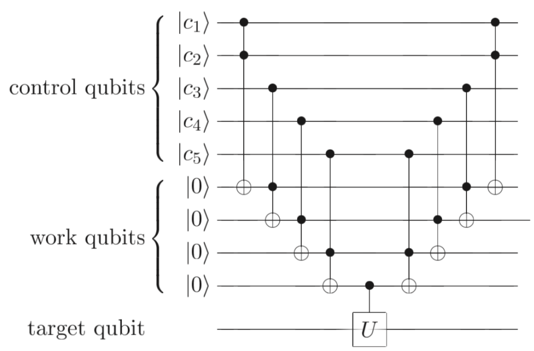

Figure 4.10. Network implementing the $C^n(U)$ operation, for the case $n = 5$.

Figure 2: Implementation of $C^n(U)$ gate

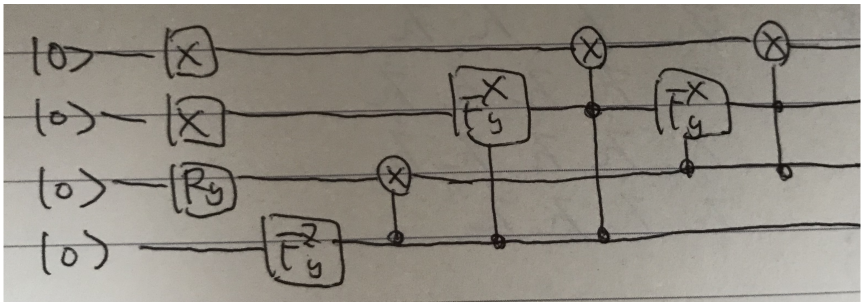

Figure 3: Implementation of circuit which generate CIS state for $(2e, 2o)$

1.3.2 Example of 4 spin-orbitals 2 electron state

Consider the case where the number of spin-orbitals $n = 4$ and the number of electrons $m = 2$. Applying the circuit shown in Fig on $|0\rangle^{\otimes 4}$ gives

$$
\begin{aligned}
&|0\rangle^{\otimes 4} \xrightarrow{R_y(2\theta_0)X_0X_0} \cos(\theta_0)\,|0011\rangle + \sin(\theta_0)\,|0111\rangle \\
&\xrightarrow{CF_y^Z(\theta_1)} \cos(\theta_0)\,|0011\rangle + \sin(\theta_0)\,(\cos(\theta_1)\,|0111\rangle + \sin(\theta_1)\,|1111\rangle) \\
&\xrightarrow{\mathrm{CNOT}_{32}} \cos(\theta_0)\,|0011\rangle + \sin(\theta_0)\,(\cos(\theta_1)\,|0111\rangle + \sin(\theta_1)\,|1011\rangle) \\
&\xrightarrow{CF_y^X(\theta_2)_{31}} \cos(\theta_0)\,|0011\rangle + \sin(\theta_0)\cos(\theta_1)\,|0111\rangle + \sin(\theta_0)\sin(\theta_1)(\cos(\theta_2)\,|1001\rangle + \sin(\theta_2)\,|1011\rangle) \\
&\xrightarrow{\mathrm{Toffoli}_{310}} \cos(\theta_0)\,|0011\rangle + \sin(\theta_0)\cos(\theta_1)\,|0111\rangle + \sin(\theta_0)\sin(\theta_1)(\cos(\theta_2)\,|1001\rangle + \sin(\theta_2)\,|1010\rangle) \\
&\xrightarrow{CF_y^X(\theta_3)_{21}} \cos(\theta_0)\,|0011\rangle + \sin(\theta_0)\cos(\theta_1)(\cos(\theta_3)\,|0101\rangle + \sin(\theta_3)\,|0111\rangle) + \sin(\theta_0)\sin(\theta_1)(\cos(\theta_2)\,|1001\rangle \\
&\xrightarrow{\mathrm{Toffoli}_{210}} \cos(\theta_0)\,|0011\rangle + \sin(\theta_0)\cos(\theta_1)(\cos(\theta_3)\,|0101\rangle + \sin(\theta_3)\,|0110\rangle) \\
&+ \sin(\theta_0)\sin(\theta_1)(\cos(\theta_2)\,|1001\rangle + \sin(\theta_2)\,|1010\rangle)
\end{aligned}
$$

$$
|\mathrm{CIS}\rangle = \alpha_0\,|0011\rangle + \alpha_1\,|1001\rangle + \alpha_2\,|1010\rangle + \alpha_3\,|0101\rangle + \alpha_4\,|0110\rangle \tag{19}
$$

where

$$
\begin{aligned}
\alpha_0 &= \cos(\theta_0) \\
\alpha_1 &= \sin(\theta_0)\sin(\theta_1)\cos(\theta_2) \\
\alpha_2 &= \sin(\theta_0)\sin(\theta_1)\sin(\theta_2) \\
\alpha_3 &= \sin(\theta_0)\cos(\theta_1)\cos(\theta_3) \\
\alpha_4 &= \sin(\theta_0)\cos(\theta_1)\sin(\theta_3)
\end{aligned}
$$

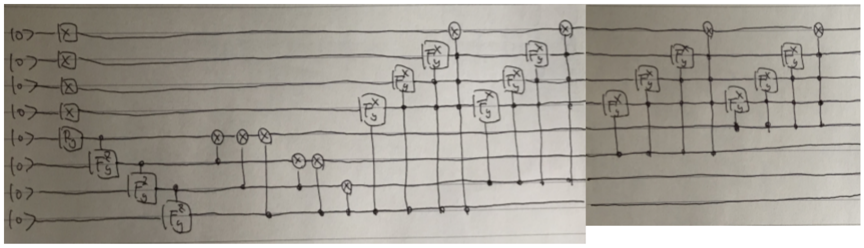

Figure 4: Implementation of circuit which generate CIS state for $(4e, 4o)$

1.3.3 Example of 8 spin-orbitals 4 electron state

Consider the case where the number of spin-orbitals $n = 8$ and the number of electrons $m = 4$. Applying the circuit shown in Fig on $|0\rangle^{\otimes 8}$ gives CIS state for such electron state.

The circuit can be divided into six parts:

$$
\begin{aligned}
|0\rangle^{\otimes 8} &\xrightarrow{R_{y_4}(2\theta_0)X_3X_2X_1X_0} c_0\,|00001111\rangle + s_0\,|00011111\rangle \\
&\xrightarrow{CF_y^Z(\theta_1)} c_0\,|00001111\rangle + s_0(c_1\,|00011111\rangle + s_1\,|00111111\rangle) \\
&\xrightarrow{CF_y^Z(\theta_2)} c_0\,|00001111\rangle + s_0c_1\,|00011111\rangle + s_0s_1(c_2\,|00111111\rangle + s_2\,|01111111\rangle) \\
&\xrightarrow{CF_y^Z(\theta_3)} c_0\,|00001111\rangle + s_0c_1\,|00011111\rangle + s_0s_1c_2\,|00111111\rangle + s_0s_1s_2(c_3\,|01111111\rangle + s_3\,|11111111\rangle) \\
&= |\psi_1\rangle
\end{aligned}
$$

$$
\begin{aligned}
|\psi_1\rangle &\xrightarrow{\mathrm{CNOT}_{74}\mathrm{CNOT}_{64}\mathrm{CNOT}_{54}} c_0\,|00001111\rangle + s_0c_1\,|00011111\rangle + s_0s_1c_2\,|00101111\rangle \\
&\qquad + s_0s_1s_2(c_3\,|01101111\rangle + s_3\,|11101111\rangle) \\
&\xrightarrow{\mathrm{CNOT}_{65}\mathrm{CNOT}_{75}} c_0\,|00001111\rangle + s_0c_1\,|00011111\rangle + s_0s_1c_2\,|00101111\rangle \\
&\qquad + s_0s_1s_2(c_3\,|01001111\rangle + s_3\,|11001111\rangle) \\
&\xrightarrow{\mathrm{CNOT}_{76}} c_0\,|00001111\rangle + s_0c_1\,|00011111\rangle + s_0s_1c_2\,|00101111\rangle + s_0s_1s_2(c_3\,|01001111\rangle + s_3\,|10001111\rangle) \\
&= |\psi_2\rangle
\end{aligned}
$$

$$
\begin{aligned}
|\psi_2\rangle \xrightarrow{CF_y^X(\theta_4)} & c_0\,|00001111\rangle + s_0c_1\,|00011111\rangle + s_0s_1c_2\,|00101111\rangle + s_0s_1s_2c_3\,|01001111\rangle \\
& + s_0s_1s_2s_3(c_4\,|10000111\rangle + s_4\,|10001111\rangle) \\
\xrightarrow{C^2F_y^X(\theta_5)} & c_0\,|00001111\rangle + s_0c_1\,|00011111\rangle + s_0s_1c_2\,|00101111\rangle + s_0s_1s_2c_3\,|01001111\rangle \\
& + s_0s_1s_2s_3c_4\,|10000111\rangle + s_0s_1s_2s_3s_4(c_5\,|10001011\rangle + s_5\,|10001111\rangle) \\
\xrightarrow{C^3F_y^X(\theta_6)} & c_0\,|00001111\rangle + s_0c_1\,|00011111\rangle + s_0s_1c_2\,|00101111\rangle + s_0s_1s_2c_3\,|01001111\rangle \\
& + s_0s_1s_2s_3c_4\,|10000111\rangle + s_0s_1s_2s_3s_4c_5\,|10001011\rangle \\
& + s_0s_1s_2s_3s_4s_5(c_6\,|10001101\rangle + s_6\,|10001111\rangle) \\
\xrightarrow{\text{Toffoli}_{73210}} & c_0\,|00001111\rangle + s_0c_1\,|00011111\rangle + s_0s_1c_2\,|00101111\rangle + s_0s_1s_1c_3\,|01001111\rangle \\
& + s_0s_1s_2s_3c_4\,|10000111\rangle + s_0s_1s_2s_3s_4c_5\,|10001011\rangle \\
& + s_0s_1s_2s_3s_4s_5(c_6\,|10001101\rangle + s_6\,|10001110\rangle) \\
= |\psi_3\rangle &
\end{aligned}
$$

$$
\begin{aligned}
|\psi_3\rangle \xrightarrow{CF_y^X(\theta_7)} & c_0\,|00001111\rangle + s_0c_1\,|00011111\rangle + s_0s_1c_2\,|00101111\rangle + s_0s_1s_2c_3(c_7\,|01000111\rangle + s_7\,|01001111\rangle) \\
& + s_0s_1s_2s_3c_4\,|10000111\rangle + s_0s_1s_2s_3s_4c_5\,|10001011\rangle \\
& + s_0s_1s_2s_3s_4s_5(c_6\,|10001101\rangle + s_6\,|10001110\rangle) \\
\xrightarrow{C^2F_y^X(\theta_8)} & c_0\,|00001111\rangle + s_0c_1\,|00011111\rangle + s_0s_1c_2\,|00101111\rangle + s_0s_1s_2c_3c_7\,|01000111\rangle \\
& + s_0s_1s_2c_3s_7(c_8\,|01001011\rangle + s_8\,|01001111\rangle) + s_0s_1s_2s_3c_4\,|10000111\rangle \\
& + s_0s_1s_2s_3s_4c_5\,|10001011\rangle + s_0s_1s_2s_3s_4s_5(c_6\,|10001101\rangle + s_6\,|10001110\rangle) \\
\xrightarrow{C^3F_y^X(\theta_9)} & c_0\,|00001111\rangle + s_0c_1\,|00011111\rangle + s_0s_1c_2\,|00101111\rangle + s_0s_1s_2c_3c_7\,|01000111\rangle \\
& + s_0s_1s_2c_3s_7c_8\,|01001011\rangle + s_0s_1s_2c_3s_7s_8(c_9\,|01001101\rangle + s_9\,|01001111\rangle) \\
& + s_0s_1s_2s_3c_4\,|10000111\rangle + s_0s_1s_2s_3s_4c_5\,|10001011\rangle \\
& + s_0s_1s_2s_3s_4s_5(c_6\,|10001101\rangle + s_6\,|10001110\rangle) \\
\xrightarrow{\text{Toffoli}_{63210}} & c_0\,|00001111\rangle + s_0c_1\,|00011111\rangle + s_0s_1c_2\,|00101111\rangle + s_0s_1s_2c_3c_7\,|01000111\rangle \\
& + s_0s_1s_2c_3s_7c_8\,|01001011\rangle + s_0s_1s_2c_3s_7s_8(c_9\,|01001101\rangle + s_9\,|01001110\rangle) \\
& + s_0s_1s_2s_3c_4\,|10000111\rangle + s_0s_1s_2s_3s_4c_5\,|10001011\rangle \\
& + s_0s_1s_2s_3s_4s_5(c_6\,|10001101\rangle + s_6\,|10001110\rangle) \\
= |\psi_4\rangle &
\end{aligned}
$$

$$
\begin{aligned}
|\psi_4\rangle \xrightarrow{CF_y^X(\theta_{10})}\ & c_0\,|00001111\rangle + s_0c_1\,|00011111\rangle + s_0s_1c_2(c_{10}\,|00100111\rangle + s_{10}\,|00101111\rangle) \\
&+ s_0s_1s_2c_3c_7\,|01000111\rangle + s_0s_1s_2c_3s_7c_8\,|01001011\rangle \\
&+ s_0s_1s_2c_3s_7s_8(c_9\,|01001101\rangle + s_9\,|01001110\rangle) \\
&+ s_0s_1s_2s_3c_4\,|10000111\rangle + s_0s_1s_2s_3s_4c_5\,|10001011\rangle \\
&+ s_0s_1s_2s_3s_4s_5(c_6\,|10001101\rangle + s_6\,|10001110\rangle) \\
\xrightarrow{C^2F_y^X(\theta_{11})}\ & c_0\,|00001111\rangle + s_0c_1\,|00011111\rangle + s_0s_1c_2c_{10}\,|00100111\rangle \\
&+ s_0s_1c_2s_{10}(c_{11}\,|00101011\rangle + s_{11}\,|00101111\rangle) \\
&+ s_0s_1s_2c_3c_7\,|01000111\rangle + s_0s_1s_2c_3s_7c_8\,|01001011\rangle \\
&+ s_0s_1s_2c_3s_7s_8(c_9\,|01001101\rangle + s_9\,|01001110\rangle) \\
&+ s_0s_1s_2s_3c_4\,|10000111\rangle + s_0s_1s_2s_3s_4c_5\,|10001011\rangle \\
&+ s_0s_1s_2s_3s_4s_5(c_6\,|10001101\rangle + s_6\,|10001110\rangle) \\
\xrightarrow{C^3F_y^X(\theta_{12})}\ & c_0\,|00001111\rangle + s_0c_1\,|00011111\rangle + s_0s_1c_2c_{10}\,|00100111\rangle + s_0s_1c_2s_{10}c_{11}\,|00101011\rangle \\
&+ s_0s_1c_2s_{10}s_{11}(c_{12}\,|00101101\rangle + s_{12}\,|00101111\rangle) \\
&+ s_0s_1s_2c_3c_7\,|01000111\rangle + s_0s_1s_2c_3s_7c_8\,|01001011\rangle \\
&+ s_0s_1s_2c_3s_7s_8(c_9\,|01001101\rangle + s_9\,|01001110\rangle) \\
&+ s_0s_1s_2s_3c_4\,|10000111\rangle + s_0s_1s_2s_3s_4c_5\,|10001011\rangle \\
&+ s_0s_1s_2s_3s_4s_5(c_6\,|10001101\rangle + s_6\,|10001110\rangle) \\
\xrightarrow{\text{Toffoli}_{53210}}\ & c_0\,|00001111\rangle + s_0c_1\,|00011111\rangle + s_0s_1c_2c_{10}\,|00100111\rangle + s_0s_1c_2s_{10}c_{11}\,|00101011\rangle \\
&+ s_0s_1c_2s_{10}s_{11}(c_{12}\,|00101101\rangle + s_{12}\,|00101110\rangle) \\
&+ s_0s_1s_2c_3c_7\,|01000111\rangle + s_0s_1s_2c_3s_7c_8\,|01001011\rangle \\
&+ s_0s_1s_2c_3s_7s_8(c_9\,|01001101\rangle + s_9\,|01001110\rangle) \\
&+ s_0s_1s_2s_3c_4\,|10000111\rangle + s_0s_1s_2s_3s_4c_5\,|10001011\rangle \\
&+ s_0s_1s_2s_3s_4s_5(c_6\,|10001101\rangle + s_6\,|10001110\rangle) \\
=\ & |\psi_5\rangle
\end{aligned}
$$

$$
\begin{aligned}
|\psi_5\rangle \xrightarrow{CF_y^X(\theta_{13})}\; & c_0\,|00001111\rangle + s_0c_1(c_{13}\,|00010111\rangle + s_{13}\,|00011111\rangle) + s_0s_1c_2c_{10}\,|00100111\rangle \\
& + s_0s_1c_2s_{10}c_{11}\,|00101011\rangle + s_0s_1c_2s_{10}s_{11}(c_{12}\,|00101101\rangle + s_{12}\,|00101110\rangle) \\
& + s_0s_1s_2c_3c_7\,|01000111\rangle + s_0s_1s_2c_3s_7c_8\,|01001011\rangle \\
& + s_0s_1s_2c_3s_7s_8(c_9\,|01001101\rangle + s_9\,|01001110\rangle) \\
& + s_0s_1s_2s_3c_4\,|10000111\rangle + s_0s_1s_2s_3s_4c_5\,|10001011\rangle \\
& + s_0s_1s_2s_3s_4s_5(c_6\,|10001101\rangle + s_6\,|10001110\rangle) \\
\xrightarrow{C^2F_y^X(\theta_{14})}\; & c_0\,|00001111\rangle + s_0c_1c_{13}\,|00010111\rangle + s_0c_1s_{13}(c_{14}\,|00011011\rangle + s_{14}\,|00011111\rangle) \\
& + s_0s_1c_2c_{10}\,|00100111\rangle + s_0s_1c_2s_{10}c_{11}\,|00101011\rangle \\
& + s_0s_1c_2s_{10}s_{11}(c_{12}\,|00101101\rangle + s_{12}\,|00101110\rangle) \\
& + s_0s_1s_2c_3c_7\,|01000111\rangle + s_0s_1s_2c_3s_7c_8\,|01001011\rangle \\
& + s_0s_1s_2c_3s_7s_8(c_9\,|01001101\rangle + s_9\,|01001110\rangle) \\
& + s_0s_1s_2s_3c_4\,|10000111\rangle + s_0s_1s_2s_3s_4c_5\,|10001011\rangle \\
& + s_0s_1s_2s_3s_4s_5(c_6\,|10001101\rangle + s_6\,|10001110\rangle) \\
\xrightarrow{C^3F_y^X(\theta_{15})}\; & c_0\,|00001111\rangle + s_0c_1c_{13}\,|00010111\rangle + s_0c_1s_{13}c_{14}\,|00011011\rangle \\
& + s_0c_1s_{13}s_{14}(c_{15}\,|00011101\rangle + s_{15}\,|00011111\rangle) \\
& + s_0s_1c_2c_{10}\,|00100111\rangle + s_0s_1c_2s_{10}c_{11}\,|00101011\rangle \\
& + s_0s_1c_2s_{10}s_{11}(c_{12}\,|00101101\rangle + s_{12}\,|00101110\rangle) \\
& + s_0s_1s_2c_3c_7\,|01000111\rangle + s_0s_1s_2c_3s_7c_8\,|01001011\rangle \\
& + s_0s_1s_2c_3s_7s_8(c_9\,|01001101\rangle + s_9\,|01001110\rangle) \\
& + s_0s_1s_2s_3c_4\,|10000111\rangle + s_0s_1s_2s_3s_4c_5\,|10001011\rangle \\
& + s_0s_1s_2s_3s_4s_5(c_6\,|10001101\rangle + s_6\,|10001110\rangle) \\
\xrightarrow{\text{Toffoli}_{43210}}\; & c_0\,|00001111\rangle + s_0c_1c_{13}\,|00010111\rangle + s_0c_1s_{13}c_{14}\,|00011011\rangle \\
& + s_0c_1s_{13}s_{14}(c_{15}\,|00011101\rangle + s_{15}\,|00011110\rangle) \\
& + s_0s_1c_2c_{10}\,|00100111\rangle + s_0s_1c_2s_{10}c_{11}\,|00101011\rangle \\
& + s_0s_1c_2s_{10}s_{11}(c_{12}\,|00101101\rangle + s_{12}\,|00101110\rangle) \\
& + s_0s_1s_2c_3c_7\,|01000111\rangle + s_0s_1s_2c_3s_7c_8\,|01001011\rangle \\
& + s_0s_1s_2c_3s_7s_8(c_9\,|01001101\rangle + s_9\,|01001110\rangle) \\
& + s_0s_1s_2s_3c_4\,|10000111\rangle + s_0s_1s_2s_3s_4c_5\,|10001011\rangle \\
& + s_0s_1s_2s_3s_4s_5(c_6\,|10001101\rangle + s_6\,|10001110\rangle)
\end{aligned}
$$

Here we denote $c_i = \cos(\theta_i)$ and $s_i = \sin(\theta_i)$, and $\text{Toffoli}_{c_1c_2\cdots c_nt}$ as generalized Toffoli gate which has n control qubits $c_1 c_2 \cdots c_n$.

We see that we obtain

$$
\begin{aligned}
|\mathrm{CIS}\rangle = &\alpha_0 |00001111\rangle + \alpha_1 |00011110\rangle + \alpha_2 |00101110\rangle + \alpha_3 |01001110\rangle + \alpha_4 |10001110\rangle \\
&+ \alpha_5 |00011101\rangle + \alpha_6 |00101101\rangle + \alpha_7 |01001101\rangle + \alpha_8 |10001101\rangle \\
&+ \alpha_9 |00011011\rangle + \alpha_{10} |00101011\rangle + \alpha_{11} |01001011\rangle + \alpha_{12} |10001011\rangle \\
&+ \alpha_{13} |00010111\rangle + \alpha_{14} |00100111\rangle + \alpha_{15} |01000111\rangle + \alpha_{16} |10000111\rangle ,
\end{aligned}
$$

where

$$
\begin{aligned}
\alpha_0 &= c_0 \\
\alpha_1 &= s_0 c_1 s_{13} s_{14} s_{15} \\
\alpha_2 &= s_0 s_1 c_2 s_{10} s_{11} s_{12} \\
\alpha_3 &= s_0 s_1 s_2 c_3 s_7 s_8 s_9 \\
\alpha_4 &= s_0 s_1 s_2 s_3 s_4 s_5 s_6 \\
\alpha_5 &= s_0 c_1 s_{13} s_{14} c_{15} \\
\alpha_6 &= s_0 s_1 c_2 s_{10} s_{11} c_{12} \\
\alpha_7 &= s_0 s_1 s_2 c_3 s_7 s_8 c_9 \\
\alpha_8 &= s_0 s_1 s_2 s_3 s_4 s_5 c_6 \\
\alpha_9 &= s_0 c_1 s_{13} c_{14} \\
\alpha_{10} &= s_0 s_1 c_2 s_{10} c_{11} \\
\alpha_{11} &= s_0 s_1 s_2 c_3 s_7 c_8 \\
\alpha_{12} &= s_0 s_1 s_2 s_3 s_4 c_5 \\
\alpha_{13} &= s_0 c_1 c_{13} \\
\alpha_{14} &= s_0 s_1 c_2 c_{10} \\
\alpha_{15} &= s_0 s_1 s_2 c_3 c_7 \\
\alpha_{16} &= s_0 s_1 s_2 s_3 c_4
\end{aligned}
$$

1.3.4 Resource estimation for general cases

Consider the case where the number of qubits n and the number of electrons m. As can be seen from the above examples, we need m X-gates, one R_y-gate, $(n-m-1)$ CF_y^Z gates, $(n-m-1)(n-m)/2$ CNOT gates, $(n-m)$ $CF_y^X, C^2F_y^X, \cdots C^{m-1}F_y^X$ gates, and $(n-m)$ $\text{Toffoli}_{c_1c_2\cdots c_m t}$ gates. Note that each $C^{m-1}F_y^X$ gate consists of $m-1$ ancilla qubits, $2(m-1)$ Toffoli gates and one CF_y^X gate, and each $(n-m)$ $\text{Toffoli}_{c_1c_2\cdots c_m t}$ gate consists of $m-2$ ancilla qubits, $(2m-1)$ Toffoli gates.