Encoding of the Fermi-Hubbard model operators for N, 2, and 4 lattice sites:

Encoding of the Fermi-Hubbard model operators for N lattice sites:
1. Hamiltonian encoding:
Fermi-Hubbard Model Hamiltonian

$$\hat{H} = -t\sum_{i,j}\sum_{\sigma}\left(\hat{a}_{i\sigma}^{\dagger}\hat{a}_{j\sigma} + \hat{a}_{j\sigma}^{\dagger}\hat{a}_{i\sigma}\right) + U\sum_{i}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$$

Where $\sigma \in \{\uparrow, \downarrow\}$, and $\hat{n}_{i\sigma} = \hat{a}_{i\sigma}^{\dagger}\hat{a}_{i\sigma}$.
Definition

$$\sigma^- = |0\rangle\langle 1| = \frac{1}{2}(X + iY)$$
$$\sigma^+ = |1\rangle\langle 0| = \frac{1}{2}(X - iY)$$

Where $X = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $Y = \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$. Note that in quantum computing, $|0\rangle := \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $|1\rangle := \begin{pmatrix} 0 \\ 1 \end{pmatrix}$, so the definition $\sigma^- = \frac{1}{2}(X + iY)$ differs in notation from that in conventional quantum mechanics.

The following relations are used in the derivation:

$$\begin{aligned}
\sigma^+ \cdot \sigma_z &= \sigma^+ \\
\sigma_z \cdot \sigma^- &= \sigma^- \\
\sigma_x \cdot \sigma_x &= I \\
\sigma_y \cdot \sigma_y &= I \\
\sigma_z \cdot \sigma_z &= I \\
\sigma_x \cdot \sigma_y &= i\sigma_z \\
\sigma_y \cdot \sigma_x &= -i\sigma_z
\end{aligned}$$

In a rectangular lattice with N sites,

$$\begin{aligned}
\hat{a}_{i\uparrow} &= Z_0 \otimes Z_1 \otimes \cdots \otimes Z_{i-1} \otimes \sigma_i^- \otimes I_{i+1} \otimes I_{i+2} \otimes \cdots \otimes I_{N-1} \otimes I_N \otimes I_{N+1} \otimes \cdots \otimes I_{2N-1} \\
&= \prod_{k=0}^{i-1} Z_k \otimes \sigma_i^- \otimes \prod_{k=i+1}^{N-1} I_k \otimes \prod_{k=N}^{2N-1} I_k \\
&= \prod_{k=0}^{i-1} Z_k \otimes \sigma_i^- \otimes \prod_{k=i+1}^{2N-1} I_k
\end{aligned}$$

Here, $\prod_{k=m}^{n} O_k$ denotes the sequential tensor product of operators, i.e., $\prod_{k=m}^{n} O_k = O_m \otimes O_{m+1} \otimes \cdots \otimes O_n$.

$$\hat{a}_{i\uparrow}^{\dagger} = \prod_{k=0}^{i-1} Z_k \otimes \sigma_i^+ \otimes \prod_{k=i+1}^{2N-1} I_k$$

$$\hat{a}_{i\downarrow} = \prod_{k=0}^{N-1} I_k \otimes \prod_{k=N}^{i-1+N} Z_k \otimes \sigma_{i+N}^- \otimes \prod_{k=i+1+N}^{2N-1} I_k$$

$$\hat{a}_{i\downarrow}^{\dagger} = \prod_{k=0}^{N-1} I_k \otimes \prod_{k=N}^{i-1+N} Z_k \otimes \sigma_{i+N}^+ \otimes \prod_{k=i+1+N}^{2N-1} I_k$$

Let $i < j$, then we have

$$\begin{aligned}
\hat{a}_{i\uparrow}^{\dagger}\hat{a}_{j\uparrow} &= \left(\prod_{k=0}^{i-1} Z_k \otimes \sigma_i^+ \otimes \prod_{k=i+1}^{2N-1} I_k\right)\left(\prod_{k=0}^{j-1} Z_k \otimes \sigma_j^- \otimes \prod_{k=j+1}^{2N-1} I_k\right) \\
&= \prod_{k=0}^{i-1} I_k \otimes \sigma_i^+ \otimes \prod_{k=i+1}^{j-1} Z_k \otimes \sigma_j^- \otimes \prod_{k=j+1}^{2N-1} I_k \\
&= \prod_{k=0}^{i-1} I_k \otimes \frac{1}{2}(X_i - iY_i) \otimes \prod_{k=i+1}^{j-1} Z_k \otimes \frac{1}{2}(X_j + iY_j) \otimes \prod_{k=j+1}^{2N-1} I_k \\
&= \prod_{k=0}^{i-1} I_k \otimes \frac{1}{2}\left(X_i \otimes \prod_{k=i+1}^{j-1} Z_k - iY_i \otimes \prod_{k=i+1}^{j-1} Z_k\right) \otimes \frac{1}{2}(X_j + iY_j) \otimes \prod_{k=j+1}^{2N-1} I_k \\
&= \frac{1}{4}\prod_{k=0}^{i-1} I_k \otimes \left[X_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes (X_j + iY_j) - iY_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes (X_j + iY_j)\right] \otimes \prod_{k=j+1}^{2N-1} I_k \\
&= \frac{1}{4}\prod_{k=0}^{i-1} I_k \otimes \left(X_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes X_j + X_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes iY_j - iY_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes X_j - iY_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes iY_j\right) \otimes \prod_{k=j+1}^{2N-1} I_k
\end{aligned}$$

Note that for two vector spaces R_1, R_2, and operators $A, B \in R_1$, $L, M \in R_2$, the relation $(A \otimes L)(B \otimes M) = AB \otimes LM$ holds.

$$\begin{aligned}
\hat{a}_{j\uparrow}^{\dagger}\hat{a}_{i\uparrow} &= \left(\prod_{k=0}^{j-1} Z_k \otimes \sigma_j^+ \otimes \prod_{k=j+1}^{2N-1} I_k\right)\left(\prod_{k=0}^{i-1} Z_k \otimes \sigma_i^- \otimes \prod_{k=i+1}^{2N-1} I_k\right) \\
&= \prod_{k=0}^{i-1} I_k \otimes \sigma_i^- \otimes \prod_{k=i+1}^{j-1} Z_k \otimes \sigma_j^+ \otimes \prod_{k=j+1}^{2N-1} I_k \\
&= \prod_{k=0}^{i-1} I_k \otimes \frac{1}{2}(X_i + iY_i) \otimes \prod_{k=i+1}^{j-1} Z_k \otimes \frac{1}{2}(X_j - iY_j) \otimes \prod_{k=j+1}^{2N-1} I_k \\
&= \prod_{k=0}^{i-1} I_k \otimes \frac{1}{2}\left(X_i \otimes \prod_{k=i+1}^{j-1} Z_k + iY_i \otimes \prod_{k=i+1}^{j-1} Z_k\right) \otimes \frac{1}{2}(X_j - iY_j) \otimes \prod_{k=j+1}^{2N-1} I_k \\
&= \frac{1}{4}\prod_{k=0}^{i-1} I_k \otimes \left[X_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes (X_j - iY_j) + iY_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes (X_j - iY_j)\right] \otimes \prod_{k=j+1}^{2N-1} I_k \\
&= \frac{1}{4}\prod_{k=0}^{i-1} I_k \otimes \left(X_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes X_j - X_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes iY_j + iY_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes X_j - iY_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes iY_j\right) \otimes \prod_{k=j+1}^{2N-1} I_k
\end{aligned}$$

or

$$\begin{aligned}
\hat{a}^\dagger_{j\uparrow}\hat{a}_{i\uparrow} &= \left(\hat{a}^\dagger_{i\uparrow}\hat{a}_{j\uparrow}\right)^\dagger \\
&= \left[\frac{1}{4}\prod_{k=0}^{i-1} I_k \otimes \left(X_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes X_j + X_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes iY_j - iY_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes X_j + Y_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes Y_j\right) \otimes \prod_{k=j+1}^{2N-1} I_k\right]^\dagger \\
&= \frac{1}{4}\prod_{k=0}^{i-1} I_k \otimes \left(X_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes X_j - X_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes iY_j + iY_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes X_j + Y_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes Y_j\right) \otimes \prod_{k=j+1}^{2N-1} I_k
\end{aligned}$$

We have

$$\begin{aligned}
\hat{a}^\dagger_{i\uparrow}\hat{a}_{j\uparrow} + \hat{a}^\dagger_{j\uparrow}\hat{a}_{i\uparrow} &= \frac{1}{4}\prod_{k=0}^{i-1} I_k \otimes \left(X_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes X_j + X_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes iY_j - iY_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes X_j - iY_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes iY_j\right) \otimes \prod_{k=j+1}^{2N-1} I_k \\
&\quad + \frac{1}{4}\prod_{k=0}^{i-1} I_k \otimes \left(X_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes X_j - X_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes iY_j + iY_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes X_j - iY_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes iY_j\right) \otimes \prod_{k=j+1}^{2N-1} I_k \\
&= \frac{1}{4}\prod_{k=0}^{i-1} I_k \otimes \left(2X_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes X_j - 2iY_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes iY_j\right) \otimes \prod_{k=j+1}^{2N-1} I_k \\
&= \frac{1}{2}\prod_{k=0}^{i-1} I_k \otimes \left(X_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes X_j + Y_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes Y_j\right) \otimes \prod_{k=j+1}^{2N-1} I_k
\end{aligned}$$

For terms like $X_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes X_j$, consider the following explanation: First, $i < j$. When $j = i+1$, we have $X_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes X_j = X_i \otimes X_{i+1}$. When $j = i+2$, $X_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes X_j = X_i \otimes Z_{i+1} \otimes X_{i+2}$, and so on.

For terms like $\prod_{k=0}^{i-1} I_k$: When $i = 0$, the term $\prod_{k=0}^{i-1} I_k$ does not exist, leading to $\hat{a}^\dagger_{0\uparrow}\hat{a}_{j\uparrow} + \hat{a}^\dagger_{j\uparrow}\hat{a}_{0\uparrow} = \frac{1}{2}\left(X_0 \otimes \prod_{k=1}^{j-1} Z_k \otimes X_j + Y_0 \otimes \prod_{k=1}^{j-1} Z_k \otimes Y_j\right) \otimes \prod_{k=j+1}^{2N-1} I_k$. When $i = 1$, $\prod_{k=0}^{i-1} I_k = I_0$, and so forth. The term $\prod_{k=j+1}^{2N-1} I_k$ follows a similar pattern.

$$\begin{aligned}
\hat{a}^\dagger_{i\downarrow}\hat{a}_{j\downarrow} &= \left(\prod_{k=0}^{N-1} I_k \otimes \prod_{k=N}^{i-1+N} Z_k \otimes \sigma^+_{i+N} \otimes \prod_{k=i+1+N}^{2N-1} I_k\right)\left(\prod_{k=0}^{N-1} I_k \otimes \prod_{k=N}^{j-1+N} Z_k \otimes \sigma^-_{j+N} \otimes \prod_{k=j+1+N}^{2N-1} I_k\right) \\
&= \prod_{k=0}^{N-1} I_k \otimes \prod_{k=N}^{i-1+N} I_k \otimes \sigma^+_{i+N} \otimes \prod_{k=i+1+N}^{j-1+N} Z_k \otimes \sigma^-_{j+N} \otimes \prod_{k=j+1+N}^{2N-1} I_k \\
&= \prod_{k=0}^{i-1+N} I_k \otimes \frac{1}{2}\left(X_{i+N} - iY_{i+N}\right) \otimes \prod_{k=i+1+N}^{j-1+N} Z_k \otimes \frac{1}{2}\left(X_{j+N} + iY_{j+N}\right) \otimes \prod_{k=j+1+N}^{2N-1} I_k \\
&= \frac{1}{4}\prod_{k=0}^{i-1+N} I_k \otimes \left(X_{i+N} \otimes \prod_{k=i+1+N}^{j-1+N} Z_k - iY_{i+N} \otimes \prod_{k=i+1+N}^{j-1+N} Z_k\right) \otimes \left(X_{j+N} + iY_{j+N}\right) \otimes \prod_{k=j+1+N}^{2N-1} I_k \\
&= \frac{1}{4}\prod_{k=0}^{i-1+N} I_k \otimes \left[X_{i+N} \otimes \prod_{k=i+1+N}^{j-1+N} Z_k \otimes \left(X_{j+N} + iY_{j+N}\right) - iY_{i+N} \otimes \prod_{k=i+1+N}^{j-1+N} Z_k \otimes \left(X_{j+N} + iY_{j+N}\right)\right] \otimes \prod_{k=j+1+N}^{2N-1} I_k \\
&= \frac{1}{4}\prod_{k=0}^{i-1+N} I_k \otimes \left(X_{i+N} \otimes \prod_{k=i+1+N}^{j-1+N} Z_k \otimes X_{j+N} + X_{i+N} \otimes \prod_{k=i+1+N}^{j-1+N} Z_k \otimes iY_{j+N} - iY_{i+N} \otimes \prod_{k=i+1+N}^{j-1+N} Z_k \otimes X_{j+N} - iY_{i+N} \otimes \prod_{k=i+1+N}^{j-1+N} Z_k \otimes iY_{j+N}\right) \otimes \prod_{k=j+1+N}^{2N-1} I_k
\end{aligned}$$

$$\begin{aligned}
\hat{a}^\dagger_{j\downarrow}\hat{a}_{i\downarrow} &= \left(\prod_{k=0}^{N-1} I_k \otimes \prod_{k=N}^{j-1+N} Z_k \otimes \sigma^+_{j+N} \otimes \prod_{k=j+1+N}^{2N-1} I_k\right)\left(\prod_{k=0}^{N-1} I_k \otimes \prod_{k=N}^{i-1+N} Z_k \otimes \sigma^-_{i+N} \otimes \prod_{k=i+1+N}^{2N-1} I_k\right) \\
&= \prod_{k=0}^{N-1} I_k \otimes \prod_{k=N}^{i-1+N} I_k \otimes \sigma^-_{i+N} \otimes \prod_{k=i+1+N}^{j-1+N} Z_k \otimes \sigma^+_{j+N} \otimes \prod_{k=j+1+N}^{2N-1} I_k \\
&= \prod_{k=0}^{i-1+N} I_k \otimes \frac{1}{2}\left(X_{i+N} + iY_{i+N}\right) \otimes \prod_{k=i+1+N}^{j-1+N} Z_k \otimes \frac{1}{2}\left(X_{j+N} - iY_{j+N}\right) \otimes \prod_{k=j+1+N}^{2N-1} I_k \\
&= \frac{1}{4}\prod_{k=0}^{i-1+N} I_k \otimes \left(X_{i+N} \otimes \prod_{k=i+1+N}^{j-1+N} Z_k + iY_{i+N} \otimes \prod_{k=i+1+N}^{j-1+N} Z_k\right) \otimes \left(X_{j+N} - iY_{j+N}\right) \otimes \prod_{k=j+1+N}^{2N-1} I_k \\
&= \frac{1}{4}\prod_{k=0}^{i-1+N} I_k \otimes \left[X_{i+N} \otimes \prod_{k=i+1+N}^{j-1+N} Z_k \otimes \left(X_{j+N} - iY_{j+N}\right) + iY_{i+N} \otimes \prod_{k=i+1+N}^{j-1+N} Z_k \otimes \left(X_{j+N} - iY_{j+N}\right)\right] \otimes \prod_{k=j+1+N}^{2N-1} I_k \\
&= \frac{1}{4}\prod_{k=0}^{i-1+N} I_k \otimes \left(X_{i+N} \otimes \prod_{k=i+1+N}^{j-1+N} Z_k \otimes X_{j+N} - X_{i+N} \otimes \prod_{k=i+1+N}^{j-1+N} Z_k \otimes iY_{j+N} + iY_{i+N} \otimes \prod_{k=i+1+N}^{j-1+N} Z_k \otimes X_{j+N} - iY_{i+N} \otimes \prod_{k=i+1+N}^{j-1+N} Z_k \otimes iY_{j+N}\right) \otimes \prod_{k=j+1+N}^{2N-1} I_k
\end{aligned}$$

We have

$$\begin{aligned}
\hat{a}^\dagger_{i\downarrow}\hat{a}_{j\downarrow} + \hat{a}^\dagger_{j\downarrow}\hat{a}_{i\downarrow} &= \frac{1}{4}\prod_{k=0}^{i-1+N} I_k \otimes \left(X_{i+N} \otimes \prod_{k=i+1+N}^{j-1+N} Z_k \otimes X_{j+N} + X_{i+N} \otimes \prod_{k=i+1+N}^{j-1+N} Z_k \otimes iY_{j+N} - iY_{i+N} \otimes \prod_{k=i+1+N}^{j-1+N} Z_k \otimes X_{j+N} - iY_{i+N} \otimes \prod_{k=i+1+N}^{j-1+N} Z_k \otimes iY_{j+N}\right) \otimes \prod_{k=j+1+N}^{2N-1} I_k \\
&\quad + \frac{1}{4}\prod_{k=0}^{i-1+N} I_k \otimes \left(X_{i+N} \otimes \prod_{k=i+1+N}^{j-1+N} Z_k \otimes X_{j+N} - X_{i+N} \otimes \prod_{k=i+1+N}^{j-1+N} Z_k \otimes iY_{j+N} + iY_{i+N} \otimes \prod_{k=i+1+N}^{j-1+N} Z_k \otimes X_{j+N} - iY_{i+N} \otimes \prod_{k=i+1+N}^{j-1+N} Z_k \otimes iY_{j+N}\right) \otimes \prod_{k=j+1+N}^{2N-1} I_k \\
&= \frac{1}{4}\prod_{k=0}^{i-1+N} I_k \otimes \left(2X_{i+N} \otimes \prod_{k=i+1+N}^{j-1+N} Z_k \otimes X_{j+N} - 2iY_{i+N} \otimes \prod_{k=i+1+N}^{j-1+N} Z_k \otimes iY_{j+N}\right) \otimes \prod_{k=j+1+N}^{2N-1} I_k \\
&= \frac{1}{2}\prod_{k=0}^{i-1+N} I_k \otimes \left(X_{i+N} \otimes \prod_{k=i+1+N}^{j-1+N} Z_k \otimes X_{j+N} + Y_{i+N} \otimes \prod_{k=i+1+N}^{j-1+N} Z_k \otimes Y_{j+N}\right) \otimes \prod_{k=j+1+N}^{2N-1} I_k
\end{aligned}$$

$$
\begin{aligned}
\hat{n}_{i\downarrow} &= \hat{a}_{i\downarrow}^{\dagger}\hat{a}_{i\downarrow} \\
&= \left(\prod_{k=0}^{N-1} I_k \otimes \prod_{k=N}^{i-1+N} Z_k \otimes \sigma_{i+N}^{+} \otimes \prod_{k=i+1+N}^{2N-1} I_k\right)\left(\prod_{k=0}^{N-1} I_k \otimes \prod_{k=N}^{i-1+N} Z_k \otimes \sigma_{i+N}^{-} \otimes \prod_{k=i+1+N}^{2N-1} I_k\right) \\
&= \prod_{k=0}^{i-1+N} I_k \otimes \sigma_{i+N}^{+} \cdot \sigma_{i+N}^{-} \otimes \prod_{k=i+1+N}^{2N-1} I_k \\
&= \frac{1}{2}\prod_{k=0}^{i-1+N} I_k \otimes (I_{i+N} - Z_{i+N}) \otimes \prod_{k=i+1+N}^{2N-1} I_k
\end{aligned}
$$

Where

$$
\begin{aligned}
\sigma_{i+N}^{+} \cdot \sigma_{i+N}^{-} &= \frac{1}{2}\left(X_{i+N} - iY_{i+N}\right) \cdot \frac{1}{2}\left(X_{i+N} + iY_{i+N}\right) \\
&= \frac{1}{4}\left(X_{i+N}X_{i+N} + iX_{i+N}Y_{i+N} - iY_{i+N}X_{i+N} + Y_{i+N}Y_{i+N}\right) \\
&= \frac{1}{4}\left[I_{i+N} + i\left(iZ_{i+N}\right) - i\left(-iZ_{i+N}\right) + I_{i+N}\right] \\
&= \frac{1}{2}\left(I_{i+N} - Z_{i+N}\right)
\end{aligned}
$$

or

$$
\begin{aligned}
\sigma_{i+N}^{+} \cdot \sigma_{i+N}^{-} &= \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}_{i+N} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}_{i+N} \\
&= \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}_{i+N} \\
&= \frac{1}{2}\left[\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}_{i+N} - \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_{i+N}\right] \\
&= \frac{1}{2}\left(I_{i+N} - Z_{i+N}\right)
\end{aligned}
$$

Similarly,

$$
\begin{aligned}
\hat{n}_{i\uparrow} &= \hat{a}_{i\uparrow}^{\dagger}\hat{a}_{i\uparrow} \\
&= \left(\prod_{k=0}^{i-1} Z_k \otimes \sigma_i^{+} \otimes \prod_{k=i+1}^{2N-1} I_k\right)\left(\prod_{k=0}^{i-1} Z_k \otimes \sigma_i^{-} \otimes \prod_{k=i+1}^{2N-1} I_k\right) \\
&= \prod_{k=0}^{i-1} I_k \otimes \sigma_i^{+} \cdot \sigma_i^{-} \otimes \prod_{k=i+1}^{2N-1} I_k \\
&= \frac{1}{2}\prod_{k=0}^{i-1} I_k \otimes (I_i - Z_i) \otimes \prod_{k=i+1}^{2N-1} I_k
\end{aligned}
$$

We have

$$
\begin{aligned}
\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} &= \left[\frac{1}{2}\prod_{k=0}^{i-1} I_k \otimes (I_i - Z_i) \otimes \prod_{k=i+1}^{2N-1} I_k\right] \cdot \left[\frac{1}{2}\prod_{k=0}^{i-1+N} I_k \otimes (I_{i+N} - Z_{i+N}) \otimes \prod_{k=i+1+N}^{2N-1} I_k\right] \\
&= \frac{1}{4}\prod_{k=0}^{i-1} I_k \otimes (I_i - Z_i) \otimes \prod_{k=i+1}^{i-1+N} I_k \otimes (I_{i+N} - Z_{i+N}) \otimes \prod_{k=i+1+N}^{2N-1} I_k \\
&= \frac{1}{4}\prod_{k=0}^{i-1} I_k \otimes \left(I_i \otimes \prod_{k=i+1}^{i-1+N} I_k - Z_i \otimes \prod_{k=i+1}^{i-1+N} I_k\right) \otimes (I_{i+N} - Z_{i+N}) \otimes \prod_{k=i+1+N}^{2N-1} I_k \\
&= \frac{1}{4}\prod_{k=0}^{i-1} I_k \otimes \left[I_i \otimes \prod_{k=i+1}^{i-1+N} I_k \otimes (I_{i+N} - Z_{i+N}) - Z_i \otimes \prod_{k=i+1}^{i-1+N} I_k \otimes (I_{i+N} - Z_{i+N})\right] \otimes \prod_{k=i+1+N}^{2N-1} I_k \\
&= \frac{1}{4}\prod_{k=0}^{i-1} I_k \otimes \left(I_i \otimes \prod_{k=i+1}^{i-1+N} I_k \otimes I_{i+N} - I_i \otimes \prod_{k=i+1}^{i-1+N} I_k \otimes Z_{i+N} - Z_i \otimes \prod_{k=i+1}^{i-1+N} I_k \otimes I_{i+N} + Z_i \otimes \prod_{k=i+1}^{i-1+N} I_k \otimes Z_{i+N}\right) \otimes \prod_{k=i+1+N}^{2N-1} I_k
\end{aligned}
$$

In summary, we have

$$
\hat{a}_{i\uparrow}^{\dagger}\hat{a}_{j\uparrow} + \hat{a}_{j\uparrow}^{\dagger}\hat{a}_{i\uparrow} = \frac{1}{2}\prod_{k=0}^{i-1} I_k \otimes \left(X_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes X_j + Y_i \otimes \prod_{k=i+1}^{j-1} Z_k \otimes Y_j\right) \otimes \prod_{k=j+1}^{2N-1} I_k
$$

$$
\hat{a}_{i\downarrow}^{\dagger}\hat{a}_{j\downarrow} + \hat{a}_{j\downarrow}^{\dagger}\hat{a}_{i\downarrow} = \frac{1}{2}\prod_{k=0}^{i-1+N} I_k \otimes \left(X_{i+N} \otimes \prod_{k=i+1+N}^{j-1+N} Z_k \otimes X_{j+N} + Y_{i+N} \otimes \prod_{k=i+1+N}^{j-1+N} Z_k \otimes Y_{j+N}\right) \otimes \prod_{k=j+1+N}^{2N-1} I_k
$$

$$
\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} = \frac{1}{4}\prod_{k=0}^{i-1} I_k \otimes \left(I_i \otimes \prod_{k=i+1}^{i-1+N} I_k \otimes I_{i+N} - I_i \otimes \prod_{k=i+1}^{i-1+N} I_k \otimes Z_{i+N} - Z_i \otimes \prod_{k=i+1}^{i-1+N} I_k \otimes I_{i+N} + Z_i \otimes \prod_{k=i+1}^{i-1+N} I_k \otimes Z_{i+N}\right) \otimes \prod_{k=i+1+N}^{2N-1} I_k
$$

2. Particle number operator encoding:

$$
\begin{aligned}
\hat{N} &= \sum_{i,\sigma\in\{\uparrow,\downarrow\}} \hat{a}_{i\sigma}^{\dagger}\hat{a}_{i\sigma} \\
&= \sum_i \left(\hat{a}_{i\uparrow}^{\dagger}\hat{a}_{i\uparrow} + \hat{a}_{i\downarrow}^{\dagger}\hat{a}_{i\downarrow}\right) \\
&= \sum_i \left[\frac{1}{2}\prod_{k=0}^{i-1} I_k \otimes (I_i - Z_i) \otimes \prod_{k=i+1}^{2N-1} I_k + \frac{1}{2}\prod_{k=0}^{i-1+N} I_k \otimes (I_{i+N} - Z_{i+N}) \otimes \prod_{k=i+1+N}^{2N-1} I_k\right] \\
&= \frac{1}{2}\sum_i \prod_{k=0}^{i-1} I_k \otimes \left[(I_i - Z_i) \otimes \prod_{k=i+1}^{i+N} I_k + \prod_{k=i}^{i-1+N} I_k \otimes (I_{i+N} - Z_{i+N})\right] \otimes \prod_{k=i+1+N}^{2N-1} I_k \\
&= \frac{1}{2}\sum_i \prod_{k=0}^{i-1} I_k \otimes \left[I_i \otimes \prod_{k=i+1}^{i+N} I_k - Z_i \otimes \prod_{k=i+1}^{i+N} I_k + \prod_{k=i}^{i-1+N} I_k \otimes I_{i+N} - \prod_{k=i}^{i-1+N} I_k \otimes Z_{i+N}\right] \otimes \prod_{k=i+1+N}^{2N-1} I_k
\end{aligned}
$$

3. z-component of the total spin operator encoding:

$$
\begin{aligned}
\hat{S}_z &= \frac{1}{2}\sum_i \left(\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}\right) \\
&= \frac{1}{2}\sum_i \left[\frac{1}{2}\prod_{k=0}^{i-1} I_k \otimes (I_i - Z_i) \otimes \prod_{k=i+1}^{2N-1} I_k - \frac{1}{2}\prod_{k=0}^{i-1+N} I_k \otimes (I_{i+N} - Z_{i+N}) \otimes \prod_{k=i+1+N}^{2N-1} I_k\right] \\
&= \frac{1}{4}\sum_i \left\{\prod_{k=0}^{i-1} I_k \otimes \left[(I_i - Z_i) \otimes \prod_{k=i+1}^{i+N} I_k - \prod_{k=i}^{i-1+N} I_k \otimes (I_{i+N} - Z_{i+N})\right] \otimes \prod_{k=i+1+N}^{2N-1} I_k\right\} \\
&= \frac{1}{4}\sum_i \prod_{k=0}^{i-1} I_k \otimes \left[I_i \otimes \prod_{k=i+1}^{i+N} I_k - Z_i \otimes \prod_{k=i+1}^{i+N} I_k - \prod_{k=i}^{i-1+N} I_k \otimes I_{i+N} + \prod_{k=i}^{i-1+N} I_k \otimes Z_{i+N}\right] \otimes \prod_{k=i+1+N}^{2N-1} I_k
\end{aligned}
$$

Fermi-Hubbard model with two lattice sites:

1. Hamiltonian encoding:

For $\sum_{i,j}\sum_\sigma \left(\hat{a}_{i\sigma}^\dagger \hat{a}_{j\sigma} + \hat{a}_{j\sigma}^\dagger \hat{a}_{i\sigma}\right)$, we have

$$\sum_{i,j}\sum_\sigma \left(\hat{a}_{i\sigma}^\dagger \hat{a}_{j\sigma} + \hat{a}_{j\sigma}^\dagger \hat{a}_{i\sigma}\right) = \left(\hat{a}_{0\uparrow}^\dagger \hat{a}_{1\uparrow} + \hat{a}_{1\uparrow}^\dagger \hat{a}_{0\uparrow}\right) + \left(\hat{a}_{0\downarrow}^\dagger \hat{a}_{1\downarrow} + \hat{a}_{1\downarrow}^\dagger \hat{a}_{0\downarrow}\right)$$

Where

$$\hat{a}_{0\uparrow}^\dagger \hat{a}_{1\uparrow} + \hat{a}_{1\uparrow}^\dagger \hat{a}_{0\uparrow} = \frac{1}{2}\left(X_0 \otimes X_1 + Y_0 \otimes Y_1\right) \otimes \prod_{k=2}^{3} I_k$$

$$\hat{a}_{0\downarrow}^\dagger \hat{a}_{1\downarrow} + \hat{a}_{1\downarrow}^\dagger \hat{a}_{0\downarrow} = \frac{1}{2}\prod_{k=0}^{1} I_k \otimes \left(X_2 \otimes X_3 + Y_2 \otimes Y_3\right)$$

For $\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$, we have

$$\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} = \hat{n}_{0\uparrow}\hat{n}_{0\downarrow} + \hat{n}_{1\uparrow}\hat{n}_{1\downarrow}$$

Where

$$\hat{n}_{0\uparrow}\hat{n}_{0\downarrow} = \frac{1}{4}\left(I_0 \otimes I_1 \otimes I_2 - I_0 \otimes I_1 \otimes Z_2 - Z_0 \otimes I_1 \otimes I_2 + Z_0 \otimes I_1 \otimes Z_2\right) \otimes I_3$$

$$\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} = \frac{1}{4} I_0 \otimes \left(I_1 \otimes I_2 \otimes I_3 - I_1 \otimes I_2 \otimes Z_3 - Z_1 \otimes I_2 \otimes I_3 + Z_1 \otimes I_2 \otimes Z_3\right)$$

2. Particle number operator encoding:

$$\hat{N} = \sum_{i=0}^{1} n_i$$

$$n_0 = \frac{1}{2}\left(I_0 \otimes \prod_{k=1}^{2} I_k - Z_0 \otimes \prod_{k=1}^{2} I_k + \prod_{k=0}^{1} I_k \otimes I_2 - \prod_{k=0}^{1} I_k \otimes Z_2\right) \otimes I_3$$

$$n_1 = \frac{1}{2} I_0 \otimes \left(I_1 \otimes \prod_{k=2}^{3} I_k - Z_1 \otimes \prod_{k=2}^{3} I_k + \prod_{k=1}^{2} I_k \otimes I_3 - \prod_{k=1}^{2} I_k \otimes Z_3\right)$$

3. z-component of the total spin operator encoding:

$$\hat{S}_z = \sum_{i=0}^{1} s_i^z$$

Where

$$s_0^z = \frac{1}{4}\left(I_0 \otimes \prod_{k=1}^{2} I_k - Z_0 \otimes \prod_{k=1}^{2} I_k - \prod_{k=0}^{1} I_k \otimes I_2 + \prod_{k=0}^{1} I_k \otimes Z_2\right) \otimes I_3$$

$$s_1^z = \frac{1}{4} I_0 \otimes \left(I_1 \otimes \prod_{k=2}^{3} I_k - Z_1 \otimes \prod_{k=2}^{3} I_k - \prod_{k=1}^{2} I_k \otimes I_3 + \prod_{k=1}^{2} I_k \otimes Z_3\right)$$

Fermi-Hubbard model with four lattice sites:

1. Hamiltonian encoding:

For a rectangular lattice with four sites, for the expression $\sum_{i,j}\sum_\sigma \left(\hat{a}_{i\sigma}^\dagger \hat{a}_{j\sigma} + \hat{a}_{j\sigma}^\dagger \hat{a}_{i\sigma}\right)$, we have

$$
\begin{aligned}
\sum_{i,j}\sum_\sigma \left(\hat{a}_{i\sigma}^\dagger \hat{a}_{j\sigma} + \hat{a}_{j\sigma}^\dagger \hat{a}_{i\sigma}\right) &= \left(\hat{a}_{0\uparrow}^\dagger \hat{a}_{1\uparrow} + \hat{a}_{1\uparrow}^\dagger \hat{a}_{0\uparrow}\right) + \left(\hat{a}_{0\uparrow}^\dagger \hat{a}_{3\uparrow} + \hat{a}_{3\uparrow}^\dagger \hat{a}_{0\uparrow}\right) \\
&\quad + \left(\hat{a}_{1\uparrow}^\dagger \hat{a}_{2\uparrow} + \hat{a}_{2\uparrow}^\dagger \hat{a}_{1\uparrow}\right) + \left(\hat{a}_{2\uparrow}^\dagger \hat{a}_{3\uparrow} + \hat{a}_{3\uparrow}^\dagger \hat{a}_{2\uparrow}\right) \\
&\quad + \left(\hat{a}_{0\downarrow}^\dagger \hat{a}_{1\downarrow} + \hat{a}_{1\downarrow}^\dagger \hat{a}_{0\downarrow}\right) + \left(\hat{a}_{0\downarrow}^\dagger \hat{a}_{3\downarrow} + \hat{a}_{3\downarrow}^\dagger \hat{a}_{0\downarrow}\right) \\
&\quad + \left(\hat{a}_{1\downarrow}^\dagger \hat{a}_{2\downarrow} + \hat{a}_{2\downarrow}^\dagger \hat{a}_{1\downarrow}\right) + \left(\hat{a}_{2\downarrow}^\dagger \hat{a}_{3\downarrow} + \hat{a}_{3\downarrow}^\dagger \hat{a}_{2\downarrow}\right)
\end{aligned}
$$

Where

$$\hat{a}_{0\uparrow}^\dagger \hat{a}_{1\uparrow} + \hat{a}_{1\uparrow}^\dagger \hat{a}_{0\uparrow} = \frac{1}{2}\left(X_0 \otimes X_1 + Y_0 \otimes Y_1\right) \otimes \prod_{k=2}^{7} I_k$$

$$\hat{a}_{0\uparrow}^\dagger \hat{a}_{3\uparrow} + \hat{a}_{3\uparrow}^\dagger \hat{a}_{0\uparrow} = \frac{1}{2}\left(X_0 \otimes Z_1 \otimes Z_2 \otimes X_3 + Y_0 \otimes Z_1 \otimes Z_2 \otimes Y_3\right) \otimes \prod_{k=4}^{7} I_k$$

$$\hat{a}_{1\uparrow}^\dagger \hat{a}_{2\uparrow} + \hat{a}_{2\uparrow}^\dagger \hat{a}_{1\uparrow} = \frac{1}{2} I_0 \otimes \left(X_1 \otimes X_2 + Y_1 \otimes Y_2\right) \otimes \prod_{k=3}^{7} I_k$$

$$\hat{a}_{2\uparrow}^\dagger \hat{a}_{3\uparrow} + \hat{a}_{3\uparrow}^\dagger \hat{a}_{2\uparrow} = \frac{1}{2} I_0 \otimes I_1 \otimes \left(X_2 \otimes X_3 + Y_2 \otimes Y_3\right) \otimes \prod_{k=4}^{7} I_k$$

$$\hat{a}_{0\downarrow}^{\dagger}\hat{a}_{1\downarrow}+\hat{a}_{1\downarrow}^{\dagger}\hat{a}_{0\downarrow}=\frac{1}{2}\prod_{k=0}^{3}I_k\otimes(X_4\otimes X_5+Y_4\otimes Y_5)\otimes\prod_{k=6}^{7}I_k$$

$$\hat{a}_{0\downarrow}^{\dagger}\hat{a}_{3\downarrow}+\hat{a}_{3\downarrow}^{\dagger}\hat{a}_{0\downarrow}=\frac{1}{2}\prod_{k=0}^{3}I_k\otimes\left(X_4\otimes\prod_{k=5}^{6}Z_k\otimes X_7+Y_4\otimes\prod_{k=5}^{6}Z_k\otimes Y_7\right)$$

$$\hat{a}_{1\downarrow}^{\dagger}\hat{a}_{2\downarrow}+\hat{a}_{2\downarrow}^{\dagger}\hat{a}_{1\downarrow}=\frac{1}{2}\prod_{k=0}^{4}I_k\otimes(X_5\otimes X_6+Y_5\otimes Y_6)\otimes I_7$$

$$\hat{a}_{2\downarrow}^{\dagger}\hat{a}_{3\downarrow}+\hat{a}_{3\downarrow}^{\dagger}\hat{a}_{2\downarrow}=\frac{1}{2}\prod_{k=0}^{5}I_k\otimes(X_6\otimes X_7+Y_6\otimes Y_7)$$

For $\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$, we have

$$\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}=\hat{n}_{0\uparrow}\hat{n}_{0\downarrow}+\hat{n}_{1\uparrow}\hat{n}_{1\downarrow}+\hat{n}_{2\uparrow}\hat{n}_{2\downarrow}+\hat{n}_{3\uparrow}\hat{n}_{3\downarrow}$$

Where

$$\hat{n}_{0\uparrow}\hat{n}_{0\downarrow}=\frac{1}{4}\left(I_0\otimes\prod_{k=1}^{3}I_k\otimes I_4-I_0\otimes\prod_{k=1}^{3}I_k\otimes Z_4-Z_0\otimes\prod_{k=1}^{3}I_k\otimes I_4+Z_0\otimes\prod_{k=1}^{3}I_k\otimes Z_4\right)\otimes\prod_{k=5}^{7}I_k$$

$$\hat{n}_{1\uparrow}\hat{n}_{1\downarrow}=\frac{1}{4}I_0\otimes\left(I_1\otimes\prod_{k=2}^{4}I_k\otimes I_5-I_1\otimes\prod_{k=2}^{4}I_k\otimes Z_5-Z_1\otimes\prod_{k=2}^{4}I_k\otimes I_5+Z_1\otimes\prod_{k=2}^{4}I_k\otimes Z_5\right)\otimes\prod_{k=6}^{7}I_k$$

$$\hat{n}_{2\uparrow}\hat{n}_{2\downarrow}=\frac{1}{4}\prod_{k=0}^{1}I_k\otimes\left(I_2\otimes\prod_{k=3}^{5}I_k\otimes I_6-I_2\otimes\prod_{k=3}^{5}I_k\otimes Z_6-Z_2\otimes\prod_{k=3}^{5}I_k\otimes I_6+Z_2\otimes\prod_{k=3}^{5}I_k\otimes Z_6\right)\otimes I_7$$

$$\hat{n}_{3\uparrow}\hat{n}_{3\downarrow}=\frac{1}{4}\prod_{k=0}^{2}I_k\otimes\left(I_3\otimes\prod_{k=4}^{6}I_k\otimes I_7-I_3\otimes\prod_{k=4}^{6}I_k\otimes Z_7-Z_3\otimes\prod_{k=4}^{6}I_k\otimes I_7+Z_3\otimes\prod_{k=4}^{6}I_k\otimes Z_7\right)$$

2. Particle number operator encoding:

$$\hat{N}=\sum_{i=0}^{3}n_i$$

Where

$$n_0=\frac{1}{2}\left(I_0\otimes\prod_{k=1}^{4}I_k-Z_0\otimes\prod_{k=1}^{4}I_k+\prod_{k=0}^{3}I_k\otimes I_4-\prod_{k=0}^{3}I_k\otimes Z_4\right)\otimes\prod_{k=5}^{7}I_k$$

$$n_1=\frac{1}{2}I_0\otimes\left(I_1\otimes\prod_{k=2}^{5}I_k-Z_1\otimes\prod_{k=2}^{5}I_k+\prod_{k=1}^{4}I_k\otimes I_5-\prod_{k=1}^{4}I_k\otimes Z_5\right)\otimes\prod_{k=6}^{7}I_k$$

$$n_2=\frac{1}{2}\prod_{k=0}^{1}I_k\otimes\left(I_2\otimes\prod_{k=3}^{6}I_k-Z_2\otimes\prod_{k=3}^{6}I_k+\prod_{k=2}^{5}I_k\otimes I_6-\prod_{k=2}^{5}I_k\otimes Z_6\right)\otimes I_7$$

$$n_3=\frac{1}{2}\prod_{k=0}^{2}I_k\otimes\left(I_3\otimes\prod_{k=4}^{7}I_k-Z_3\otimes\prod_{k=4}^{7}I_k+\prod_{k=3}^{6}I_k\otimes I_7-\prod_{k=3}^{6}I_k\otimes Z_7\right)$$

3. z-component of the total spin operator encoding:

$$\hat{S}_z=\sum_{i=0}^{3}s_i^z$$

Where

$$s_0^z=\frac{1}{4}\left(I_0\otimes\prod_{k=1}^{4}I_k-Z_0\otimes\prod_{k=1}^{4}I_k-\prod_{k=0}^{3}I_k\otimes I_4+\prod_{k=0}^{3}I_k\otimes Z_4\right)\otimes\prod_{k=5}^{7}I_k$$

$$s_1^z=\frac{1}{4}I_0\otimes\left(I_1\otimes\prod_{k=2}^{5}I_k-Z_1\otimes\prod_{k=2}^{5}I_k-\prod_{k=1}^{4}I_k\otimes I_5+\prod_{k=1}^{4}I_k\otimes Z_5\right)\otimes\prod_{k=6}^{7}I_k$$

$$s_2^z=\frac{1}{4}\prod_{k=0}^{1}I_k\otimes\left(I_2\otimes\prod_{k=3}^{6}I_k-Z_2\otimes\prod_{k=3}^{6}I_k-\prod_{k=2}^{5}I_k\otimes I_6+\prod_{k=2}^{5}I_k\otimes Z_6\right)\otimes I_7$$

$$s_3^z=\frac{1}{4}\prod_{k=0}^{2}I_k\otimes\left(I_3\otimes\prod_{k=4}^{7}I_k-Z_3\otimes\prod_{k=4}^{7}I_k-\prod_{k=3}^{6}I_k\otimes I_7+\prod_{k=3}^{6}I_k\otimes Z_7\right)$$