The initial states used in the computation processes.

Fermi-Hubbard model with two lattice sites:

The following uses $|\alpha\rangle, |\beta\rangle, |\gamma\rangle, \ldots$ to represent the ground state, first excited state, second excited state, and so on. The subscripts denote the eigenvalues of the particle number operator and the total spin z-component operator for each eigenstate. For example, $|\alpha_{2,0}\rangle$ represents the ground state with eigenvalue $\alpha_{2,0}$.

$$
\begin{aligned}
|\psi^+\rangle &= \frac{1}{\sqrt{2}}\left(|01\rangle + |10\rangle\right) \\
|\psi^-\rangle &= \frac{1}{\sqrt{2}}\left(|01\rangle - |10\rangle\right)
\end{aligned}
$$

$|\alpha_{2,0}\rangle$: $n = 2, M = 0$

$$
\begin{aligned}
|\psi_0\rangle &= |\psi^+\rangle \otimes |\psi^+\rangle \\
&= \frac{1}{\sqrt{2}}\left(|01\rangle + |10\rangle\right) \otimes \frac{1}{\sqrt{2}}\left(|01\rangle + |10\rangle\right) \\
&= \frac{1}{2}\left(|0101\rangle + |0110\rangle + |1001\rangle + |1010\rangle\right)
\end{aligned}
$$

$|\beta_{1,-1/2}\rangle$: $n = 1, M = -\frac{1}{2}$

$$
\begin{aligned}
|\psi_1\rangle &= |00\rangle \otimes |\psi^+\rangle \\
&= \frac{1}{\sqrt{2}}\left(|0001\rangle + |0010\rangle\right)
\end{aligned}
$$

$|\beta_{1,1/2}\rangle$: $n = 1, M = \frac{1}{2}$

$$
\begin{aligned}
|\psi_2\rangle &= |\psi^+\rangle \otimes |00\rangle \\
&= \frac{1}{\sqrt{2}}\left(|0100\rangle + |1000\rangle\right)
\end{aligned}
$$

$|\gamma_{2,-1}\rangle$: $n = 2, M = -1$

$$|\psi_3\rangle = |0011\rangle$$

$|\gamma_{0,0}\rangle$: $n = 0, M = 0$

$$|\psi_4\rangle = |0000\rangle$$

$|\gamma_{2,1}\rangle$: $n = 2, M = 1$

$$|\psi_5\rangle = |1100\rangle$$

$|\gamma_{2,0}\rangle$: $n = 2, M = 0$

$$
\begin{aligned}
|\psi_6\rangle &= |\psi^+\rangle \otimes |\psi^-\rangle \\
&= \frac{1}{\sqrt{2}}\left(|01\rangle + |10\rangle\right) \otimes \frac{1}{\sqrt{2}}\left(|01\rangle - |10\rangle\right) \\
&= \frac{1}{2}\left(|0101\rangle - |0110\rangle + |1001\rangle - |1010\rangle\right)
\end{aligned}
$$

$|\delta_{3,-1/2}\rangle$: $n = 3, M = -\frac{1}{2}$

$$
\begin{aligned}
|\psi_7\rangle &= |\psi^+\rangle \otimes |11\rangle \\
&= \frac{1}{\sqrt{2}}\left(|0111\rangle + |1011\rangle\right)
\end{aligned}
$$

$|\delta_{1,1/2}\rangle$: $n = 1, M = \frac{1}{2}$

$$
\begin{aligned}
|\psi_8\rangle &= |\psi^-\rangle \otimes |00\rangle \\
&= \frac{1}{\sqrt{2}}\left(|0100\rangle - |1000\rangle\right)
\end{aligned}
$$

$|\delta_{1,-1/2}\rangle$: $n=1, M=-\frac{1}{2}$

$$\begin{aligned}|\psi_9\rangle &= |00\rangle\otimes|\psi^-\rangle \\ &= \frac{1}{\sqrt{2}}\left(|0001\rangle-|0010\rangle\right)\end{aligned}$$

$|\delta_{3,1/2}\rangle$: $n=3, M=\frac{1}{2}$

$$\begin{aligned}|\psi_{10}\rangle &= |11\rangle\otimes|\psi^+\rangle \\ &= \frac{1}{\sqrt{2}}\left(|1101\rangle+|1110\rangle\right)\end{aligned}$$

$|\varepsilon_{2,0}\rangle$: $n=2, M=0$

$$\begin{aligned}|\psi_{11}\rangle &= |\psi^-\rangle\otimes|\psi^+\rangle \\ &= \frac{1}{\sqrt{2}}\left(|01\rangle-|10\rangle\right)\otimes\frac{1}{\sqrt{2}}\left(|01\rangle+|10\rangle\right) \\ &= \frac{1}{2}\left(|0101\rangle+|0110\rangle-|1001\rangle-|1010\rangle\right)\end{aligned}$$

$|\zeta_{3,-1/2}\rangle$: $n=3, M=-\frac{1}{2}$

$$\begin{aligned}|\psi_{12}\rangle &= |\psi^-\rangle\otimes|11\rangle \\ &= \frac{1}{\sqrt{2}}\left(|0111\rangle-|1011\rangle\right)\end{aligned}$$

$|\zeta_{3,1/2}\rangle$: $n=3, M=\frac{1}{2}$

$$\begin{aligned}|\psi_{13}\rangle &= |11\rangle\otimes|\psi^-\rangle \\ &= \frac{1}{\sqrt{2}}\left(|1101\rangle-|1110\rangle\right)\end{aligned}$$

$|\eta_{2,0}\rangle$: $n=2, M=0$

$$\begin{aligned}|\psi_{14}\rangle &= |\psi^-\rangle\otimes|\psi^-\rangle \\ &= \frac{1}{\sqrt{2}}\left(|01\rangle-|10\rangle\right)\otimes\frac{1}{\sqrt{2}}\left(|01\rangle-|10\rangle\right) \\ &= \frac{1}{2}\left(|0101\rangle-|0110\rangle-|1001\rangle+|1010\rangle\right)\end{aligned}$$

$|\theta_{4,0}\rangle$: $n=4, M=0$

$$|\psi_{15}\rangle = |1111\rangle$$

Fermi-Hubbard model with four lattice sites:

The following uses $|\iota\rangle, |\kappa\rangle, |\lambda\rangle$ to represent the ground state, first excited state, second excited state, and so on. The subscripts denote the eigenvalues of the particle number operator and the total spin z-component operator for each eigenstate. For example, $|\iota_{2,0}\rangle$ represents the ground state with eigenvalue $\iota_{2,0}$. In the first excited state, the subscripts 1 and 2 are labels used because no quantum numbers were found to distinguish between different degenerate states, and they have no physical meaning. In the paper, only the ground state $|\iota_{2,0}\rangle$ and the second excited state $|\lambda_{4,0}\rangle$ are used.

$|\iota_{2,0}\rangle$: $n=2, M=0$

$$|\phi_0\rangle = \frac{1}{2}\big(|00\rangle\otimes|\psi^+\rangle+|\psi^+\rangle\otimes|00\rangle\big)\otimes\big(|00\rangle\otimes|\psi^+\rangle+|\psi^+\rangle\otimes|00\rangle\big)$$

Specifically,

$$
\begin{aligned}
|\phi_0\rangle &= \frac{1}{\sqrt{16}}\Big(|00\rangle\otimes\sqrt{2}|\psi^+\rangle\otimes|00\rangle\otimes\sqrt{2}|\psi^+\rangle \\
&\quad +|00\rangle\otimes\sqrt{2}|\psi^+\rangle\otimes\sqrt{2}|\psi^+\rangle\otimes|00\rangle \\
&\quad +\sqrt{2}|\psi^+\rangle\otimes|00\rangle\otimes|00\rangle\otimes\sqrt{2}|\psi^+\rangle \\
&\quad +\sqrt{2}|\psi^+\rangle\otimes|00\rangle\otimes\sqrt{2}|\psi^+\rangle\otimes|00\rangle\Big) \\
&= \frac{1}{\sqrt{16}}\Big[|00\rangle\otimes\sqrt{2}|\psi^+\rangle\otimes\Big(|00\rangle\otimes\sqrt{2}|\psi^+\rangle+\sqrt{2}|\psi^+\rangle\otimes|00\rangle\Big) \\
&\quad +\sqrt{2}|\psi^+\rangle\otimes|00\rangle\otimes\Big(|00\rangle\otimes\sqrt{2}|\psi^+\rangle+\sqrt{2}|\psi^+\rangle\otimes|00\rangle\Big)\Big] \\
&= \frac{1}{2}\big(|00\rangle\otimes|\psi^+\rangle+|\psi^+\rangle\otimes|00\rangle\big)\otimes\big(|00\rangle\otimes|\psi^+\rangle+|\psi^+\rangle\otimes|00\rangle\big) \\
&= \frac{1}{4}\left(|00010001\rangle+|00010010\rangle+|00010100\rangle+|00011000\rangle\right. \\
&\quad +|00100001\rangle+|00100010\rangle+|00100100\rangle+|00101000\rangle \\
&\quad +|01000001\rangle+|01000010\rangle+|01000100\rangle+|01001000\rangle \\
&\quad \left.+|10000001\rangle+|10000010\rangle+|10000100\rangle+|10001000\rangle\right)
\end{aligned}
$$

$|\kappa_{3,1/2,1}\rangle$: $n=3, M=\frac{1}{2}$

$$
|\phi_1\rangle = \frac{1}{\sqrt{12}}\big(|00\rangle\otimes|11\rangle+|11\rangle\otimes|00\rangle+2|\psi^+\rangle\otimes|\psi^+\rangle\big)\otimes\big(|00\rangle\otimes|\psi^+\rangle+|\psi^+\rangle\otimes|00\rangle\big)
$$

Specifically,

$$
\begin{aligned}
|\phi_1\rangle &= \frac{1}{\sqrt{24}}\Big(|00\rangle\otimes|11\rangle\otimes|00\rangle\otimes\sqrt{2}|\psi^+\rangle \\
&\quad +|00\rangle\otimes|11\rangle\otimes\sqrt{2}|\psi^+\rangle\otimes|00\rangle \\
&\quad +|11\rangle\otimes|00\rangle\otimes|00\rangle\otimes\sqrt{2}|\psi^+\rangle \\
&\quad +|11\rangle\otimes|00\rangle\otimes\sqrt{2}|\psi^+\rangle\otimes|00\rangle \\
&\quad +\sqrt{2}|\psi^+\rangle\otimes\sqrt{2}|\psi^+\rangle\otimes|00\rangle\otimes\sqrt{2}|\psi^+\rangle \\
&\quad +\sqrt{2}|\psi^+\rangle\otimes\sqrt{2}|\psi^+\rangle\otimes\sqrt{2}|\psi^+\rangle\otimes|00\rangle\Big) \\
&= \frac{1}{\sqrt{24}}\Big[|00\rangle\otimes|11\rangle\otimes\Big(|00\rangle\otimes\sqrt{2}|\psi^+\rangle+\sqrt{2}|\psi^+\rangle\otimes|00\rangle\Big) \\
&\quad +|11\rangle\otimes|00\rangle\otimes\Big(|00\rangle\otimes\sqrt{2}|\psi^+\rangle+\sqrt{2}|\psi^+\rangle\otimes|00\rangle\Big) \\
&\quad +\sqrt{2}|\psi^+\rangle\otimes\sqrt{2}|\psi^+\rangle\otimes\Big(|00\rangle\otimes\sqrt{2}|\psi^+\rangle+\sqrt{2}|\psi^+\rangle\otimes|00\rangle\Big)\Big] \\
&= \frac{1}{\sqrt{12}}\big(|00\rangle\otimes|11\rangle+|11\rangle\otimes|00\rangle+2|\psi^+\rangle\otimes|\psi^+\rangle\big)\otimes\big(|00\rangle\otimes|\psi^+\rangle+|\psi^+\rangle\otimes|00\rangle\big) \\
&= \frac{1}{\sqrt{24}}\left(|00110001\rangle+|00110010\rangle+|00110100\rangle+|00111000\rangle\right. \\
&\quad +|11000001\rangle+|11000010\rangle+|11000100\rangle+|11001000\rangle \\
&\quad +|01010001\rangle+|01010010\rangle+|01010100\rangle+|01011000\rangle \\
&\quad +|01100001\rangle+|01100010\rangle+|01100100\rangle+|01101000\rangle \\
&\quad +|10010001\rangle+|10010010\rangle+|10010100\rangle+|10011000\rangle \\
&\quad \left.+|10100001\rangle+|10100010\rangle+|10100100\rangle+|10101000\rangle\right)
\end{aligned}
$$

$|\kappa_{3,-1/2,1}\rangle$: $n=3, M=-\frac{1}{2}$

$$
|\phi_2\rangle = \frac{1}{\sqrt{12}}\big(|00\rangle\otimes|\psi^+\rangle+|\psi^+\rangle\otimes|00\rangle\big)\otimes\big(|00\rangle\otimes|11\rangle+|11\rangle\otimes|00\rangle+2|\psi^+\rangle\otimes|\psi^+\rangle\big)
$$

Specifically,

$$
\begin{aligned}
|\phi_2\rangle &= \frac{1}{\sqrt{24}}\Big(|00\rangle\otimes\sqrt{2}|\psi^+\rangle\otimes|00\rangle\otimes|11\rangle \\
&\quad +\sqrt{2}|\psi^+\rangle\otimes|00\rangle\otimes|00\rangle\otimes|11\rangle \\
&\quad +|00\rangle\otimes\sqrt{2}|\psi^+\rangle\otimes|11\rangle\otimes|00\rangle \\
&\quad +\sqrt{2}|\psi^+\rangle\otimes|00\rangle\otimes|11\rangle\otimes|00\rangle \\
&\quad +|00\rangle\otimes\sqrt{2}|\psi^+\rangle\otimes\sqrt{2}|\psi^+\rangle\otimes\sqrt{2}|\psi^+\rangle \\
&\quad +\sqrt{2}|\psi^+\rangle\otimes|00\rangle\otimes\sqrt{2}|\psi^+\rangle\otimes\sqrt{2}|\psi^+\rangle\Big) \\
&= \frac{1}{\sqrt{24}}\Big[\Big(|00\rangle\otimes\sqrt{2}|\psi^+\rangle+\sqrt{2}|\psi^+\rangle\otimes|00\rangle\Big)\otimes|00\rangle\otimes|11\rangle \\
&\quad +\Big(|00\rangle\otimes\sqrt{2}|\psi^+\rangle+\sqrt{2}|\psi^+\rangle\otimes|00\rangle\Big)\otimes|11\rangle\otimes|00\rangle \\
&\quad +\Big(|00\rangle\otimes\sqrt{2}|\psi^+\rangle+\sqrt{2}|\psi^+\rangle\otimes|00\rangle\Big)\otimes\sqrt{2}|\psi^+\rangle\otimes\sqrt{2}|\psi^+\rangle\Big] \\
&= \frac{1}{\sqrt{12}}\left(|00\rangle\otimes|\psi^+\rangle+|\psi^+\rangle\otimes|00\rangle\right)\otimes\left(|00\rangle\otimes|11\rangle+|11\rangle\otimes|00\rangle+2|\psi^+\rangle\otimes|\psi^+\rangle\right) \\
&= \frac{1}{\sqrt{24}}(|00010011\rangle+|00100011\rangle+|01000011\rangle+|10000011\rangle \\
&\quad +|00011100\rangle+|00101100\rangle+|01001100\rangle+|10001100\rangle \\
&\quad +|00010101\rangle+|00100101\rangle+|01000101\rangle+|10000101\rangle \\
&\quad +|00010110\rangle+|00100110\rangle+|01000110\rangle+|10000110\rangle \\
&\quad +|00011001\rangle+|00101001\rangle+|01001001\rangle+|10001001\rangle \\
&\quad +|00011010\rangle+|00101010\rangle+|01001010\rangle+|10001010\rangle)
\end{aligned}
$$

$|\kappa_{3,-1/2,2}\rangle$: $n=3, M=-\frac{1}{2}$

$$
|\phi_3\rangle = \frac{1}{\sqrt{12}}\left(|00\rangle\otimes|\psi^-\rangle+|\psi^-\rangle\otimes|00\rangle\right)\otimes\left(|00\rangle\otimes|11\rangle+|11\rangle\otimes|00\rangle+2|\psi^-\rangle\otimes|\psi^-\rangle\right)
$$

Specifically,

$$
\begin{aligned}
|\phi_3\rangle &= \frac{1}{\sqrt{24}}\Big(|00\rangle\otimes\sqrt{2}|\psi^-\rangle\otimes|00\rangle\otimes|11\rangle \\
&\quad +\sqrt{2}|\psi^-\rangle\otimes|00\rangle\otimes|00\rangle\otimes|11\rangle \\
&\quad +|00\rangle\otimes\sqrt{2}|\psi^-\rangle\otimes|11\rangle\otimes|00\rangle \\
&\quad +\sqrt{2}|\psi^-\rangle\otimes|00\rangle\otimes|11\rangle\otimes|00\rangle \\
&\quad +|00\rangle\otimes\sqrt{2}|\psi^-\rangle\otimes\sqrt{2}|\psi^-\rangle\otimes\sqrt{2}|\psi^-\rangle \\
&\quad +\sqrt{2}|\psi^-\rangle\otimes|00\rangle\otimes\sqrt{2}|\psi^-\rangle\otimes\sqrt{2}|\psi^-\rangle\Big) \\
&= \frac{1}{\sqrt{12}}\left(|00\rangle\otimes|\psi^-\rangle+|\psi^-\rangle\otimes|00\rangle\right)\otimes\left(|00\rangle\otimes|11\rangle+|11\rangle\otimes|00\rangle+2|\psi^-\rangle\otimes|\psi^-\rangle\right) \\
&= \frac{1}{\sqrt{24}}(|00010011\rangle-|00100011\rangle+|01000011\rangle-|10000011\rangle \\
&\quad +|00011100\rangle-|00101100\rangle+|01001100\rangle-|10001100\rangle \\
&\quad +|00010101\rangle-|00100101\rangle+|01000101\rangle-|10000101\rangle \\
&\quad -|00010110\rangle+|00100110\rangle-|01000110\rangle+|10000110\rangle \\
&\quad -|00011001\rangle+|00101001\rangle-|01001001\rangle+|10001001\rangle \\
&\quad +|00011010\rangle-|00101010\rangle+|01001010\rangle-|10001010\rangle)
\end{aligned}
$$

$|\kappa_{3,1/2,2}\rangle$: $n=3, M=\frac{1}{2}$

$$
|\phi_4\rangle = \frac{1}{\sqrt{12}}\left(|00\rangle\otimes|11\rangle+|11\rangle\otimes|00\rangle+2|\psi^-\rangle\otimes|\psi^-\rangle\right)\otimes\left(|00\rangle\otimes|\psi^-\rangle+|\psi^-\rangle\otimes|00\rangle\right)
$$

$$\begin{aligned}
|\phi_4\rangle &= \frac{1}{\sqrt{24}}\Big(|00\rangle\otimes|11\rangle\otimes|00\rangle\otimes\sqrt{2}|\psi^-\rangle \\
&\quad +|00\rangle\otimes|11\rangle\otimes\sqrt{2}|\psi^-\rangle\otimes|00\rangle \\
&\quad +|11\rangle\otimes|00\rangle\otimes|00\rangle\otimes\sqrt{2}|\psi^-\rangle \\
&\quad +|11\rangle\otimes|00\rangle\otimes\sqrt{2}|\psi^-\rangle\otimes|00\rangle \\
&\quad +\sqrt{2}|\psi^-\rangle\otimes\sqrt{2}|\psi^-\rangle\otimes|00\rangle\otimes\sqrt{2}|\psi^-\rangle \\
&\quad +\sqrt{2}|\psi^-\rangle\otimes\sqrt{2}|\psi^-\rangle\otimes\sqrt{2}|\psi^-\rangle\otimes|00\rangle\Big) \\
&= \frac{1}{\sqrt{12}}\big(|00\rangle\otimes|11\rangle+|11\rangle\otimes|00\rangle+2|\psi^-\rangle\otimes|\psi^-\rangle\big)\otimes\big(|00\rangle\otimes|\psi^-\rangle+|\psi^-\rangle\otimes|00\rangle\big) \\
&= \frac{1}{\sqrt{24}}(|00110001\rangle-|00110010\rangle+|00110100\rangle-|00111000\rangle \\
&\quad +|11000001\rangle-|11000010\rangle+|11000100\rangle-|11001000\rangle \\
&\quad +|01010001\rangle-|01010010\rangle+|01010100\rangle-|01011000\rangle \\
&\quad -|01100001\rangle+|01100010\rangle-|01100100\rangle+|01101000\rangle \\
&\quad -|10010001\rangle+|10010010\rangle-|10010100\rangle+|10011000\rangle \\
&\quad +|10100001\rangle-|10100010\rangle+|10100100\rangle-|10101000\rangle)
\end{aligned}$$

$|\lambda_{4,0}\rangle$: $n=4, M=0$

$$|\phi_5\rangle=\frac{1}{6}\big(|00\rangle\otimes|11\rangle+|11\rangle\otimes|00\rangle+2|\psi^+\rangle\otimes|\psi^+\rangle\big)\otimes\big(|00\rangle\otimes|11\rangle+|11\rangle\otimes|00\rangle+2|\psi^+\rangle\otimes|\psi^+\rangle\big)$$

$$\begin{aligned}
|\phi_5\rangle &= \frac{1}{\sqrt{36}}(|00\rangle\otimes|11\rangle\otimes|00\rangle\otimes|11\rangle \\
&\quad +|00\rangle\otimes|11\rangle\otimes|11\rangle\otimes|00\rangle \\
&\quad +|00\rangle\otimes|11\rangle\otimes\sqrt{2}|\psi^+\rangle\otimes\sqrt{2}|\psi^+\rangle \\
&\quad +|11\rangle\otimes|00\rangle\otimes|00\rangle\otimes|11\rangle \\
&\quad +|11\rangle\otimes|00\rangle\otimes|11\rangle\otimes|00\rangle \\
&\quad +|11\rangle\otimes|00\rangle\otimes\sqrt{2}|\psi^+\rangle\otimes\sqrt{2}|\psi^+\rangle \\
&\quad +\sqrt{2}|\psi^+\rangle\otimes\sqrt{2}|\psi^+\rangle\otimes|00\rangle\otimes|11\rangle \\
&\quad +\sqrt{2}|\psi^+\rangle\otimes\sqrt{2}|\psi^+\rangle\otimes|11\rangle\otimes|00\rangle \\
&\quad +\sqrt{2}|\psi^+\rangle\otimes\sqrt{2}|\psi^+\rangle\otimes\sqrt{2}|\psi^+\rangle\otimes\sqrt{2}|\psi^+\rangle\Big) \\
&= \frac{1}{6}\big(|00\rangle\otimes|11\rangle\otimes\big(|00\rangle\otimes|11\rangle+|11\rangle\otimes|00\rangle+2|\psi^+\rangle\otimes|\psi^+\rangle\big) \\
&\quad +|11\rangle\otimes|00\rangle\otimes\big(|00\rangle\otimes|11\rangle+|11\rangle\otimes|00\rangle+2|\psi^+\rangle\otimes|\psi^+\rangle\big) \\
&\quad +2|\psi^+\rangle\otimes|\psi^+\rangle\otimes\big(|00\rangle\otimes|11\rangle+|11\rangle\otimes|00\rangle+2|\psi^+\rangle\otimes|\psi^+\rangle\big)\big) \\
&= \frac{1}{6}\big(|00\rangle\otimes|11\rangle+|11\rangle\otimes|00\rangle+2|\psi^+\rangle\otimes|\psi^+\rangle\big)\otimes\big(|00\rangle\otimes|11\rangle+|11\rangle\otimes|00\rangle+2|\psi^+\rangle\otimes|\psi^+\rangle\big) \\
&= \frac{1}{6}(|00110011\rangle+|00111100\rangle+|00110101\rangle+|00110110\rangle+|00111001\rangle+|00111010\rangle \\
&\quad +|11000011\rangle+|11001100\rangle+|11000101\rangle+|11000110\rangle+|11001001\rangle+|11001010\rangle \\
&\quad +|01010011\rangle+|01011100\rangle+|01010101\rangle+|01010110\rangle+|01011001\rangle+|01011010\rangle \\
&\quad +|01100011\rangle+|01101100\rangle+|01100101\rangle+|01100110\rangle+|01101001\rangle+|01101010\rangle \\
&\quad +|10010011\rangle+|10011100\rangle+|10010101\rangle+|10010110\rangle+|10011001\rangle+|10011010\rangle \\
&\quad +|10100011\rangle+|10101100\rangle+|10100101\rangle+|10100110\rangle+|10101001\rangle+|10101010\rangle)
\end{aligned}$$