The rotated Hamiltonian in the $N = 2$ subspace is coming out as

$$\mathcal{H}_{\text{rot}} = U\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + U(1-\hat{n}_{1\uparrow})\hat{n}_{2\uparrow}\hat{n}_{2\downarrow} + \hat{n}_{1\uparrow}\left[\frac{U+\Delta}{2}\hat{n}_{2\uparrow} + \frac{U-\Delta}{2}\hat{n}_{2\downarrow}\right] \tag{1}$$

I defined

$$\begin{aligned} f_1^C &= \begin{pmatrix} c_{1\uparrow} \\ c_{2\downarrow}^\dagger \end{pmatrix}, f_2^C = \begin{pmatrix} c_{2\uparrow} \\ c_{1\downarrow}^\dagger \end{pmatrix} \\ f_1^S &= \begin{pmatrix} c_{1\uparrow} \\ c_{2\downarrow} \end{pmatrix}, f_2^S = \begin{pmatrix} c_{2\uparrow} \\ c_{1\downarrow} \end{pmatrix} \end{aligned} \tag{2}$$

These give

$$\begin{aligned} C_1^z &= (f_1^C)^\dagger \sigma_z f_1^C = \hat{n}_{1\uparrow} + \hat{n}_{2\downarrow} - 1 \\ C_2^z &= (f_2^C)^\dagger \sigma_z f_2^C = \hat{n}_{1\downarrow} + \hat{n}_{2\uparrow} - 1 \\ S_1^z &= (f_1^S)^\dagger \sigma_z f_1^S = \hat{n}_{1\uparrow} - \hat{n}_{2\downarrow} \\ S_2^z &= (f_2^S)^\dagger \sigma_z f_2^S = \hat{n}_{1\downarrow} - \hat{n}_{2\uparrow} \end{aligned} \tag{3}$$

But if I try to substitute these C and S instead of the number operators in the rotated Hamiltonian, it becomes extremely complicated. Do you have any idea where I might be going wrong?

$$\begin{aligned} \mathcal{H}_{\text{rot}} = &\frac{U}{4}(C_1^z + S_1^z + 1)(C_2^z - S_2^z + 1) + \\ &\frac{U}{8}(1 - C_1^z - S_1^z)(C_1^z - S_1^z + 1)(C_2^z + S_2^z + 1) + \\ &\frac{C_1^z + S_1^z + 1}{8}\left[U(C_1^z - S_1^z + C_2^z - S_2^z + 2) + \Delta(C_1^z - S_1^z - C_2^z + S_2^z)\right] \end{aligned} \tag{4}$$