

In the simple example, you write down the expression for  $\eta^\dagger$  from the *first off-diagonal equation*, take its conjugate to find  $\eta$  and go on to find the correct eigenvalues (and eigenvectors). An issue apparently arises if I take, instead, the *second off-diagonal equation* to calculate  $\eta$ , hence calculate  $\eta^\dagger$  and try to find the eigenstates and values.

## Eigenvalues

From second-off diagonal equation,

$$\begin{aligned}
\eta_1 &= \frac{-t}{\omega + \mu \hat{n}_2(1 - \hat{n}_1)} c_2^\dagger c_1 \\
\Rightarrow \eta_1^\dagger &= c_1^\dagger c_2 \frac{-t}{\omega + \mu \hat{n}_2(1 - \hat{n}_1)} \\
\eta_1 \eta_1^\dagger &= 1 - \hat{n}_1 \Rightarrow 1 - \hat{n}_1 = \frac{1}{\omega + \mu \hat{n}_2(1 - \hat{n}_1)} t^2 \hat{n}_2(1 - \hat{n}_1) \frac{1}{\omega + \mu \hat{n}_2(1 - \hat{n}_1)} \\
\Rightarrow [\omega + \mu \hat{n}_2(1 - \hat{n}_1)]^2 (1 - \hat{n}_1) &= t^2 \hat{n}_2(1 - \hat{n}_1) \\
\Rightarrow \overline{\omega(1 - \hat{n}_1) = t \hat{n}_2(1 - \hat{n}_1) - \mu \hat{n}_2(1 - \hat{n}_1)}
\end{aligned} \tag{1}$$

From what I understand,  $\omega = \begin{pmatrix} \hat{E}_1 & \\ & \hat{E}_1 \end{pmatrix}$ , so  $\omega(1 - \hat{n}_1)$  should just be the eigenblock  $\hat{E}_1 = (V - 2\mu)\hat{n}_2 + (t - \mu)(1 - \hat{n}_2)$ . In that case, there is a contradiction between the two methods.

## Eigenstates

The correct eigenstate corresponding to  $|10\rangle$  is  $U^\dagger |10\rangle = |10\rangle - |01\rangle$ , where  $|10\rangle$  means  $|\hat{n}_1 = 1, \hat{n}_2 = 0\rangle$ . If I now attempt to calculate the eigenstates using the alternative approach (just as I did for the eigenvalues), the following happens:

$$\begin{aligned}
U^\dagger |10\rangle &= (1 - \eta + \eta^\dagger) |10\rangle = |10\rangle - \eta |10\rangle & (\eta^\dagger |10\rangle = 0) \\
\text{Now, } \eta |10\rangle &= \frac{-t}{\omega + \mu \hat{n}_2(1 - \hat{n}_1)} c_2^\dagger c_1 |10\rangle = \frac{-t}{\omega + \mu \hat{n}_2(1 - \hat{n}_1)} |01\rangle \\
\text{But, } (\omega + \mu \hat{n}_2(1 - \hat{n}_1)) |01\rangle &= \left[ \begin{pmatrix} \hat{E}_1 & \\ & \hat{E}_1 \end{pmatrix} + \mu \right] \begin{pmatrix} 0 \\ |\hat{n}_2 = 1\rangle \end{pmatrix} = \begin{pmatrix} 0 \\ (\hat{E}_1 + \mu) |\hat{n}_2 = 1\rangle \end{pmatrix}
\end{aligned} \tag{2}$$

Using  $\hat{E}_1 |\hat{n}_2 = 1\rangle = [(V - 2\mu)\hat{n}_2 + (t - \mu)(1 - \hat{n}_2)] |\hat{n}_2 = 1\rangle = (V - 2\mu) |\hat{n}_2 = 1\rangle$ , the final expression for  $(\omega + \mu \hat{n}_2(1 - \hat{n}_1)) |10\rangle$  becomes

$$\begin{aligned}
(\omega + \mu \hat{n}_2(1 - \hat{n}_1)) |10\rangle &= \begin{pmatrix} 0 \\ (V - 2\mu + \mu) |\hat{n}_2 = 1\rangle \end{pmatrix} = (V - \mu) |01\rangle \\
\text{therefore, } \eta |10\rangle &= \frac{-t}{V - \mu} |01\rangle
\end{aligned} \tag{3}$$

$$\text{which means, } \overline{U^\dagger |10\rangle = |10\rangle + \frac{t}{V - \mu} |01\rangle}$$

This is in conflict with the actual eigenvalue  $|10\rangle - |01\rangle$ .