

For 2 momentum Hubbard model, we have :-

$$H = \sum_{k\sigma} (\epsilon_{k\sigma}^0 - \mu_{eff}) \hat{n}_{k\sigma} + U_0 (\tilde{\mathbf{C}}^2 - \tilde{\mathbf{S}}^2)$$

Here, $\tilde{\mathbf{C}} = \sum_{k\sigma} \vec{C}_{k\sigma}$, and $\tilde{\mathbf{S}} = \sum_{k\sigma} \vec{S}_{k\sigma}$. $\vec{S}_{k\sigma} = \frac{1}{2} f_k^s \vec{\sigma} f_k^s$ and $\vec{C}_{k\sigma} = \frac{1}{2} f_k^{c\dagger} \vec{\sigma} f_k^c$. The f^s and f^c are defined as :-

$$f_k^s = \begin{bmatrix} c_{k\uparrow} \\ c_{-k\downarrow} \end{bmatrix}$$

and

$$f_k^c = \begin{bmatrix} c_{k\uparrow} \\ c_{-k\downarrow}^\dagger \end{bmatrix}$$

Using this notation, we ultimately get the Hamiltonian as (for $\mu_{eff} = 0$) :-

$$H = \begin{bmatrix} H_{\Lambda\downarrow,e} n_{\Lambda\downarrow} & c_{\Lambda\downarrow}^\dagger T_{\Lambda\downarrow} \\ T_{\Lambda\downarrow}^\dagger c_{\Lambda\downarrow} & H_{\Lambda\downarrow,h} (1 - n_{\Lambda\downarrow}) \end{bmatrix}$$

where

$$\begin{aligned} H_{\Lambda\downarrow,e} &= \epsilon_0 + \frac{1}{2} + \frac{1}{4} [n_{\Lambda\downarrow} - n_{\Lambda\uparrow} + n_{-\Lambda\downarrow} - n_{-\Lambda\uparrow}] \\ H_{\Lambda\downarrow,h} &= \frac{1}{2} + \frac{1}{4} [(1 - n_{\Lambda\downarrow}) - n_{\Lambda\uparrow} + (1 - n_{-\Lambda\downarrow}) - n_{-\Lambda\uparrow}] \\ T_{\Lambda\downarrow} &= (c_{-\Lambda\uparrow}^\dagger c_{\Lambda\uparrow} - c_{\Lambda\uparrow}^\dagger c_{-\Lambda\uparrow}) c_{-\Lambda\downarrow} \end{aligned}$$

Now, we have

$$\hat{\eta} = \frac{1}{(E_{\Lambda\downarrow,h} - H_{\Lambda\downarrow,h} (1 - n_{\Lambda\downarrow}))} T_{\Lambda\downarrow}^\dagger c_{\Lambda\downarrow} = G_h E_{\Lambda\downarrow} T_{\Lambda\downarrow}^\dagger c_{\Lambda\downarrow}$$

and

$$U = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & \hat{\eta}^\dagger \\ -\hat{\eta} & 1 \end{bmatrix}$$

We want to rotate away the $\Lambda\downarrow$ node, i.e. block diagonalize the H-matrix.

After applying the unitary transformation, we have :-

$$\begin{aligned} & H^{(1)} \\ &= U H U^\dagger \\ &= \begin{bmatrix} H_{\Lambda\downarrow,e} n_{\Lambda\downarrow} + \hat{\eta}^\dagger T_{\Lambda\downarrow}^\dagger c_{\Lambda\downarrow} + c_{\Lambda\downarrow}^\dagger T_{\Lambda\downarrow} \hat{\eta} + \hat{\eta}^\dagger H_{\Lambda\downarrow,h} (1 - n_{\Lambda\downarrow}) \hat{\eta} & c_{\Lambda\downarrow}^\dagger T_{\Lambda\downarrow} - H_{\Lambda\downarrow,e} n_{\Lambda\downarrow} \hat{\eta}^\dagger - \hat{\eta}^\dagger T_{\Lambda\downarrow}^\dagger c_{\Lambda\downarrow} \hat{\eta} + \hat{\eta}^\dagger H_{\Lambda\downarrow,h} (1 - n_{\Lambda\downarrow}) \\ T_{\Lambda\downarrow}^\dagger c_{\Lambda\downarrow} - \hat{\eta} H_{\Lambda\downarrow,e} n_{\Lambda\downarrow} - \hat{\eta}^\dagger c_{\Lambda\downarrow}^\dagger T_{\Lambda\downarrow} \hat{\eta} + H_{\Lambda\downarrow,h} (1 - n_{\Lambda\downarrow}) \hat{\eta} & H_{\Lambda\downarrow,h} (1 - n_{\Lambda\downarrow}) + \hat{\eta} H_{\Lambda\downarrow,e} n_{\Lambda\downarrow} \hat{\eta}^\dagger - T_{\Lambda\downarrow}^\dagger c_{\Lambda\downarrow} \hat{\eta}^\dagger - \hat{\eta} c_{\Lambda\downarrow}^\dagger T_{\Lambda\downarrow} \end{bmatrix} \end{aligned}$$

Calculating the off-diagonal element term by term, we get :-

$$\begin{aligned} \hat{\eta}^\dagger T_{\Lambda\downarrow}^\dagger c_{\Lambda\downarrow} \hat{\eta} &= -c_{\Lambda\downarrow}^\dagger T_{\Lambda\downarrow} G_h E_{\Lambda\downarrow} T_{\Lambda\downarrow} c_{\Lambda\downarrow} c_{\Lambda\downarrow}^\dagger T_{\Lambda\downarrow} G_h E_{\Lambda\downarrow} = -c_{\Lambda\downarrow}^\dagger T_{\Lambda\downarrow} \left[\frac{1}{(E_{\Lambda\downarrow} - H_{\Lambda\downarrow,h})^2 (1 - n_{\Lambda\downarrow})} \{ n_{\Lambda\uparrow} (1 - n_{-\Lambda\uparrow}) + n_{-\Lambda\uparrow} (1 - n_{\Lambda\uparrow}) \} n_{-\Lambda\downarrow} \right] \\ H_{\Lambda\downarrow,e} n_{\Lambda\downarrow} \hat{\eta}^\dagger &= c_{\Lambda\downarrow}^\dagger T_{\Lambda\downarrow} \frac{\epsilon_0 - H_{\Lambda\downarrow,h}}{(\epsilon_0 - E_{\Lambda\downarrow}) - H_{\Lambda\downarrow,h}} \\ \hat{\eta}^\dagger H_{\Lambda\downarrow,h} (1 - n_{\Lambda\downarrow}) &= c_{\Lambda\downarrow}^\dagger T_{\Lambda\downarrow} \frac{H_{\Lambda\downarrow,h}}{(E_{\Lambda\downarrow}) - H_{\Lambda\downarrow,h}} \end{aligned}$$

This gives an equation for $E_{\Lambda\downarrow}$, whose solution is the required operator-valued eigenvalue for the block diagonalization.