$$
\begin{aligned}
\therefore \hat{n}_{N\sigma}\mathcal{H}_{2N}\hat{P}(1-\hat{n}_{N\sigma}) &= \frac{1}{2}(H_e\hat{n}_{N\sigma}+c^\dagger\hat{T})(1+\eta^\dagger)(1-\hat{n}_{N\sigma}) \\
&= \frac{1}{2}(H_e\hat{n}_{N\sigma}+H_e\hat{n}_{N\sigma}\eta^\dagger+c^\dagger T+c^\dagger T\eta^\dagger)(1-\hat{n}_{N\sigma}) \\
&= \frac{1}{2}H_e\hat{n}_{N\sigma}\eta^\dagger(1-\hat{n}_{N\sigma})+c^\dagger T(1-\hat{n}_{N\sigma})+\frac{1}{2}c^\dagger T\eta^\dagger(1-\hat{n}_{N\sigma}) \\
&= \frac{1}{2}H_e\hat{n}_{N\sigma}\eta^\dagger+\frac{1}{2}c^\dagger T \\
&\Big(\because \eta^\dagger(1-\hat{n}_{N\sigma})=\eta^\dagger, c^\dagger(1-\hat{n}_{N\sigma})=c^\dagger, c^\dagger\eta^\dagger=0\Big)
\end{aligned} \tag{68}
$$

Combining the final equations of 66 and 68, we get

$$
c^\dagger_{N\sigma}\hat{T}_{N\sigma}+H_e\hat{n}_{N\sigma}\eta^\dagger_{N\sigma}=\mathcal{H}'\eta^\dagger_{N\sigma} \implies \eta^\dagger_{N\sigma}=\frac{1}{\mathcal{H}'-H_e\hat{n}_{N\sigma}}c^\dagger_{N\sigma}\hat{T}_{N\sigma} \tag{69}
$$

Defining $\hat{G}_e(\hat{E}_{N\sigma})=\frac{1}{\mathcal{H}'-H_e\hat{n}_{N\sigma}}$,

$$
\boxed{\eta^\dagger_{N\sigma}=\hat{G}_e(\hat{E}_{N\sigma})c^\dagger_{N\sigma}\hat{T}_{N\sigma}} \tag{70}
$$

This expresses the electron-hole transition operator in terms of the eigenblock $\hat{E}_{N\sigma}$.

The expression for η is obtained using $(1-\hat{n}_{N\sigma})\mathcal{H}_{2N}\hat{P}\hat{n}_{N\sigma}=(1-\hat{n}_{N\sigma})\mathcal{H}'\hat{P}\hat{n}_{N\sigma}$

$$
\hat{P}\hat{n}_{N\sigma}=\frac{1}{2}(1+\eta+\eta^\dagger)\hat{n}_{N\sigma}=\frac{1}{2}(\hat{n}_{N\sigma}+\eta) \quad \Big(\because \eta\hat{n}_{N\sigma}=\eta, \eta^\dagger\hat{n}_{N\sigma}=0\Big) \tag{71}
$$

$$
(1-\hat{n}_{N\sigma})\mathcal{H}_{2N}=(H_h(1-\hat{n}_{N\sigma})+\hat{T}^\dagger c) \tag{72}
$$

$$
(1-\hat{n}_{N\sigma})\mathcal{H}_{2N}\hat{P}\hat{n}_{N\sigma}=\frac{1}{2}H_h(1-\hat{n}_{N\sigma})\eta+\frac{1}{2}\hat{T}^\dagger c\hat{n}_{N\sigma}+\frac{1}{2}\hat{T}^\dagger c\eta=\frac{1}{2}H_h(1-\hat{n}_{N\sigma})\eta+\frac{1}{2}\hat{T}^\dagger c \quad (\because c\hat{n}_{N\sigma}=c, c\eta=0) \tag{73}
$$

$$
(1-\hat{n}_{N\sigma})\mathcal{H}'\hat{P}\hat{n}_{N\sigma}=\frac{1}{2}\mathcal{H}'(1-\hat{n}_{N\sigma})\eta=\frac{1}{2}\mathcal{H}'\eta \tag{74}
$$

Combining 73 and 74, we get

$$
\boxed{\eta_{N\sigma}=G_h(\hat{E}_{N\sigma})\hat{T}^\dagger_{N\sigma}c_{N\sigma}} \tag{75}
$$

where $G_h(\hat{E}_{N\sigma}=\frac{1}{\mathcal{H}'-H_h(1-\hat{n}_{N\sigma})}$

The expression for the eigenblock $\hat{E}_{N\sigma}$ is obtained using $\hat{n}_{N\sigma}\mathcal{H}_{2N}\hat{P}\hat{n}_{N\sigma} = \hat{n}_{N\sigma}\mathcal{H}'\hat{P}\hat{n}_{N\sigma}$

$$
\begin{aligned}
\hat{n}_{N\sigma}\mathcal{H}_{2N}\hat{P}\hat{n}_{N\sigma} &= \frac{1}{2}(H_e\hat{n}_{N\sigma} + c^\dagger\hat{T})(\hat{n}_{N\sigma} + \eta) = \frac{1}{2}\left(H_e\hat{n}_{N\sigma} + H_e\hat{n}_{N\sigma}\eta + c^\dagger T\hat{n}_{N\sigma} + c^\dagger T\eta\right)\\
&= \frac{1}{2}\left(H_e\hat{n}_{N\sigma} + c^\dagger T\eta\right)\\
&\left(\because \hat{n}_{N\sigma}\eta = 0, c^\dagger\hat{T}\hat{n}_{N\sigma} = \hat{T}c^\dagger\hat{n}_{N\sigma} = 0\right)\\
\hat{n}_{N\sigma}\mathcal{H}'\hat{P}\hat{n}_{N\sigma} &= \frac{1}{2}\hat{n}_{N\sigma}\mathcal{H}'(\hat{n}_{N\sigma} + \eta) = \frac{1}{2}\left(\hat{n}_{N\sigma}\mathcal{H}'\hat{n}_{N\sigma} + \hat{n}_{N\sigma}\mathcal{H}'\eta\right) = \frac{1}{2}\hat{E}_{N\sigma}\hat{n}_{N\sigma}\\
&\left(\because \hat{n}_{N\sigma}\mathcal{H}'\hat{n}_{N\sigma} = \hat{E}\hat{n}_{N\sigma}, \hat{n}_{N\sigma}\mathcal{H}'\eta = \mathcal{H}'\hat{n}_{N\sigma}\eta = 0\right)
\end{aligned}
\tag{76}
$$

Combining,

$$
\boxed{\hat{E}_{N\sigma}\hat{n}_{N\sigma} = H_e\hat{n}_{N\sigma} + c^\dagger_{N\sigma}\hat{T}_{N\sigma}\eta_{N\sigma}} \tag{77}
$$

The expression for the lower eigenblock $\hat{E}'_{N\sigma}$ is obtained by repeating the last stuff with $\mathcal{H}''$:

$$
\begin{aligned}
&\mathcal{H}_{2N}(1-\hat{P}) = \mathcal{H}''(1-\hat{P})\\
\implies &(1-\hat{n}_{N\sigma})\mathcal{H}_{2N}(1-\hat{P})(1-\hat{n}_{N\sigma}) = (1-\hat{n}_{N\sigma})\mathcal{H}''(1-\hat{P})(1-\hat{n}_{N\sigma})
\end{aligned}
\tag{78}
$$

Now,

$$
(1-\hat{P})(1-\hat{n}_{N\sigma}) = \frac{1}{2}(1-\eta-\eta^\dagger)(1-\hat{n}_{N\sigma}) = \frac{1}{2}\left((1-\hat{n}_{N\sigma}) - \eta^\dagger\right) \tag{79}
$$

Therefore,

$$
\begin{aligned}
(1-\hat{n}_{N\sigma})\mathcal{H}_{2N}(1-\hat{P})(1-\hat{n}_{N\sigma}) &= \frac{1}{2}(H_h(1-\hat{n}_{N\sigma}) + \hat{T}^\dagger c)(1-\hat{n}_{N\sigma} - \eta^\dagger)\\
&= \frac{1}{2}\left(H_h(1-\hat{n}_{N\sigma}) - \hat{T}^\dagger c\eta^\dagger\right)\\
&\left(\because (1-\hat{n}_{N\sigma})\eta^\dagger = 0, c(1-\hat{n}_{N\sigma}) = 0\right)\\
(1-\hat{n}_{N\sigma})\mathcal{H}''(1-\hat{P})(1-\hat{n}_{N\sigma}) &= \frac{1}{2}\hat{(}1-\hat{n}_{N\sigma})H''(1-\hat{n}_{N\sigma}) = \frac{1}{2}\hat{E}'(1-\hat{n}_{N\sigma})
\end{aligned}
\tag{80}
$$

Combining the last two equations,

$$
\boxed{\hat{E}'_{N\sigma}(1-\hat{n}_{N\sigma}) = H_h(1-\hat{n}_{N\sigma}) - \hat{T}^\dagger_{N\sigma}c_{N\sigma}\eta^\dagger_{N\sigma}} \tag{81}
$$

3.4 A Simple Example

$$\mathcal{H} = -t\left(c_2^\dagger c_1 + c_1^\dagger c_2\right) + V\hat{n}_1\hat{n}_2 - \mu(\hat{n}_1+\hat{n}_2) \quad \hat{n}_i = c_i^\dagger c_i = \begin{pmatrix} V-2\mu & 0 & 0 & 0 \\ 0 & -\mu & -t & 0 \\ 0 & -t & \mu & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{82}$$

The basis used is the ordered set $\{|11\rangle, |10\rangle, |01\rangle, |00\rangle\}$

For this problem, we take $N\sigma \equiv 1$. 1 refers to the first site. First step is to represent the Hamiltonian in block matrix form (equation 49).

$$\begin{aligned} \hat{H}_{1,e} &= Tr_1[\mathcal{H}\hat{n}_1] \\ &= Tr_1[V\hat{n}_1\hat{n}_2 - \mu(\hat{n}_1+\hat{n}_2)] \quad \left(c \text{ and } c^\dagger \text{ will not conserve the eigenvalue of } \hat{n}\right) \\ &= V\hat{n}_2 - \mu(1+\hat{n}_2) \qquad\qquad (Tr_1[V\hat{n}_1\hat{n}_2] = VTr_1[\hat{n}_1]\hat{n}_2 = V\hat{n}_2) \\ &= (V-2\mu)\hat{n}_2 - \mu(1-\hat{n}_2) \end{aligned} \tag{83}$$

Next is calculation of $\hat{H}_{1,h}$:

$$\hat{H}_{1,h} = Tr_1[\mathcal{H}(1-\hat{n}_1)] = -\mu\hat{n}_2 \tag{84}$$

Next is calculation of $T_{1,e-h}$.

$$\begin{aligned} T_{1,e-h} &= Tr_1[\mathcal{H}c_1] \\ &= Tr_1[-tc_1^\dagger c_2 c_1] = -tc_2 \quad \text{(the only term that conserves eigenvalue of } \hat{n}) \end{aligned} \tag{85}$$

Therefore, $T^\dagger_{1,e-h} = -tc_2^\dagger$. The block matrix form becomes

$$\mathcal{H} = \begin{pmatrix} (V-2\mu)\hat{n}_2 - \mu(1-\hat{n}_2) & -tc_2 \\ -tc_2^\dagger & -\mu\hat{n}_2 \end{pmatrix} \tag{86}$$

The block-diagonal form is, as usual, $\overline{\mathcal{H}} = \begin{pmatrix} \hat{E}_1 & 0 \\ 0 & \hat{E}'_1 \end{pmatrix}$

The expression of $\eta^\dagger$ is $\hat{\eta}^\dagger = \hat{G}_e c_1^\dagger \hat{T}_{1,e-h} = G_e c_1^\dagger(-tc_2)$. Hence, $\eta = -tc_2^\dagger c_1 G_e^\dagger$. Since $H_e^\dagger = H_e$ for this problem, we have $\eta = -tc_2^\dagger c_1 G_e$. It was proved in the formalism that $\eta^\dagger\eta = \hat{n}_1$. Therefore,

$$\begin{aligned} t^2 G_e c_1^\dagger c_2 c_2^\dagger c_1 G_e = \hat{n}_1 &\implies t^2\hat{n}_1(1-\hat{n}_2) = \hat{n}_1\{G_e^{-1}\}^2 = \hat{n}_1(\mathcal{H}' - H_e\hat{n}_1)^2 \\ &\implies t^2\hat{n}_1^2(1-\hat{n}_2)^2 = (\mathcal{H}'\hat{n}_1 - H_e\hat{n}_1)^2 \\ &\implies \mathcal{H}'\hat{n}_1 = H_e\hat{n}_1 + t\hat{n}_1(1-\hat{n}_2) = (V-2\mu)\hat{n}_1\hat{n}_2 + (t-\mu)\hat{n}_1(1-\hat{n}_2) \end{aligned} \tag{87}$$

This equation gives the upper block of the diagonalised Hamiltonian. Why the upper block? Because it is multiplied by $\hat{n}_1$, and hence can give non-zero contribution only in the upper block. It is also obvious that the upper block itself is internally diagonal in $\hat{n}_2$; this is seen from the fact that the expression of $\mathcal{H}'\hat{n}_1$ has no c_2 or $c_2^\dagger$, only $\hat{n}_2$. The term multiplying $\hat{n}_2$ becomes the upper matrix element in the block of $\hat{n}_2$, while that multiplying $1-\hat{n}_2$ becomes the lower element. Summarizing,

$$\overline{\mathcal{H}} = \mathcal{H}'\hat{n}_1 + \mathcal{H}''(1-\hat{n}_1) = \begin{pmatrix} \begin{matrix} V-2\mu & 0 \\ 0 & t-\mu \end{matrix} & \mathbf{0}_{2x2} \\ \mathbf{0}_{2x2} & (\hat{E}_1')_{2x2} \end{pmatrix} \tag{88}$$

The $\hat{E}'$ is the contribution from $\mathcal{H}''$; just as $\mathcal{H}\hat{n}_1$ gives the upper block contribution, $\mathcal{H}''$ gives the lower contribution. And since $\mathcal{H}'' = \begin{pmatrix} \hat{E}' & 0 \\ 0 & \hat{E}' \end{pmatrix}$, we end up with $\hat{E}'$ in the lower block of $\overline{\mathcal{H}}$. It still remains to compute $\mathcal{H}''(1-\hat{n}_1) = \hat{E}'(1-\hat{n}_1)$. But that is easy because we already have the expression for that, equation 81.

$$E_1'(1-\hat{n}_1) = H_h(1-\hat{n}_1) - \hat{T}_1^\dagger c_1 \eta^\dagger = -\mu(1-\hat{n}_1)\hat{n}_2 - t^2 c_2^\dagger c_1 G_e c_1^\dagger \hat{c}_2 \tag{89}$$

This is the expression for the lower block. But to get the final matrix elements, we need to resolve it in $\hat{n}_2$. That is, the upper matrix element of the lower block will be $\langle 01| E'(1-\hat{n}_1) |01\rangle$ and the lower element will be $\langle 00| E'(1-\hat{n}_1) |00\rangle$. The bra and ket are written in the notation $\langle n_1, n_2|, |n_1, n_2\rangle$. Since this is the lower block in the representation of $\hat{n}_1$, n_1 will always be zero while calculating the elements of $\hat{E}'$. $n_2 = 1(0)$ means the upper(lower) diagonal element. Similarly, $\langle 01| E'(1-\hat{n}_1) |00\rangle$ is an off-diagonal element.

It is easy to see that the off-diagonal terms will be zero. The lower diagonal term will also be zero: $\hat{n}_2 |n_1, 0\rangle = c_2 |n_1, 0\rangle = 0$. Thus the only non-zero term is

$$\langle 01| E'(1-\hat{n}_1) |01\rangle = -\mu - t^2 \langle 10| G_e |10\rangle \tag{90}$$

Now,

$$\begin{aligned} \langle 10| G_e^{-1} |10\rangle &= \langle 10| H' - (V-\mu)\hat{n}_1\hat{n}_2 + \mu\hat{n}_1 |10\rangle \\ &= \langle 10| \mathcal{H}' |10\rangle + \mu = \langle 10| \mathcal{H}'\hat{n}_1 |10\rangle + \mu \\ &= \langle 10| (V-2\mu)\hat{n}_1\hat{n}_2 + (t-\mu)\hat{n}_1(1-\hat{n}_2) |10\rangle + \mu \\ &= t - \mu + \mu = t \\ \therefore \langle 10| G_e |10\rangle &= \frac{1}{t} \end{aligned} \tag{91}$$

Therefore, $\langle 01| E'(1-\hat{n}_1)|01\rangle = -\mu - t^2\frac{1}{t} = -\mu - t$. The final diagonalized matrix becomes

$$\overline{\mathcal{H}} = \begin{array}{c} \begin{array}{cccc} |11\rangle & |10\rangle & |01\rangle & |00\rangle \end{array} \\ \begin{pmatrix} (V-2\mu) & 0 & 0 & 0 \\ \\ 0 & (t-\mu) & 0 & 0 \\ \\ 0 & 0 & -(\mu+t) & 0 \\ \\ 0 & 0 & 0 & 0 \end{pmatrix} \end{array} \tag{92}$$

3.4.1 The Eigenstates

The unitarily transformed Hamiltonian, $\overline{\mathcal{H}}$ is diagonal in the basis of $\hat{n}$. This implies that the eigenstates of the original Hamiltonian $\mathcal{H}$ are the unitarily transformed versions of the eigenkets of $\hat{n}$:

$$\mathcal{H}(\hat{U}^\dagger_{N\sigma}|n_1,n_2\rangle) = \hat{U}^\dagger_{N\sigma}\overline{\mathcal{H}}|n_1,n_2\rangle = \hat{U}^\dagger_{N\sigma}E_{n_1,n_2}|n_1,n_2\rangle = E_{n_1,n_2}(\hat{U}^\dagger_{N\sigma}|n_1,n_2\rangle) \tag{93}$$

To find the eigenvectors $\hat{U}^\dagger_{N\sigma}|n_1,n_2\rangle$, we need to find the $\hat{U}_{N\sigma}$. From equation ??, we have $\hat{U}_{N\sigma} = \frac{1}{\sqrt{2}}\left(1+\hat{\eta}^\dagger-\hat{\eta}\right)$.
To get the eigenstates of $\mathcal{H}$, I act with $U^\dagger$ on the eigenstates ($|n_1,n_2\rangle$):

$$\hat{U}^\dagger_{N\sigma}|11\rangle = |11\rangle \tag{94}$$

$$\hat{U}^\dagger_{N\sigma}|00\rangle = |00\rangle, \tag{95}$$

$$\begin{aligned}\hat{U}^\dagger_{N\sigma}|10\rangle = \frac{1}{2}(|10\rangle - \eta|10\rangle) = \frac{1}{2}\left(|10\rangle + tc_2^\dagger c_1\hat{G}_e|10\rangle\right) = \frac{1}{2}\left(|10\rangle + tc_2^\dagger c_1\frac{1}{t}|01\rangle\right) \\ = \frac{1}{2}(|10\rangle + |01\rangle)\end{aligned} \tag{96}$$

$$\hat{U}^\dagger_{N\sigma}|01\rangle = \frac{1}{2}\left(|01\rangle + \eta^\dagger|01\rangle\right) = \frac{1}{2}\left(|01\rangle - t\hat{G}_e c_1^\dagger c_2|01\rangle\right) = \frac{1}{2}(|01\rangle - |10\rangle) \tag{97}$$

The eigenstates come out to be (upto a normalizaiton):

$$\begin{aligned} &|00\rangle \\ &|10\rangle + |01\rangle \\ &|01\rangle - |10\rangle \\ &|11\rangle \end{aligned} \tag{98}$$

3.5 Applying the RG on the Hubbard dimer

$$
\begin{aligned}
\mathcal{H} &= -t\sum_\sigma (c^\dagger_{1\sigma}c_{2\sigma} + c^\dagger_{2\sigma}c_{1\sigma}) + U\left(\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow}\right)\\
H_e &= Tr_{\hat{n}_{1\uparrow}}(\mathcal{H}\hat{n}_{1\uparrow}) = U(\hat{n}_{1\downarrow} + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow}) - t(c^\dagger_{1\downarrow}c_{2\downarrow} + c^\dagger_{2\downarrow}c_{1\downarrow})\\
H_h &= Tr_{\hat{n}_{1\uparrow}}(\mathcal{H}(1-\hat{n}_{1\uparrow})) = U\hat{n}_{2\uparrow}\hat{n}_{2\downarrow} - t(c^\dagger_{1\downarrow}c_{2\downarrow} + c^\dagger_{2\downarrow}c_{1\downarrow})\\
T &= Tr_{\hat{n}_{1\uparrow}}(\mathcal{H}c_{1\uparrow}) = -tc_{2\uparrow}\\
T^\dagger &= Tr_{\hat{n}_{1\uparrow}}(c^\dagger_{1\uparrow}\mathcal{H}) = -tc^\dagger_{2\uparrow}\\
\eta^\dagger_{1\uparrow} &= G_e c^\dagger_{1\uparrow}T = -t\hat{G}_e c^\dagger_{1\uparrow}c_{2\uparrow} = -t(\mathcal{H}'_{1\uparrow} - H_e\hat{n})^{-1}c^\dagger_{1\uparrow}c_{2\uparrow}\\
\therefore \eta_{1\uparrow} &= -tc^\dagger_{2\uparrow}c_{1\uparrow}(\mathcal{H}'_{1\uparrow} - H_e\hat{n})^{-1}\\
\eta^\dagger_{1\uparrow}\eta_{1\uparrow} = \hat{n}_{1\uparrow} &\implies t^2(1-\hat{n}_{2\uparrow}) = (\mathcal{H}'_{1\uparrow} - H_e\hat{n}_{1\uparrow})^2\hat{n}_{1\uparrow} \implies \mathcal{H}'_{1\uparrow}\hat{n}_{1\uparrow} = H_e\hat{n}_{1\uparrow} + t(1-\hat{n}_{2\uparrow})\hat{n}_{1\uparrow}
\end{aligned}
\tag{99}
$$

$$
\mathcal{H}'_{1\uparrow}\hat{n}_{1\uparrow} = U\hat{n}_{1\uparrow}(\hat{n}_{1\downarrow} + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow}) + t\hat{n}_{1\uparrow}(1 - \hat{n}_{2\uparrow} - c^\dagger_{1\downarrow}c_{2\downarrow} - c_{1\downarrow}c^\dagger_{2\downarrow}) \tag{100}
$$

The upper block is not diagonal, and has to be further diagonalised. The block is given by

$$
\boxed{\hat{E}_{1\uparrow} = \langle\hat{n}_{1\uparrow} = 1|\,\mathcal{H}'_{1\uparrow}\hat{n}_{1\uparrow}\,|\hat{n}_{1\uparrow} = 1\rangle = U(\hat{n}_{1\downarrow} + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow}) + t(1 - \hat{n}_{2\uparrow} - c^\dagger_{1\downarrow}c_{2\uparrow} - c^\dagger_{2\uparrow}c_{1\downarrow})} \tag{101}
$$

To calculate the eigenvalues of the upper block, we take $\hat{E}_{1\uparrow}$ as the new Hamiltonian $\mathcal{H}_{1\downarrow}$and this time trace out $\hat{n}_{1\downarrow}$.

$$
\begin{aligned}
H_e &= Tr_{\hat{n}_{1\downarrow}}(\mathcal{H}_{1\downarrow}\hat{n}_{1\downarrow}) = U(1 + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow}) + t(1-\hat{n}_{2\uparrow})\\
H_h &= U\hat{n}_{2\uparrow}\hat{n}_{2\downarrow} + t(1-\hat{n}_{2\uparrow})\\
T &= -tc_{2\downarrow}\\
T^\dagger &= -tc^\dagger_{2\downarrow}\\
\eta^\dagger_{1\downarrow} &= \hat{G}_e c^\dagger_{1\downarrow}T = -t\hat{G}_e c^\dagger_{1\downarrow}c_{2\downarrow}\\
\implies \eta_{1\downarrow} &= -tc^\dagger_{2\downarrow}c_{1\downarrow}\hat{G}_e
\end{aligned}
\tag{102}
$$

Then,

$$
\eta^\dagger_{1\downarrow}\eta_{1\downarrow} = \hat{n}_{1\downarrow} \implies \mathcal{H}'_{1\downarrow}\hat{n}_{1\downarrow} = H_e\hat{n}_{1\downarrow} + t\hat{n}_{1\downarrow}(1-\hat{n}_{2\downarrow}) = U\hat{n}_{1\downarrow}(1 + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow}) + 2t\hat{n}_{1\downarrow}(1-\hat{n}_{2\downarrow}) \tag{103}
$$

This gives the upper block of the $\hat{n}_{1\uparrow} = 1$ sector (that is, the $\hat{n}_{1\uparrow} = 1, \hat{n}_{1\downarrow} = 1$ sector); the matrix element is given by $\hat{E}_{1\downarrow} = \langle\hat{n}_{1\downarrow} = 1|\,\mathcal{H}'_{1\downarrow}\hat{n}_{1\downarrow}\,|\hat{n}_{1\downarrow} = 1\rangle$

$$E_{\hat{n}_{1\downarrow}} = U(\hat{n}_{2\uparrow}\hat{n}_{2\downarrow}+1) + 2t(1-\hat{n}_{2\downarrow}) = \begin{pmatrix} 2U & & & \\ & U+2t & & \\ & & U & \\ & & & U+2t \end{pmatrix} \tag{104}$$

The lower block of $\hat{n}_{1\uparrow}=1$ sector($\hat{n}_{1\uparrow}=1, \hat{n}_{1\downarrow}=0$), that is, $E'_{1\downarrow}$, can again be determined using the formula for the lower blocks.

$$\mathcal{H}''_{1\downarrow}\hat{n}_{1\downarrow} = H_h(1-\hat{n}_{1\downarrow}) - T^\dagger c_{1\downarrow}\eta^\dagger_{1\downarrow} = H_h(1-\hat{n}_{1\downarrow}) - t^2 c^\dagger_{2\downarrow}c_{1\downarrow}G_e c^\dagger_{1\downarrow}c_{2\downarrow} \tag{105}$$

The matrix element, $\hat{E}'_{1\downarrow} = \langle \hat{n}_{1\downarrow}=0|\,\mathcal{H}''(1-\hat{n}_{1\downarrow})\,|\hat{n}_{1\downarrow}=0\rangle = H_h - t^2 c^\dagger_{2\downarrow}\langle 1|\,G_e\,|1\rangle\, c_{2\downarrow}$

$$\begin{aligned} \langle 1|\,G_e^{-1}\,|1\rangle = \langle 1|\,\mathcal{H}'_{1\downarrow} - H_e\hat{n}_{1\downarrow}\,|1\rangle = \langle 1|\,\mathcal{H}'_{1\downarrow}\hat{n}_{1\downarrow} - H_e\hat{n}_{1\downarrow}\,|1\rangle = t(1-\hat{n}_{2\downarrow}) \\ \therefore \hat{E}'_{1\downarrow} = H_h - tc^\dagger_{2\downarrow}\frac{1}{1-\hat{n}_{2\downarrow}}c_{2\downarrow} = H_h - t\hat{n}_{2\downarrow} = U\hat{n}_{2\uparrow}\hat{n}_{2\downarrow} + t(1-\hat{n}_{2\uparrow}\hat{n}_{2\downarrow}) \end{aligned} \tag{106}$$

$$E'_{1\downarrow} = H_h - t\hat{n}_{2\downarrow} = U\hat{n}_{2\uparrow}\hat{n}_{2\downarrow} + t(1-\hat{n}_{2\uparrow}\hat{n}_{2\downarrow}) = \begin{pmatrix} U-t & & & \\ & 0 & & \\ & & 0 & \\ & & & -t \end{pmatrix} \tag{107}$$

The $\hat{n}_{1\uparrow} = 1$ part of the diagonalised Hamiltonian is

$$E'_{1\hat{n}_{1\downarrow}} = \begin{pmatrix} 2U & & & & & & & \\ & U+2t & & & & & & \\ & & U & & & & & \\ & & & U+2t & & & & \\ & & & & 2U-t & & & \\ & & & & & U-t & & \\ & & & & & & U & \\ & & & & & & & U \end{pmatrix} \tag{108}$$

3.5.1 Eigenvectors of $\hat{n}_{1\uparrow} = 1$ sector

To get the first eight eigenvectors, I first find the eigenvectors in the space of $\hat{n}_{1\downarrow}$. There are 8 eigenvectors in the space of $\hat{n}_{1\downarrow}$, that is $|\hat{n}_{1\downarrow}, \hat{n}_{2\uparrow}, \hat{n}_{2\downarrow}\rangle$. The η for this space is

$$\eta_{1\downarrow} = -tc^\dagger_{2\downarrow}c_{1\downarrow}\hat{G}_e,\ \eta^\dagger_{1\downarrow} = -t\hat{G}_e c^\dagger_{1\downarrow}c_{2\downarrow} \tag{109}$$

The required eigenvectors are $U^\dagger_{1\downarrow}|\hat{n}_{1\downarrow}\hat{n}_{2\uparrow}\hat{n}_{2\downarrow}\rangle = \frac{1}{2}(1 - \eta_{1\downarrow} + \eta^\dagger_{1\downarrow})|\hat{n}_{1\downarrow}\hat{n}_{2\uparrow}\hat{n}_{2\downarrow}\rangle$
Note that η acting on $|\hat{n}_{1\downarrow}\hat{n}_{2\uparrow}\hat{n}_{2\downarrow}\rangle$ will give non-zero only when $\hat{n}_{1\downarrow} = 1, \hat{n}_{2\downarrow} = 0$ and $\eta^\dagger$ will give non-zero only when $\hat{n}_{1\downarrow} = 0, \hat{n}_{2\downarrow} = 1$.

$$\begin{aligned}\eta^\dagger_{1\downarrow}|0, \hat{n}_{2\uparrow}, 1\rangle = -t\hat{G}_e|1, \hat{n}_{2\uparrow}, 0\rangle = \frac{-t}{\mathcal{H}'_{1\downarrow} - H_e\hat{n}_{1\downarrow}}|1, \hat{n}_{2\uparrow}, 0\rangle = \frac{-t}{\mathcal{H}'_{1\downarrow}\hat{n}_{1\downarrow} - H_e\hat{n}_{1\downarrow}}|1, \hat{n}_{2\uparrow}, 0\rangle \\ = \frac{-t}{t\hat{n}_{1\downarrow}(1 - \hat{n}_{2\downarrow})}|1, \hat{n}_{2\uparrow}, 0\rangle = -|1, \hat{n}_{2\uparrow}, 0\rangle\end{aligned} \tag{110}$$

Similarly,

$$\eta_{1\downarrow}|1, \hat{n}_{2\uparrow}, 0\rangle = -tc^\dagger_{2\downarrow}c_{1\downarrow}\hat{G}_e|1, \hat{n}_{2\uparrow}, 0\rangle = -tc^\dagger_{2\downarrow}c_{1\downarrow}\frac{1}{t}|1, \hat{n}_{2\uparrow}, 0\rangle = -|0, \hat{n}_{2\uparrow}, 1\rangle \tag{111}$$

Therefore,

$$\begin{aligned} U^\dagger_{1\downarrow}|1, \hat{n}_{2\uparrow}, 0\rangle &= (1 - \eta_{1\downarrow})|1, \hat{n}_{2\uparrow}, 0\rangle = |1, \hat{n}_{2\uparrow}, 0\rangle + |0, \hat{n}_{2\uparrow}, 1\rangle \\ U^\dagger_{1\downarrow}|0, \hat{n}_{2\uparrow}, 1\rangle &= (1 + \eta^\dagger_{1\downarrow})|0, \hat{n}_{2\uparrow}, 1\rangle = |0, \hat{n}_{2\uparrow}, 1\rangle - |1, \hat{n}_{2\uparrow}, 0\rangle \\ U^\dagger_{1\downarrow}|1, \hat{n}_{2\uparrow}, 1\rangle &= |1, \hat{n}_{2\uparrow}, 1\rangle \\ U^\dagger_{1\downarrow}|0, \hat{n}_{2\uparrow}, 0\rangle &= |0, \hat{n}_{2\uparrow}, 0\rangle \end{aligned} \tag{112}$$

Eigenvectors for $\hat{n}_{1\uparrow} = 1$ sector:

$\hat{n}_{1\downarrow}$	$\hat{n}_{2\uparrow}$	$\hat{n}_{2\downarrow}$	Eigenvector	Eigenvalue
1	1	1	$\|111\rangle$	2U
1	1	0	$\|110\rangle + \|011\rangle$	U+2t
1	0	1	$\|101\rangle$	U
1	0	0	$\|100\rangle + \|001\rangle$	U+2t
0	1	1	$\|011\rangle - \|110\rangle$	U-t
0	1	0	$\|010\rangle$	0
0	0	1	$\|001\rangle - \|100\rangle$	0
0	0	0	$\|000\rangle$	-t

Now we need to find the eigenvectors in the space of $\hat{n}_{1\uparrow} = 1$. To do this, we will act with $U^{\dagger}_{1\uparrow}$ on the previously obtained eigenvectors.

$$\begin{aligned}
\eta^{\dagger}_{1\uparrow} = -t\hat{G}_e c^{\dagger}_{1\uparrow}c_{2\uparrow},\ \eta_{1\uparrow} = -tc^{\dagger}_{2\uparrow}c_{1\uparrow}\hat{G}_e \\
\eta^{\dagger}_{1\uparrow}\left|\hat{n}_{1\uparrow} = 0, \hat{n}_{1\downarrow}, \hat{n}_{2\uparrow} = 1, \hat{n}_{2\downarrow}\right\rangle = -\left|1, \hat{n}_{1\downarrow}, 0, \hat{n}_{2\downarrow}\right\rangle \\
\eta_{1\uparrow}\left|\hat{n}_{1\uparrow} = 1, \hat{n}_{1\downarrow}, \hat{n}_{2\uparrow} = 0, \hat{n}_{2\downarrow}\right\rangle = -\left|0, \hat{n}_{1\downarrow}, 1, \hat{n}_{2\downarrow}\right\rangle
\end{aligned} \tag{113}$$

Applying these on the previously obtained eigenvectors give

$\hat{n}_{1\uparrow}$	$\hat{n}_{1\downarrow}$	$\hat{n}_{2\uparrow}$	$\hat{n}_{2\downarrow}$	Eigenvector	Match?	Evalue(Exact Evalue)
1	1	1	1	$\|1111\rangle$	Y	2U(same)
1	1	1	0	$\|1110\rangle + \|1011\rangle$	Y	U+2t(U-t)
1	1	0	1	$\|1101\rangle - \|0111\rangle$	Y	U(U+t)
1	1	0	0	$\|1100\rangle + \|1001\rangle - \|0110\rangle - \|0011\rangle$	N	U+2t(U+t)
1	0	1	1	$\|1011\rangle - \|1110\rangle$	Y	U-t(...)
1	0	1	0	$\|1010\rangle$	Y	0(same)
1	0	0	1	$\|1001\rangle - \|1100\rangle - \|0011\rangle + \|0110\rangle$	N	0(...)
1	0	0	0	$\|1000\rangle - \|0010\rangle$	Y	-t(t)