Title

Contents

1 Exact diagonalization of the two-site Hubbard model

The Hamiltonian

$$\mathcal{H} = -t \sum_{\sigma} \left(c^{\dagger}_{1\sigma} c_{2\sigma} + c^{\dagger}_{2\sigma} c_{1\sigma} \right) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \mu \hat{N} \tag{1}$$

a_a I have two lattice sites, indexed by 1 and 2, occupied by electrons. μ is the chemical potential, $c^{\dagger}_{i\sigma}$ and $c_{i\sigma}$ are the fermionic creation and annihilation operators at the i^{th} site, with spin-index σ. σ can take values $\uparrow$ and $\downarrow$, denoting spin-up and spin-down states respectively. $\hat{n}_{i\sigma} = c^{\dagger}_{i\sigma} c_{i\sigma}$ is the number operator for the i^{th} site and at spin-index σ; it counts the number of fermions with the designated quantum numbers. $\hat{N} = \sum_{i\sigma} \hat{n}_{i\sigma}$ is the total number operator; it counts the total number of fermions at all sites and spin-indices. t is the hopping strength; the more the t, the more are the electrons likely to hop between sites. U is the on-site repulsion cost; it represents the increase in energy when two electrons occupy the same site.

1.1 Symmetries of the problem

The following operators commute with the Hamiltonian.

1. **Total number operator**: $\left[\mathcal{H}, \hat{N}\right] = 0$.

   Proof. The last term in the Hamiltonian is the number operator itself. Ignoring that, there are three terms that I need to individually consider.

   - $c^{\dagger}_{1\sigma} c_{2\sigma}$

$$\begin{aligned}
\left[c^{\dagger}_{1\sigma} c_{2\sigma}, \hat{n}_{i\sigma'}\right] &= \left[c^{\dagger}_{1\sigma} c_{2\sigma}, c^{\dagger}_{i\sigma'} c_{i\sigma'}\right] \\
&= c^{\dagger}_{1\sigma} \left[c_{2\sigma}, c^{\dagger}_{i\sigma'} c_{i\sigma'}\right] + \left[c^{\dagger}_{1\sigma}, c^{\dagger}_{i\sigma'} c_{i\sigma'}\right] c_{2\sigma} \\
&= \delta_{i,2}\, c^{\dagger}_{1\sigma} \left[c_{2\sigma}, c^{\dagger}_{2\sigma'} c_{2\sigma'}\right] + \delta_{i,1} \left[c^{\dagger}_{1\sigma}, c^{\dagger}_{1\sigma'} c_{1\sigma'}\right] c_{2\sigma} \\
&= \delta_{i,2}\, c^{\dagger}_{1\sigma} \left\{c_{2\sigma}, c^{\dagger}_{2\sigma'}\right\} c_{2\sigma'} - \delta_{i,1} c^{\dagger}_{1\sigma'} \left\{c_{1\sigma'}, c^{\dagger}_{1\sigma}\right\} c_{2\sigma} \\
&= \delta_{\sigma,\sigma'} c^{\dagger}_{1\sigma} c_{1\sigma} \left(\delta_{i,2} - \delta_{i,1}\right)
\end{aligned} \tag{2}$$

     The third line follows because the electrons on different sites are distinguishable and hence, the *creation and anhillation operators of different sites will commute among themselves.* Therefore,

$$\left[c^{\dagger}_{1\sigma} c_{2\sigma}, \hat{N}\right] = \sum_{i\sigma'} \left[c^{\dagger}_{1\sigma} c_{2\sigma}, \hat{n}_{i\sigma'}\right] = c^{\dagger}_{1\sigma} c_{1\sigma} \sum_{i=\{1,2\}} \left(\delta_{i,2} - \delta_{i,1}\right) = 0 \tag{3}$$

   - $c^{\dagger}_{2\sigma} c_{1\sigma}$: Since the operator $\hat{N}$ is symmetric with respect to the site indices 1 and 2, I can go through the last proof again with the site indices 1 and 2 exchanged and since the proof does not depend on the site indices, this commutator will also be zero.

- $\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$:

$$\begin{aligned}
[\hat{n}_{i\uparrow}\hat{n}_{j\downarrow}, \hat{n}_{j\sigma}] &= \hat{n}_{i\uparrow}[\hat{n}_{i\downarrow}, \hat{n}_{j\sigma}] - [\hat{n}_{i\uparrow}, \hat{n}_{j\sigma}]\,\hat{n}_{i\downarrow} \\
&= \delta_{ij}\left(\hat{n}_{i\uparrow}[\hat{n}_{i\downarrow}, \hat{n}_{i\sigma}] - [\hat{n}_{i\uparrow}, \hat{n}_{i\sigma}]\,\hat{n}_{i\downarrow}\right) \\
&= \delta_{ij}\left(\delta_{\sigma\uparrow}\hat{n}_{i\uparrow}[\hat{n}_{i\downarrow}, \hat{n}_{i\uparrow}] - \delta_{\sigma\downarrow}[\hat{n}_{i\uparrow}, \hat{n}_{i\downarrow}]\,\hat{n}_{i\downarrow}\right) \\
&= \delta_{ij}\left(\delta_{\sigma\downarrow}\hat{n}_{i\downarrow} - \delta_{\sigma\uparrow}\hat{n}_{i\uparrow}\right)[\hat{n}_{i\uparrow}, \hat{n}_{i\downarrow}] \\
&= \delta_{ij}\left(\delta_{\sigma\downarrow}\hat{n}_{i\downarrow} - \delta_{\sigma\uparrow}\hat{n}_{i\uparrow}\right)\left(c^\dagger_{i\uparrow}c_{i\uparrow}c^\dagger_{i\downarrow}c_{i\downarrow} - c^\dagger_{i\downarrow}c_{i\downarrow}c^\dagger_{i\uparrow}c_{i\uparrow}\right) \\
&= \delta_{ij}\left(\delta_{\sigma\downarrow}\hat{n}_{i\downarrow} - \delta_{\sigma\uparrow}\hat{n}_{i\uparrow}\right)\left(c^\dagger_{i\downarrow}c_{i\downarrow}c^\dagger_{i\uparrow}c_{i\uparrow} - c^\dagger_{i\downarrow}c_{i\downarrow}c^\dagger_{i\uparrow}c_{i\uparrow}\right) = 0
\end{aligned} \tag{4}$$

  Therefore, $\left[\hat{n}_{i\uparrow}\hat{n}_{j\downarrow}, \hat{N}\right] = \sum_{j,\sigma}[\hat{n}_{i\uparrow}\hat{n}_{j\downarrow}, \hat{n}_{j\sigma}] = 0$

The total Hamiltonian is just a sum of the three terms; since the number operator commutes individually with these terms, it obviously commutes with the total Hamiltonian. □

2. **Magnetization operator**: $\hat{S}^z_{tot} \equiv \frac{1}{2}\sum_i(\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})$, $\left[\mathcal{H}, \hat{S}^z_{tot}\right] = 0$.

   Proof. The magnetization operator can be rewritten as $\hat{S}^z_{tot} = \frac{1}{2}\sum_i(\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow} - 2\hat{n}_{i\downarrow}) = \hat{N} - 2\sum_i \hat{n}_{i\downarrow}$. Since $\hat{N}$ commutes with $\mathcal{H}$, I just need to prove that $[\mathcal{H}, \sum_i \hat{n}_{i\downarrow}]$. From eq. 2,

$$\left[c^\dagger_{1\sigma}c_{2\sigma}, \sum_i \hat{n}_{i\downarrow}\right] = c^\dagger_{1\downarrow}c_{1\downarrow}\sum_{i=\{1,2\}}(\delta_{i,2} - \delta_{i,1}) = 0 \tag{5}$$

   Again using the symmetry of the magnetization operator with the exchange of indices, its obvious that $\left[c^\dagger_{2\sigma}c_{1\sigma}, \sum_i \hat{n}_{i\downarrow}\right] = 0$

   Using eq. 4, $[\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}, \hat{n}_{i\downarrow}] = 0$.

   Finally, $[N, \hat{n}_{i\downarrow}] = \sum_{j\sigma}[\hat{n}_{j\sigma}, \hat{n}_{i\downarrow}] = [\hat{n}_{i\uparrow}, \hat{n}_{i\downarrow}] = c^\dagger_{i\uparrow}c_{i\uparrow}c^\dagger_{i\downarrow}c_{i\downarrow} - c^\dagger_{i\downarrow}c_{i\downarrow}c^\dagger_{i\uparrow}c_{i\uparrow} = 0$. Since $\hat{S}^z_{tot}$ commutes with each part individually, it commutes with the total Hamiltonian. □

3. **Two-site parity operator** $\hat{P}$: The action of $\hat{P}$ is defined as follows. If $|\Psi_{\alpha\beta}\rangle$ is a wavefunction with site indices α and β,

$$\hat{P}\,|\Psi(\alpha, \beta)\rangle = |\Psi(\beta, \alpha)\rangle \tag{6}$$

   That is, it operates on each electron and reverses it's site indices.

   Proof. I now rewrite the Hamiltonian by explcitly showing the two site indices:

$$\mathcal{H}(\alpha, \beta) = -t\sum_\sigma(c^\dagger_{\alpha\sigma}c_{\beta\sigma} + c^\dagger_{\beta\sigma}c_{\alpha\sigma}) + U(n_{\alpha\uparrow}n_{\alpha\downarrow} + n_{\beta\uparrow}n_{\beta\downarrow}) - \mu\sum_\sigma(n_{\alpha\sigma} + n_{\beta\sigma}) \tag{7}$$

Its obvious that $\mathcal{H}$ is symmetric in the site indices: $\mathcal{H}(\alpha, \beta) = \mathcal{H}(\beta, \alpha)$. This means that the eigenvalues also have this symmetry. Let $|\Phi(\alpha, \beta)\rangle$ be an eigenstate of $\mathcal{H}(\alpha, \beta)$ with eigenvalue $E(\alpha, \beta)$. Then,

$$\begin{aligned} \hat{P}\mathcal{H}\,|\Phi(\alpha,\beta)\rangle &= E(\alpha,\beta)\hat{P}\,|\Phi(\alpha,\beta)\rangle = E(\beta,\alpha)\,|\Phi(\beta,\alpha)\rangle \\ &= \mathcal{H}\,|\Phi(\beta,\alpha)\rangle = \mathcal{H}\hat{P}\,|\Phi(\alpha,\beta)\rangle \\ \implies \mathcal{H}\hat{P}\,|\Phi(\alpha,\beta)\rangle &= \hat{P}\mathcal{H}\,|\Phi(\alpha,\beta)\rangle \end{aligned} \tag{8}$$

Since any general wavefunction can be expanded in terms of these wavefunctions and since both the operator are linear, the above result will also hold for a general wavefunction $|\Psi(\alpha, \beta)\rangle$:

$$\mathcal{H}\hat{P}\,|\Psi(\alpha,\beta)\rangle = \hat{P}\mathcal{H}\,|\Psi(\alpha,\beta)\rangle \implies [\mathcal{H}, \hat{P}] = 0 \tag{9}$$

□

1.2 Partitioning the Hilbert space

THe Hamiltonian commutes with the three operators. This means that is possible to simultaneously diagonalize these four operators: $\mathcal{H}, \hat{N}, S_z^{tot}, \hat{P}$. I will be able to label the eigenstates of the total Hamiltonian using the eigenvalues of these operatos. First take the total number operator. $\hat{N}$ can take four values for a two-site system, 1 through 4. The eigenstates labelled by a particular number, say N=2 will be orthogonal to the eigenstates labelled by another number, say N=4. This means each eigenvalue of $\hat{N}$ will have a distinct subspace orthogonal to the other values of $\hat{N}$. I will be able to diagonalize each such subspace independently of each other, because they will not have any overlap. This feature enables us to block-diagonalize the total Hamiltonian into four blocks, each block belonging to each value $\hat{N}$.

Inside each block, I will be able to repeat the procedure by next using the eigenvalues of S_z^{tot}. Each block of the Hamiltonian will again break up to smaller blocks for each value of the total magnetization. The eigenvalues of parity operator provide a further partitioning of the blocks of magnetization.

From this point, all the states I will work with will necessarily be eigenfunctions of $\hat{N}$, so it doesn't make sense to keep the last term in the Hamiltonian, $\mu\hat{N}$. I redefine the Hamiltonian by absorbing this term: $\mathcal{H} \to \mathcal{H} + \mu\hat{N} = -t\sum_\sigma \left(c_{1\sigma}^\dagger c_{2\sigma} + c_{2\sigma}^\dagger c_{1\sigma}\right) + U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$. This will keep the eigenvectors unaltered, but will increase the eigenvalues by μN, where N is the number of particles in the eigenstate I are considering.

1.3 N = 1

For writing the state kets, I use the following notation: $|\uparrow, \downarrow\rangle$ means electron on site 1 has spin up and that on site 2 has spin-down. $|\downarrow, 0\rangle$ means electron on site 1 has spin-down and there is no electron on site 2.

For one electron on two lattice sites, I start by writing down the eigenstates of S_z^{tot}. For odd number of electrons, zero magnetization is not possible. So,

- $S_z^{tot} = -1$: $|\downarrow, 0\rangle, |0, \downarrow\rangle$
- $S_z^{tot} = +1$: $|\uparrow, 0\rangle, |0, \uparrow\rangle$

Each eigenvalue will have a separate subspace and can be separately diagonalized. I need to find the matrix elements of $\mathcal{H}$ in these eigenkets. Since there is no possibility of two electrons occupying same site, I ignore the U-term for the time being.

1.3.1 $S_z^{tot} = -1$

Let us first see the action of the Hamiltonian on the eigenfunctions with $S_z^{tot} = -1$.

$$\begin{aligned}\mathcal{H}|\downarrow, 0\rangle &= -tc_{2\downarrow}^\dagger c_{1\downarrow}|\downarrow, 0\rangle = -t|0, \downarrow\rangle \\ \mathcal{H}|0, \downarrow\rangle &= -tc_{1\downarrow}^\dagger c_{2\downarrow}|0, \downarrow\rangle = -t|\downarrow, 0\rangle\end{aligned} \tag{10}$$

We get the following matrix for this tiny subspace of the Hamiltonian:

$$\begin{array}{c c} & \begin{array}{cc} |\downarrow, 0\rangle & |0, \downarrow\rangle \end{array} \\ \begin{array}{c} |\downarrow, 0\rangle \\ \\ |0, \downarrow\rangle \end{array} & \begin{pmatrix} 0 & -t \\ \\ -t & 0 \end{pmatrix} \end{array} \tag{11}$$

The eigenvalues and eigenvectors of this matrix are $\frac{|\downarrow,0\rangle \pm |0,\downarrow\rangle}{\sqrt{2}}$, with eigenvalues $\mp t$. These are also the eigenvalues of the parity operator, as expected.

$$\begin{aligned}\hat{P}(|\downarrow, 0\rangle + |0, \downarrow\rangle) = |0, \downarrow\rangle + |\downarrow, 0\rangle \implies \hat{P} = 1 \\ \hat{P}(|\downarrow, 0\rangle - |0, \downarrow\rangle) = |0, \downarrow\rangle - |\downarrow, 0\rangle \implies \hat{P} = -1\end{aligned} \tag{12}$$

1.3.2 $S_z^{tot} = +1$

Now I look at the spin-up states.

$$\begin{aligned}\mathcal{H}|\uparrow, 0\rangle &= -tc_{2\uparrow}^\dagger c_{1\uparrow}|\uparrow, 0\rangle = -t|0, \uparrow\rangle \\ \mathcal{H}|0, \uparrow\rangle &= -tc_{1\uparrow}^\dagger c_{2\uparrow}|0, \uparrow\rangle = -t|\uparrow, 0\rangle\end{aligned} \tag{13}$$

Clearly, this gives the same matrix as the spin-down states:

$$\begin{array}{c c} & \begin{array}{cc} |\uparrow, 0\rangle & |0, \uparrow\rangle \end{array} \\ \begin{array}{c} |\uparrow, 0\rangle \\ \\ |0, \uparrow\rangle \end{array} & \begin{pmatrix} 0 & -t \\ \\ -t & 0 \end{pmatrix} \end{array} \tag{14}$$

and hence similar eigenfunctions: $\frac{|\uparrow,0\rangle \pm |0,\uparrow\rangle}{\sqrt{2}}$, with eigenvalues $\mp t$.

1.4 N=3

I once again write down the eigenstates of S_z^{tot}, this time with three electrons.

- $S_z^{tot} = -1$: $|\uparrow\downarrow, \downarrow\rangle, |\downarrow, \uparrow\downarrow\rangle$
- $S_z^{tot} = +1$: $|\uparrow\downarrow, \uparrow\rangle, |\uparrow, \uparrow\downarrow\rangle$

1.4.1 $S_z^{tot} = -1$

$$\begin{aligned}
\mathcal{H}\,|\uparrow\downarrow, \downarrow\rangle &= -tc_{2\uparrow}^{\dagger}c_{1\uparrow}\,|\uparrow\downarrow, \downarrow\rangle + U\,|\uparrow\downarrow, \downarrow\rangle = -t\,|\downarrow, \uparrow\downarrow\rangle + U\,|\uparrow\downarrow, \downarrow\rangle \\
\mathcal{H}\,|\downarrow, \uparrow\downarrow\rangle &= -tc_{1\uparrow}^{\dagger}c_{2\uparrow}\,|\downarrow, \uparrow\downarrow\rangle + U\,|\downarrow, \uparrow\downarrow\rangle = -t\,|\uparrow\downarrow, \downarrow\rangle + U\,|\downarrow, \uparrow\downarrow\rangle
\end{aligned} \tag{15}$$

$$\begin{array}{c c}
 & \begin{array}{cc} |\uparrow\downarrow, \downarrow\rangle & |\downarrow, \uparrow\downarrow\rangle \end{array} \\
\begin{array}{c} |\uparrow\downarrow, \downarrow\rangle \\ \\ |\downarrow, \uparrow\downarrow\rangle \end{array} & \begin{pmatrix} U & -t \\ & \\ -t & U \end{pmatrix}
\end{array} \tag{16}$$

This matrix has eigenvalues $U \mp t$, and corresponding eigenvectors $\frac{|\uparrow\downarrow, \downarrow\rangle \pm |\downarrow, \uparrow\downarrow\rangle}{\sqrt{2}}$

1.4.2 $S_z^{tot} = +1$

$$\begin{aligned}
\mathcal{H}\,|\uparrow\downarrow, \uparrow\rangle &= -tc_{2\downarrow}^{\dagger}c_{1\downarrow}\,|\uparrow\downarrow, \uparrow\rangle + U\,|\uparrow\downarrow, \uparrow\rangle = tc_{2\downarrow}^{\dagger}c_{1\downarrow}\,|\downarrow\uparrow, \uparrow\rangle + U\,|\uparrow\downarrow, \uparrow\rangle \\
&= t\,|\uparrow, \downarrow\uparrow\rangle + U\,|\uparrow\downarrow, \uparrow\rangle = -t\,|\uparrow, \uparrow\downarrow\rangle + U\,|\uparrow\downarrow, \uparrow\rangle \\
\mathcal{H}\,|\uparrow, \uparrow\downarrow\rangle &= -tc_{1\downarrow}^{\dagger}c_{2\downarrow}\,|\uparrow, \uparrow\downarrow\rangle + U\,|\uparrow, \uparrow\downarrow\rangle = tc_{1\downarrow}^{\dagger}c_{2\downarrow}\,|\uparrow, \downarrow\uparrow\rangle + U\,|\uparrow, \uparrow\downarrow\rangle \\
&= t\,|\downarrow\uparrow, \uparrow\rangle + U\,|\uparrow, \uparrow\downarrow\rangle = -t\,|\uparrow\downarrow, \uparrow\rangle + U\,|\uparrow, \uparrow\downarrow\rangle
\end{aligned} \tag{17}$$

$$\begin{array}{c c}
 & \begin{array}{cc} |\uparrow\downarrow, \uparrow\rangle & |\uparrow, \uparrow\downarrow\rangle \end{array} \\
\begin{array}{c} |\uparrow\downarrow, \uparrow\rangle \\ \\ |\uparrow, \uparrow\downarrow\rangle \end{array} & \begin{pmatrix} U & -t \\ & \\ -t & U \end{pmatrix}
\end{array} \tag{18}$$

This matrix has eigenvalues $U \mp t$, and corresponding eigenvectors $\frac{|\uparrow\downarrow, \uparrow\rangle \pm |\uparrow, \uparrow\downarrow\rangle}{\sqrt{2}}$

1.5 N=4

With four electrons, the only possible state is $|\uparrow\downarrow, \uparrow\downarrow\rangle$. Its easy to find the eigenvalue. Since all states are filled, no hopping can take place, so the hopping term is zero. Therefore,

$$\mathcal{H}\,|\uparrow\downarrow, \uparrow\downarrow\rangle = 2U\,|\uparrow\downarrow, \uparrow\downarrow\rangle \tag{19}$$

So, $|\uparrow\downarrow, \uparrow\downarrow\rangle$ is an eigenvector with eigenvalue $2U$.

1.6 N=2

This is the eigenvalue that has the largest subspace.

- $S_z^{tot} = -1$: $|\downarrow,\downarrow\rangle$
- $S_z^{tot} = +1$: $|\uparrow,\uparrow\rangle$
- $S_z^{tot} = 0$: $|\uparrow,\downarrow\rangle, |\downarrow,\uparrow\rangle, |0,\uparrow\downarrow\rangle, |\uparrow\downarrow,0\rangle$

1.6.1 $S_z^{tot} = \pm 1$

These two subspaces have a single state each, so theya are obviously eigenstates. Since they both have identical spins on both sites, the hopping term is 0, and the U-term is also zero because of single occupation. As a result, they both have zero eigenvalue

$$\mathcal{H}\,|\downarrow,\downarrow\rangle = \mathcal{H}\,|\uparrow,\uparrow\rangle = 0 \tag{20}$$

1.6.2 $S_z^{tot} = 0$

This subspace has four eigenvectors,

$$|\uparrow,\downarrow\rangle, \qquad |\downarrow,\uparrow\rangle, \qquad |0,\uparrow\downarrow\rangle, \qquad |\uparrow\downarrow,0\rangle \tag{21}$$

so it is not possible to directly diagonalize this subspace. First we organize these states into eigenstates of parity. It is easy by inspection.

$$\begin{aligned}\hat{P}\left(|\uparrow,\downarrow\rangle \pm |\downarrow,\uparrow\rangle\right) &= \pm\left(|\uparrow,\downarrow\rangle \pm |\downarrow,\uparrow\rangle\right)\\ \hat{P}\left(|\uparrow\downarrow,0\rangle \pm |0,\uparrow\downarrow\rangle\right) &= \pm\left(|\uparrow\downarrow,0\rangle \pm |0,\uparrow\downarrow\rangle\right)\end{aligned} \tag{22}$$

I have the parity eigenstates for this subspace, so its most convenient to work in the basis of these eigenstates

- $\hat{P} = 1 : \frac{|\uparrow,\downarrow\rangle+|\downarrow,\uparrow\rangle}{\sqrt{2}}, \qquad \frac{|\uparrow\downarrow,0\rangle+|0,\uparrow\downarrow\rangle}{\sqrt{2}}$
- $\hat{P} = -1 : \frac{|\uparrow,\downarrow\rangle-|\downarrow,\uparrow\rangle}{\sqrt{2}}, \qquad \frac{|\uparrow\downarrow,0\rangle-|0,\uparrow\downarrow\rangle}{\sqrt{2}}$

Each eigenvalue subspace can now be diagonalized separately. First I look at the eigenstates of $\hat{P} = 1$. I find the matrix of $\mathcal{H}$ in the subspace spanned by these two vectors and then diagonalize that subspace.

$$\begin{aligned}\mathcal{H}\,\frac{|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle}{\sqrt{2}} &= -\frac{t}{\sqrt{2}}\left\{\left(c^\dagger_{1\downarrow}c_{2\downarrow} + c^\dagger_{2\uparrow}c_{1\uparrow}\right)|\uparrow,\downarrow\rangle + \left(c^\dagger_{1\uparrow}c_{2\uparrow} + c^\dagger_{2\downarrow}c_{1\downarrow}\right)|\downarrow,\uparrow\rangle\right\}\\ &= -\frac{t}{\sqrt{2}}\left\{|\downarrow\uparrow,0\rangle + |0,\uparrow\downarrow\rangle + |\uparrow\downarrow,0\rangle + |0,\downarrow\uparrow\rangle\right\} = 0\\ \mathcal{H}\,\frac{|\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle}{\sqrt{2}} &= -\frac{t}{\sqrt{2}}\left\{\left(c^\dagger_{2\uparrow}c_{1\uparrow} + c^\dagger_{2\downarrow}c_{1\downarrow}\right)|\uparrow\downarrow,0\rangle + \left(c^\dagger_{1\uparrow}c_{2\uparrow} + c^\dagger_{1\downarrow}c_{2\downarrow}\right)|0,\uparrow\downarrow\rangle\right\} + U\frac{|\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle}{\sqrt{2}}\\ &= -\frac{t}{\sqrt{2}}\left\{|\downarrow,\uparrow\rangle - |\uparrow,\downarrow\rangle + |\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\right\} + U\frac{|\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle}{\sqrt{2}} = U\frac{|\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle}{\sqrt{2}}\end{aligned} \tag{23}$$

We get the following matrix

$$\begin{array}{cc} & \begin{array}{cc} \frac{|\uparrow,\downarrow\rangle+|\downarrow,\uparrow\rangle}{\sqrt{2}} & \frac{|\uparrow\downarrow,0\rangle+|0,\uparrow\downarrow\rangle}{\sqrt{2}} \end{array} \\ \begin{array}{c} \frac{|\uparrow,\downarrow\rangle+|\downarrow,\uparrow\rangle}{\sqrt{2}} \\ \\ \frac{|\uparrow\downarrow,0\rangle+|0,\uparrow\downarrow\rangle}{\sqrt{2}} \end{array} & \left(\begin{array}{cc} 0 & 0 \\ \\ 0 & U \end{array} \right) \end{array} \tag{24}$$

As it appears, the subspace is already diagonal in the eigenbasis of $\hat{P}$. The $\hat{P} = 1$ eigenstates are eigenstates of $\mathcal{H}$, with eigenvalues 0 and U. Next I look at the eigenstates of $\hat{P} = -1$.

$$\begin{aligned}
\mathcal{H}\,\frac{|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle}{\sqrt{2}} &= -\frac{t}{\sqrt{2}}\left\{\left(c^\dagger_{1\downarrow}c_{2\downarrow}c^\dagger_{2\uparrow}c_{1\uparrow}\right)|\uparrow,\downarrow\rangle - \left(c^\dagger_{1\uparrow}c_{2\uparrow} + c^\dagger_{2\downarrow}c_{1\downarrow}\right)|\downarrow,\uparrow\rangle\right\} \\
&= -\frac{t}{\sqrt{2}}\left\{|\downarrow\uparrow,0\rangle + |0,\uparrow\downarrow\rangle - |\uparrow\downarrow,0\rangle - |0,\downarrow\uparrow\rangle\right\} \\
&= 2t\frac{|\uparrow\downarrow,0\rangle - |0,\uparrow\downarrow\rangle}{\sqrt{2}} \\
\mathcal{H}\,\frac{|\uparrow\downarrow,0\rangle - |0,\uparrow\downarrow\rangle}{\sqrt{2}} &= -\frac{t}{\sqrt{2}}\left\{\left(c^\dagger_{2\uparrow}c_{1\uparrow} + c^\dagger_{2\downarrow}c_{1\downarrow}\right)|\uparrow\downarrow,0\rangle - \left(c^\dagger_{1\uparrow}c_{2\uparrow} + c^\dagger_{1\downarrow}c_{2\downarrow}\right)|0,\uparrow\downarrow\rangle\right\} + U\frac{|\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle}{\sqrt{2}} \\
&= -\frac{t}{\sqrt{2}}\left\{|\downarrow,\uparrow\rangle - |\uparrow,\downarrow\rangle - |\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle\right\} + U\frac{|\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle}{\sqrt{2}} \\
&= 2t\frac{|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle}{2} + U\frac{|\uparrow\downarrow,0\rangle - |0,\uparrow\downarrow\rangle}{\sqrt{2}}
\end{aligned} \tag{25}$$

$$\begin{array}{cc} & \begin{array}{cc} \frac{|\uparrow,\downarrow\rangle-|\downarrow,\uparrow\rangle}{\sqrt{2}} & \frac{|\uparrow\downarrow,0\rangle-|0,\uparrow\downarrow\rangle}{\sqrt{2}} \end{array} \\ \begin{array}{c} \frac{|\uparrow,\downarrow\rangle-|\downarrow,\uparrow\rangle}{\sqrt{2}} \\ \\ \frac{|\uparrow\downarrow,0\rangle-|0,\uparrow\downarrow\rangle}{\sqrt{2}} \end{array} & \left(\begin{array}{cc} 0 & 2t \\ \\ 2t & U \end{array} \right) \end{array} \tag{26}$$

This subspace is not automatically diagonal, but is easily diagonalized. The eigenvectors are

$$\begin{aligned}
&\frac{1}{N_\pm}\left\{2t\frac{(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle)}{\sqrt{2}} + \frac{U \pm \sqrt{U^2+16t^2}}{2}\frac{(|\uparrow\downarrow,0\rangle - |0,\uparrow\downarrow\rangle)}{\sqrt{2}}\right\} \\
&N_\pm = \left\{\frac{U}{2}\left[U \pm \sqrt{U^2+16t^2}\right] + 16t^2\right\}^{\frac{1}{2}}
\end{aligned} \tag{27}$$

with eigenvalues $\frac{U\pm\sqrt{U^2+16t^2}}{2}$ respectively.

1.7 The total spectrum

The final spectrum is already obtained. One final thing to do is to just add the respective values of $-\mu N$ to the eigenvalues.

2 Exact diagonalization of the Anderson molecule

The Hamiltonian

$$\mathcal{H} = -t\sum_{\sigma}\left(c^{\dagger}_{1\sigma}c_{2\sigma} + c^{\dagger}_{2\sigma}c_{1\sigma}\right) + U\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + \epsilon_s\sum_{\sigma}\hat{n}_{2\sigma} + \epsilon_d\sum_{\sigma}\hat{n}_{1\sigma} \tag{28}$$

I have two lattice sites, indexed by 1 and 2, occupied by electrons. μ is the chemical potential, $c^{\dagger}_{i\sigma}$ and $c_{i\sigma}$ are the fermionic creation and annihilation operators at the i$^{\text{th}}$ site, with spin-index σ. σ can take values $\uparrow$ and $\downarrow$, denoting spin-up and spin-down states respectively. $\hat{n}_{i\sigma} = c^{\dagger}_{i\sigma}c_{i\sigma}$ is the number operator for the i^{th} site and at spin-index σ; it counts the number of fermions with the designated quantum numbers. $\hat{N} = \sum_{i\sigma}\hat{n}_{i\sigma}$ is the total number operator; it counts the total number of fermions at all sites and spin-indices. t is the hopping strength; the more the t, the more are the electrons likely to hop between sites. U is the on-site repulsion cost; it represents the increase in energy when two electrons occupy the same site. The model has on-site repulsion only for the first site. The sites have energies of ϵ_s and ϵ_s respectively.

2.1 Symmetries of the problem

The following operators commute with the Hamiltonian.

1. **Total number operator**: $\left[\mathcal{H}, \hat{N}\right] = 0$.

2. **Magnetization operator**: $\left[\mathcal{H}, \hat{S}^z_{tot}\right] = 0$.

3. **Total Spin Operator**: Total spin angular momentum operator,

$$\hat{S}^2_{tot} = \hat{(}S^x_{tot})^2 + \hat{(}S^y_{tot})^2 + \hat{(}S^z_{tot})^2 = S^+_{tot}S^-_{tot} - \hbar S^z_{tot} + (S^z_{tot})^2 \tag{29}$$

   Since all the terms in the Hamiltonian are spin-preserving (all events conserve the number of particles having a definite spin σ), total angular momentum will be conserved. It's obvious that the number operator term do so. The hopping term does so as well; $c^{\dagger}_{i\sigma}c_{j\sigma}$ destroys a particle of spin σ and creates a particle of the same spin; the total angular momentum remain conserved in the process, although the number of particles at a particular site is not conserved. Thus, $\left[\hat{S}^2_{tot}, \mathcal{H}\right] = 0$.

2.2 N = 1

- $S^z_{tot} = -1$: $\left|\downarrow, 0\right\rangle, \left|0, \downarrow\right\rangle$
- $S^z_{tot} = +1$: $\left|\uparrow, 0\right\rangle, \left|0, \uparrow\right\rangle$

2.2.1 $S^z_{tot} = -1$

Let us first see the action of the Hamiltonian on the eigenfunctions with $S^z_{tot} = -1$.

$$\begin{aligned}\mathcal{H}\left|\downarrow, 0\right\rangle &= \epsilon_d\left|\downarrow, 0\right\rangle - t\left|0, \downarrow\right\rangle \\ \mathcal{H}\left|0, \downarrow\right\rangle &= \epsilon_s\left|0, \downarrow\right\rangle - t\left|\downarrow, 0\right\rangle\end{aligned} \tag{30}$$

We get the following matrix for this tiny subspace of the Hamiltonian:

$$\begin{array}{c|c} & \begin{array}{cc} |\downarrow,0\rangle & |0,\downarrow\rangle \end{array} \\ \begin{array}{c} |\downarrow,0\rangle \\ \\ |0,\downarrow\rangle \end{array} & \begin{pmatrix} \epsilon_d & -t \\ \\ -t & \epsilon_s \end{pmatrix} \end{array} \tag{31}$$

Eigenvalues: $\frac{1}{2}\left[\epsilon_d + \epsilon_s \pm \sqrt{(\epsilon_d - \epsilon_s)^2 + 4t^2}\right]$. For $\epsilon_s = \epsilon_d + \frac{U}{2}$ and $\Delta = \sqrt{U^2 + 16t^2}$, eigenvalues, $\lambda_\pm = \epsilon_d + \frac{1}{4}(U \pm \Delta)$.
The eigenvectors are $\frac{1}{N_\pm}\left(t\,|\downarrow,0\rangle - \frac{1}{4}(U \pm \Delta)\,|0,\downarrow\rangle\right)$, where $N_\pm^2 = t^2 + (\frac{U\pm\Delta}{4})^2$

2.2.2 $S^z_{tot} = +1$

$$\begin{aligned} \mathcal{H}\,|\uparrow,0\rangle &= \epsilon_d\,|\uparrow,0\rangle - t\,|0,\uparrow\rangle \\ \mathcal{H}\,|0,\uparrow\rangle &= \epsilon_s\,|0,\uparrow\rangle - t\,|\uparrow,0\rangle \end{aligned} \tag{32}$$

Clearly, this gives the same matrix as the spin-down states. So, the eigenvalues will be exactly the same, and the eigenvectors will be correspondingly modified in the new basis.
eigenvectors : $\frac{1}{N_\pm}\left(t\,|\uparrow,0\rangle + (\epsilon_d - \lambda_\pm)\,|0,\uparrow\rangle\right)$

2.3 N=3

- $S^z_{tot} = -1$: $|\uparrow\downarrow,\downarrow\rangle, |\downarrow,\uparrow\downarrow\rangle$
- $S^z_{tot} = +1$: $|\uparrow\downarrow,\uparrow\rangle, |\uparrow,\uparrow\downarrow\rangle$

2.3.1 $S^z_{tot} = -1$

$$\begin{aligned} \mathcal{H}\,|\uparrow\downarrow,\downarrow\rangle &= -t\,|\downarrow,\uparrow\downarrow\rangle + (2\epsilon_d + \epsilon_s + U)\,|\uparrow\downarrow,\downarrow\rangle \\ \mathcal{H}\,|\downarrow,\uparrow\downarrow\rangle &= -t\,|\uparrow\downarrow,\downarrow\rangle + (2\epsilon_s + \epsilon_d)\,|\downarrow,\uparrow\downarrow\rangle \end{aligned} \tag{33}$$

$$\begin{array}{c|c} & \begin{array}{cc} |\uparrow\downarrow,\downarrow\rangle & |\downarrow,\uparrow\downarrow\rangle \end{array} \\ \begin{array}{c} |\uparrow\downarrow,\downarrow\rangle \\ \\ |\downarrow,\uparrow\downarrow\rangle \end{array} & \begin{pmatrix} 2\epsilon_d + \epsilon_s + U & -t \\ \\ -t & 2\epsilon_s + \epsilon_d \end{pmatrix} \end{array} \tag{34}$$

Again setting $\epsilon_s = \epsilon_d + \frac{U}{2}$, eigenvalues: $3\epsilon_d + \frac{5}{4}U \pm \frac{1}{4}\Delta$.
Corresponding eigenvectors $\frac{1}{N_\pm}(t\,|\uparrow\downarrow,\downarrow\rangle - \frac{1}{4}(U \pm \Delta)\,|\downarrow,\uparrow\downarrow\rangle)$

2.3.2 $S^z_{tot} = +1$

$$\begin{aligned} \mathcal{H}\,|\uparrow\downarrow,\uparrow\rangle &= -t\,|\uparrow,\uparrow\downarrow\rangle + (2\epsilon_d + \epsilon_s + U)\,|\uparrow\downarrow,\uparrow\rangle \\ \mathcal{H}\,|\uparrow,\uparrow\downarrow\rangle &= -t\,|\uparrow\downarrow,\uparrow\rangle + (2\epsilon_s + \epsilon_d)\,|\uparrow,\uparrow\downarrow\rangle \end{aligned} \tag{35}$$

Again the same matrix. Hence the eigenvalues are same. Eigenvectors are $\frac{1}{N_\pm}(t\,|\uparrow\downarrow,\uparrow\rangle - \frac{1}{4}(U \pm \Delta)\,|\uparrow,\uparrow\downarrow\rangle)$

2.4 N=2

This is the eigenvalue that has the largest subspace.

- $S^z_{tot} = -1$: $|\downarrow, \downarrow\rangle$
- $S^z_{tot} = +1$: $|\uparrow, \uparrow\rangle$
- $S^z_{tot} = 0$: $|\uparrow, \downarrow\rangle, |\downarrow, \uparrow\rangle, |0, \uparrow\downarrow\rangle, |\uparrow\downarrow, 0\rangle$

2.4.1 $S^z_{tot} = \pm 1$

These two subspaces have a single state each, so theya are obviously eigenstates. Since they both have identical spins on both sites, the hopping term is 0, and the U-term is also zero because of single occupation. As a result, they both have zero eigenvalue

$$\mathcal{H}|\downarrow, \downarrow\rangle = \mathcal{H}|\uparrow, \uparrow\rangle = \epsilon_s + \epsilon_d \tag{36}$$

2.4.2 $S^z_{tot} = 0$

This subspace has four eigenvectors,

$$|\uparrow, \downarrow\rangle, \qquad |\downarrow, \uparrow\rangle, \qquad |0, \uparrow\downarrow\rangle, \qquad |\uparrow\downarrow, 0\rangle \tag{37}$$

so it is easier to first find eigenstates of S^2_{tot}. Since these are states with zero S^z, S^2_{tot} for these states is just S^+S^-

$$\begin{aligned} S^+S^-|\uparrow, \downarrow\rangle = S^+S^-|\downarrow, \uparrow\rangle = |\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle \\ S^+S^-|\uparrow\downarrow, 0\rangle = S^+S^-|0, \uparrow\downarrow\rangle = 0 \end{aligned} \tag{38}$$

The eigenstates are

$$\frac{|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle}{\sqrt{2}}(S^2_{tot} = 1), \qquad \left\{\frac{|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle}{\sqrt{2}}, |\uparrow\downarrow, 0\rangle, |0, \uparrow\downarrow\rangle\right\}(S^2_{tot} = 0) \tag{39}$$

$S^2_{tot} = 1$ immediately delivers an eigenstate:

$$\mathcal{H}\frac{|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle}{\sqrt{2}} = (\epsilon_d + \epsilon_s)\left(\frac{|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle}{\sqrt{2}}\right) \tag{40}$$

Next I diagonalize the subspace $S^2_{tot} = 0$.

$$\begin{aligned} \mathcal{H}\frac{|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle}{\sqrt{2}} &= (\epsilon_d + \epsilon_s)\left(\frac{|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle}{\sqrt{2}}\right) + \sqrt{2}t(|\uparrow\downarrow, 0\rangle - |0, \uparrow\downarrow\rangle) \\ \mathcal{H}|\uparrow\downarrow, 0\rangle &= (2\epsilon_d + U)|\uparrow\downarrow, 0\rangle + \sqrt{2}t\frac{|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle}{\sqrt{2}} \\ \mathcal{H}|0, \uparrow\downarrow\rangle &= (2\epsilon_d + U)|0, \uparrow\downarrow\rangle - \sqrt{2}t\frac{|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle}{\sqrt{2}} \end{aligned} \tag{41}$$

We get the following matrix

$$\begin{pmatrix} 2\epsilon_d + \frac{U}{2} & \sqrt{2}t & -\sqrt{2}t \\ \sqrt{2}t & 2\epsilon_d + U & 0 \\ -\sqrt{2}t & 0 & 2\epsilon_d + U \end{pmatrix} \tag{42}$$

The eigenvectors are

- $|\uparrow\downarrow, 0\rangle - |0, \uparrow\downarrow\rangle : 2\epsilon_d + U$
- $\frac{U-\Delta}{4\sqrt{2}t} \frac{|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle}{\sqrt{2}} - |\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle : 2\epsilon_d + \frac{3}{4}U + \frac{1}{2}\Delta(\frac{U}{2}, t)$
- $\frac{U+\Delta}{4\sqrt{2}t} \frac{|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle}{\sqrt{2}} - |\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle : 2\epsilon_d + \frac{3}{4}U - \frac{1}{2}\Delta(\frac{U}{2}, t)$

2.5 The total spectrum

The final spectrum is already obtained. One final thing to do is to just add the respective values of $-\mu N$ to the eigenvalues.

3 Block diagonalization of a Fermionic Hamiltonian in single Fermion number occupancy basis

3.1 The Problem

You have a system of N spin-half fermions. The corresponding Hamiltonian $\mathcal{H}_{2N}$ comprises $2N$ fermionic single particle degrees of freedom defined in the number occupancy basis of $\hat{n}_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$, for all $[i\sigma] \in [1, N] \times [\sigma, -\sigma]$. The corresponding Hilbert space has a dimension of 2^{2N}. i represents some external degree of freedom like site-index for electrons on a lattice or the electron momentum if we go to momentum-space. This Hamiltonian is in general non-diagonal in the occupancy basis of a certain degree of freedom $N\sigma$. $N\sigma$ can be taken to be any degree of freedom, like say, the first lattice site or the largest momentum (Fermi momentum for a fermi gas). Equivalenty, for a general $\mathcal{H}$, $[\mathcal{H}, \hat{n}_{N\sigma}] \neq 0$. The goal is to diagonalize this Hamiltonian.

Theorem 1. *This Hamiltonian can be transformed using a certain unitary transformation $\hat{U}_{N\sigma}$, into $\overline{\mathcal{H}} = \hat{U}_{N\sigma} \mathcal{H} \hat{U}^\dagger_{N\sigma}$ such that this transformed Hamiltonian is diagonal in the occupancy basis of $\hat{n}_{N\sigma}$. A rephrased statement is, there exists a unitary operator $\hat{U}_{N\sigma}$ such that* $\left[\hat{U}_{N\sigma} \mathcal{H}_{2N} \hat{U}^\dagger_{N\sigma}, \hat{n}_{N\sigma}\right] = 0$.

3.2 Warming Up - Writing the Hamiltonian as blocks

The Hamiltonian $\mathcal{H}_{2N}$ in general has off-diagonal terms and can be written as the following general matrix in the occupancy basis of $N\sigma$:

$$\mathcal{H}_{2N} = \begin{array}{c c} & \begin{array}{cc} |1\rangle & |0\rangle \end{array} \\ \begin{array}{c} \langle 1| \\ \\ \langle 0| \end{array} & \begin{pmatrix} H_1 & H_2 \\ & \\ H_3 & H_4 \end{pmatrix} \end{array} \tag{43}$$

where $|1\rangle \equiv |\hat{n}_{N\sigma} = 1\rangle$ (occupied). Note that the H_i are not scalars but matrices(blocks), of dimension half that of $\mathcal{H}_{2N}$, that is 2^{2N-1}. Its clear that since, for example, $H_2 = \langle 1| \mathcal{H}_{2N} |0\rangle$, we have

$$\mathcal{H}_{2N} = H_1\hat{n}_{N\sigma} + c^{\dagger}_{N\sigma}H_2 + H_3c_{N\sigma} + H_4(1-\hat{n}_{N\sigma}) \tag{44}$$

Its trivial to check that this definition of $\mathcal{H}_{2N}$ indeed gives back the mentioned matrix elements. The expression for these matrix elements is quite easy to calculate. First, we define the partial trace over the subspace $N\sigma$

$$Tr_{N\sigma}\left(\mathcal{H}_{2N}\right) \equiv \sum_{|N\sigma\rangle} \langle N\sigma| \mathcal{H}_{2N} |N\sigma\rangle \tag{45}$$

The sum is over the possible states of $N\sigma$, that is, $\hat{n}_{N\sigma} = 0$ and $\hat{n}_{N\sigma} = 1$. Applying this partial trace to equation 44, after multiplying throughout with $\hat{n}_{N\sigma}$ from the right, gives

$$Tr_{N\sigma}\left(\mathcal{H}_{2N}\hat{n}_{N\sigma}\right) = Tr_{N\sigma}\left[H_1\hat{n}_{N\sigma}\hat{n}_{N\sigma} + c^{\dagger}_{N\sigma}H_2\hat{n}_{N\sigma} + H_3c_{N\sigma}\hat{n}_{N\sigma} + H_4(1-\hat{n}_{N\sigma})\hat{n}_{N\sigma}\right] \tag{46}$$

Recall the following: $\hat{n}^2_{N\sigma} = \hat{n}_{N\sigma}$, $(1-\hat{n}_{N\sigma})\hat{n}_{N\sigma} = 0$.

Also, since H_i are matrix elements with respect to $\hat{n}_{N\sigma}$, they will commute with the creation and annihilation operators. Hence, $Tr_{N\sigma}(c^{\dagger}_{N\sigma}H_2\hat{n}_{N\sigma}) = H_2Tr_{N\sigma}(c^{\dagger}_{N\sigma}\hat{n}_{N\sigma}) = 0$, because $c^{\dagger}_{N\sigma}\hat{n}_{N\sigma} = 0$.

Lastly, $Tr_{N\sigma}(H_3c_{N\sigma}\hat{n}_{N\sigma}) = H_3Tr_{N\sigma}(c_{N\sigma}\hat{n}_{N\sigma}) = H_3Tr_{N\sigma}(\hat{n}_{N\sigma}c_{N\sigma}) = 0$, because $\hat{n}_{N\sigma}c_{N\sigma} = 0$. So,

$$Tr_{N\sigma}\left(\mathcal{H}_{2N}\hat{n}_{N\sigma}\right) = Tr_{N\sigma}\left[H_1\hat{n}_{N\sigma}\right] = H_1Tr_{N\sigma}\hat{n}_{N\sigma} = H_1 \tag{47}$$

This gives the expression for H_1. Similarly, by taking partial trace of $\mathcal{H}(1-\hat{n}_{N\sigma})$, $\mathcal{H}c_{N\sigma}$ and $c^{\dagger}_{N\sigma}\mathcal{H}$, we get the expressions for all the blocks. They are listed here.

$$\begin{aligned} H_1 &\equiv \hat{H}_{N\sigma,e} = Tr_{N\sigma}\left[\mathcal{H}_{2N}\hat{n}_{N\sigma}\right] \\ H_2 &\equiv \hat{T}_{N\sigma,e-h} = Tr_{N\sigma}\left[\mathcal{H}_{2N}c_{N\sigma}\right] \\ H_3 &\equiv T^{\dagger}_{N\sigma,e-h} = Tr_{N\sigma}\left[c^{\dagger}_{N\sigma}\mathcal{H}_{2N}\right] \\ H_4 &\equiv \hat{H}_{N\sigma,h} = Tr_{N\sigma}\left[\mathcal{H}_{2N}(1-\hat{n}_{N\sigma})\right] \end{aligned} \tag{48}$$

We get the following block decomposition of the Hamiltonian.

$$\mathcal{H}_{2N} = \begin{array}{c c} & \begin{array}{cc} |1\rangle & |0\rangle \end{array} \\ \begin{array}{c} \langle 1| \\ \\ \langle 0| \end{array} & \begin{pmatrix} \hat{H}_{N\sigma,e} & \hat{T}_{N\sigma,e-h} \\ \\ T^{\dagger}_{N\sigma,e-h} & \hat{H}_{N\sigma,h} \end{pmatrix} \end{array} = \begin{array}{c c} & \begin{array}{cc} |1\rangle & |0\rangle \end{array} \\ \begin{array}{c} \langle 1| \\ \\ \langle 0| \end{array} & \begin{pmatrix} Tr_{N\sigma}\left[\mathcal{H}_{2N}\hat{n}_{N\sigma}\right] & Tr_{N\sigma}\left[\mathcal{H}_{2N}c_{N\sigma}\right] \\ \\ Tr_{N\sigma}\left[c^{\dagger}_{N\sigma}\mathcal{H}_{2N}\right] & Tr_{N\sigma}\left[\mathcal{H}_{2N}(1-\hat{n}_{N\sigma})\right] \end{pmatrix} \end{array} \tag{49}$$

$$\begin{aligned} \mathcal{H}_{2N} = Tr_{N\sigma}\left[\mathcal{H}_{2N}\hat{n}_{N\sigma}\right]\hat{n}_{N\sigma} + c^{\dagger}_{N\sigma}Tr_{N\sigma}\left[\mathcal{H}_{2N}c_{N\sigma}\right] + Tr_{N\sigma}\left[c^{\dagger}_{N\sigma}\mathcal{H}_{2N}\right]c_{N\sigma} \\ + Tr_{N\sigma}\left[\mathcal{H}_{2N}(1-\hat{n}_{N\sigma})\right](1-\hat{n}_{N\sigma}) \end{aligned} \tag{50}$$

3.3 Proof of the theorem

Define an operator $\hat{P_{N\sigma}} = \hat{U}^{\dagger}_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma}$. This is the roated version of the number operator. What this does will be apparent from the following demonstration.

$$\begin{aligned} \left[\mathcal{H}_{2N}, \hat{P_{N\sigma}}\right] &= \left[\mathcal{H}_{2N}, \hat{U}^{\dagger}_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma}\right] = \mathcal{H}_{2N}\hat{U}^{\dagger}_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma} - \hat{U}^{\dagger}_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma}\mathcal{H}_{2N} \\ &= \hat{U}^{\dagger}_{N\sigma}\overline{\mathcal{H}_{2N}}\hat{n}_{N\sigma}\hat{U}_{N\sigma} - \hat{U}^{\dagger}_{N\sigma}\hat{n}_{N\sigma}\overline{\mathcal{H}_{2N}}\hat{U}_{N\sigma} = \hat{U}^{\dagger}_{N\sigma}\left[\mathcal{H}_{2N}, \hat{n}_{N\sigma}\right]\hat{U}_{N\sigma} \\ &= 0 \end{aligned} \tag{51}$$

We see that $\hat{P_{N\sigma}}$ is the operator that commutes with the original Hamiltonian. Note that here we are not transforming the Hamiltonian. Instead we are changing the single particle basis; $\hat{P_{N\sigma}}$ is not the single-particle occupation basis $\hat{n}_{N\sigma}$, rather a unitarily transformed version of that.This operator projects out the eigensubspaces of the diagonal Hamlitonian. $\hat{n}_{N\sigma}\mathcal{H}_{2N}\hat{n}_{N\sigma}$ will project out the subspace of the Hamiltonian in which the particle states are occupied, but since the $\mathcal{H}_{2N}$ is not diagonal, these will not be the eigensubspace. Instead, $\hat{P_{N\sigma}}\mathcal{H}_{2N}\hat{P_{N\sigma}}$ will project out the eigensubspace.
Both the approaches are mathematically equivalent; the matrix of $\mathcal{H}_{2N}$in the basis of $\hat{P_{N\sigma}}$ and the matrix of $\overline{\mathcal{H}_{2N}}$ in the basis of $\hat{n}_{N\sigma}$ will be identical; they will both be block-diagonal with the same blocks in the diagonal.

$\hat{P_{N\sigma}}$ also has the following properties:

- $\hat{P_{N\sigma}}^2 = \hat{U}^{\dagger}_{N\sigma}\hat{n}^2_{N\sigma}\hat{U}_{N\sigma} = \hat{U}^{\dagger}_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma} = \hat{P_{N\sigma}}$

- $\hat{P_{N\sigma}}(1-\hat{P_{N\sigma}}) = \hat{U}^{\dagger}_{N\sigma}\hat{n}_{N\sigma}(1-\hat{n}_{N\sigma})\hat{U}_{N\sigma} = 0$

Let the block-diagonal form of the Hamiltonian be

$$\overline{\mathcal{H}_{2N}} = \begin{pmatrix} \hat{E_{N\sigma}} & 0 \\ \\ 0 & \hat{E'_{N\sigma}} \end{pmatrix} \tag{52}$$

The block diagonal equations for $\overline{\mathcal{H}_{2N}}$ are then, very simply,:

$$\begin{aligned} \overline{\mathcal{H}_{2N}}\,|1\rangle &= \hat{E_{N\sigma}}\,|1\rangle \\ \overline{\mathcal{H}_{2N}}\,|0\rangle &= \hat{E'_{N\sigma}}\,|0\rangle \end{aligned} \tag{53}$$

$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ is the eigenstate of $\hat{n}_{N\sigma}$for the occupied state. Similarly, $|0\rangle$ is the vacant eigenstate. The goal is to construct expressions for the blocks $\hat{E_{N\sigma}}$ and $\hat{E'_{N\sigma}}$.

Its easy to see that if any matrix $\hat{A}$ is written in the basis of some operator $\hat{m}$, $\hat{m}\hat{A}\hat{m}$ returns the upper diagonal element of $\hat{A}$ and $(1-\hat{m})\hat{A}(1-\hat{m})$ returns the lower diagonal element. For example, to get the upper diagonal element,

$$\hat{A} = \begin{pmatrix} 1 & -1 \\ 2 & 0 \end{pmatrix} \implies \hat{m}\hat{A}\hat{m} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \times \begin{pmatrix} 1 & -1 \\ 2 & 0 \end{pmatrix} \times \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{54}$$

Similarly,

$$\hat{m}\hat{A}(1-\hat{m}) = \begin{pmatrix} 0 & -1 \\ 0 & 0 \end{pmatrix}, (1-\hat{m})\hat{A}\hat{m} = \begin{pmatrix} 0 & 0 \\ 2 & 0 \end{pmatrix}, (1-\hat{m})\hat{A}(1-\hat{m}) = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \tag{55}$$

We hence have the equation

$$\begin{aligned} \hat{n}_{N\sigma}\overline{\mathcal{H}_{2N}}\hat{n}_{N\sigma} = \hat{P_{N\sigma}}\mathcal{H}_{2N}\hat{P_{N\sigma}} &= \begin{pmatrix} \hat{E_{N\sigma}} & 0 \\ 0 & 0 \end{pmatrix} \\ (1-\hat{n}_{N\sigma})\overline{\mathcal{H}_{2N}}(1-\hat{n}_{N\sigma}) = (1-\hat{P_{N\sigma}})\mathcal{H}_{2N}(1-\hat{P_{N\sigma}}) &= \begin{pmatrix} 0 & 0 \\ 0 & \hat{E'_{N\sigma}} \end{pmatrix} \end{aligned} \tag{56}$$

Here, we have used the fact that the diagonal blocks remain invariant under unitary transformations.

Define two matrices diagonal in $\hat{n}_{N\sigma}$:

$$\mathcal{H}' = \hat{E_{N\sigma}} \otimes \mathbf{I} = \begin{pmatrix} \hat{E_{N\sigma}} & 0 \\ 0 & \hat{E_{N\sigma}} \end{pmatrix} \tag{57}$$

$$\mathcal{H}'' = \hat{E'_{N\sigma}} \otimes \mathbf{I} = \begin{pmatrix} \hat{E'_{N\sigma}} & 0 \\ 0 & \hat{E'_{N\sigma}} \end{pmatrix} \tag{58}$$

This enables us to derive the following equation between $\mathcal{H}_{2N}$ and $\mathcal{H}'$:

$$\begin{aligned} \mathcal{H}_{2N}\hat{P_{N\sigma}} = \mathcal{H}_{2N}\hat{U}^{\dagger}_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma} = \hat{U}^{\dagger}_{N\sigma}\overline{\mathcal{H}_{2N}}\hat{n}_{N\sigma}\hat{U}_{N\sigma} = \hat{U}^{\dagger}_{N\sigma}\begin{pmatrix} \hat{E_{N\sigma}} & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\hat{U}_{N\sigma} \\ = \hat{U}^{\dagger}_{N\sigma}\begin{pmatrix} \hat{E_{N\sigma}} & 0 \\ 0 & \hat{E_{N\sigma}} \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\hat{U}_{N\sigma} = \hat{U}^{\dagger}_{N\sigma}\hat{E_{N\sigma}} \otimes \mathbb{I}\ \hat{n}_{N\sigma}\hat{U}_{N\sigma} = \hat{E_{N\sigma}} \otimes \mathbb{I}\ \hat{U}^{\dagger}_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma} = \mathcal{H}'\hat{P_{N\sigma}} \end{aligned} \tag{59}$$

$$\therefore \mathcal{H}_{2N}\hat{P_{N\sigma}} = \mathcal{H}'\hat{P_{N\sigma}} \tag{60}$$

Similar;y, performing the calculation with $\mathcal{H}''$ gives

$$\therefore \mathcal{H}_{2N}(1 - \hat{P_{N\sigma}}) = \mathcal{H}''(1 - \hat{P_{N\sigma}}) \tag{61}$$

A general unitary matrix $\hat{U}_{N\sigma}$ has the form (in basis of $\hat{n}_{N\sigma}$)

$$\hat{U}_{N\sigma} = \begin{bmatrix} e^{\iota\phi_1}\cos\theta & e^{\iota\phi_2}\sin\theta \\ -e^{-\iota\phi_2}\sin\theta & e^{-\iota\phi_1}\cos\theta \end{bmatrix} \tag{62}$$

This provides a form for the matrix of the projection operator in the basis of $\hat{n}_{N\sigma}$:

$$\begin{aligned} \hat{P_{N\sigma}} = \hat{U}^{\dagger}_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma} = \begin{bmatrix} e^{-\iota\phi_1}\cos\theta & -e^{\iota\phi_2}\sin\theta \\ e^{-\iota\phi_2}\sin\theta & e^{\iota\phi_1}\cos\theta \end{bmatrix} \times \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \times \begin{bmatrix} e^{\iota\phi_1}\cos\theta & e^{\iota\phi_2}\sin\theta \\ -e^{-\iota\phi_2}\sin\theta & e^{-\iota\phi_1}\cos\theta \end{bmatrix} \\ = \begin{bmatrix} \cos^2\theta & \cos\theta\sin\theta e^{-\iota(\phi_1-\phi_2)} \\ \cos\theta\sin\theta e^{\iota(\phi_1-\phi_2)} & \sin^2\theta \end{bmatrix} \end{aligned} \tag{63}$$

The diagonal terms represent the particle(occupied) and hole(vacant) contributions; owing to symmetry, we set them equal $\cos^2\theta = \sin^2\theta = \frac{1}{2}$. Call the off-diagonal elements $\hat{\eta}_{01}$ and $\hat{\eta}^{\dagger}_{01}$. The final form becomes

$$\hat{P_{N\sigma}} = \frac{1}{2}\begin{bmatrix} 1 & \hat{\eta}^{\dagger}_{01} \\ \hat{\eta}_{01} & 1 \end{bmatrix} = \frac{1}{2}\left(\mathbf{I} + \eta_{N\sigma} + \eta^{\dagger}_{N\sigma}\right) \tag{64}$$

$$\mathbf{I} - \hat{P_{N\sigma}} = \frac{1}{2}\begin{bmatrix} 1 & -\hat{\eta}_{01}^{\dagger} \\ & \\ -\hat{\eta}_{01} & 1 \end{bmatrix} = \frac{1}{2}\left(\mathbf{I} - \eta_{N\sigma} - \eta_{N\sigma}^{\dagger}\right) \tag{65}$$

$\hat{\eta}_{N\sigma} = \hat{\eta}_{01} c_{N\sigma}$ is the electron to hole transition operator. $\hat{\eta}_{N\sigma}^{\dagger} = \hat{\eta}_{01}^{\dagger} c_{N\sigma}$ is the hole to electron transition operator. Hence, they are defined to have some pretty obvious properties.

1. $\hat{\eta}_{N\sigma}^2 = \hat{\eta_{N\sigma}^{\dagger}}^2 = 0$: once an electron or hole has undergone transition, there is no other to transition.

2. $(1 - \hat{n}_{N\sigma})\hat{\eta}_{N\sigma}\hat{n}_{N\sigma} = \eta_{N\sigma}$: this is expected from the fact that $\hat{\eta}_{N\sigma}$ acts with non-zero result only states of particle-number 1, and hence, $\hat{n}_{N\sigma}$ will just give 1; after the action of $\hat{\eta}_{N\sigma}$, we will get a state with hole (particle-number zero), so $(1 - \hat{n}_{N\sigma})$ will just give 1.

3. $\hat{n}_{N\sigma}\hat{\eta}_{N\sigma}(1 - \hat{n}_{N\sigma}) = 0$: this is expected because $1 - \hat{n}_{N\sigma}$ will give non-zero result only on hole states, but those states will give zero when acted upon by $\hat{\eta}_{N\sigma}$, because there won't be any electron to transition from.

These defining properties have many corrolaries in terms of properties of $\hat{\eta}_{N\sigma}$:

- $\hat{n}_{N\sigma}\hat{\eta}_{N\sigma} = \hat{\eta}_{N\sigma}^{\dagger}\hat{n}_{N\sigma} = 0$: act with $\hat{n}_{N\sigma}$ from left on property 2.
- $\hat{\eta}_{N\sigma}(1 - \hat{n}_{N\sigma}) = (1 - \hat{n}_{N\sigma})\hat{\eta}_{N\sigma}^{\dagger} = 0$: act with $1 - \hat{n}_{N\sigma}$ from right on property 2.
- $\hat{\eta}_{N\sigma}\hat{n}_{N\sigma} = (1 - \hat{n}_{N\sigma})\hat{\eta}_{N\sigma} = \eta_{N\sigma}$: act with $\hat{n}_{N\sigma}$ from right on property 2.

To construct the diagonalised Hamiltonian and get some properties of the $\eta_{N\sigma}$, we will use equations 60 and 61.

First of all, $\mathcal{H}_{2N}\hat{P}_{N\sigma} = \mathcal{H}' P_{N\sigma} \implies \hat{n}_{N\sigma}\mathcal{H}_{2N}\hat{P}_{N\sigma}(1 - \hat{n}_{N\sigma}) = \hat{n}_{N\sigma}\mathcal{H}'\hat{P}_{N\sigma}(1 - \hat{n}_{N\sigma})$.

The RHS simplifies as

$$\begin{aligned} \hat{P}_{N\sigma}(1 - \hat{n}_{N\sigma}) &= \frac{1}{2}(1 + \eta + \eta^{\dagger})(1 - \hat{n}_{N\sigma}) = \frac{1}{2}(1 + \eta^{\dagger})(1 - \hat{n}_{N\sigma}) \qquad (\because \eta_{N\sigma}(1 - \hat{n}_{N\sigma}) = 0) \\ \therefore \hat{n}_{N\sigma}\mathcal{H}'\hat{P}_{N\sigma}(1 - \hat{n}_{N\sigma}) &= \frac{1}{2}\hat{n}_{N\sigma}\mathcal{H}'(1 + \eta_{N\sigma}^{\dagger})(1 - \hat{n}_{N\sigma}) = \frac{1}{2}\mathcal{H}'\eta_{N\sigma}^{\dagger} \quad (\because \hat{n}_{N\sigma}\eta^{\dagger}(1 - \hat{n}_{N\sigma}) = \eta^{\dagger}) \end{aligned} \tag{66}$$

The LHS simplifies as

$$\begin{aligned} \hat{n}_{N\sigma}\mathcal{H}_{2N} &= (\hat{n}_{N\sigma}H_e\hat{n}_{N\sigma} + \hat{n}_{N\sigma}c^{\dagger}\hat{T} + \hat{n}_{N\sigma}\hat{T}^{\dagger}c + \hat{n}_{N\sigma}H_h(1 - \hat{n}_{N\sigma})) \\ &= H_e\hat{n}_{N\sigma} + c^{\dagger}\hat{T} \\ \Big(\because \hat{n}_{N\sigma}c^{\dagger} = c^{\dagger}, \hat{n}_{N\sigma}\hat{T}^{\dagger}c &= \hat{T}^{\dagger}\hat{n}_{N\sigma}c = 0, \hat{n}_{N\sigma}H_h(1 - \hat{n}_{N\sigma}) = H_h\hat{n}_{N\sigma}(1 - \hat{n}_{N\sigma}) = 0\Big) \end{aligned} \tag{67}$$

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

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 Determining the $\hat{U}_{N\sigma}$

The starting equation for the above construction was equation 60. That will also provide an expression for the $\hat{U}_{N\sigma}$. Operating equation 60 to the right of $|1\rangle$ (occupied eigenstate of

$\hat{n}_{N\sigma}$) gives

$$
\begin{aligned}
&\mathcal{H}_{2N}\hat{P}_{N\sigma}\left|1\right\rangle = \hat{E}_{N\sigma}\otimes\mathbf{I}\;\hat{P}_{N\sigma}\mathcal{H}_{2N}\left|1\right\rangle = \hat{E}_{N\sigma}\hat{P}_{N\sigma}\left|1\right\rangle \\
&\implies \mathcal{H}_{2N}\hat{U}^{\dagger}_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma}\left|1\right\rangle = \hat{E}_{N\sigma}\hat{U}^{\dagger}_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma}\left|1\right\rangle \qquad \left(\text{substituting expression of } \hat{P}_{N\sigma}\right) \\
&\implies \hat{U}_{N\sigma}\mathcal{H}_{2N}\hat{U}^{\dagger}_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma}\left|1\right\rangle = \hat{U}_{N\sigma}\hat{E}_{N\sigma}\hat{U}^{\dagger}_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma}\left|1\right\rangle \quad \left(\text{operating } \hat{U}_{N\sigma} \text{ from left}\right) \\
&\implies \overline{\mathcal{H}_{2N}}\hat{n}_{N\sigma}\hat{U}_{N\sigma}\left|1\right\rangle = \hat{U}_{N\sigma}\hat{E}_{N\sigma}\hat{U}^{\dagger}_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma}\left|1\right\rangle
\end{aligned}
\tag{82}
$$

Compare the last equation with 53. In order to satisfy the first equation of 53, we need the following two equations,

$$
\begin{aligned}
\hat{n}_{N\sigma}\hat{U}_{N\sigma}\left|1\right\rangle &\propto \left|1\right\rangle \\
\hat{U}_{N\sigma}\hat{E}_{N\sigma}\hat{U}^{\dagger}_{N\sigma} &= E_{N\sigma}
\end{aligned}
\tag{83}
$$

The second equations says

$$
\left[E_{N\sigma},\hat{U}_{N\sigma}\right] = 0 \tag{84}
$$

The $\hat{U}_{N\sigma}$ that satisfies the first equation is $\hat{U}_{N\sigma} = \kappa\left(1-\hat{\eta}+\hat{\eta}^{\dagger}\right)$. κ is a constant determined by the unitarity condition $\hat{U}_{N\sigma}\hat{U}^{\dagger}_{N\sigma} = \mathbf{I}$. To check that this satisfies 83,

$$
\begin{aligned}
\hat{n}_{N\sigma}\hat{U}_{N\sigma}\left|1\right\rangle &= \begin{pmatrix}\mathbf{I} & 0\\ 0 & 0\end{pmatrix}\kappa\begin{pmatrix}\mathbf{I} & \eta^{\dagger}_{01}\\ -\eta_{01} & \mathbf{I}\end{pmatrix}\begin{pmatrix}\mathbf{I}\\ 0\end{pmatrix} \\
&= \kappa\begin{pmatrix}\mathbf{I}\\ 0\end{pmatrix} \propto \left|1\right\rangle
\end{aligned}
\tag{85}
$$

To find κ,

$$
\begin{aligned}
\hat{U}_{N\sigma}\hat{U}^{\dagger}_{N\sigma} &= \kappa^2\begin{pmatrix}\mathbf{I} & \eta^{\dagger}_{01}\\ -\eta_{01} & \mathbf{I}\end{pmatrix}\begin{pmatrix}\mathbf{I} & -\eta^{\dagger}_{01}\\ \eta_{01} & \mathbf{I}\end{pmatrix} = \kappa^2\begin{pmatrix}\mathbf{I}+\eta^{\dagger}_{01}\eta_{01} & 0\\ 0 & \mathbf{I}+\eta^{\dagger}_{01}\eta_{01}\end{pmatrix} \\
&= \kappa^2\begin{pmatrix}\mathbf{I}+\eta^{\dagger}_{01}\eta_{01} & 0\\ 0 & \mathbf{I}+\eta^{\dagger}_{01}\eta_{01}\end{pmatrix} = 2\kappa^2\begin{pmatrix}\mathbf{I} & 0\\ 0 & \mathbf{I}\end{pmatrix} \left(\text{check } \textbf{??},\textbf{??} \text{ for } \eta^{\dagger}_{01}\eta_{01},\eta_{01}\eta^{\dagger}_{01}\right) \\
\implies \kappa &= \frac{1}{\sqrt{2}}
\end{aligned}
\tag{86}
$$

$$
\boxed{\hat{U}_{N\sigma} = \frac{1}{\sqrt{2}}\left(1-\hat{\eta}+\hat{\eta}^{\dagger}\right)} \tag{87}
$$

3.5 A corrolary: $\left[\hat{G}_e(\hat{E}_{N\sigma}), \hat{E}_{N\sigma}\right] = 0$

First note,

$$\hat{T}^\dagger_{N\sigma,e-h}\left[\hat{E}_{N\sigma}, \hat{G}_e(\hat{E}_{N\sigma})\right] = T^\dagger_{N\sigma,e-h}\hat{E}_{N\sigma}\hat{G}_e(\hat{E}_{N\sigma}) - T^\dagger_{N\sigma,e-h}\hat{G}_e(\hat{E}_{N\sigma})\hat{E}_{N\sigma} \tag{88}$$

Now,

$$T^\dagger_{N\sigma,e-h}\hat{G}_e(\hat{E}_{N\sigma})\hat{E}_{N\sigma} = \hat{\eta}_{01}\hat{E}_{N\sigma} \tag{89}$$

Also,

$$\begin{aligned}
T^\dagger_{N\sigma,e-h}\hat{E}_{N\sigma}\hat{G}_e(\hat{E}_{N\sigma}) &= T^\dagger_{N\sigma,e-h}\left[\hat{H}_{N\sigma,e} + \hat{T}_{N\sigma,e-h}\hat{\eta}_{01}\right]\hat{G}_e(\hat{E}_{N\sigma}) \\
&= T^\dagger_{N\sigma,e-h}\left[\hat{H}_{N\sigma,e}\hat{G}_e(\hat{E}_{N\sigma}) + \hat{T}_{N\sigma,e-h}\hat{G}_h(\hat{E}_{N\sigma})\hat{T}^\dagger_{N\sigma,e-h}\hat{G}_e(\hat{E}_{N\sigma})\right] \\
&= T^\dagger_{N\sigma,e-h}\hat{H}_{N\sigma,e}\hat{G}_e(\hat{E}_{N\sigma}) + T^\dagger_{N\sigma,e-h}
\end{aligned} \tag{90}$$

The last line follows because $\hat{T}_{N\sigma,e-h}\hat{G}_h(\hat{E}_{N\sigma})\hat{T}^\dagger_{N\sigma,e-h}\hat{G}_e(\hat{E}_{N\sigma}) = \mathbf{1}$. From **??**, we have

$$\begin{aligned}
\hat{E}_{N\sigma} - \hat{H}_{N\sigma,e} = \hat{T}_{N\sigma,e-h}\hat{\eta}_{01} &\implies \hat{G}_e^{-1}(\hat{E}_{N\sigma}) = \hat{T}_{N\sigma,e-h}\hat{G}_h(\hat{E}_{N\sigma})\hat{T}^\dagger_{N\sigma,e-h} \\
&\implies \mathbf{1} = \hat{T}_{N\sigma,e-h}\hat{G}_h(\hat{E}_{N\sigma})\hat{T}^\dagger_{N\sigma,e-h}\hat{G}_e(\hat{E}_{N\sigma})
\end{aligned} \tag{91}$$

Continuing from 90,

$$\begin{aligned}
T^\dagger_{N\sigma,e-h}\hat{E}_{N\sigma}\hat{G}_e(\hat{E}_{N\sigma}) &= T^\dagger_{N\sigma,e-h}\hat{H}_{N\sigma,e}\hat{G}_e(\hat{E}_{N\sigma}) + T^\dagger_{N\sigma,e-h} \\
&= \hat{H}_{N\sigma,h}T^\dagger_{N\sigma,e-h}\hat{G}_e(\hat{E}_{N\sigma}) + T^\dagger_{N\sigma,e-h}
\end{aligned} \tag{92}$$

The last line follows from equation **??**:

$$\begin{aligned}
&\hat{T}^\dagger_{N\sigma,e-h}\hat{G}_e(\hat{E}_{N\sigma}) = \hat{G}_h(\hat{E}_{N\sigma})\hat{T}^\dagger_{N\sigma,e-h} \\
&\implies (\hat{E}_{N\sigma} - \hat{H}_{N\sigma,h})\hat{T}^\dagger_{N\sigma,e-h} = \hat{T}^\dagger_{N\sigma,e-h}(\hat{E}_{N\sigma} - \hat{H}_{N\sigma,e}) \\
&\implies \hat{E}_{N\sigma}\hat{T}^\dagger_{N\sigma,e-h} - \hat{H}_{N\sigma,h}\hat{T}^\dagger_{N\sigma,e-h} = \hat{T}^\dagger_{N\sigma,e-h}\hat{E}_{N\sigma} - \hat{T}^\dagger_{N\sigma,e-h}\hat{H}_{N\sigma,e} \\
&\implies \hat{H}_{N\sigma,h}\hat{T}^\dagger_{N\sigma,e-h} = \hat{T}^\dagger_{N\sigma,e-h}\hat{H}_{N\sigma,e} \qquad \left(\because \hat{E}_{N\sigma}\hat{T}^\dagger_{N\sigma,e-h} = \hat{T}^\dagger_{N\sigma,e-h}\hat{E}_{N\sigma}\right)
\end{aligned} \tag{93}$$

Again continuing from 92,

$$\begin{aligned}
&T^\dagger_{N\sigma,e-h}\hat{E}_{N\sigma}\hat{G}_e(\hat{E}_{N\sigma}) = \hat{H}_{N\sigma,h}T^\dagger_{N\sigma,e-h}\hat{G}_e(\hat{E}_{N\sigma}) + T^\dagger_{N\sigma,e-h} \\
&= \hat{H}_{N\sigma,h}\hat{G}_h(\hat{E}_{N\sigma})T^\dagger_{N\sigma,e-h} + T^\dagger_{N\sigma,e-h} && \text{(from eq ??)} \\
&= \hat{H}_{N\sigma,h}\hat{G}_h(\hat{E}_{N\sigma})T^\dagger_{N\sigma,e-h} + T^\dagger_{N\sigma,e-h}G_e(\hat{E}_{N\sigma})T_{N\sigma,e-h}G_h(\hat{E}_{N\sigma})T^\dagger_{N\sigma,e-h} && \text{(from eq 91)} \\
&= \left(\hat{H}_{N\sigma,h} + T^\dagger_{N\sigma,e-h}G_e(\hat{E}_{N\sigma})T_{N\sigma,e-h}\right)\hat{G}_h(\hat{E}_{N\sigma})T^\dagger_{N\sigma,e-h} \\
&= \left(\hat{H}_{N\sigma,h} + T^\dagger_{N\sigma,e-h}\hat{\eta}^\dagger_{01}\right)\hat{G}_h(\hat{E}_{N\sigma})T^\dagger_{N\sigma,e-h} \\
&= \hat{E}_{N\sigma}\hat{G}_h(\hat{E}_{N\sigma})T^\dagger_{N\sigma,e-h} \\
&= \hat{E}_{N\sigma}\hat{\eta}_{01}
\end{aligned} \tag{94}$$

Therefore,

$$T^{\dagger}_{N\sigma,e-h}\hat{E}_{N\sigma}\hat{G}_e(\hat{E}_{N\sigma}) = \hat{E}_{N\sigma}\hat{\eta}_{01} \tag{95}$$

Substituting equations 89 and 95 in equation 88, we have

$$\begin{aligned} \hat{T}^{\dagger}_{N\sigma,e-h}\left[\hat{E}_{N\sigma}, \hat{G}_e(\hat{E}_{N\sigma})\right] &= \hat{E}_{N\sigma}\hat{\eta}_{01} - \hat{\eta}_{01}\hat{E}_{N\sigma} = \left[\hat{E}_{N\sigma}, \hat{\eta}_{01}\right] \\ &= 0 \qquad \text{(from equation 84)} \end{aligned} \tag{96}$$

Therefore,

$$\boxed{\left[\hat{E}_{N\sigma}, \hat{G}_e(\hat{E}_{N\sigma})\right] = 0} \tag{97}$$

3.6 A Simple Example

$$\mathcal{H} = -t\left(c_2^{\dagger}c_1 + c_1^{\dagger}c_2\right) + V\hat{n}_1\hat{n}_2 - \mu(\hat{n}_1 + \hat{n}_2) \quad \hat{n}_i = c_i^{\dagger}c_i = \begin{pmatrix} V-2\mu & 0 & 0 & 0 \\ 0 & -\mu & -t & 0 \\ 0 & -t & \mu & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{98}$$

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).

$$\begin{aligned} \hat{H}_{1,e} &= Tr_1[\mathcal{H}\hat{n}_1] \\ &= Tr_1[V\hat{n}_1\hat{n}_2 - \mu(\hat{n}_1 + \hat{n}_2)] \quad \left(c \text{ and } c^{\dagger} \text{ will not conserve the eigenvalue of } \hat{n}\right) \\ &= V\hat{n}_2 - \mu(1 + \hat{n}_2) \qquad (Tr_1[V\hat{n}_1\hat{n}_2] = VTr_1[\hat{n}_1]\hat{n}_2 = V\hat{n}_2) \\ &= (V - 2\mu)\hat{n}_2 - \mu(1 - \hat{n}_2) \end{aligned} \tag{99}$$

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

$$\hat{H}_{1,h} = Tr_1[\mathcal{H}(1 - \hat{n}_1)] = -\mu\hat{n}_2 \tag{100}$$

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

$$\begin{aligned} T_{1,e-h} &= Tr_1[\mathcal{H}c_1] \\ &= Tr_1[-tc_1^{\dagger}c_2c_1] = -tc_2 \quad \text{(the only term that conserves eigenvalue of } \hat{n}) \end{aligned} \tag{101}$$

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

$$\mathcal{H} = \begin{pmatrix} (V-2\mu)\hat{n}_2 - \mu(1-\hat{n}_2) & -tc_2 \\ -tc_2^{\dagger} & -\mu\hat{n}_2 \end{pmatrix} \tag{102}$$

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,

$$
\begin{aligned}
t^2 G_e c_1^\dagger c_2 c_2^\dagger c_1 G_e = \hat{n}_1 &\implies t^2\hat{n}_1(1-\hat{n}_2) = \hat{n}_1\{G_e^{-1}\}^2 = \hat{n}_1(\mathcal{H}' - H_e\hat{n}_1)^2 \\
&\implies t^2\hat{n}_1^2(1-\hat{n}_2)^2 = (\mathcal{H}'\hat{n}_1 - H_e\hat{n}_1)^2 \\
&\implies \mathcal{H}'\hat{n}_1 = H_e\hat{n}_1 + t\hat{n}_1(1-\hat{n}_2) = (V-2\mu)\hat{n}_1\hat{n}_2 + (t-\mu)\hat{n}_1(1-\hat{n}_2)
\end{aligned}
\tag{103}
$$

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,

$$
\overline{\mathcal{H}} = \mathcal{H}'\hat{n}_1 + \mathcal{H}''(1-\hat{n}_1) = \begin{pmatrix} \begin{matrix} V-2\mu & 0 \\ 0 & t-\mu \end{matrix} & \mathbf{0}_{2x2} \\ \mathbf{0}_{2x2} & (\hat{E}'_1)_{2x2} \end{pmatrix} \tag{104}
$$

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.

$$
E'_1(1-\hat{n}_1) = H_h(1-\hat{n}_1) - \hat{T}_1^\dagger c_1\eta^\dagger = -\mu(1-\hat{n}_1)\hat{n}_2 - t^2 c_2^\dagger c_1 G_e c_1^\dagger \hat{c}_2 \tag{105}
$$

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

$$
\langle 01| E'(1-\hat{n}_1) |01\rangle = -\mu - t^2 \langle 10| G_e |10\rangle \tag{106}
$$

Now,

$$\begin{aligned}\langle 10| G_e^{-1} |10\rangle &= \langle 10| H' - (V-\mu)\hat{n}_1\hat{n}_2 + \mu\hat{n}_1 |10\rangle \\ &= \langle 10| \mathcal{H}' |10\rangle + \mu = \langle 10| \mathcal{H}'\hat{n}_1 |10\rangle + \mu \\ &= \langle 10| (V-2\mu)\hat{n}_1\hat{n}_2 + (t-\mu)\hat{n}_1(1-\hat{n}_2) |10\rangle + \mu \\ &= t - \mu + \mu = t \\ \therefore \langle 10| G_e |10\rangle &= \frac{1}{t}\end{aligned} \tag{107}$$

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

$$\overline{\mathcal{H}} = \begin{array}{c} \begin{array}{cccc} |11\rangle & |10\rangle & |01\rangle & |00\rangle \end{array} \\ \begin{pmatrix} (V-2\mu) & 0 & 0 & 0 \\ 0 & (t-\mu) & 0 & 0 \\ 0 & 0 & -(\mu+t) & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \end{array} \tag{108}$$

3.6.1 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 $\hat{n}$:

$$\mathcal{H}(\hat{U}^\dagger_{N\sigma} |n_1, n_2\rangle) = \hat{U}^\dagger_{N\sigma}\overline{\mathcal{H}} |n_1, n_2\rangle = \hat{U}^\dagger_{N\sigma} E_{n_1,n_2} |n_1, n_2\rangle = E_{n_1,n_2}(\hat{U}^\dagger_{N\sigma} |n_1, n_2\rangle) \tag{109}$$

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 87, 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 ($|n_1, n_2\rangle$):

$$\hat{U}^\dagger_{N\sigma} |11\rangle = |11\rangle \tag{110}$$

$$\hat{U}^\dagger_{N\sigma} |00\rangle = |00\rangle\,, \tag{111}$$

$$\begin{aligned}\hat{U}^\dagger_{N\sigma} |10\rangle = \frac{1}{2}\left(|10\rangle - \eta |10\rangle\right) = \frac{1}{2}\left(|10\rangle + tc_2^\dagger c_1 \hat{G}_e |10\rangle\right) &= \frac{1}{2}\left(|10\rangle + tc_2^\dagger c_1 \frac{1}{t} |01\rangle\right) \\ &= \frac{1}{2}\left(|10\rangle + |01\rangle\right)\end{aligned} \tag{112}$$

$$\hat{U}^\dagger_{N\sigma} |01\rangle = \frac{1}{2}\left(|01\rangle + \eta^\dagger |01\rangle\right) = \frac{1}{2}\left(|01\rangle - t\hat{G}_e c_1^\dagger c_2 |01\rangle\right) = \frac{1}{2}\left(|01\rangle - |10\rangle\right) \tag{113}$$

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

$$\begin{aligned} &|00\rangle \\ &|10\rangle + |01\rangle \\ &|01\rangle - |10\rangle \\ &|11\rangle \end{aligned} \tag{114}$$

3.7 Applying the RG on the Hubbard dimer

$$\mathcal{H} = -t\sum_\sigma (c^\dagger_{1\sigma}c_{2\sigma} + c^\dagger_{2\sigma}c_{1\sigma}) + U\left(\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow}\right)$$
$$H_e = Tr_{\hat{n}_{1\uparrow}}(\mathcal{H}\hat{n}_{1\uparrow}) = U(\hat{n}_{1\downarrow} + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow}) - t(c^\dagger_{1\downarrow}c_{2\downarrow} + c^\dagger_{2\downarrow}c_{1\downarrow})$$
$$H_h = Tr_{\hat{n}_{1\uparrow}}(\mathcal{H}(1-\hat{n}_{1\uparrow})) = U\hat{n}_{2\uparrow}\hat{n}_{2\downarrow} - t(c^\dagger_{1\downarrow}c_{2\downarrow} + c^\dagger_{2\downarrow}c_{1\downarrow})$$
$$T = Tr_{\hat{n}_{1\uparrow}}(\mathcal{H}c_{1\uparrow}) = -tc_{2\uparrow}$$
$$T^\dagger = Tr_{\hat{n}_{1\uparrow}}(c^\dagger_{1\uparrow}\mathcal{H}) = -tc^\dagger_{2\uparrow}$$
$$\eta^\dagger_{1\uparrow} = G_e c^\dagger_{1\uparrow}T = -t\hat{G}_e c^\dagger_{1\uparrow}c_{2\uparrow} = -t(\mathcal{H}'_{1\uparrow} - H_e\hat{n})^{-1}c^\dagger_{1\uparrow}c_{2\uparrow}$$
$$\therefore \eta_{1\uparrow} = -tc^\dagger_{2\uparrow}c_{1\uparrow}(\mathcal{H}'_{1\uparrow} - H_e\hat{n})^{-1}$$
$$\eta^\dagger_{1\uparrow}\eta_{1\uparrow} = \hat{n}_{1\uparrow} \implies t^2(1-\hat{n}_{2\uparrow}) = (\mathcal{H}'_{1\uparrow} - H_e\hat{n}_{1\uparrow})^2\hat{n}_{1\uparrow} \implies \mathcal{H}'_{1\uparrow}\hat{n}_{1\uparrow} = H_e\hat{n}_{1\uparrow} + t(1-\hat{n}_{2\uparrow})\hat{n}_{1\uparrow} \tag{115}$$
$$\mathcal{H}'_{1\uparrow}\hat{n}_{1\uparrow} = U\hat{n}_{1\uparrow}(\hat{n}_{1\downarrow} + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow}) + t\hat{n}_{1\uparrow}(1 - \hat{n}_{2\uparrow} - c^\dagger_{1\downarrow}c_{2\downarrow} - c_{1\downarrow}c^\dagger_{2\downarrow}) \tag{116}$$

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

$$\hat{E}_{1\uparrow} = \langle\hat{n}_{1\uparrow} = 1|\,\mathcal{H}'_{1\uparrow}\hat{n}_{1\uparrow}\,|\hat{n}_{1\uparrow} = 1\rangle = U(\hat{n}_{1\downarrow} + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow}) + t(1 - \hat{n}_{2\uparrow} - c^\dagger_{1\downarrow}c_{2\uparrow} - c^\dagger_{2\uparrow}c_{1\downarrow}) \tag{117}$$

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 $\hat{n}_{1\downarrow}$.

$$\begin{aligned} H_e &= Tr_{\hat{n}_{1\downarrow}}(\mathcal{H}_{1\downarrow}\hat{n}_{1\downarrow}) = U(1 + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow}) + t(1-\hat{n}_{2\uparrow}) \\ H_h &= U\hat{n}_{2\uparrow}\hat{n}_{2\downarrow} + t(1-\hat{n}_{2\uparrow}) \\ T &= -tc_{2\downarrow} \\ T^\dagger &= -tc^\dagger_{2\downarrow} \\ \eta^\dagger_{1\downarrow} &= \hat{G}_e c^\dagger_{1\downarrow}T = -t\hat{G}_e c^\dagger_{1\downarrow}c_{2\downarrow} \\ \implies \eta_{1\downarrow} &= -tc^\dagger_{2\downarrow}c_{1\downarrow}\hat{G}_e \end{aligned} \tag{118}$$

Then,

$$\eta^\dagger_{1\downarrow}\eta_{1\downarrow} = \hat{n}_{1\downarrow} \implies \mathcal{H}'_{1\downarrow}\hat{n}_{1\downarrow} = H_e\hat{n}_{1\downarrow} + t\hat{n}_{1\downarrow}(1-\hat{n}_{2\downarrow}) = U\hat{n}_{1\downarrow}(1 + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow}) + 2t\hat{n}_{1\downarrow}(1-\hat{n}_{2\downarrow}) \tag{119}$$

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 $\hat{E}_{1\downarrow} = \langle\hat{n}_{1\downarrow} = 1|\,\mathcal{H}'_{1\downarrow}\hat{n}_{1\downarrow}\,|\hat{n}_{1\downarrow} = 1\rangle$

$$E_{\hat{n}_{1\downarrow}} = U(\hat{n}_{2\uparrow}\hat{n}_{2\downarrow} + 1) + 2t(1 - \hat{n}_{2\downarrow}) = \begin{pmatrix} 2U & & & \\ & U+2t & & \\ & & U & \\ & & & U+2t \end{pmatrix} \tag{120}$$

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.

$$\mathcal{H}''_{1\downarrow}\hat{n}_{1\downarrow} = H_h(1 - \hat{n}_{1\downarrow}) - T^\dagger c_{1\downarrow}\eta^\dagger_{1\downarrow} = H_h(1 - \hat{n}_{1\downarrow}) - t^2 c^\dagger_{2\downarrow} c_{1\downarrow} G_e c^\dagger_{1\downarrow} c_{2\downarrow} \tag{121}$$

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

$$\begin{aligned} \langle 1 | G_e^{-1} | 1 \rangle = \langle 1 | \mathcal{H}'_{1\downarrow} - H_e \hat{n}_{1\downarrow} | 1 \rangle = \langle 1 | \mathcal{H}'_{1\downarrow}\hat{n}_{1\downarrow} - H_e \hat{n}_{1\downarrow} | 1 \rangle = t(1 - \hat{n}_{2\downarrow}) \\ \therefore \hat{E}'_{1\downarrow} = H_h - t c^\dagger_{2\downarrow} \frac{1}{1 - \hat{n}_{2\downarrow}} c_{2\downarrow} = H_h - t\hat{n}_{2\downarrow} = U\hat{n}_{2\uparrow}\hat{n}_{2\downarrow} + t(1 - \hat{n}_{2\uparrow}\hat{n}_{2\downarrow}) \end{aligned} \tag{122}$$

$$E'_{1\downarrow} = H_h - t\hat{n}_{2\downarrow} = U\hat{n}_{2\uparrow}\hat{n}_{2\downarrow} + t(1 - \hat{n}_{2\uparrow}\hat{n}_{2\downarrow}) = \begin{pmatrix} U-t & & & \\ & 0 & & \\ & & 0 & \\ & & & -t \end{pmatrix} \tag{123}$$

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

$$E'_{1\hat{n}_{1\downarrow}} = \begin{pmatrix} 2U & & & & & & & \\ & U+2t & & & & & & \\ & & U & & & & & \\ & & & U+2t & & & & \\ & & & & 2U-t & & & \\ & & & & & U-t & & \\ & & & & & & U & \\ & & & & & & & U \end{pmatrix} \tag{124}$$

3.7.1 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

$$\eta_{1\downarrow} = -tc^{\dagger}_{2\downarrow}c_{1\downarrow}\hat{G}_e,\ \eta^{\dagger}_{1\downarrow} = -t\hat{G}_e c^{\dagger}_{1\downarrow}c_{2\downarrow} \tag{125}$$

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 $\hat{n}_{1\downarrow} = 0, \hat{n}_{2\downarrow} = 1$.

$$\begin{aligned} \eta^{\dagger}_{1\downarrow}|0,\hat{n}_{2\uparrow},1\rangle = -t\hat{G}_e|1,\hat{n}_{2\uparrow},0\rangle = \frac{-t}{\mathcal{H}'_{1\downarrow} - H_e\hat{n}_{1\downarrow}}|1,\hat{n}_{2\uparrow},0\rangle &= \frac{-t}{\mathcal{H}'_{1\downarrow}\hat{n}_{1\downarrow} - H_e\hat{n}_{1\downarrow}}|1,\hat{n}_{2\uparrow},0\rangle \\ &= \frac{-t}{t\hat{n}_{1\downarrow}(1-\hat{n}_{2\downarrow})}|1,\hat{n}_{2\uparrow},0\rangle = -|1,\hat{n}_{2\uparrow},0\rangle \end{aligned} \tag{126}$$

Similarly,

$$\eta_{1\downarrow}|1,\hat{n}_{2\uparrow},0\rangle = -tc^{\dagger}_{2\downarrow}c_{1\downarrow}\hat{G}_e|1,\hat{n}_{2\uparrow},0\rangle = -tc^{\dagger}_{2\downarrow}c_{1\downarrow}\frac{1}{t}|1,\hat{n}_{2\uparrow},0\rangle = -|0,\hat{n}_{2\uparrow},1\rangle \tag{127}$$

Therefore,

$$\begin{aligned} U^{\dagger}_{1\downarrow}|1,\hat{n}_{2\uparrow},0\rangle &= (1-\eta_{1\downarrow})|1,\hat{n}_{2\uparrow},0\rangle = |1,\hat{n}_{2\uparrow},0\rangle + |0,\hat{n}_{2\uparrow},1\rangle \\ U^{\dagger}_{1\downarrow}|0,\hat{n}_{2\uparrow},1\rangle &= (1+\eta^{\dagger}_{1\downarrow})|0,\hat{n}_{2\uparrow},1\rangle = |0,\hat{n}_{2\uparrow},1\rangle - |1,\hat{n}_{2\uparrow},0\rangle \\ U^{\dagger}_{1\downarrow}|1,\hat{n}_{2\uparrow},1\rangle &= |1,\hat{n}_{2\uparrow},1\rangle \\ U^{\dagger}_{1\downarrow}|0,\hat{n}_{2\uparrow},0\rangle &= |0,\hat{n}_{2\uparrow},0\rangle \end{aligned} \tag{128}$$

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.

$$\begin{aligned} \eta^\dagger_{1\uparrow} = -t\hat{G}_e c^\dagger_{1\uparrow} c_{2\uparrow},\ \eta_{1\uparrow} = -tc^\dagger_{2\uparrow} c_{1\uparrow}\hat{G}_e \\ \eta^\dagger_{1\uparrow} \left|\hat{n}_{1\uparrow} = 0, \hat{n}_{1\downarrow}, \hat{n}_{2\uparrow} = 1, \hat{n}_{2\downarrow}\right\rangle = -\left|1, \hat{n}_{1\downarrow}, 0, \hat{n}_{2\downarrow}\right\rangle \\ \eta_{1\uparrow} \left|\hat{n}_{1\uparrow} = 1, \hat{n}_{1\downarrow}, \hat{n}_{2\uparrow} = 0, \hat{n}_{2\downarrow}\right\rangle = -\left|0, \hat{n}_{1\downarrow}, 1, \hat{n}_{2\downarrow}\right\rangle \end{aligned} \tag{129}$$

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)

Exact Diagonalization of Hubbard Dimer

$\hat{N}$	S_z^{tot}	$\hat{P}$	E	$\|\Phi\rangle$
0	-	-	0	$\|0,0\rangle$
1	-1	1	-t-μ	$\frac{\|\downarrow,0\rangle+\|0,\downarrow\rangle}{\sqrt{2}}$
		-1	t-μ	$\frac{\|\downarrow,0\rangle-\|0,\downarrow\rangle}{\sqrt{2}}$
	1	1	-t-μ	$\frac{\|\uparrow,0\rangle+\|0,\uparrow\rangle}{\sqrt{2}}$
		-1	t-μ	$\frac{\|\uparrow,0\rangle-\|0,\uparrow\rangle}{\sqrt{2}}$
2	-1	1	0-2μ	$\|\downarrow,\downarrow\rangle$
	0	1	0-2μ	$\frac{\|\uparrow,\downarrow\rangle+\|\downarrow,\uparrow\rangle}{\sqrt{2}}$
		1	U-2μ	$\frac{\|\uparrow\downarrow,0\rangle+\|0,\uparrow\downarrow\rangle}{\sqrt{2}}$
		-1	$\frac{U+\sqrt{U^2+16t^2}}{2}-2\mu$	$\frac{1}{N_\pm}\left\{2t\frac{(\|\uparrow,\downarrow\rangle-\|\downarrow,\uparrow\rangle)}{\sqrt{2}}+\frac{U\pm\sqrt{U^2+16t^2}}{2}\frac{(\|\uparrow\downarrow,0\rangle-\|0,\uparrow\downarrow\rangle)}{\sqrt{2}}\right\}$
		-1	$\frac{U-\sqrt{U^2+16t^2}}{2}-2\mu$	$\frac{1}{N_-}\left\{2t\frac{(\|\uparrow,\downarrow\rangle-\|\downarrow,\uparrow\rangle)}{\sqrt{2}}+\frac{U-\sqrt{U^2+16t^2}}{2}\frac{(\|\uparrow\downarrow,0\rangle-\|0,\uparrow\downarrow\rangle)}{\sqrt{2}}\right\}$
	1	1	0-2μ	$\|\uparrow,\uparrow\rangle$
3	-1	1	U-t-3μ	$\frac{\|\uparrow\downarrow,\downarrow\rangle+\|\downarrow,\uparrow\downarrow\rangle}{\sqrt{2}}$
		-1	U+t-3μ	$\frac{\|\uparrow\downarrow,\downarrow\rangle-\|\downarrow,\uparrow\downarrow\rangle}{\sqrt{2}}$
	1	1	U-t-3μ	$\frac{\|\uparrow\downarrow,\uparrow\rangle+\|\uparrow,\uparrow\downarrow\rangle}{\sqrt{2}}$
		-1	U+t-3μ	$\frac{\|\uparrow\downarrow,\uparrow\rangle-\|\uparrow,\uparrow\downarrow\rangle}{\sqrt{2}}$
4	0	1	2U-4μ	$\|\uparrow\downarrow,\uparrow\downarrow\rangle$

Exact Diagonalization of Anderson Molecule			
$\hat{N}$	S^z_{tot}	E	$\vert\Phi\rangle$
0	-	0	$\vert 0,0\rangle$
1	-1	$\epsilon_d + \frac{1}{4}(U \pm \Delta)$	$\frac{1}{N_\pm}\left(t\vert\downarrow,0\rangle - \frac{1}{4}(U\pm\Delta)\vert 0,\downarrow\rangle\right)$
	1	$\epsilon_d + \frac{1}{4}(U \pm \Delta)$	$\frac{1}{N_\pm}\left(t\vert\downarrow,0\rangle - \frac{1}{4}(U\pm\Delta)\vert 0,\downarrow\rangle\right)$
2	-1	$2\epsilon_d + \frac{U}{2}$	$\vert\downarrow,\downarrow\rangle$
	1	$2\epsilon_d + \frac{U}{2}$	$\vert\uparrow,\uparrow\rangle$
	0	$2\epsilon_d + \frac{U}{2}$	$\frac{\vert\uparrow,\downarrow\rangle + \vert\downarrow,\uparrow\rangle}{\sqrt{2}}$
		$2\epsilon_d + U$	$\frac{\vert\uparrow\downarrow,0\rangle + \vert 0,\uparrow\downarrow\rangle}{\sqrt{2}}$
		$2\epsilon_d + \frac{3}{4}U \pm \frac{1}{2}\Delta(\frac{U}{2},t)$	$\frac{U\mp\Delta}{4\sqrt{2}t}\frac{\vert\uparrow,\downarrow\rangle - \vert\downarrow,\uparrow\rangle}{\sqrt{2}} - \vert\uparrow\downarrow,0\rangle + \vert 0,\uparrow\downarrow\rangle$
3	-1	$3\epsilon_d + \frac{5}{4}U \pm \frac{1}{4}\Delta$	$\frac{1}{N_\pm}(t\vert\uparrow\downarrow,\downarrow\rangle - \frac{1}{4}(U\pm\Delta)\vert\downarrow,\uparrow\downarrow\rangle)$
	1	$3\epsilon_d + \frac{5}{4}U \pm \frac{1}{4}\Delta$	$\frac{1}{N_\pm}(t\vert\uparrow\downarrow,\downarrow\rangle - \frac{1}{4}(U\pm\Delta)\vert\downarrow,\uparrow\downarrow\rangle)$
4	0	$2(\epsilon_s + \epsilon_d) + U$	$\vert\uparrow\downarrow,\uparrow\downarrow\rangle$