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1 Exact diagonalization of the two-site Hubbard model

The Hamiltonian

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

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.

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,

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

- $c^\dagger_{2\sigma}c_{1\sigma}$: 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.
- $\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$:

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

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

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: $\mathcal{H}, \hat{N}, S^{tot}_z, \hat{P}$. 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.

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

1.3.2 $S_z^{tot} = +1$

Now I look at the spin-up states.

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

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 $S_z^{tot} = -1$

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

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

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

1.4.2 $S_z^{tot} = +1$

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

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

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

1.5 N=4

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

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

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

1.6 N=2

This is the eigenvalue that has the largest subspace.

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

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

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

1.6.2 $S_z^{tot} = 0$

This subspace has four eigenvectors,

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

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

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

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

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

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

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

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 $\hat{P}=-1$.

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

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

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^{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

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

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

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

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

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 $N^2_\pm = t^2 + (\frac{U \pm \Delta}{4})^2$

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

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

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 : $\frac{1}{N_\pm}\left(t\left|\uparrow,0\right\rangle + (\epsilon_d - \lambda_\pm)\left|0,\uparrow\right\rangle\right)$

2.3 N=3

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

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

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

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

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

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

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

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

2.4 N=2

This is the eigenvalue that has the largest subspace.

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

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

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, $Tr_{N\sigma}(H_3 c_{N\sigma}\hat{n}_{N\sigma}) = H_3 Tr_{N\sigma}(c_{N\sigma}\hat{n}_{N\sigma}) = H_3 Tr_{N\sigma}(\hat{n}_{N\sigma}c_{N\sigma}) = 0$, because $\hat{n}_{N\sigma}c_{N\sigma} = 0$. So,

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

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,:

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

$\left|1\right\rangle = \begin{pmatrix} 1 \\ \\ 0 \end{pmatrix}$ is the eigenstate of $\hat{n}_{N\sigma}$for the occupied state. Similarly, $\left|0\right\rangle$ 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 $\mathcal{H}'$:

$$\mathcal{H}_{2N}\hat{P}_{N\sigma} = \mathcal{H}_{2N}\hat{U}^{\dagger}_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma} = \hat{U}^{\dagger}_{N\sigma}\overline{\mathcal{H}_{2N}}\hat{n}_{N\sigma}\hat{U}_{N\sigma} = \hat{U}^{\dagger}_{N\sigma}\begin{pmatrix} \hat{E}_{N\sigma} & 0 \\ & \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ & \\ 0 & 0 \end{pmatrix}\hat{U}_{N\sigma}$$

$$= \hat{U}^{\dagger}_{N\sigma}\begin{pmatrix} \hat{E}_{N\sigma} & 0 \\ & \\ 0 & \hat{E}_{N\sigma} \end{pmatrix}\begin{pmatrix} 1 & 0 \\ & \\ 0 & 0 \end{pmatrix}\hat{U}_{N\sigma} = \hat{U}^{\dagger}_{N\sigma}\hat{E}_{N\sigma} \otimes \mathbb{I}\ \hat{n}_{N\sigma}\hat{U}_{N\sigma} = \hat{E}_{N\sigma} \otimes \mathbb{I}\ \hat{U}^{\dagger}_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma} = \mathcal{H}' P \tag{59}$$

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

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

$\hat{n}_{N\sigma}$:

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

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

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

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

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

1. $\hat{\eta}^2_{N\sigma} = \hat{\eta^\dagger_{N\sigma}}^2 = 0$: 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 $\hat{\eta}_{N\sigma}$:

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

Using 60 and the matrix form of $\hat{P_{N\sigma}}$, $\mathcal{H}_{2N}$ and $\mathcal{H}'$ (64, 49 and 57), we get

$$\begin{pmatrix} \hat{H}_{N\sigma,e} & \hat{T}_{N\sigma,e-h} \\ T^\dagger_{N\sigma,e-h} & \hat{H}_{N\sigma,h} \end{pmatrix} \begin{pmatrix} 1 & \hat{\eta}^\dagger_{01} \\ \hat{\eta}_{01} & 1 \end{pmatrix} = \hat{E}_{N\sigma}\mathbf{I} \begin{pmatrix} 1 & \hat{\eta}^\dagger_{01} \\ \hat{\eta}_{01} & 1 \end{pmatrix}$$
$$\Longrightarrow \begin{pmatrix} \hat{H}_{N\sigma,e} + \hat{T}_{N\sigma,e-h}\hat{\eta}_{01} & \hat{H}_{N\sigma,e}\hat{\eta}^\dagger_{01} + \hat{T}_{N\sigma,e-h} \\ \hat{H}_{N\sigma,h}\hat{\eta}_{01} + T^\dagger_{N\sigma,e-h} & \hat{H}_{N\sigma,h} + T^\dagger_{N\sigma,e-h}\hat{\eta}^\dagger_{01} \end{pmatrix} = \begin{pmatrix} \hat{E}_{N\sigma} & \hat{E}_{N\sigma}\hat{\eta}^\dagger_{01} \\ \hat{E}_{N\sigma}\hat{\eta}_{01} & \hat{E}_{N\sigma} \end{pmatrix} \tag{66}$$

The off-diagonal equations give expressions for the $\hat{\eta}_{N\sigma}$.

$$\begin{aligned} \hat{E}_{N\sigma}\hat{\eta}^\dagger_{01} = \hat{H}_{N\sigma,e}\hat{\eta}^\dagger_{01} + \hat{T}_{N\sigma,e-h} \implies \hat{\eta}^\dagger_{01} &= \frac{1}{\hat{E}_{N\sigma} - \hat{H}_{N\sigma,e}}\hat{T}_{N\sigma,e-h} = \hat{G}_e(\hat{E}_{N\sigma})\hat{T}_{N\sigma,e-h} \\ \implies \hat{\eta}^\dagger_{N\sigma} &= c^\dagger_{N\sigma}\hat{\eta}^\dagger_{01} = c^\dagger_{N\sigma}\hat{G}_e(\hat{E}_{N\sigma})\hat{T}_{N\sigma,e-h} \end{aligned} \tag{67}$$

$$\begin{aligned} \hat{E}_{N\sigma}\hat{\eta}_{01} = \hat{H}_{N\sigma,h}\hat{\eta}_{01} + T^\dagger_{N\sigma,e-h} \implies \hat{\eta}_{01} &= \frac{1}{\hat{E}_{N\sigma} - \hat{H}_{N\sigma,h}}T^\dagger_{N\sigma,e-h} = \hat{G}_h(\hat{E}_{N\sigma})T^\dagger_{N\sigma,e-h} \\ \implies \hat{\eta}_{N\sigma} &= \hat{\eta}_{01}c_{N\sigma} = \hat{G}_h(\hat{E}_{N\sigma})T^\dagger_{N\sigma,e-h}c_{N\sigma} \end{aligned} \tag{68}$$

where

$$\hat{G}_e(\hat{E}_{N\sigma}) \equiv \frac{1}{\hat{E}_{N\sigma} - \hat{H}_{N\sigma,e}}.\ \hat{G}_h(\hat{E}_{N\sigma}) \equiv \frac{1}{\hat{E}_{N\sigma} - \hat{H}_{N\sigma,h}} \tag{69}$$

Comparing the definitions of $\hat{\eta}_{N\sigma}$ and $\hat{\eta}^\dagger_{N\sigma}$, 67 and 68, gives us a consistency equation:

$$\hat{G}_h(\hat{E}_{N\sigma})T^\dagger_{N\sigma,e-h} = T^\dagger_{N\sigma,e-h}\hat{G}_e(\hat{E}_{N\sigma}) \tag{70}$$

The diagonal equations gives an equation for $\hat{E}_{N\sigma}$:

$$\hat{E}_{N\sigma} = \hat{H}_{N\sigma,e} + \hat{T}_{N\sigma,e-h}\hat{\eta}_{01} \tag{71}$$

$$\hat{E}_{N\sigma} = \hat{H}_{N\sigma,h} + T^{\dagger}_{N\sigma,e-h}\hat{\eta}^{\dagger}_{01} \tag{72}$$

These equations provide the commutator and anticommutator of the $\hat{\eta}_{N\sigma}$ and $\hat{\eta}^{\dagger}_{N\sigma}$. From eq 71,

$$\begin{aligned} \hat{E}_{N\sigma} - \hat{H}_{N\sigma,e} = \hat{T}_{N\sigma,e-h}\hat{\eta}_{01} &\implies \hat{G}_e(\hat{E}_{N\sigma})^{-1} = \hat{T}_{N\sigma,e-h}\hat{\eta}_{01} \\ &\implies \mathbf{1} = \hat{G}_e(\hat{E}_{N\sigma})\hat{T}_{N\sigma,e-h}\hat{\eta}_{01} = \hat{\eta}^{\dagger}_{01}\hat{\eta}_{01} \end{aligned} \tag{73}$$

$$\hat{\eta}^{\dagger}\hat{\eta} = c^{\dagger}_{N\sigma}\hat{\eta}^{\dagger}_{01}\hat{\eta}_{01}c_{N\sigma} = c^{\dagger}_{N\sigma}c_{N\sigma} = \hat{n}_{N\sigma} \tag{74}$$

From 72,

$$\begin{aligned} \hat{E}_{N\sigma} - \hat{H}_{N\sigma,h} = T^{\dagger}_{N\sigma,e-h}\hat{\eta}^{\dagger}_{01} &\implies \hat{G}_h(\hat{E}_{N\sigma})^{-1} = T^{\dagger}_{N\sigma,e-h}\hat{\eta}^{\dagger}_{01} \\ &\implies \mathbf{1} = \hat{G}_h(\hat{E}_{N\sigma})T^{\dagger}_{N\sigma,e-h}\hat{\eta}^{\dagger}_{01} = \hat{\eta}_{01}\hat{\eta}^{\dagger}_{01} \end{aligned} \tag{75}$$

$$\hat{\eta}\hat{\eta}^{\dagger} = c_{N\sigma}\hat{\eta}_{01}\hat{\eta}^{\dagger}_{01}c^{\dagger}_{N\sigma} = c_{N\sigma}c^{\dagger}_{N\sigma} = 1 - \hat{n}_{N\sigma} \tag{76}$$

Combining equations 74 and 76,

$$\begin{aligned} \left[\hat{\eta}, \hat{\eta}^{\dagger}\right] &= 1 - 2\hat{n}_{N\sigma} \\ \left\{\hat{\eta}, \hat{\eta}^{\dagger}\right\} &= 1 \end{aligned} \tag{77}$$

Equation 71 provides an expression for the upper block of the diagonalised Hamiltonian,

$$\boxed{\hat{E}_{N\sigma} = \hat{H}_{N\sigma,e} + \hat{T}_{N\sigma,e-h}\hat{\eta}_{01}} \tag{78}$$

This expression has $\hat{E}_{N\sigma}$ on both sides, so it has to be solved using the consistency equations. The goal of this exercise was to show that it is possible to consistently construct an expression for the diagonalised Hamiltonian purely from the blocks of the original Hamiltonian, namely $\hat{H}_{N\sigma,h}$, $\hat{H}_{N\sigma,e}$, $\hat{T}_{N\sigma,e-h}$ and $T^{\dagger}_{N\sigma,e-h}$. We have shown that for the upper block.

The lower block can be constructed similarly, starting from 61. We again write the matrices in the basis of $\hat{n}_{N\sigma}$ (using 49, 65, 58) and compare the matrix elements.

$$\begin{pmatrix} \hat{H}_{N\sigma,e} & \hat{T}_{N\sigma,e-h} \\ \\ T^{\dagger}_{N\sigma,e-h} & \hat{H}_{N\sigma,h} \end{pmatrix} \begin{pmatrix} 1 & -\hat{\eta}^{\dagger}_{01} \\ \\ -\hat{\eta}_{01} & 1 \end{pmatrix} = \hat{E'}_{N\sigma}\mathbf{I} \begin{pmatrix} 1 & -\hat{\eta}^{\dagger}_{01} \\ \\ -\hat{\eta}_{01} & 1 \end{pmatrix}$$

$$\implies \begin{pmatrix} \hat{H}_{N\sigma,e} - \hat{T}_{N\sigma,e-h}\hat{\eta}_{01} & -\hat{H}_{N\sigma,e}\hat{\eta}^{\dagger}_{01} + \hat{T}_{N\sigma,e-h} \\ \\ -\hat{H}_{N\sigma,h}\hat{\eta}_{01} + T^{\dagger}_{N\sigma,e-h} & \hat{H}_{N\sigma,h} - T^{\dagger}_{N\sigma,e-h}\hat{\eta}^{\dagger}_{01} \end{pmatrix} = \begin{pmatrix} \hat{E'}_{N\sigma} & -\hat{E'}_{N\sigma}\hat{\eta}^{\dagger}_{01} \\ \\ -\hat{E'}_{N\sigma}\hat{\eta}_{01} & \hat{E'}_{N\sigma} \end{pmatrix} \tag{79}$$

The off-diagonal equations again give expressions for $\hat{\eta}_{N\sigma}$ and $\hat{\eta}^{\dagger}_{N\sigma}$ which when compared with the previous expressions will give two more consistency equations.

$$\hat{E'}_{N\sigma}\hat{\eta}^{\dagger}_{01} = \hat{H}_{N\sigma,e}\hat{\eta}^{\dagger}_{01} - \hat{T}_{N\sigma,e-h} \implies \hat{\eta}^{\dagger}_{01} = \frac{-1}{\hat{E'}_{N\sigma} - \hat{H}_{N\sigma,e}}\hat{T}_{N\sigma,e-h} = -\hat{G}_e\left(\hat{E}'_{N\sigma}\right)\hat{T}_{N\sigma,e-h} \tag{80}$$

$$\hat{E'}_{N\sigma}\hat{\eta}_{01} = \hat{H}_{N\sigma,h}\hat{\eta}_{01} - T^{\dagger}_{N\sigma,e-h} \implies \hat{\eta}_{01} = \frac{-1}{\hat{E'}_{N\sigma} - \hat{H}_{N\sigma,h}}T^{\dagger}_{N\sigma,e-h} = -\hat{G}_h\left(\hat{E}'_{N\sigma}\right)T^{\dagger}_{N\sigma,e-h} \tag{81}$$

Comparing equation 80 to equation 67 and equation 81 to equation 68, we get the following consistency equations:

$$\begin{aligned} -\hat{G}_e\left(\hat{E}'_{N\sigma}\right)\hat{T}_{N\sigma,e-h} &= \hat{G}_e\left(\hat{E}_{N\sigma}\right)\hat{T}_{N\sigma,e-h} \\ -\hat{G}_h\left(\hat{E}'_{N\sigma}\right)T^{\dagger}_{N\sigma,e-h} &= \hat{G}_h\left(\hat{E}_{N\sigma}\right)T^{\dagger}_{N\sigma,e-h} \end{aligned} \tag{82}$$

The diagonal element gives an expression for the lower block of $\overline{\mathcal{H}_{2N}}$.

$$\boxed{\hat{E}'_{N\sigma} = \hat{H}_{N\sigma,e} - \hat{T}_{N\sigma,e-h}\hat{\eta}_{01} \qquad (83)}$$

Looking at equations 78 and 83, we can write down the diagonalised Hamiltonian in the basis of $\hat{n}_{N\sigma}$:

$$\begin{aligned}\overline{\mathcal{H}_{2N}} = \hat{U}_{N\sigma}\mathcal{H}_{2N}\hat{U}^{\dagger}_{N\sigma} &= \begin{pmatrix} \hat{E_{N\sigma}} & 0 \\ \\ 0 & \hat{E'_{N\sigma}} \end{pmatrix} \\ &= \begin{pmatrix} \hat{H}_{N\sigma,e} + \hat{T}_{N\sigma,e-h}\hat{\eta}_{01} & 0 \\ \\ 0 & \hat{H}_{N\sigma,e} - \hat{T}_{N\sigma,e-h}\hat{\eta}_{01} \end{pmatrix}\end{aligned} \tag{84}$$

This concludes the construction of the diagonalised Hamiltonian.

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

$$\begin{aligned}&\mathcal{H}_{2N}\hat{P}_{N\sigma}|1\rangle = \hat{E}_{N\sigma}\otimes\mathbf{I}\,\hat{P}_{N\sigma}\mathcal{H}_{2N}|1\rangle = \hat{E}_{N\sigma}\hat{P}_{N\sigma}|1\rangle \\ &\implies \mathcal{H}_{2N}\hat{U}^{\dagger}_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma}|1\rangle = \hat{E}_{N\sigma}\hat{U}^{\dagger}_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma}|1\rangle \qquad \Big(\text{substituting expression of } \hat{P}_{N\sigma}\Big) \\ &\implies \hat{U}_{N\sigma}\mathcal{H}_{2N}\hat{U}^{\dagger}_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma}|1\rangle = \hat{U}_{N\sigma}\hat{E}_{N\sigma}\hat{U}^{\dagger}_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma}|1\rangle \quad \Big(\text{operating } \hat{U}_{N\sigma} \text{ from left}\Big) \\ &\implies \overline{\mathcal{H}_{2N}}\hat{n}_{N\sigma}\hat{U}_{N\sigma}|1\rangle = \hat{U}_{N\sigma}\hat{E}_{N\sigma}\hat{U}^{\dagger}_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma}|1\rangle\end{aligned} \tag{85}$$

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

$$\begin{aligned}\hat{n}_{N\sigma}\hat{U}_{N\sigma}|1\rangle &\propto |1\rangle \\ \hat{U}_{N\sigma}\hat{E}_{N\sigma}\hat{U}^{\dagger}_{N\sigma} &= E_{N\sigma}\end{aligned} \tag{86}$$

The second equations says

$$\Big[E_{N\sigma}, \hat{U}_{N\sigma}\Big] = 0 \tag{87}$$

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 86,

$$\hat{n}_{N\sigma}\hat{U}_{N\sigma}|1\rangle = \begin{pmatrix} \mathbf{I} & 0 \\ 0 & 0 \end{pmatrix} \kappa \begin{pmatrix} \mathbf{I} & \eta_{01}^{\dagger} \\ -\eta_{01} & \mathbf{I} \end{pmatrix} \begin{pmatrix} \mathbf{I} \\ 0 \end{pmatrix}$$
$$= \kappa \begin{pmatrix} \mathbf{I} \\ 0 \end{pmatrix} \propto |1\rangle \tag{88}$$

To find κ,

$$\hat{U}_{N\sigma}\hat{U}_{N\sigma}^{\dagger} = \kappa^2 \begin{pmatrix} \mathbf{I} & \eta_{01}^{\dagger} \\ -\eta_{01} & \mathbf{I} \end{pmatrix} \begin{pmatrix} \mathbf{I} & -\eta_{01}^{\dagger} \\ \eta_{01} & \mathbf{I} \end{pmatrix} = \kappa^2 \begin{pmatrix} \mathbf{I} + \eta_{01}^{\dagger}\eta_{01} & 0 \\ 0 & \mathbf{I} + \eta_{01}^{\dagger}\eta_{01} \end{pmatrix}$$
$$= \kappa^2 \begin{pmatrix} \mathbf{I} + \eta_{01}^{\dagger}\eta_{01} & 0 \\ 0 & \mathbf{I} + \eta_{01}^{\dagger}\eta_{01} \end{pmatrix} = 2\kappa^2 \begin{pmatrix} \mathbf{I} & 0 \\ 0 & \mathbf{I} \end{pmatrix} \left(\text{check 73,75 for } \eta_{01}^{\dagger}\eta_{01}, \eta_{01}\eta_{01}^{\dagger}\right)$$
$$\implies \kappa = \frac{1}{\sqrt{2}} \tag{89}$$

$$\boxed{\hat{U}_{N\sigma} = \frac{1}{\sqrt{2}}\left(1 - \hat{\eta} + \hat{\eta}^{\dagger}\right)} \tag{90}$$

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

First note,

$$\hat{T}_{N\sigma,e-h}^{\dagger}\left[\hat{E}_{N\sigma}, \hat{G}_e(\hat{E}_{N\sigma})\right] = T_{N\sigma,e-h}^{\dagger}\hat{E}_{N\sigma}\hat{G}_e(\hat{E}_{N\sigma}) - T_{N\sigma,e-h}^{\dagger}\hat{G}_e(\hat{E}_{N\sigma})\hat{E}_{N\sigma} \tag{91}$$

Now,

$$T_{N\sigma,e-h}^{\dagger}\hat{G}_e(\hat{E}_{N\sigma})\hat{E}_{N\sigma} = \hat{\eta}_{01}\hat{E}_{N\sigma} \tag{92}$$

Also,

$$\begin{aligned}
T^{\dagger}_{N\sigma,e-h}\hat{E}_{N\sigma}\hat{G}_e(\hat{E}_{N\sigma}) &= T^{\dagger}_{N\sigma,e-h}\left[\hat{H}_{N\sigma,e} + \hat{T}_{N\sigma,e-h}\hat{\eta}_{01}\right]\hat{G}_e(\hat{E}_{N\sigma}) \\
&= T^{\dagger}_{N\sigma,e-h}\left[\hat{H}_{N\sigma,e}\hat{G}_e(\hat{E}_{N\sigma}) + \hat{T}_{N\sigma,e-h}\hat{G}_h(\hat{E}_{N\sigma})\hat{T}^{\dagger}_{N\sigma,e-h}\hat{G}_e(\hat{E}_{N\sigma})\right] \\
&= T^{\dagger}_{N\sigma,e-h}\hat{H}_{N\sigma,e}\hat{G}_e(\hat{E}_{N\sigma}) + T^{\dagger}_{N\sigma,e-h}
\end{aligned} \tag{93}$$

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 71, we have

$$\begin{aligned}
\hat{E}_{N\sigma} - \hat{H}_{N\sigma,e} = \hat{T}_{N\sigma,e-h}\hat{\eta}_{01} &\implies \hat{G}_e^{-1}(\hat{E}_{N\sigma}) = \hat{T}_{N\sigma,e-h}\hat{G}_h(\hat{E}_{N\sigma})\hat{T}^{\dagger}_{N\sigma,e-h} \\
&\implies \mathbf{1} = \hat{T}_{N\sigma,e-h}\hat{G}_h(\hat{E}_{N\sigma})\hat{T}^{\dagger}_{N\sigma,e-h}\hat{G}_e(\hat{E}_{N\sigma})
\end{aligned} \tag{94}$$

Continuing from 93,

$$\begin{aligned}
T^{\dagger}_{N\sigma,e-h}\hat{E}_{N\sigma}\hat{G}_e(\hat{E}_{N\sigma}) &= T^{\dagger}_{N\sigma,e-h}\hat{H}_{N\sigma,e}\hat{G}_e(\hat{E}_{N\sigma}) + T^{\dagger}_{N\sigma,e-h} \\
&= \hat{H}_{N\sigma,h}T^{\dagger}_{N\sigma,e-h}\hat{G}_e(\hat{E}_{N\sigma}) + T^{\dagger}_{N\sigma,e-h}
\end{aligned} \tag{95}$$

The last line follows from equation 70:

$$\begin{aligned}
&\hat{T}^{\dagger}_{N\sigma,e-h}\hat{G}_e(\hat{E}_{N\sigma}) = \hat{G}_h(\hat{E}_{N\sigma})\hat{T}^{\dagger}_{N\sigma,e-h} \\
&\implies (\hat{E}_{N\sigma} - \hat{H}_{N\sigma,h})\hat{T}^{\dagger}_{N\sigma,e-h} = \hat{T}^{\dagger}_{N\sigma,e-h}(\hat{E}_{N\sigma} - \hat{H}_{N\sigma,e}) \\
&\implies \hat{E}_{N\sigma}\hat{T}^{\dagger}_{N\sigma,e-h} - \hat{H}_{N\sigma,h}\hat{T}^{\dagger}_{N\sigma,e-h} = \hat{T}^{\dagger}_{N\sigma,e-h}\hat{E}_{N\sigma} - \hat{T}^{\dagger}_{N\sigma,e-h}\hat{H}_{N\sigma,e} \\
&\implies \hat{H}_{N\sigma,h}\hat{T}^{\dagger}_{N\sigma,e-h} = \hat{T}^{\dagger}_{N\sigma,e-h}\hat{H}_{N\sigma,e} \qquad \left(\because \hat{E}_{N\sigma}\hat{T}^{\dagger}_{N\sigma,e-h} = \hat{T}^{\dagger}_{N\sigma,e-h}\hat{E}_{N\sigma}\right)
\end{aligned} \tag{96}$$

Again continuing from 95,

$$\begin{aligned}
&T^{\dagger}_{N\sigma,e-h}\hat{E}_{N\sigma}\hat{G}_e(\hat{E}_{N\sigma}) = \hat{H}_{N\sigma,h}T^{\dagger}_{N\sigma,e-h}\hat{G}_e(\hat{E}_{N\sigma}) + T^{\dagger}_{N\sigma,e-h} \\
&= \hat{H}_{N\sigma,h}\hat{G}_h(\hat{E}_{N\sigma})T^{\dagger}_{N\sigma,e-h} + T^{\dagger}_{N\sigma,e-h} && \text{(from eq 70)} \\
&= \hat{H}_{N\sigma,h}\hat{G}_h(\hat{E}_{N\sigma})T^{\dagger}_{N\sigma,e-h} + T^{\dagger}_{N\sigma,e-h}G_e(\hat{E}_{N\sigma})T_{N\sigma,e-h}G_h(\hat{E}_{N\sigma})T^{\dagger}_{N\sigma,e-h} && \text{(from eq 94)} \\
&= \left(\hat{H}_{N\sigma,h} + T^{\dagger}_{N\sigma,e-h}G_e(\hat{E}_{N\sigma})T_{N\sigma,e-h}\right)\hat{G}_h(\hat{E}_{N\sigma})T^{\dagger}_{N\sigma,e-h} \\
&= \left(\hat{H}_{N\sigma,h} + T^{\dagger}_{N\sigma,e-h}\hat{\eta}^{\dagger}_{01}\right)\hat{G}_h(\hat{E}_{N\sigma})T^{\dagger}_{N\sigma,e-h} \\
&= \hat{E}_{N\sigma}\hat{G}_h(\hat{E}_{N\sigma})T^{\dagger}_{N\sigma,e-h} \\
&= \hat{E}_{N\sigma}\hat{\eta}_{01}
\end{aligned} \tag{97}$$

Therefore,

$$T^{\dagger}_{N\sigma,e-h}\hat{E}_{N\sigma}\hat{G}_e(\hat{E}_{N\sigma}) = \hat{E}_{N\sigma}\hat{\eta}_{01} \tag{98}$$

Substituting equations 92 and 98 in equation 91, we have

$$\begin{aligned}\hat{T}^{\dagger}_{N\sigma,e-h}\left[\hat{E}_{N\sigma}, \hat{G}_e(\hat{E}_{N\sigma})\right] &= \hat{E}_{N\sigma}\hat{\eta}_{01} - \hat{\eta}_{01}\hat{E}_{N\sigma} = \left[\hat{E}_{N\sigma}, \hat{\eta}_{01}\right] \\ &= 0 \qquad\qquad \text{(from equation 87)}\end{aligned} \tag{99}$$

Therefore,

$$\boxed{\left[\hat{E}_{N\sigma}, \hat{G}_e(\hat{E}_{N\sigma})\right] = 0} \tag{100}$$

3.6 A Simple Example

$$\mathcal{H} = -t\left(c_2^{\dagger}c_1 + c_1^{\dagger}c_2\right) + V\hat{n}_1\hat{n}_2 - \mu(\hat{n}_1 + \hat{n}_2) \quad \hat{n}_i = c_i^{\dagger}c_i \tag{101}$$

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).

$$\begin{aligned}\hat{H}_{1,e} &= Tr_1[\mathcal{H}\hat{n}_1] \\ &= Tr_1[V\hat{n}_1\hat{n}_2 - \mu(\hat{n}_1 + \hat{n}_2)] \quad \left(c \text{ and } c^{\dagger} \text{ will not conserve the eigenvalue of } \hat{n}\right) \\ &= V\hat{n}_2 - \mu(1 + \hat{n}_2) \qquad\quad (Tr_1[V\hat{n}_1\hat{n}_2] = VTr_1[\hat{n}_1]\hat{n}_2 = V\hat{n}_2)\end{aligned} \tag{102}$$

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

$$\hat{H}_{1,h} = Tr_1[\mathcal{H}(1 - \hat{n}_1)] = -\mu\hat{n}_2 \tag{103}$$

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

$$\begin{aligned}T_{1,e-h} &= Tr_1[\mathcal{H}c_1] \\ &= Tr_1[-tc_1^{\dagger}c_2c_1] = -tc_2 \quad \text{(the only term that conserves eigenvalue of } \hat{n})\end{aligned} \tag{104}$$

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

$$\mathcal{H} = \begin{pmatrix} V\hat{n}_2 - \mu(1 + \hat{n}_2) & -tc_2 \\ \\ -tc_2^{\dagger} & -\mu\hat{n}_2 \end{pmatrix} \tag{105}$$

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

From equations 67 and 68, $\hat{\eta}_{01}^\dagger = \hat{G}_e \hat{T}_{1,e-h}$ and $\hat{\eta}_{01} = \hat{G}_h \hat{T}_{1,e-h}^\dagger$. Equation 73 gives

$$\hat{\eta}_{01}^\dagger \hat{\eta}_{01} = 1 \implies \hat{G}_e \hat{T}_{1,e-h} \hat{G}_h \hat{T}_{1,e-h}^\dagger = 1 \tag{106}$$

Again, from equation 70, $\hat{G}_h \hat{T}_{1,e-h}^\dagger = \hat{T}_{1,e-h}^\dagger \hat{G}_e$. With this modification, equation 106 becomes

$$\hat{G}_e \hat{T}_{1,e-h} \hat{T}_{1,e-h}^\dagger \hat{G}_e = 1 \implies \hat{T}_{1,e-h} \hat{T}_{1,e-h}^\dagger = \left(\hat{G}_e^{-1}\right)^2 \tag{107}$$

For this problem,

$$\begin{aligned} \hat{T}_{1,e-h} \hat{T}_{1,e-h}^\dagger &= t^2 c_2 c_2^\dagger = t^2 (1 - \hat{n}_2) = t^2 (1 - \hat{n}_2)^2 \\ \left(\hat{G}_e^{-1}\right)^2 &= \left(\hat{E}_1 - \hat{H}_{1,e}\right)^2 = \left(\hat{E}_1 - V \hat{n}_2 + \mu(1 + \hat{n}_2)\right)^2 \end{aligned} \tag{108}$$

Substituting these expressions in equation 107,

$$t^2 \left(1 - \hat{n}_2\right)^2 = \left(\hat{E}_1 - V \hat{n}_2 + \mu(1 + \hat{n}_2)\right)^2 \tag{109}$$

This has a solution, $\hat{E}_1 - V\hat{n}_2 + \mu(1 + \hat{n}_2) = t\left(1 - \hat{n}_2\right)$, that is,

$$\boxed{\hat{E}_1 = V\hat{n}_2 - \mu(1 + \hat{n}_2) + t\left(1 - \hat{n}_2\right) = (V - 2\mu)\hat{n}_2 + (t - \mu)(1 - \hat{n}_2)} \tag{110}$$

The lower diagonal block $\hat{E}'$can be determined as follows. First note that in the original Hamiltonian, only the upper 3×3 portion is interacting among themselves, the 4^{th} row and 4^{th} column of the Hamiltonian do not interact with the rest. This means that the lower element of $\hat{E}'$ is zero. Also note that the unitary transformations do not alter the partial trace of the matrix. Specifically,

$$Tr_1\left(\overline{\mathcal{H}}\right) = Tr_1\left(\hat{U}_{N\sigma} \mathcal{H} \hat{U}_{N\sigma}^\dagger\right) = Tr_1\left(\hat{U}_{N\sigma}^\dagger \hat{U}_{N\sigma} \mathcal{H}\right) = Tr_1\left(\mathcal{H}\right) \tag{111}$$

Since we know the expression of $\hat{E}_1$ and the structure of $\hat{E}'_1$, we can write down the structure of $\overline{\mathcal{H}}$:

$$\overline{\mathcal{H}} = \begin{pmatrix} V-2\mu & & & \\ & t-\mu & & \\ & & \hat{E}'_1 & \\ & & & 0 \end{pmatrix} \tag{112}$$

Therefore,

$$\hat{E}'_1 \hat{n}_2 = -(\mu + t)\hat{n}_2 \tag{113}$$

This gives nothing

$$\begin{aligned} \overline{\mathcal{H}} &= \begin{array}{c} \begin{array}{cc} |\hat{n}_1 = 1\rangle & \qquad\qquad |\hat{n}_1 = 0\rangle \end{array} \\ \begin{pmatrix} (V-2\mu)\hat{n}_2 + (t-\mu)(1-\hat{n}_2) & 0 \\ 0 & -(\mu+t)\hat{n}_2 \end{pmatrix} \end{array} \\ &= \begin{array}{c} \begin{array}{cccc} |11\rangle & |10\rangle & |01\rangle & |00\rangle \end{array} \\ \begin{pmatrix} (V-2\mu) & 0 & 0 & 0 \\ 0 & (t-\mu) & 0 & 0 \\ 0 & 0 & -(\mu+t) & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \end{array} \end{aligned} \tag{114}$$

The EigenstatesHaHa 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 $\hat{n}$:

$$\mathcal{H}(\hat{U}^\dagger_{N\sigma} |n_1, n_2\rangle) = \hat{U}^\dagger_{N\sigma} \overline{\mathcal{H}} |n_1, n_2\rangle = \hat{U}^\dagger_{N\sigma} E_{n_1,n_2} |n_1, n_2\rangle = E_{n_1,n_2}(\hat{U}^\dagger_{N\sigma} |n_1, n_2\rangle) \tag{115}$$

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 **??**.

$\hat{N}$	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	$\frac{\|\uparrow\downarrow,\uparrow\rangle-\|\uparrow,\uparrow\downarrow\rangle}{\sqrt{2}}$

$\hat{N}$	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	$2(\epsilon_s + \epsilon_d) + U$	$\vert\uparrow\downarrow,\uparrow\downarrow\rangle$