Title

Contents

1 Exact diagonalization of the two-site Hubbard model

The Hamiltonian

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

a_a I have two lattice sites, indexed by 1 and 2, occupied by electrons. μ is the chemical potential, $c_{i\sigma}^{\dagger}$ 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. $\hat{n}_{i\sigma} = c_{i\sigma}^{\dagger} c_{i\sigma}$ 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.

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

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

   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,

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

   - $c_{2\sigma}^{\dagger} c_{1\sigma}$: 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.

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

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

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

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

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

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:

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

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:

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

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 $S_z^{tot} = -1$

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

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

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 $S_z^{tot} = +1$

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

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

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.

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

We get the following matrix

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

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 $\hat{P}=-1$.

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

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

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.

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	$\frac{U+\sqrt{U^2+16t^2}}{2}-2\mu$	$\frac{1}{N_+}\left\{2t\frac{(\|\uparrow,\downarrow\rangle-\|\downarrow,\uparrow\rangle)}{\sqrt{2}}+\frac{U+\sqrt{U^2+16t^2}}{2}\frac{(\|\uparrow\downarrow,0\rangle-\|0,\uparrow\downarrow\rangle)}{\sqrt{2}}\right\}$
		-1	$\frac{U-\sqrt{U^2+16t^2}}{2}-2\mu$	$\frac{1}{N_-}\left\{2t\frac{(\|\uparrow,\downarrow\rangle-\|\downarrow,\uparrow\rangle)}{\sqrt{2}}+\frac{U-\sqrt{U^2+16t^2}}{2}\frac{(\|\uparrow\downarrow,0\rangle-\|0,\uparrow\downarrow\rangle)}{\sqrt{2}}\right\}$
	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	$\|\uparrow\downarrow,\uparrow\downarrow\rangle$

1.8 The Mott-insulating limit

In the limit of $U \gg t$, the $N = 2$ part of the spectrum groups itself roughly into two bands:

$$\frac{U + \sqrt{U^2 + 16t^2}}{2} = \frac{U + U\sqrt{1 + \frac{16t^2}{U}}}{2} \approx \frac{U + U(1 + \frac{8t^2}{U^2})}{2} = U + \frac{4t^2}{U} \tag{28}$$

$$\frac{U - \sqrt{U^2 + 16t^2}}{2} = \frac{U - U\sqrt{1 + \frac{16t^2}{U}}}{2} \approx \frac{U - U(1 + \frac{8t^2}{U^2})}{2} = -\frac{4t^2}{U} \tag{29}$$

lower	$\frac{-4t^2}{U}$	$\frac{\lvert\uparrow,\downarrow\rangle - \lvert\downarrow,\uparrow\rangle}{\sqrt{2}}$
	0	$\lvert\uparrow,\uparrow\rangle, \lvert\downarrow,\downarrow\rangle, \frac{\lvert\uparrow,\downarrow\rangle + \lvert\downarrow,\uparrow\rangle}{\sqrt{2}}$
upper	U	$\frac{\lvert\uparrow\downarrow,0\rangle + \lvert 0,\uparrow\downarrow\rangle}{\sqrt{2}}$
	$U + \frac{4t^2}{U}$	$\frac{\lvert\uparrow\downarrow,0\rangle - \lvert 0,\uparrow\downarrow\rangle}{\sqrt{2}}$

- The separation between the two bands is $\Delta = U$. The kets in the lower band are formed mostly of superpositions of the Neel states (singly occupied states with opposite spin) as well as the polarised states (singly occupied states with same spin). This is expected because for very large U, it becomes the only determining factor, and states with single occupation will be appreciably lower in energy compared to the doubly occupied states, and hence will gather in the lower band.
- For exactly the same reason, the upper band will be formed mostly by superpositions of holon-doublon states (two electrons on one site and none on the other), because they will incur the heavy cost of the on-site repulsion energy, and will hence assemble in the upper band.
- The lower band is a collection of three states: the ground state is the singlet state $|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle$, with an energy of $-\frac{4t^2}{U}$, while the other three , $|\uparrow,\uparrow\rangle, |\downarrow,\downarrow\rangle, |\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle$, form a degenerate triplet of first excited states with 0 energy.

1.9 Comparison with the antiferromagnetic Heisenberg model

$$\mathcal{H}_{\text{Heisenberg}} = J\vec{\sigma_1} \cdot \vec{\sigma_2} - J, \quad \text{with } J = -\frac{t^2}{U} < 0 \tag{30}$$

To diagonalise this Hamiltonian, we rewrite the pauli matrix vectors using σ^z and $\sigma^{\pm}$:

$$\vec{\sigma_1} \cdot \vec{\sigma_2} = \sigma_1^z \sigma_2^z + \frac{\sigma_1^+ \sigma_2^- + \sigma_1^- \sigma_2^+}{2} \tag{31}$$

where $\sigma_i^{\pm} = \sigma_i^x \pm \iota \sigma_i^y$. Note that

$$\sigma^+ |\uparrow\rangle = \sigma^- |\downarrow\rangle = 0 \tag{32}$$

$$\sigma^+ |\downarrow\rangle = 2 |\uparrow\rangle \tag{33}$$

$$\sigma^- |\uparrow\rangle = 2 |\downarrow\rangle \tag{34}$$

Using these properties, it is easy to write down the 4×4 matrix of the Hamiltonian in the basis of $|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle$.

$$\mathcal{H} = J \begin{pmatrix} 1 & & & \\ & -1 & 2 & \\ & 2 & -1 & \\ & & & 1 \end{pmatrix} - J \tag{35}$$

The $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ form eigenkets with eigenvalues J each. The middle 2×2 matrix can easily be diagonalised. It gives two other eigenvectors $|\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle$, with eigenvalues $J, -3J$. After adding the constant term $-J$ to these eigenvalues, the final spectrum becomes

- $|\uparrow\uparrow\rangle : 0$
- $|\downarrow\downarrow\rangle : 0$
- $|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle : 0$
- $|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle : -4J$

Recognizing J as $-\frac{t^2}{U}$, we get the same spectrum as the lower block.

2 Exact diagonalization of the Anderson molecule

The Hamiltonian

$$\mathcal{H} = -t \sum_{\sigma} \left(c^{\dagger}_{1\sigma} c_{2\sigma} + c^{\dagger}_{2\sigma} c_{1\sigma} \right) + U \hat{n}_{1\uparrow} \hat{n}_{1\downarrow} + \epsilon_s \sum_{\sigma} \hat{n}_{2\sigma} + \epsilon_d \sum_{\sigma} \hat{n}_{1\sigma} \tag{36}$$

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,

$$\hat{S}^2_{tot} = \hat{(S^x_{tot})}^2 + \hat{(S^y_{tot})}^2 + \hat{(S^z_{tot})}^2 = S^+_{tot}S^-_{tot} - \hbar S^z_{tot} + (S^z_{tot})^2 \tag{37}$$

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

$$\begin{aligned} \mathcal{H}|\downarrow, 0\rangle &= \epsilon_d |\downarrow, 0\rangle - t|0, \downarrow\rangle \\ \mathcal{H}|0, \downarrow\rangle &= \epsilon_s |0, \downarrow\rangle - t|\downarrow, 0\rangle \end{aligned} \tag{38}$$

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

$$\begin{array}{c} \\ |\downarrow, 0\rangle \\ \\ |0, \downarrow\rangle \end{array} \begin{array}{c} \begin{array}{cc} |\downarrow, 0\rangle & |0, \downarrow\rangle \end{array} \\ \begin{pmatrix} \epsilon_d & -t \\ \\ -t & \epsilon_s \end{pmatrix} \end{array} \tag{39}$$

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 $S^z_{tot} = +1$

$$\begin{aligned} \mathcal{H}|\uparrow, 0\rangle &= \epsilon_d |\uparrow, 0\rangle - t|0, \uparrow\rangle \\ \mathcal{H}|0, \uparrow\rangle &= \epsilon_s |0, \uparrow\rangle - t|\uparrow, 0\rangle \end{aligned} \tag{40}$$

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 $S^z_{tot} = -1$

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

$$\begin{array}{c} \\ |\uparrow\downarrow,\downarrow\rangle \\ \\ |\downarrow,\uparrow\downarrow\rangle \end{array} \begin{array}{c} \begin{array}{cc} |\uparrow\downarrow,\downarrow\rangle & \quad |\downarrow,\uparrow\downarrow\rangle \end{array} \\ \begin{pmatrix} 2\epsilon_d + \epsilon_s + U & -t \\ -t & 2\epsilon_s + \epsilon_d \end{pmatrix} \end{array} \tag{42}$$

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 $S^z_{tot} = +1$

$$\begin{aligned} \mathcal{H}|\uparrow\downarrow,\uparrow\rangle &= -t|\uparrow,\uparrow\downarrow\rangle + (2\epsilon_d + \epsilon_s + U)|\uparrow\downarrow,\uparrow\rangle \\ \mathcal{H}|\uparrow,\uparrow\downarrow\rangle &= -t|\uparrow\downarrow,\uparrow\rangle + (2\epsilon_s + \epsilon_d)|\uparrow,\uparrow\downarrow\rangle \end{aligned} \tag{43}$$

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

$$\mathcal{H}|\downarrow,\downarrow\rangle = \mathcal{H}|\uparrow,\uparrow\rangle = \epsilon_s + \epsilon_d \tag{44}$$

2.4.2 $S^z_{tot} = 0$

This subspace has four eigenvectors,

$$|\uparrow,\downarrow\rangle, \quad |\downarrow,\uparrow\rangle, \quad |0,\uparrow\downarrow\rangle, \quad |\uparrow\downarrow,0\rangle \tag{45}$$

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^-

$$\begin{aligned} S^+S^- |\uparrow,\downarrow\rangle &= S^+S^- |\downarrow,\uparrow\rangle = |\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle \\ S^+S^- |\uparrow\downarrow,0\rangle &= S^+S^- |0,\uparrow\downarrow\rangle = 0 \end{aligned} \tag{46}$$

The eigenstates are

$$\frac{|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle}{\sqrt{2}}(S^2_{tot}=1), \quad \left\{\frac{|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle}{\sqrt{2}}, |\uparrow\downarrow,0\rangle, |0,\uparrow\downarrow\rangle\right\}(S^2_{tot}=0) \tag{47}$$

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

$$\mathcal{H}\frac{|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle}{\sqrt{2}} = (\epsilon_d + \epsilon_s)\left(\frac{|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle}{\sqrt{2}}\right) \tag{48}$$

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

$$\begin{aligned} \mathcal{H}\frac{|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle}{\sqrt{2}} &= (\epsilon_d + \epsilon_s)\left(\frac{|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle}{\sqrt{2}}\right) + \sqrt{2}t(|\uparrow\downarrow,0\rangle - |0,\uparrow\downarrow\rangle) \\ \mathcal{H}|\uparrow\downarrow,0\rangle &= (2\epsilon_d + U)|\uparrow\downarrow,0\rangle + \sqrt{2}t\frac{|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle}{\sqrt{2}} \\ \mathcal{H}|0,\uparrow\downarrow\rangle &= (2\epsilon_d + U)|0,\uparrow\downarrow\rangle - \sqrt{2}t\frac{|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle}{\sqrt{2}} \end{aligned} \tag{49}$$

We get the following matrix

$$\begin{pmatrix} 2\epsilon_d + \frac{U}{2} & \sqrt{2}t & -\sqrt{2}t \\ \sqrt{2}t & 2\epsilon_d + U & 0 \\ -\sqrt{2}t & 0 & 2\epsilon_d + U \end{pmatrix} \tag{50}$$

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.

Exact Diagonalization of Anderson Molecule

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

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 $N\sigma$:

$$\mathcal{H}_{2N} = \begin{array}{c} \\ \langle 1| \\ \langle 0| \end{array} \begin{array}{c} \begin{array}{cc} |1\rangle & |0\rangle \end{array} \\ \begin{pmatrix} H_1 & H_2 \\ H_3 & H_4 \end{pmatrix} \end{array} \tag{51}$$

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

$$\mathcal{H}_{2N} = H_1\hat{n}_{N\sigma} + c^{\dagger}_{N\sigma}H_2 + H_3c_{N\sigma} + H_4(1 - \hat{n}_{N\sigma}) \tag{52}$$

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 $N\sigma$

$$Tr_{N\sigma}\left(\mathcal{H}_{2N}\right) \equiv \sum_{|N\sigma\rangle} \langle N\sigma| \mathcal{H}_{2N} |N\sigma\rangle \tag{53}$$

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 52, after multiplying throughout with $\hat{n}_{N\sigma}$ from the right, gives

$$Tr_{N\sigma}\left(\mathcal{H}_{2N}\hat{n}_{N\sigma}\right) = Tr_{N\sigma}\left[H_1\hat{n}_{N\sigma}\hat{n}_{N\sigma} + c^{\dagger}_{N\sigma}H_2\hat{n}_{N\sigma} + H_3c_{N\sigma}\hat{n}_{N\sigma} + H_4(1 - \hat{n}_{N\sigma})\hat{n}_{N\sigma}\right] \tag{54}$$

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,

$$Tr_{N\sigma}\left(\mathcal{H}_{2N}\hat{n}_{N\sigma}\right) = Tr_{N\sigma}\left[H_1\hat{n}_{N\sigma}\right] = H_1 Tr_{N\sigma}\hat{n}_{N\sigma} = H_1 \tag{55}$$

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.

$$\begin{aligned}
H_1 &\equiv \hat{H}_{N\sigma,e} = Tr_{N\sigma}\left[\mathcal{H}_{2N}\hat{n}_{N\sigma}\right] \\
H_2 &\equiv \hat{T}_{N\sigma,e-h} = Tr_{N\sigma}\left[\mathcal{H}_{2N}c_{N\sigma}\right] \\
H_3 &\equiv T^\dagger_{N\sigma,e-h} = Tr_{N\sigma}\left[c^\dagger_{N\sigma}\mathcal{H}_{2N}\right] \\
H_4 &\equiv \hat{H}_{N\sigma,h} = Tr_{N\sigma}\left[\mathcal{H}_{2N}(1-\hat{n}_{N\sigma})\right]
\end{aligned} \tag{56}$$

We get the following block decomposition of the Hamiltonian.

$$\mathcal{H}_{2N} = \begin{array}{c} \\ \langle 1| \\ \langle 0| \end{array} \begin{array}{c} \begin{array}{cc} |1\rangle & |0\rangle \end{array} \\ \begin{pmatrix} \hat{H}_{N\sigma,e} & \hat{T}_{N\sigma,e-h} \\ T^\dagger_{N\sigma,e-h} & \hat{H}_{N\sigma,h} \end{pmatrix} \end{array} = \begin{array}{c} \\ \langle 1| \\ \langle 0| \end{array} \begin{array}{c} \begin{array}{cc} |1\rangle & |0\rangle \end{array} \\ \begin{pmatrix} Tr_{N\sigma}\left[\mathcal{H}_{2N}\hat{n}_{N\sigma}\right] & Tr_{N\sigma}\left[\mathcal{H}_{2N}c_{N\sigma}\right] \\ Tr_{N\sigma}\left[c^\dagger_{N\sigma}\mathcal{H}_{2N}\right] & Tr_{N\sigma}\left[\mathcal{H}_{2N}(1-\hat{n}_{N\sigma})\right] \end{pmatrix} \end{array} \tag{57}$$

$$\begin{aligned}
\mathcal{H}_{2N} = Tr_{N\sigma}\left[\mathcal{H}_{2N}\hat{n}_{N\sigma}\right]\hat{n}_{N\sigma} + c^\dagger_{N\sigma}Tr_{N\sigma}\left[\mathcal{H}_{2N}c_{N\sigma}\right] + Tr_{N\sigma}\left[c^\dagger_{N\sigma}\mathcal{H}_{2N}\right]c_{N\sigma} \\
+Tr_{N\sigma}\left[\mathcal{H}_{2N}(1-\hat{n}_{N\sigma})\right](1-\hat{n}_{N\sigma})
\end{aligned} \tag{58}$$

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.

$$\begin{aligned}
\left[\mathcal{H}_{2N}, \hat{P_{N\sigma}}\right] &= \left[\mathcal{H}_{2N}, \hat{U}^\dagger_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma}\right] = \mathcal{H}_{2N}\hat{U}^\dagger_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma} - \hat{U}^\dagger_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma}\mathcal{H}_{2N} \\
&= \hat{U}^\dagger_{N\sigma}\overline{\mathcal{H}_{2N}}\hat{n}_{N\sigma}\hat{U}_{N\sigma} - \hat{U}^\dagger_{N\sigma}\hat{n}_{N\sigma}\overline{\mathcal{H}_{2N}}\hat{U}_{N\sigma} = \hat{U}^\dagger_{N\sigma}\left[\mathcal{H}_{2N}, \hat{n}_{N\sigma}\right]\hat{U}_{N\sigma} \\
&= 0
\end{aligned} \tag{59}$$

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

$$\overline{\mathcal{H}_{2N}} = \begin{pmatrix} \hat{E_{N\sigma}} & 0 \\ 0 & \hat{E'_{N\sigma}} \end{pmatrix} \tag{60}$$

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

$$\begin{aligned} \overline{\mathcal{H}_{2N}}\,|1\rangle &= \hat{E_{N\sigma}}\,|1\rangle \\ \overline{\mathcal{H}_{2N}}\,|0\rangle &= \hat{E'_{N\sigma}}\,|0\rangle \end{aligned} \tag{61}$$

$|1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ 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,

$$\hat{A} = \begin{pmatrix} 1 & -1 \\ 2 & 0 \end{pmatrix} \implies \hat{m}\hat{A}\hat{m} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \times \begin{pmatrix} 1 & -1 \\ 2 & 0 \end{pmatrix} \times \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{62}$$

Similarly,

$$\hat{m}\hat{A}(1-\hat{m}) = \begin{pmatrix} 0 & -1 \\ 0 & 0 \end{pmatrix}, (1-\hat{m})\hat{A}\hat{m} = \begin{pmatrix} 0 & 0 \\ 2 & 0 \end{pmatrix}, (1-\hat{m})\hat{A}(1-\hat{m}) = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \tag{63}$$

We hence have the equation

$$\begin{aligned} \hat{n}_{N\sigma}\overline{\mathcal{H}_{2N}}\hat{n}_{N\sigma} = \hat{P_{N\sigma}}\mathcal{H}_{2N}\hat{P_{N\sigma}} &= \begin{pmatrix} \hat{E_{N\sigma}} & 0 \\ 0 & 0 \end{pmatrix} \\ (1-\hat{n}_{N\sigma})\overline{\mathcal{H}_{2N}}(1-\hat{n}_{N\sigma}) = (1-\hat{P_{N\sigma}})\mathcal{H}_{2N}(1-\hat{P_{N\sigma}}) &= \begin{pmatrix} 0 & 0 \\ 0 & \hat{E'_{N\sigma}} \end{pmatrix} \end{aligned} \tag{64}$$

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

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

$$\mathcal{H}' = \hat{E_{N\sigma}} \otimes \mathbf{I} = \begin{pmatrix} \hat{E_{N\sigma}} & 0 \\ 0 & \hat{E_{N\sigma}} \end{pmatrix} \tag{65}$$

$$\mathcal{H}'' = \hat{E'_{N\sigma}} \otimes \mathbf{I} = \begin{pmatrix} \hat{E'_{N\sigma}} & 0 \\ 0 & \hat{E'_{N\sigma}} \end{pmatrix} \tag{66}$$

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

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

$$= \hat{U}^{\dagger}_{N\sigma}\begin{pmatrix} \hat{E_{N\sigma}} & 0 \\ 0 & \hat{E_{N\sigma}} \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}\hat{U}_{N\sigma} = \hat{U}^{\dagger}_{N\sigma}\hat{E_{N\sigma}} \otimes \mathbb{I}\ \hat{n}_{N\sigma}\hat{U}_{N\sigma} = \hat{E_{N\sigma}} \otimes \mathbb{I}\ \hat{U}^{\dagger}_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma} = \mathcal{H}'\hat{P_{N\sigma}} \tag{67}$$

$$\therefore \mathcal{H}_{2N}\hat{P_{N\sigma}} = \mathcal{H}'\hat{P_{N\sigma}} \tag{68}$$

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

$$\therefore \mathcal{H}_{2N}(1 - \hat{P_{N\sigma}}) = \mathcal{H}''(1 - \hat{P_{N\sigma}}) \tag{69}$$

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

$$\hat{U}_{N\sigma} = \begin{bmatrix} e^{\iota\phi_1}\cos\theta & e^{\iota\phi_2}\sin\theta \\ -e^{-\iota\phi_2}\sin\theta & e^{-\iota\phi_1}\cos\theta \end{bmatrix} \tag{70}$$

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

$$\hat{P_{N\sigma}} = \hat{U}^{\dagger}_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma} = \begin{bmatrix} e^{-\iota\phi_1}\cos\theta & -e^{\iota\phi_2}\sin\theta \\ e^{-\iota\phi_2}\sin\theta & e^{\iota\phi_1}\cos\theta \end{bmatrix} \times \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \times \begin{bmatrix} e^{\iota\phi_1}\cos\theta & e^{\iota\phi_2}\sin\theta \\ -e^{-\iota\phi_2}\sin\theta & e^{-\iota\phi_1}\cos\theta \end{bmatrix}$$
$$= \begin{bmatrix} \cos^2\theta & \cos\theta\sin\theta e^{-\iota(\phi_1-\phi_2)} \\ \cos\theta\sin\theta e^{\iota(\phi_1-\phi_2)} & \sin^2\theta \end{bmatrix} \tag{71}$$

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

$$\hat{P_{N\sigma}} = \frac{1}{2}\begin{bmatrix} 1 & \hat{\eta}^{\dagger}_{01} \\ \hat{\eta}_{01} & 1 \end{bmatrix} = \frac{1}{2}\left(\mathbf{I} + \eta_{N\sigma} + \eta^{\dagger}_{N\sigma}\right) \tag{72}$$

$$\mathbf{I} - \hat{P_{N\sigma}} = \frac{1}{2}\begin{bmatrix} 1 & -\hat{\eta}^{\dagger}_{01} \\ -\hat{\eta}_{01} & 1 \end{bmatrix} = \frac{1}{2}\left(\mathbf{I} - \eta_{N\sigma} - \eta^{\dagger}_{N\sigma}\right) \tag{73}$$

$\hat{\eta}_{N\sigma} = \hat{\eta}_{01}c_{N\sigma}$ 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.

To construct the diagonalised Hamiltonian and get some properties of the $\eta_{N\sigma}$, we will use equations 68 and 69.

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

$$\begin{aligned}
\hat{P}_{N\sigma}(1-\hat{n}_{N\sigma}) &= \frac{1}{2}(1+\eta+\eta^\dagger)(1-\hat{n}_{N\sigma}) = \frac{1}{2}(1+\eta^\dagger)(1-\hat{n}_{N\sigma}) \qquad (\because \eta_{N\sigma}(1-\hat{n}_{N\sigma}) = 0) \\
\therefore \hat{n}_{N\sigma}\mathcal{H}'\hat{P}_{N\sigma}(1-\hat{n}_{N\sigma}) &= \frac{1}{2}\hat{n}_{N\sigma}\mathcal{H}'(1+\eta^\dagger_{N\sigma})(1-\hat{n}_{N\sigma}) = \frac{1}{2}\mathcal{H}'\eta^\dagger_{N\sigma} \quad \left(\because \hat{n}_{N\sigma}\eta^\dagger(1-\hat{n}_{N\sigma}) = \eta^\dagger\right)
\end{aligned} \tag{74}$$

The LHS simplifies as

$$\begin{aligned}
\hat{n}_{N\sigma}\mathcal{H}_{2N} &= (\hat{n}_{N\sigma}H_e\hat{n}_{N\sigma} + \hat{n}_{N\sigma}c^\dagger\hat{T} + \hat{n}_{N\sigma}\hat{T}^\dagger c + \hat{n}_{N\sigma}H_h(1-\hat{n}_{N\sigma})) \\
&= H_e\hat{n}_{N\sigma} + c^\dagger\hat{T}
\end{aligned} \tag{75}$$

$$\left(\because \hat{n}_{N\sigma}c^\dagger = c^\dagger, \hat{n}_{N\sigma}\hat{T}^\dagger c = \hat{T}^\dagger\hat{n}_{N\sigma}c = 0, \hat{n}_{N\sigma}H_h(1-\hat{n}_{N\sigma}) = H_h\hat{n}_{N\sigma}(1-\hat{n}_{N\sigma}) = 0\right)$$

$$\begin{aligned}
\therefore \hat{n}_{N\sigma}\mathcal{H}_{2N}\hat{P}(1-\hat{n}_{N\sigma}) &= \frac{1}{2}(H_e\hat{n}_{N\sigma} + c^\dagger\hat{T})(1+\eta^\dagger)(1-\hat{n}_{N\sigma}) \\
&= \frac{1}{2}(H_e\hat{n}_{N\sigma} + H_e\hat{n}_{N\sigma}\eta^\dagger + c^\dagger T + c^\dagger T\eta^\dagger)(1-\hat{n}_{N\sigma}) \\
&= \frac{1}{2}H_e\hat{n}_{N\sigma}\eta^\dagger(1-\hat{n}_{N\sigma}) + c^\dagger T(1-\hat{n}_{N\sigma}) + \frac{1}{2}c^\dagger T\eta^\dagger(1-\hat{n}_{N\sigma}) \\
&= \frac{1}{2}H_e\hat{n}_{N\sigma}\eta^\dagger + \frac{1}{2}c^\dagger T \\
&\left(\because \eta^\dagger(1-\hat{n}_{N\sigma}) = \eta^\dagger, c^\dagger(1-\hat{n}_{N\sigma}) = c^\dagger, c^\dagger\eta^\dagger = 0\right)
\end{aligned} \tag{76}$$

Combining the final equations of 74 and 76, we get

$$c^\dagger_{N\sigma}\hat{T}_{N\sigma} + H_e\hat{n}_{N\sigma}\eta^\dagger_{N\sigma} = \mathcal{H}'\eta^\dagger_{N\sigma} \implies \eta^\dagger_{N\sigma} = \frac{1}{\mathcal{H}' - H_e\hat{n}_{N\sigma}}c^\dagger_{N\sigma}\hat{T}_{N\sigma} \tag{77}$$

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

$$\eta^\dagger_{N\sigma} = \hat{G}_e(\hat{E}_{N\sigma})c^\dagger_{N\sigma}\hat{T}_{N\sigma} \tag{78}$$

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

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

$$\hat{P}\hat{n}_{N\sigma} = \frac{1}{2}(1+\eta+\eta^\dagger)\hat{n}_{N\sigma} = \frac{1}{2}(\hat{n}_{N\sigma}+\eta) \quad \left(\because \eta\hat{n}_{N\sigma} = \eta, \eta^\dagger\hat{n}_{N\sigma} = 0\right) \tag{79}$$

$$(1-\hat{n}_{N\sigma})\mathcal{H}_{2N} = (H_h(1-\hat{n}_{N\sigma}) + \hat{T}^\dagger c) \tag{80}$$

$$(1-\hat{n}_{N\sigma})\mathcal{H}_{2N}\hat{P}\hat{n}_{N\sigma} = \frac{1}{2}H_h(1-\hat{n}_{N\sigma})\eta + \frac{1}{2}\hat{T}^\dagger c\hat{n}_{N\sigma} + \frac{1}{2}\hat{T}^\dagger c\eta = \frac{1}{2}H_h(1-\hat{n}_{N\sigma})\eta + \frac{1}{2}\hat{T}^\dagger c$$
$$(\because c\hat{n}_{N\sigma} = c, c\eta = 0) \tag{81}$$

$$(1-\hat{n}_{N\sigma})\mathcal{H}'\hat{P}\hat{n}_{N\sigma} = \frac{1}{2}\mathcal{H}'(1-\hat{n}_{N\sigma})\eta = \frac{1}{2}\mathcal{H}'\eta \tag{82}$$

Combining 81 and 82, we get

$$\eta_{N\sigma} = G_h(\hat{E}_{N\sigma})\hat{T}^\dagger_{N\sigma}c_{N\sigma} \tag{83}$$

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 $\hat{n}_{N\sigma}\mathcal{H}_{2N}\hat{P}\hat{n}_{N\sigma} = \hat{n}_{N\sigma}\mathcal{H}'\hat{P}\hat{n}_{N\sigma}$

$$\begin{aligned}
\hat{n}_{N\sigma}\mathcal{H}_{2N}\hat{P}\hat{n}_{N\sigma} &= \frac{1}{2}(H_e\hat{n}_{N\sigma} + c^\dagger\hat{T})(\hat{n}_{N\sigma} + \eta) = \frac{1}{2}\left(H_e\hat{n}_{N\sigma} + H_e\hat{n}_{N\sigma}\eta + c^\dagger T\hat{n}_{N\sigma} + c^\dagger T\eta\right) \\
&= \frac{1}{2}\left(H_e\hat{n}_{N\sigma} + c^\dagger T\eta\right) \\
&\left(\because \hat{n}_{N\sigma}\eta = 0, c^\dagger\hat{T}\hat{n}_{N\sigma} = \hat{T}c^\dagger\hat{n}_{N\sigma} = 0\right) \\
\hat{n}_{N\sigma}\mathcal{H}'\hat{P}\hat{n}_{N\sigma} &= \frac{1}{2}\hat{n}_{N\sigma}\mathcal{H}'(\hat{n}_{N\sigma} + \eta) = \frac{1}{2}\left(\hat{n}_{N\sigma}\mathcal{H}'\hat{n}_{N\sigma} + \hat{n}_{N\sigma}\mathcal{H}'\eta\right) = \frac{1}{2}\hat{E}_{N\sigma}\hat{n}_{N\sigma} \\
&\left(\because \hat{n}_{N\sigma}\mathcal{H}'\hat{n}_{N\sigma} = \hat{E}\hat{n}_{N\sigma}, \hat{n}_{N\sigma}\mathcal{H}'\eta = \mathcal{H}'\hat{n}_{N\sigma}\eta = 0\right)
\end{aligned} \tag{84}$$

Combining,

$$\hat{E}_{N\sigma}\hat{n}_{N\sigma} = H_e\hat{n}_{N\sigma} + c^\dagger_{N\sigma}\hat{T}_{N\sigma}\eta_{N\sigma} \tag{85}$$

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

$$\begin{aligned}
&\mathcal{H}_{2N}(1-\hat{P}) = \mathcal{H}''(1-\hat{P}) \\
\implies &(1-\hat{n}_{N\sigma})\mathcal{H}_{2N}(1-\hat{P})(1-\hat{n}_{N\sigma}) = (1-\hat{n}_{N\sigma})\mathcal{H}''(1-\hat{P})(1-\hat{n}_{N\sigma})
\end{aligned} \tag{86}$$

Now,

$$(1-\hat{P})(1-\hat{n}_{N\sigma}) = \frac{1}{2}(1-\eta-\eta^\dagger)(1-\hat{n}_{N\sigma}) = \frac{1}{2}\left((1-\hat{n}_{N\sigma}) - \eta^\dagger\right) \tag{87}$$

Therefore,

$$\begin{aligned}
(1-\hat{n}_{N\sigma})\mathcal{H}_{2N}(1-\hat{P})(1-\hat{n}_{N\sigma}) &= \frac{1}{2}(H_h(1-\hat{n}_{N\sigma}) + \hat{T}^\dagger c)(1-\hat{n}_{N\sigma} - \eta^\dagger) \\
&= \frac{1}{2}\left(H_h(1-\hat{n}_{N\sigma}) - \hat{T}^\dagger c\eta^\dagger\right) \\
&\left(\because (1-\hat{n}_{N\sigma})\eta^\dagger = 0, c(1-\hat{n}_{N\sigma}) = 0\right) \\
(1-\hat{n}_{N\sigma})\mathcal{H}''(1-\hat{P})(1-\hat{n}_{N\sigma}) &= \frac{1}{2}\hat{(}1-\hat{n}_{N\sigma})H''(1-\hat{n}_{N\sigma}) = \frac{1}{2}\hat{E}'(1-\hat{n}_{N\sigma})
\end{aligned} \tag{88}$$

Combining the last two equations,

$$\hat{E}'_{N\sigma}(1-\hat{n}_{N\sigma}) = H_h(1-\hat{n}_{N\sigma}) - \hat{T}^{\dagger}_{N\sigma}c_{N\sigma}\eta^{\dagger}_{N\sigma} \tag{89}$$

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

The starting equation for the above construction was equation 68. That will also provide an expression for the $\hat{U}_{N\sigma}$. Operating equation 68 to the right of $|1\rangle$ (occupied eigenstate of $\hat{n}_{N\sigma}$) gives

$$\begin{aligned}
&\mathcal{H}_{2N}\hat{P}_{N\sigma}|1\rangle = \hat{E}_{N\sigma}\otimes\mathbf{I}\,\hat{P}_{N\sigma}|1\rangle = \hat{E}_{N\sigma}\hat{P}_{N\sigma}|1\rangle \\
&\implies \mathcal{H}_{2N}\hat{U}^{\dagger}_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma}|1\rangle = \hat{E}_{N\sigma}\hat{U}^{\dagger}_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma}|1\rangle \qquad \Big(\text{substituting expression of } \hat{P}_{N\sigma}\Big) \\
&\implies \hat{U}_{N\sigma}\mathcal{H}_{2N}\hat{U}^{\dagger}_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma}|1\rangle = \hat{U}_{N\sigma}\hat{E}_{N\sigma}\hat{U}^{\dagger}_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma}|1\rangle \quad \Big(\text{operating } \hat{U}_{N\sigma} \text{ from left}\Big) \\
&\implies \overline{\mathcal{H}_{2N}}\hat{n}_{N\sigma}\hat{U}_{N\sigma}|1\rangle = \hat{U}_{N\sigma}\hat{E}_{N\sigma}\hat{U}^{\dagger}_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma}|1\rangle
\end{aligned} \tag{90}$$

Compare the last equation with 61. In order to satisfy the first equation of 61, we need the following two equations,

$$\begin{aligned}
\hat{n}_{N\sigma}\hat{U}_{N\sigma}|1\rangle &\propto |1\rangle \\
\hat{U}_{N\sigma}\hat{E}_{N\sigma}\hat{U}^{\dagger}_{N\sigma} &= E_{N\sigma}
\end{aligned} \tag{91}$$

The second equations says

$$\Big[E_{N\sigma}, \hat{U}_{N\sigma}\Big] = 0 \tag{92}$$

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 91,

$$\begin{aligned}
\hat{n}_{N\sigma}\hat{U}_{N\sigma}|1\rangle &\propto \hat{n}_{N\sigma}(1-\hat{\eta}+\hat{\eta}^{\dagger})|1\rangle \\
&= \hat{n}_{N\sigma}(1-\hat{\eta})|1\rangle && \left(\eta^{\dagger}|1\rangle = 0\right) \\
&= |1\rangle - \hat{n}\hat{\eta}|1\rangle \\
&= |1\rangle && (\hat{n}\hat{\eta} = 0)
\end{aligned} \tag{93}$$

To find κ, we will use the unitarity of $\hat{U}_{N\sigma}$:

$$\begin{aligned}
\hat{U}_{N\sigma}\hat{U}^{\dagger}_{N\sigma} &= \kappa^2(1-\eta+\eta^{\dagger})(1+\eta-\eta^{\dagger}) \\
&= \kappa^2(1+\left\{\eta,\eta^{\dagger}\right\}) && \left(\eta^2 = {\eta^{\dagger}}^2 = 0\right) \\
&= 2\kappa^2 && \left(\left\{\eta,\eta^{\dagger}\right\} = 1\right) \\
\implies \kappa &= \frac{1}{\sqrt{2}}
\end{aligned} \tag{94}$$

$$\hat{U}_{N\sigma} = \frac{1}{\sqrt{2}}\left(1-\hat{\eta}+\hat{\eta}^{\dagger}\right) \tag{95}$$

3.5 A Simple Example

$$\mathcal{H} = -t\left(c_2^\dagger c_1 + c_1^\dagger c_2\right) + V\hat{n}_1\hat{n}_2 - \mu(\hat{n}_1+\hat{n}_2) \quad \hat{n}_i = c_i^\dagger c_i = \begin{pmatrix} V-2\mu & 0 & 0 & 0 \\ 0 & -\mu & -t & 0 \\ 0 & -t & \mu & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{96}$$

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 57).

$$\begin{aligned} \hat{H}_{1,e} &= Tr_1[\mathcal{H}\hat{n}_1] \\ &= Tr_1[V\hat{n}_1\hat{n}_2 - \mu(\hat{n}_1+\hat{n}_2)] \quad \left(c \text{ and } c^\dagger \text{ will not conserve the eigenvalue of } \hat{n}\right) \\ &= V\hat{n}_2 - \mu(1+\hat{n}_2) \quad (Tr_1[V\hat{n}_1\hat{n}_2] = VTr_1[\hat{n}_1]\hat{n}_2 = V\hat{n}_2) \\ &= (V-2\mu)\hat{n}_2 - \mu(1-\hat{n}_2) \end{aligned} \tag{97}$$

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

$$\hat{H}_{1,h} = Tr_1[\mathcal{H}(1-\hat{n}_1)] = -\mu\hat{n}_2 \tag{98}$$

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

$$\begin{aligned} T_{1,e-h} &= Tr_1[\mathcal{H}c_1] \\ &= Tr_1[-tc_1^\dagger c_2 c_1] = -tc_2 \quad \text{(the only term that conserves eigenvalue of } \hat{n}) \end{aligned} \tag{99}$$

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

$$\mathcal{H} = \begin{pmatrix} (V-2\mu)\hat{n}_2 - \mu(1-\hat{n}_2) & -tc_2 \\ -tc_2^\dagger & -\mu\hat{n}_2 \end{pmatrix} \tag{100}$$

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,

$$\begin{aligned} t^2 G_e c_1^\dagger c_2 c_2^\dagger c_1 G_e = \hat{n}_1 &\implies t^2\hat{n}_1(1-\hat{n}_2) = \hat{n}_1\{G_e^{-1}\}^2 = \hat{n}_1(\mathcal{H}' - H_e\hat{n}_1)^2 \\ &\implies t^2\hat{n}_1^2(1-\hat{n}_2)^2 = (\mathcal{H}'\hat{n}_1 - H_e\hat{n}_1)^2 \\ &\implies \mathcal{H}'\hat{n}_1 = H_e\hat{n}_1 + t\hat{n}_1(1-\hat{n}_2) = (V-2\mu)\hat{n}_1\hat{n}_2 + (t-\mu)\hat{n}_1(1-\hat{n}_2) \end{aligned} \tag{101}$$

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,

$$\overline{\mathcal{H}} = \mathcal{H}'\hat{n}_1 + \mathcal{H}''(1-\hat{n}_1) = \begin{pmatrix} V-2\mu & 0 & \\ & & \mathbf{0}_{2x2} \\ 0 & t-\mu & \\ & & \\ \mathbf{0}_{2x2} & & (\hat{E}'_1)_{2x2} \end{pmatrix} \tag{102}$$

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 89.

$$E'_1(1-\hat{n}_1) = H_h(1-\hat{n}_1) - \hat{T}_1^\dagger c_1 \eta^\dagger = -\mu(1-\hat{n}_1)\hat{n}_2 - t^2 c_2^\dagger c_1 G_e c_1^\dagger \hat{c}_2 \tag{103}$$

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

$$\langle 01|\, E'(1-\hat{n}_1)\,|01\rangle = -\mu - t^2\,\langle 10|\, G_e\,|10\rangle \tag{104}$$

Now,

$$\begin{aligned} \langle 10|\, G_e^{-1}\,|10\rangle &= \langle 10|\, H' - (V-\mu)\hat{n}_1\hat{n}_2 + \mu\hat{n}_1\,|10\rangle \\ &= \langle 10|\, \mathcal{H}'\,|10\rangle + \mu = \langle 10|\, \mathcal{H}'\hat{n}_1\,|10\rangle + \mu \\ &= \langle 10|\, (V-2\mu)\hat{n}_1\hat{n}_2 + (t-\mu)\hat{n}_1(1-\hat{n}_2)\,|10\rangle + \mu \\ &= t - \mu + \mu = t \\ \therefore \langle 10|\, G_e\,|10\rangle &= \frac{1}{t} \end{aligned} \tag{105}$$

Therefore, $\langle 01|\, E'(1-\hat{n}_1)\,|01\rangle = -\mu - t^2\frac{1}{t} = -\mu - t$. The final diagonalized matrix becomes Equation **??** 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 **??**, $\hat{G}_h\hat{T}^\dagger_{1,e-h} = \hat{T}^\dagger_{1,e-h}\hat{G}_e$. With this modification, equation 106 becomes

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

For this problem,

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

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,

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

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,

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

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, $Tr_1\overline{\mathcal{H}} = (V-2\mu)\hat{n}_2 + (t-\mu)(1-\hat{n}_2) + \hat{E}'_1\hat{n}_2$. From equation 100, $Tr_1\left(\mathcal{H}\right) = V\hat{n}_2 - \mu(1+\hat{n}_2) - \mu\hat{n}_2$. Equating the two traces, we get an expression for the lower block:

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

This gives nothing

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

$$\overline{\mathcal{H}} = \begin{array}{c} \begin{matrix} |11\rangle & |10\rangle & |01\rangle & |00\rangle \end{matrix} \\ \begin{pmatrix} (V-2\mu) & 0 & 0 & 0 \\ 0 & (t-\mu) & 0 & 0 \\ 0 & 0 & -(\mu+t) & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \end{array} \tag{115}$$

3.5.1 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 $\hat{n}$:

$$\mathcal{H}(\hat{U}^\dagger_{N\sigma}|n_1,n_2\rangle) = \hat{U}^\dagger_{N\sigma}\overline{\mathcal{H}}|n_1,n_2\rangle = \hat{U}^\dagger_{N\sigma}E_{n_1,n_2}|n_1,n_2\rangle = E_{n_1,n_2}(\hat{U}^\dagger_{N\sigma}|n_1,n_2\rangle) \tag{116}$$

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 95, we have $\hat{U}_{N\sigma} = \frac{1}{\sqrt{2}}\left(1+\hat{\eta}^\dagger-\hat{\eta}\right)$.
Again, $\hat{\eta}_1 = G_h T^\dagger c_1$, and $\hat{\eta}_1^\dagger = c_1^\dagger G_e T$ Using the expression of $\hat{E}_1$. this simplifies as:

$$\begin{aligned} \eta &= \frac{1}{\hat{E}_1 - H_h}(-tc_2^\dagger)c_1 = \frac{-t}{(V-2\mu)\hat{n}_2 + (t-\mu)(1-\hat{n}_2) + \mu\hat{n}_2}c_1c_2^\dagger = \frac{-t}{V-\mu}c_1c_2^\dagger \\ \eta^\dagger &= c_1^\dagger\frac{1}{(V-2\mu)\hat{n}_2 + (t-\mu)(1-\hat{n}_2) - (V-2\mu)\hat{n}_2 + \mu(1-\hat{n}_2)}(-tc_2) = -c_1^\dagger c_2 \end{aligned} \tag{117}$$

QUESTION: How can the η in the previous equation be conjugates of each other? Where's the problem? This question boils down to the following. In order for η and $\eta^\dagger$ to be conjugates of each other, the consistency equation $G_h T^\dagger = T^\dagger G_e$ needs to be satisfied. That comes down to $c_2^\dagger\{t(1-\hat{n}_2) - 4\mu\hat{n}_2\} = \{(V-\mu)n_2^\dagger + (t-\mu)(1-\hat{n}_2)\}c_2^\dagger$, or, $tc_2^\dagger = (V-\mu)c_2^\dagger$. Why should this work out in general?

$$\therefore \hat{U}_{N\sigma} = \frac{1}{\sqrt{2}}\left[1 + \frac{t}{V-\mu}c_1c_2^\dagger - c_1^\dagger c_2\right], \hat{U}^\dagger_{N\sigma} = \frac{1}{\sqrt{2}}\left[1 + \frac{t}{V-\mu}c_1^\dagger c_2 - c_2c_1^\dagger\right] \tag{118}$$

To get the eigenstates of $\mathcal{H}$, I act with $U^\dagger$ on the eigenstates ($|n_1,n_2\rangle$):

$$\hat{U}^\dagger_{N\sigma}|11\rangle = |11\rangle \tag{119}$$

$$\hat{U}^\dagger_{N\sigma}|00\rangle = |00\rangle, \tag{120}$$

$$\begin{aligned} \hat{U}^\dagger_{N\sigma}|10\rangle = \frac{1}{2}(|10\rangle - \eta|10\rangle) = \frac{1}{2}\left(|10\rangle + tc_2^\dagger c_1\hat{G}_e|10\rangle\right) = \frac{1}{2}\left(|10\rangle + tc_2^\dagger c_1\frac{1}{t}|01\rangle\right) \\ = \frac{1}{2}(|10\rangle + |01\rangle) \end{aligned} \tag{121}$$

$$\hat{U}^{\dagger}_{N\sigma}\left|01\right\rangle = \frac{1}{2}\left(\left|01\right\rangle + \eta^{\dagger}\left|01\right\rangle\right) = \frac{1}{2}\left(\left|01\right\rangle - t\hat{G}_e c_1^{\dagger}c_2\left|01\right\rangle\right) = \frac{1}{2}\left(\left|01\right\rangle - \left|10\right\rangle\right) \tag{122}$$

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

$$\begin{aligned} &\left|00\right\rangle \\ &\left|10\right\rangle + \left|01\right\rangle \\ &\left|01\right\rangle - \left|10\right\rangle \\ &\left|11\right\rangle \end{aligned} \tag{123}$$

4 Applying the RG on the Hubbard dimer

$$\mathcal{H} = -t\sum_{\sigma}(c_{1\sigma}^{\dagger}c_{2\sigma} + c_{2\sigma}^{\dagger}c_{1\sigma}) + U\left(\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow}\right) \tag{124}$$

We begin by decoupling the first degree of freedom, namely, a spin-up electron on the first site.

$$H^{e}_{1\uparrow} = Tr_{\hat{n}_{1\uparrow}}(\mathcal{H}\hat{n}_{1\uparrow}) = U(\hat{n}_{1\downarrow} + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow}) - t(c_{1\downarrow}^{\dagger}c_{2\downarrow} + c_{2\downarrow}^{\dagger}c_{1\downarrow}) \tag{125}$$

$$H^{h}_{1\uparrow} = Tr_{\hat{n}_{1\uparrow}}(\mathcal{H}(1-\hat{n}_{1\uparrow})) = U\hat{n}_{2\uparrow}\hat{n}_{2\downarrow} - t(c_{1\downarrow}^{\dagger}c_{2\downarrow} + c_{2\downarrow}^{\dagger}c_{1\downarrow}) \tag{126}$$

$$T_{1\uparrow} = Tr_{\hat{n}_{1\uparrow}}(\mathcal{H}c_{1\uparrow}) = -tc_{2\uparrow} \tag{127}$$

$$T^{\dagger}_{1\uparrow} = Tr_{\hat{n}_{1\uparrow}}(c_{1\uparrow}^{\dagger}\mathcal{H}) = -tc_{2\uparrow}^{\dagger} \tag{128}$$

Assume that the Hamiltonian, after block-diagonalisation in the subspace of $\hat{n}_{1\uparrow}$, looks like

$$\overline{\mathcal{H}} = U_{1\uparrow}^{\dagger}\mathcal{H}U_{1\uparrow} = \begin{pmatrix} \hat{E}_{1\uparrow} & 0 \\ 0 & \hat{E}'_{1\uparrow} \end{pmatrix} \tag{129}$$

$\hat{E}_{1\uparrow}$ and $\hat{E}'_{1\uparrow}$ are the sub-Hamiltonians with one fewer degree of freedom. That is, they are the Hamiltonians in the subspaces $\hat{n}_{1\uparrow} = 1, 0$ respectively.

4.1 $\hat{n}_{1\uparrow} = 1$

Define $\hat{H}'_{1\uparrow} \equiv \hat{E}_{1\uparrow} \otimes \mathbb{I}$. Again, proceeding as in the formalism, we can derive

$$\eta_{1\uparrow} = \hat{G}_e\hat{T}^{\dagger}_{1\uparrow}c_{1\uparrow} \tag{130}$$

$$\eta^{\dagger}_{1\uparrow} = \hat{G}_h c^{\dagger}_{1\uparrow}\hat{T}_{1\uparrow} \tag{131}$$

The process of finding the eigenvalues involves using the equations for $\eta^{\dagger}\eta$ and $\eta\eta^{\dagger}$:

$$\eta^{\dagger}_{1\uparrow}\eta_{1\uparrow} = \hat{n}_{1\uparrow} \tag{132}$$

$$\eta_{1\uparrow}\eta^{\dagger}_{1\uparrow} = 1 - \hat{n}_{1\uparrow} \tag{133}$$

This subspace involves $1-\hat{n}_{1\uparrow}=0$, hence we cannot use eq. 133. We also have the choice of starting with the expression of either η or $\eta^\dagger$, but since η involves $1-\hat{n}_{1\uparrow}$ in the denominator, it doesn't lead to anything fruitful. So we start with $\eta^\dagger_{1\hat{n}_{1\uparrow}}$. Using eq. 78:

$$\eta^\dagger_{1\uparrow} = G_e c^\dagger_{1\uparrow} T_{1\uparrow} = -t\hat{G}_e c^\dagger_{1\uparrow} c_{2\uparrow} = \frac{-t}{\hat{E}_{1\uparrow}\hat{n}_{1\uparrow} - H_e\hat{n}_{1\uparrow}} c^\dagger_{1\uparrow} c_{2\uparrow} \tag{134}$$

The hole to electron operator $\eta_{1\uparrow}$ is obtained by taking the Hermitian conjugate of $\eta^\dagger_{1\uparrow}$:

$$\eta_{1\uparrow} = c^\dagger_{2\uparrow} c_{1\uparrow} \frac{-t}{\hat{E}_{1\uparrow}\hat{n}_{1\uparrow} - H_e\hat{n}_{1\uparrow}} \tag{135}$$

Here we used the fact that $H_e\hat{n}_{1\uparrow}$ is Hermitian as seen from its expression, and $\hat{E}_{1\hat{n}_{1\uparrow}}\hat{n}_{1\uparrow} \equiv \hat{E}_{1\hat{n}_{1\uparrow}} \otimes \hat{n}_{1\uparrow}$ is Hermitian because it is a sub-Hamiltonian by definition. Substituting these expressions in eq. 132,

$$\hat{n}_{1\uparrow} = \eta^\dagger_{1\uparrow}\eta_{1\uparrow} = \frac{-t}{\hat{E}_{1\uparrow}\hat{n}_{1\uparrow} - H_e\hat{n}_{1\uparrow}} \hat{n}_{1\uparrow}(1-\hat{n}_{2\uparrow}) \frac{-t}{\hat{E}_{1\uparrow}\hat{n}_{1\uparrow} - H_e\hat{n}_{1\uparrow}} \tag{136}$$

$$\implies (\hat{E}_{1\uparrow}\hat{n}_{1\uparrow} - H_e\hat{n}_{1\uparrow})^2 = t^2\hat{n}_{1\uparrow}(1-\hat{n}_{2\uparrow}) \tag{137}$$

This is the central equation(eq. 137) that will be used for determining all the eigenvalues for the $\hat{n}_{1\uparrow}=1$ subspace. Substituting the expression for H_e gives:

$$\left[\hat{E}_{1\uparrow}\hat{n}_{1\uparrow} - U\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} - U\hat{n}_{2\uparrow}\hat{n}_{2\downarrow}\hat{n}_{1\uparrow} + t(c^\dagger_{1\downarrow}c_{2\downarrow} + c^\dagger_{2\downarrow}c_{1\downarrow})\hat{n}_{1\uparrow}\right]^2 = t^2\hat{n}_{1\uparrow}(1-\hat{n}_{2\uparrow}) \tag{138}$$

4.1.1 N=2

We first look at the $N=2$ portion of the $\hat{n}_{1\uparrow}$ occupied subspace. The remaining degrees of freedom are $\hat{n}_{1\downarrow}$, $\hat{n}_{2\uparrow}$ and $\hat{n}_{2\downarrow}$. Notice that the working equation, eq. 138 involves the creation and annihilation operators only for $\hat{n}_{1\downarrow}$ and $\hat{n}_{2\downarrow}$. This means that $\hat{n}_{1\downarrow}$ and $\hat{n}_{2\downarrow}$ form a coupled degree of freedom, and this is in turn decoupled from $\hat{n}_{2\uparrow}$.Out of the two electrons ($N=2$), one electron is already there at $\hat{n}_{1\uparrow}$. This leaves us with two possible subspaces to work in:

- $\hat{\mathcal{P}} = |1100\rangle\langle 1100| + |1001\rangle\langle 1001|$

  This is the subspace in which we keep $\hat{n}_{2\uparrow}$ empty, and the second electron thus lie somewhere in the subspace spanned by $\hat{n}_{1\downarrow}$ and $\hat{n}_{2\downarrow}$. The notation is obvious: $|1100\rangle \equiv |\uparrow\downarrow, 0\rangle$ and $|1001\rangle \equiv |\uparrow,\downarrow\rangle$. In this subspace, the right hand side of eq. 138 is unity, because $\hat{n}_{1\uparrow}=1$ and $\hat{n}_{2\uparrow}=0$. Define $\hat{a}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. Clearly, $\hat{a}_x^2 = 1$. Then, in this subspace,

$$\left[\hat{E}_{1\uparrow}\hat{n}_{1\uparrow} - U\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} - U\hat{n}_{2\uparrow}\hat{n}_{2\downarrow}\hat{n}_{1\uparrow} + t(c^\dagger_{1\downarrow}c_{2\downarrow} + c^\dagger_{2\downarrow}c_{1\downarrow})\hat{n}_{1\uparrow}\right]^2 = t^2\hat{a}_x^2 \tag{139}$$

$$\implies \hat{E}_{1\uparrow}\hat{n}_{1\uparrow} - U\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} - U\hat{n}_{2\uparrow}\hat{n}_{2\downarrow}\hat{n}_{1\uparrow} + t(c^\dagger_{1\downarrow}c_{2\downarrow} + c^\dagger_{2\downarrow}c_{1\downarrow})\hat{n}_{1\uparrow} = \pm t\hat{a}_x \tag{140}$$

Next we need to write the LHS in this subspace. Taking $|1100\rangle$ and $|1001\rangle$ as the basis elements, we see that both $c^\dagger_{2\downarrow}c_{1\downarrow}$ and $c^\dagger_{1\downarrow}c_{2\downarrow}$ take one basis vector to the other, and hence

$$c^\dagger_{1\downarrow}c_{2\downarrow} + c^\dagger_{2\downarrow}c_{1\downarrow} = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \tag{141}$$

Since $\hat{n}_{2\uparrow} = 0$, the $\hat{n}_{2\uparrow}\hat{n}_{2\downarrow}\hat{n}_{1\uparrow}$ term drops out. Also,

$$\hat{n}_{1\uparrow}\hat{n}_{2\downarrow} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{142}$$

Finally, $\hat{E}_{1\uparrow,2} \equiv \mathcal{P}\hat{E}_{1\uparrow}\mathcal{P}$ is the projected Hamiltonian in this subspace. Putting all these together,

$$\hat{E}_{1\uparrow,2} - \begin{pmatrix} U & 0 \\ 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & t \\ t & 0 \end{pmatrix} = \pm \begin{pmatrix} 0 & t \\ t & 0 \end{pmatrix} \tag{143}$$

$$\implies \hat{E}_{1\uparrow,2} = \begin{pmatrix} U & 0 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix} U & 2t \\ 2t & 0 \end{pmatrix} \tag{144}$$

The first matrix gives eigenvalues $= \{U, 0\}$ and eigenvectors $= \{|\uparrow\downarrow, 0\rangle, |\uparrow, \downarrow\rangle\}$. The second matrix gives eigenvalues $E_\pm = \frac{U \pm \sqrt{U^2+16t^2}}{2}$ and eigenvectors $= \{2t\,|\uparrow, \downarrow\rangle + E_\pm\,|\uparrow\downarrow, 0\rangle\}$. Note that this is not the eigenvector for the total Hamiltonian, because it doesn't include the contribution from $\hat{n}_{1\uparrow} = 0$ sector.

- $\mathcal{P} = |1010\rangle\langle 1010|$

  In the previous subspace, we set $\hat{n}_{2\uparrow} = 0$, so here we consider $\hat{n}_{2\uparrow} = 1$: Since $\hat{n}_{1\downarrow} = \hat{n}_{2\downarrow} = 0$, we have $U(\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow}) = 0$ and $c^\dagger_{1\downarrow}c_{2\downarrow} + c^\dagger_{2\downarrow}c_{1\downarrow} = 0$. The RHS is also zero. This means that in this subspace, the only eigenvalue is $E = 0$. The eigenvector is $|\uparrow, \uparrow\rangle$.

4.1.2 N=1

This case is simpler, because the only electron is placed at $\hat{n}_{1\uparrow}$. Thus, $\hat{n}_{1\downarrow} = \hat{n}_{2\uparrow} = \hat{n}_{2\downarrow} = 0$ in this subspace. Since the subspace has just one state, it is unidimensionl, and the equation for this subspace will involve scalars instead of matrices. The RHS is hence t^2 instead of $t^2a_x^2$. Since there are no electrons in $\hat{n}_{1\downarrow}$ or $\hat{n}_{2\downarrow}$, the creation and annihilation operators in the LHS are zero:

$$\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow} = c^\dagger_{1\downarrow}c_{2\downarrow} + c^\dagger_{2\downarrow}c_{1\downarrow} = 0 \tag{145}$$

Eq. 138 thus reduces to

$$\hat{E}_{1\uparrow,1} = \pm t \tag{146}$$

$\hat{E}_{1\uparrow,1}$ is the projected Hamiltonian in this subspace. The eigenvalues in this subspace come out to be $\pm t$. Since the only state in this subspace is $|\uparrow, 0\rangle$, that is the contribution to the eigenvectors.

4.1.3 N=3

With one electron at $\hat{n}_{1\uparrow}$, we have two electrons to place. There are two options:

- $\hat{\mathcal{P}} = |1110\rangle\langle 1110| + |1011\rangle\langle 1011|$

  Since the equation is diagonal in $\hat{n}_{2\uparrow}$, it makes sense to place one electron at $\hat{n}_{2\uparrow}$, and the other electron in the coupled subspace, that is, $\hat{n}_{1\downarrow}$ and $\hat{n}_{2\downarrow}$. The corresponding projection operator is The RHS of eq. 138 in this subspace is 0, because $\hat{n}_{2\uparrow} = 1$. This also means that

$$\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow}\hat{n}_{1\uparrow} = \hat{n}_{1\downarrow} + \hat{n}_{2\downarrow} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{147}$$

$$c^\dagger_{1\downarrow}c_{2\downarrow} + c^\dagger_{2\downarrow}c_{1\downarrow} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{148}$$

  The equation becomes

$$\hat{E}_{1\uparrow,3} - \begin{pmatrix} U & 0 \\ 0 & U \end{pmatrix} + \begin{pmatrix} 0 & t \\ t & 0 \end{pmatrix} = 0 \implies \hat{E}_{1\uparrow,3} = \begin{pmatrix} U & -t \\ -t & U \end{pmatrix} \tag{149}$$

  The eigenvalues come out as $U \pm t$. The eigenvectors are $|1110\rangle \mp |1011\rangle$.

- $\hat{\mathcal{P}} = |1101\rangle$

  The other sensible choice is to keep $\hat{n}_{2\uparrow} = 0$. Since this subspace has just one state, it is unidimensional, and the equation is scalar.

$$\begin{aligned} \hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow} &= 1 \\ c^\dagger_{1\downarrow}c_{2\downarrow} + c^\dagger_{2\downarrow}c_{1\downarrow} &= 0 \\ \hat{E}_{1\uparrow,3} - U &= \pm t \end{aligned} \tag{150}$$

  The eigenvalues are $U \pm t$, and the eigenvector is $|\uparrow\downarrow, \downarrow\rangle$.

4.2 $\hat{n}_{1\uparrow} = 0$

To calculate the eigenvalues for the unoccupied sector, define $\mathcal{H}'' \equiv \hat{E}'_{1\hat{n}_{1\uparrow}} \otimes \mathbb{I}$. We can derive

$$\eta_{1\uparrow} = -\hat{G}'_h \hat{T}^\dagger_{1\uparrow} c_{1\uparrow} \tag{151}$$

$$\eta^\dagger_{1\uparrow} = -\hat{G}'_e c^\dagger_{1\uparrow} \hat{T}_{1\uparrow} \tag{152}$$

$$\eta^\dagger_{1\uparrow} \eta_{1\uparrow} = \hat{n}_{1\uparrow} \tag{153}$$

$$\eta_{1\uparrow} \eta^\dagger_{1\uparrow} = 1 - \hat{n}_{1\uparrow} \tag{154}$$

Note that $\hat{G}'$ involves $\hat{E}'$ in the denominator, because we now want to diagonalize the unoccupied block. Since $\hat{n}_{1\uparrow} = 0$ now, we need to use eq. 154 and start with the expression of $\eta_{1\uparrow}(eq.\ 151)$ instead of $\eta^\dagger_{1\uparrow}$. Substituting the expression for $\eta_{1\uparrow}$ and it's conjugate gives the following equation for the unoccupied sector:

$$\left[\hat{E}'_{1\uparrow} - U\hat{n}_{2\uparrow}\hat{n}_{2\downarrow} + t(c^\dagger_{1\downarrow}c_{2\downarrow} + c^\dagger_{2\downarrow}c_{1\downarrow})\right]^2 = t^2\hat{n}_{2\uparrow} \tag{155}$$

4.2.1 N=1

With no electron on $1,\uparrow$, the only electron can reside in a superposition of $|\downarrow, 0\rangle$ or $|0, \downarrow\rangle$:

$$\mathcal{P} = |0100\rangle\langle 0100| + |0001\rangle\langle 0001| \tag{156}$$

The right hand side is zero because $\hat{n}_{2\uparrow} = 0$. Also,

$$\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow} = 0 \tag{157}$$

$$c^\dagger_{1\downarrow}c_{2\downarrow} + c^\dagger_{2\downarrow}c_{1\downarrow} = \begin{pmatrix} 0 & t \\ t & 0 \end{pmatrix} \tag{158}$$

Putting it all together,

$$\left(E'_{1\uparrow,2} + \begin{pmatrix} 0 & t \\ t & 0 \end{pmatrix}\right)^2 = 0 \tag{159}$$

$$\implies E'_{1\uparrow,2} = \begin{pmatrix} 0 & -t \\ -t & 0 \end{pmatrix} \tag{160}$$

The eigenvalues are $\pm t$, the eigenvectors are $|\downarrow, 0\rangle \mp |0.\ \downarrow\rangle$.

4.2.2 N=2

$$\mathcal{P} = |0110\rangle \langle 0110| + |0011\rangle \langle 0011| \tag{161}$$

$$\implies E'_{1\uparrow,2} - \begin{pmatrix} 0 & 0 \\ 0 & U \end{pmatrix} - \begin{pmatrix} 0 & t \\ t & U \end{pmatrix} = \pm t a_x \tag{162}$$

$$\implies E'_{1\uparrow,2} = \begin{pmatrix} 0 & 0 \\ 0 & U \end{pmatrix}, \begin{pmatrix} 0 & 2t \\ 2t & 0 \end{pmatrix} \tag{163}$$

The eigenvalues are $0, U$ for the first matrix, with eigenvectors $|0110\rangle, |0011\rangle$, and $E_\pm = \frac{U \pm \sqrt{U^2+16t^2}}{2}$, and $2t\,|\downarrow,\uparrow\rangle + E_\pm\,|0,\uparrow\downarrow\rangle$ for the second.

Similar to the $\hat{n}_{1\uparrow} = 1$ situation,we can consider another subspace where $\hat{n}_{2\uparrow} = 0$:

$$\mathcal{P} = |0101\rangle \langle 0101| \tag{164}$$

Obviously, $\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow} = c^\dagger_{1\downarrow}c_{2\downarrow} + c^\dagger_{2\downarrow}c_{1\downarrow} = 0$. The only eigenvalue is 0, with eigenvector $|\downarrow,\downarrow\rangle$.

4.2.3 N=3

Only state in this subspace is $|0111\rangle$.

$$\mathcal{P} = |0111\rangle \tag{165}$$

$$\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + \hat{n}_{2\uparrow}\hat{n}_{2\downarrow} = 1 \tag{166}$$

$$c^\dagger_{1\downarrow}c_{2\downarrow} + c^\dagger_{2\downarrow}c_{1\downarrow} = 0 \tag{167}$$

The equation(scalar) in this subspace is

$$E'_{1\uparrow,3} - U = \pm t \tag{168}$$

The eigenvalues are $U \pm t$. The eigenvector is $|0111\rangle$.

4.3 The eigenstates

The eigenstates obtained for the various subspaces form only parts of the total eigenstates. Using the unitary operator $\hat{U}^\dagger = \frac{1}{\sqrt{2}}(1 + \eta - \eta^\dagger)$, these individual eigenstates can be combined into the total eigenstates.

4.3.1 N=1

First, consider the case of $\hat{n}_{1\uparrow} = 1$. The eigenstate for the subspace is $|\hat{n}_{1\uparrow} = 1, N = 1\rangle = |\uparrow, 0\rangle$. The total eigenstates are given by $|\psi\rangle = \hat{U}^\dagger_{1\uparrow} |\hat{n}_{1\uparrow} = 1, N = 1\rangle$. Note that since $\eta^\dagger_{1\uparrow}$ takes a hole at $\hat{n}_{1\uparrow}$ to an electron at the same quantum number, and since there is no hole at that quantum number ($\hat{n}_{1\uparrow}$ is occupied), $\eta^\dagger$ will act to give zero, so we drop it.

$$\hat{U}^\dagger_{1\uparrow} |\hat{n}_{1\uparrow} = 1, N = 1\rangle = \frac{1}{\sqrt{2}}(1 + \eta_{1\uparrow}) |\uparrow, 0\rangle \tag{169}$$

From eq. 135, $\eta_{1\uparrow} = c^\dagger_{2\uparrow} c_{1\uparrow} \frac{-t}{\hat{E}_{1\uparrow}\hat{n}_{1\uparrow} - H_e \hat{n}_{1\uparrow}}$. In the subspace we are talking about, $\hat{E}_{1\uparrow}\hat{n}_{1\uparrow} - H_e\hat{n}_{1\uparrow} = \pm t$ (see eq. 146). Therefore,

$$\eta_{1\uparrow} |\uparrow, 0\rangle = \mp c^\dagger_{2\uparrow} c_{1\uparrow} |\uparrow, 0\rangle = \mp |0, \uparrow\rangle \tag{170}$$

The total eigenstate turns out to be

$$\hat{U}^\dagger_{1\uparrow} |\hat{n}_{1\uparrow} = 1, N = 1\rangle = \frac{1}{\sqrt{2}}(|\uparrow, 0\rangle + \eta_{1\uparrow} |\uparrow, 0\rangle) = |\uparrow, 0\rangle \mp |0, \uparrow\rangle \tag{171}$$

Note that the respective eigenvalues are $\pm t$.

Now consider the case of $\hat{n}_{1\uparrow} = 0$. The eigenstates for the subspace is $|\hat{n}_{1\uparrow} = 0, N = 1\rangle = |\downarrow, 0\rangle \mp |0, \downarrow\rangle$. This time, however, since the states are missing an electron in $\hat{n}_{1\uparrow}$, η will act trivially, and we are left with

$$\hat{U}^\dagger_{1\uparrow} |\hat{n}_{1\uparrow} = 0, N = 1\rangle = \frac{1}{\sqrt{2}}(1 - \eta^\dagger_{1\uparrow}) |\hat{n}_{1\uparrow} = 0, N = 1\rangle \tag{172}$$

From eq. 151, $\eta^\dagger_{1\uparrow} = -c^\dagger_{1\uparrow} c_{2\uparrow} \hat{G}'_h = c^\dagger_{1\uparrow} c_{2\uparrow} \frac{t}{E' - H_h(1-\hat{n}_{1\uparrow})}$. Note, however, that $|\hat{n}_{1\uparrow} = 0, N = 1\rangle$ does not have any electron at $\hat{n}_{2\uparrow}$, and $c_{2\uparrow}$ in $\eta^\dagger_{1\uparrow}$ will necessarily give 0. Therefore,

$$\eta^\dagger_{1\uparrow} |\hat{n}_{1\uparrow} = 0, N = 1\rangle = 0 \tag{173}$$

which means

$$U^\dagger_{1\uparrow} |\hat{n}_{1\uparrow} = 0, N = 1\rangle = \frac{1}{\sqrt{2}} |\hat{n}_{1\uparrow} = 0, N = 1\rangle = \frac{|\downarrow, 0\rangle \mp |0, \downarrow\rangle}{\sqrt{2}} \tag{174}$$

These are thus the final eigenstates for respective eigenvalues $\pm t$.
The four eigenstates for $N = 1$ are listed in this table:

t	$\frac{\|\uparrow,0\rangle - \|0,\uparrow\rangle}{\sqrt{2}}$
$-t$	$\frac{\|\uparrow,0\rangle + \|0,\uparrow\rangle}{\sqrt{2}}$
t	$\frac{\|\downarrow,0\rangle - \|0,\downarrow\rangle}{\sqrt{2}}$
$-t$	$\frac{\|\downarrow,0\rangle + \|0,\downarrow\rangle}{\sqrt{2}}$

4.3.2 N=3

The eigenstate for the first subspace are
$|\hat{n}_{1\uparrow} = 1, N = 3\rangle = |\uparrow\downarrow, \uparrow\rangle \mp |\uparrow, \uparrow\downarrow\rangle$. The total eigenstates are given by $\hat{U}^\dagger_{1\uparrow} |\hat{n}_{1\uparrow} = 1, N = 3\rangle$. Note that since $\eta^\dagger_{1\uparrow}$ takes a hole at $\hat{n}_{1\uparrow}$ to an electron at the same quantum number, and since there is no hole at that quantum number ($\hat{n}_{1\uparrow}$ is occupied), $\eta^\dagger$ will act to give zero, so we drop it.

$$\hat{U}^\dagger_{1\uparrow} |\hat{n}_{1\uparrow} = 1, N = 3\rangle = \frac{1}{\sqrt{2}}(1 + \eta_{1\uparrow})(|\uparrow\downarrow, \uparrow\rangle \mp |\uparrow, \uparrow\downarrow\rangle) \tag{175}$$

From eq. 135, $\eta_{1\uparrow} = c^\dagger_{2\uparrow} c_{1\uparrow} \frac{-t}{\hat{E}_{1\uparrow}\hat{n}_{1\uparrow} - H_e \hat{n}_{1\uparrow}}$. Since the part before $c_{1\uparrow}$ can only attach a coefficient to the kets, and since $c^\dagger_{2\uparrow}$ will act on both $|\uparrow\downarrow, \uparrow\rangle$ and $|\uparrow, \uparrow\downarrow\rangle$ to give zero, we have

$$\eta_{1\uparrow} |\hat{n}_{1\uparrow} = 1, N = 3\rangle = 0 \tag{176}$$

The total eigenstates turn out to be

$$\hat{U}^\dagger_{1\uparrow} |\hat{n}_{1\uparrow} = 1, N = 3\rangle = \frac{1}{\sqrt{2}} |\hat{n}_{1\uparrow} = 1, N = 3\rangle + \eta_{1\uparrow} |\hat{n}_{1\uparrow} = 1, N = 3\rangle = \frac{|\uparrow\downarrow, \uparrow\rangle \mp |\uparrow, \uparrow\downarrow\rangle}{\sqrt{2}} \tag{177}$$

Note that the respective eigenvalues are $U \pm t$.

Now consider second subspace for $N = 3, \hat{n}_{1\uparrow} = 1$. The eigenstate is $|\uparrow\downarrow, \downarrow\rangle$. Here, $E - H_e = \pm t$, therefore,

$$\eta_{1\uparrow} |\uparrow\downarrow, \downarrow\rangle = c^\dagger_{2\uparrow} c_{1\downarrow} \frac{-t}{\pm t} |\uparrow\downarrow, \downarrow\rangle = \mp |\downarrow, \uparrow\downarrow\rangle \tag{178}$$

which means

$$U^\dagger_{1\uparrow} |\uparrow\downarrow, \downarrow\rangle = \frac{|\uparrow\downarrow, \downarrow\rangle \mp |\downarrow, \uparrow\downarrow\rangle}{\sqrt{2}} \tag{179}$$

These are thus the final eigenstates for respective eigenvalues $U \pm t$.
The four eigenstates for $N = 1$ are listed in this table:

$U + t$	$\frac{\|\uparrow\downarrow,\uparrow\rangle - \|\uparrow,\uparrow\downarrow\rangle}{\sqrt{2}}$
$U - t$	$\frac{\|\uparrow\downarrow,\uparrow\rangle + \|\uparrow,\uparrow\downarrow\rangle}{\sqrt{2}}$
$U + t$	$\frac{\|\uparrow\downarrow,\downarrow\rangle - \|\downarrow,\uparrow\downarrow\rangle}{\sqrt{2}}$
$U - t$	$\frac{\|\uparrow\downarrow,\downarrow\rangle + \|\downarrow,\uparrow\downarrow\rangle}{\sqrt{2}}$

4.3.3 N=2

Consider the first set of eigenstates in $\hat{n}_{1\uparrow} = 1$: $|\uparrow\downarrow, 0\rangle$ and $|\uparrow, \downarrow\rangle$. $\eta^\dagger$ can be dropped as usual. In this subspace, $\eta = -t c^\dagger_{2\uparrow} c_{1\uparrow} \frac{1}{-t\hat{a}_x} = c^\dagger_{2\uparrow} c_{1\uparrow} \hat{a}_x$ (using $\hat{a}^2_x = 1$). Applying these on the

eigenstates gives

$$\eta_{1\uparrow}|\uparrow\downarrow,0\rangle = c^\dagger_{2\uparrow}c_{1\uparrow}\hat{a}_x|\uparrow\downarrow,0\rangle = c^\dagger_{2\uparrow}c_{1\uparrow}|\uparrow,\downarrow\rangle = |0,\uparrow\downarrow\rangle \tag{180}$$

$$\eta_{1\uparrow}|\uparrow,\downarrow\rangle = c^\dagger_{2\uparrow}c_{1\uparrow}\hat{a}_x|\uparrow,\downarrow\rangle = c^\dagger_{2\uparrow}c_{1\uparrow}|\uparrow\downarrow,0\rangle = |\downarrow,\uparrow\rangle \tag{181}$$

The total eigenstates are

$$\hat{U}^\dagger_{1\uparrow}|\uparrow\downarrow,0\rangle = \frac{|\uparrow\downarrow,0\rangle + \eta_{1\uparrow}|\uparrow\downarrow,0\rangle}{\sqrt{2}} = \frac{|\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle}{\sqrt{2}} \tag{182}$$

$$\hat{U}^\dagger_{1\uparrow}|\uparrow,\downarrow\rangle = \frac{|\uparrow,\downarrow\rangle + \eta_{1\uparrow}|\uparrow,\downarrow\rangle}{\sqrt{2}} = \frac{|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle}{\sqrt{2}} \tag{183}$$

These are the total eigenstates corresponding to eigenvalues $U, 0$.Consider the corresponding eigenstates from the $\hat{n}_{1\uparrow} = 0$ sector will give the same eigenstates.
Instead, take the second set of eigenstates of $\hat{n}_{1\uparrow} = 1$: $2t|\uparrow,\downarrow\rangle + E_\pm|\uparrow\downarrow,0\rangle$ corresponding to eigenvalues $E_\pm = \frac{U\pm\sqrt{U^2+16t^2}}{2}$. Here, $\eta = -tc^\dagger_{2\uparrow}c_{1\uparrow}\frac{1}{t\hat{a}_x} = -c^\dagger_{2\uparrow}c_{1\uparrow}\hat{a}_x$.

$$\begin{aligned}\eta_{1\uparrow}(2t|\uparrow,\downarrow\rangle + E_\pm|\uparrow\downarrow,0\rangle) = -c^\dagger_{2\uparrow}c_{1\uparrow}\hat{a}_x(2t|\uparrow,\downarrow\rangle + E_\pm|\uparrow\downarrow,0\rangle) = -c^\dagger_{2\uparrow}c_{1\uparrow}(2t|\uparrow\downarrow,0\rangle + E_\pm|\uparrow,\downarrow\rangle)\\ = -2t|\downarrow,\uparrow\rangle - E_\pm|0,\uparrow\downarrow\rangle\end{aligned} \tag{184}$$

The total eigenstates are

$$\begin{aligned}\hat{U}^\dagger_{1\uparrow}(2t|\uparrow,\downarrow\rangle + E_\pm|\uparrow\downarrow,0\rangle) &= \frac{1+\eta_{1\uparrow}}{\sqrt{2}}(2t|\uparrow,\downarrow\rangle + E_\pm|\uparrow\downarrow,0\rangle)\\ &= 2t\frac{|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle}{\sqrt{2}} + E_\pm\frac{|\uparrow\downarrow,0\rangle - |0,\uparrow\downarrow\rangle}{\sqrt{2}}\end{aligned} \tag{185}$$

These are the final states corresponding to the eigenvalues $E_\pm$.

The final states to consider are the ones with zero eigenvalues, that is, $|\uparrow,\uparrow\rangle$ for $\hat{n}_{1\uparrow} = 1$ and $|\downarrow,\downarrow\rangle$ for $\hat{n}_{1\uparrow} = 0$. The action of $\hat{U}^\dagger_{1\uparrow}$ on them is easy to see. Since η or $\eta^\dagger$ annihilate one spin up electron and create another spin up electron at a different site, it is clear that they will give zero for both these states: $|\downarrow,\downarrow\rangle$ has no spin up electron to annihilate, and $|\uparrow,\uparrow\rangle$ has no free site to create a spin up electron. Hence, the final eigenstates are

$$\begin{aligned}\hat{U}^\dagger_{1\uparrow}|\uparrow,\uparrow\rangle &= |\uparrow,\uparrow\rangle\\ \hat{U}^\dagger_{1\uparrow}|\downarrow,\downarrow\rangle &= |\downarrow,\downarrow\rangle\end{aligned} \tag{186}$$

These have eigenvalues 0.

0	$\frac{\lvert\uparrow\downarrow,0\rangle+\lvert 0,\uparrow\downarrow\rangle}{\sqrt{2}}$
U	$\frac{\lvert\uparrow,\downarrow\rangle+\lvert\downarrow,\uparrow\rangle}{\sqrt{2}}$
E_+	$2t\frac{\lvert\uparrow,\downarrow\rangle-\lvert\downarrow,\uparrow\rangle}{\sqrt{2}}+E_+\frac{\lvert\uparrow\downarrow,0\rangle-\lvert 0,\uparrow\downarrow\rangle}{\sqrt{2}}$
E_-	$2t\frac{\lvert\uparrow,\downarrow\rangle-\lvert\downarrow,\uparrow\rangle}{\sqrt{2}}+E_-\frac{\lvert\uparrow\downarrow,0\rangle-\lvert 0,\uparrow\downarrow\rangle}{\sqrt{2}}$
0	$\lvert\uparrow,\uparrow\rangle$
0	$\lvert\downarrow,\downarrow\rangle$