Unitary Renormalization Group

Anirban Mukherjee
(edited by Abhirup Mukherjee)

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

1.1 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 $\left[\hat{U}_{N\sigma}\mathcal{H}_{2N}\hat{U}^\dagger_{N\sigma}, \hat{n}_{N\sigma}\right] = 0$.*

1.2 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 $N\sigma$:

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

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

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

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 $N\sigma$

$$Tr_{N\sigma}(\mathcal{H}_{2N}) \equiv \sum_{|N\sigma\rangle} \langle N\sigma| \mathcal{H}_{2N} |N\sigma\rangle \tag{3}$$

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

$$Tr_{N\sigma}\left(\mathcal{H}_{2N}\hat{n}_{N\sigma}\right) = Tr_{N\sigma}\left[H_1\hat{n}_{N\sigma}\hat{n}_{N\sigma} + c^\dagger_{N\sigma}H_2\hat{n}_{N\sigma} + H_3 c_{N\sigma}\hat{n}_{N\sigma} + H_4(1-\hat{n}_{N\sigma})\hat{n}_{N\sigma}\right] \tag{4}$$

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, $Tr_{N\sigma}(c^\dagger_{N\sigma}H_2\hat{n}_{N\sigma}) = H_2 Tr_{N\sigma}(c^\dagger_{N\sigma}\hat{n}_{N\sigma}) = 0$, 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,

$$Tr_{N\sigma}\left(\mathcal{H}_{2N}\hat{n}_{N\sigma}\right) = Tr_{N\sigma}\left[H_1\hat{n}_{N\sigma}\right] = H_1 Tr_{N\sigma}\hat{n}_{N\sigma} = H_1 \tag{5}$$

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.

$$\begin{aligned}
H_1 &\equiv \hat{H}_{N\sigma,e} = Tr_{N\sigma}\left[\mathcal{H}_{2N}\hat{n}_{N\sigma}\right] \\
H_2 &\equiv \hat{T}_{N\sigma,e-h} = Tr_{N\sigma}\left[\mathcal{H}_{2N}c_{N\sigma}\right] \\
H_3 &\equiv T^\dagger_{N\sigma,e-h} = Tr_{N\sigma}\left[c^\dagger_{N\sigma}\mathcal{H}_{2N}\right] \\
H_4 &\equiv \hat{H}_{N\sigma,h} = Tr_{N\sigma}\left[\mathcal{H}_{2N}(1-\hat{n}_{N\sigma})\right]
\end{aligned} \tag{6}$$

We get the following block decomposition of the Hamiltonian.

$$\mathcal{H}_{2N} = \begin{array}{c c} & \begin{array}{cc} |1\rangle & |0\rangle \end{array} \\ \begin{array}{c} \langle 1| \\ \\ \langle 0| \end{array} & \begin{pmatrix} \hat{H}_{N\sigma,e} & \hat{T}_{N\sigma,e-h} \\ & \\ T^\dagger_{N\sigma,e-h} & \hat{H}_{N\sigma,h} \end{pmatrix} \end{array} = \begin{array}{c c} & \begin{array}{cc} |1\rangle & |0\rangle \end{array} \\ \begin{array}{c} \langle 1| \\ \\ \langle 0| \end{array} & \begin{pmatrix} Tr_{N\sigma}\left[\mathcal{H}_{2N}\hat{n}_{N\sigma}\right] & Tr_{N\sigma}\left[\mathcal{H}_{2N}c_{N\sigma}\right] \\ & \\ Tr_{N\sigma}\left[c^\dagger_{N\sigma}\mathcal{H}_{2N}\right] & Tr_{N\sigma}\left[\mathcal{H}_{2N}(1-\hat{n}_{N\sigma})\right] \end{pmatrix} \end{array} \tag{7}$$

$$\begin{aligned}
\mathcal{H}_{2N} = Tr_{N\sigma}\left[\mathcal{H}_{2N}\hat{n}_{N\sigma}\right]\hat{n}_{N\sigma} + c^\dagger_{N\sigma}Tr_{N\sigma}\left[\mathcal{H}_{2N}c_{N\sigma}\right] + Tr_{N\sigma}\left[c^\dagger_{N\sigma}\mathcal{H}_{2N}\right]c_{N\sigma} \\
+ Tr_{N\sigma}\left[\mathcal{H}_{2N}(1-\hat{n}_{N\sigma})\right](1-\hat{n}_{N\sigma})
\end{aligned} \tag{8}$$

1.3 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.

$$\begin{aligned}
\left[\mathcal{H}_{2N}, \hat{P_{N\sigma}}\right] = \left[\mathcal{H}_{2N}, \hat{U}^\dagger_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma}\right] &= \mathcal{H}_{2N}\hat{U}^\dagger_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma} - \hat{U}^\dagger_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma}\mathcal{H}_{2N} \\
&= \hat{U}^\dagger_{N\sigma}\overline{\mathcal{H}_{2N}}\hat{n}_{N\sigma}\hat{U}_{N\sigma} - \hat{U}^\dagger_{N\sigma}\hat{n}_{N\sigma}\overline{\mathcal{H}_{2N}}\hat{U}_{N\sigma} = \hat{U}^\dagger_{N\sigma}\left[\mathcal{H}_{2N}, \hat{n}_{N\sigma}\right]\hat{U}_{N\sigma} \\
&= 0
\end{aligned} \tag{9}$$

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

$$\overline{\mathcal{H}_{2N}} = \begin{pmatrix} \hat{E_{N\sigma}} & 0 \\ 0 & \hat{E'_{N\sigma}} \end{pmatrix} \tag{10}$$

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

$$\begin{aligned} \overline{\mathcal{H}_{2N}}\,|1\rangle &= \hat{E_{N\sigma}}\,|1\rangle \\ \overline{\mathcal{H}_{2N}}\,|0\rangle &= \hat{E'_{N\sigma}}\,|0\rangle \end{aligned} \tag{11}$$

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

$$\hat{A} = \begin{pmatrix} 1 & -1 \\ 2 & 0 \end{pmatrix} \implies \hat{m}\hat{A}\hat{m} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \times \begin{pmatrix} 1 & -1 \\ 2 & 0 \end{pmatrix} \times \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{12}$$

Similarly,

$$\hat{m}\hat{A}(1-\hat{m}) = \begin{pmatrix} 0 & -1 \\ 0 & 0 \end{pmatrix}, (1-\hat{m})\hat{A}\hat{m} = \begin{pmatrix} 0 & 0 \\ 2 & 0 \end{pmatrix}, (1-\hat{m})\hat{A}(1-\hat{m}) = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \tag{13}$$

We hence have the equation

$$\begin{aligned}
\hat{n}_{N\sigma}\overline{\mathcal{H}_{2N}}\hat{n}_{N\sigma} = \hat{P_{N\sigma}}\mathcal{H}_{2N}\hat{P_{N\sigma}} = \begin{pmatrix} \hat{E_{N\sigma}} & 0 \\ \\ 0 & 0 \end{pmatrix} \\
(1-\hat{n}_{N\sigma})\overline{\mathcal{H}_{2N}}(1-\hat{n}_{N\sigma}) = (1-\hat{P_{N\sigma}})\mathcal{H}_{2N}(1-\hat{P_{N\sigma}}) = \begin{pmatrix} 0 & 0 \\ \\ 0 & \hat{E'_{N\sigma}} \end{pmatrix}
\end{aligned} \tag{14}$$

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

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

$$\mathcal{H}' = \hat{E_{N\sigma}} \otimes \mathbf{I} = \begin{pmatrix} \hat{E_{N\sigma}} & 0 \\ \\ 0 & \hat{E_{N\sigma}} \end{pmatrix} \tag{15}$$

$$\mathcal{H}'' = \hat{E'_{N\sigma}} \otimes \mathbf{I} = \begin{pmatrix} \hat{E'_{N\sigma}} & 0 \\ \\ 0 & \hat{E'_{N\sigma}} \end{pmatrix} \tag{16}$$

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

$$\begin{aligned}
\mathcal{H}_{2N}\hat{P_{N\sigma}} = \mathcal{H}_{2N}\hat{U}^{\dagger}_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma} = \hat{U}^{\dagger}_{N\sigma}\overline{\mathcal{H}_{2N}}\hat{n}_{N\sigma}\hat{U}_{N\sigma} = \hat{U}^{\dagger}_{N\sigma}\begin{pmatrix} \hat{E_{N\sigma}} & 0 \\ \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ \\ 0 & 0 \end{pmatrix}\hat{U}_{N\sigma} \\
= \hat{U}^{\dagger}_{N\sigma}\begin{pmatrix} \hat{E_{N\sigma}} & 0 \\ \\ 0 & \hat{E_{N\sigma}} \end{pmatrix}\begin{pmatrix} 1 & 0 \\ \\ 0 & 0 \end{pmatrix}\hat{U}_{N\sigma} = \hat{U}^{\dagger}_{N\sigma}\hat{E_{N\sigma}}\otimes\mathbb{I}\,\hat{n}_{N\sigma}\hat{U}_{N\sigma} = \hat{E_{N\sigma}}\otimes\mathbb{I}\,\hat{U}^{\dagger}_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma} = \mathcal{H}'\hat{P_{N\sigma}}
\end{aligned} \tag{17}$$

$$\therefore \mathcal{H}_{2N}\hat{P_{N\sigma}} = \mathcal{H}'\hat{P_{N\sigma}} \tag{18}$$

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

$$\therefore \mathcal{H}_{2N}(1-\hat{P_{N\sigma}}) = \mathcal{H}''(1-\hat{P_{N\sigma}}) \tag{19}$$

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

$$\hat{U}_{N\sigma} = \begin{bmatrix} e^{\iota\phi_1}\cos\theta & e^{\iota\phi_2}\sin\theta \\ -e^{-\iota\phi_2}\sin\theta & e^{-\iota\phi_1}\cos\theta \end{bmatrix} \tag{20}$$

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

$$\begin{aligned} \hat{P_{N\sigma}} = \hat{U}^{\dagger}_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma} &= \begin{bmatrix} e^{-\iota\phi_1}\cos\theta & -e^{\iota\phi_2}\sin\theta \\ e^{-\iota\phi_2}\sin\theta & e^{\iota\phi_1}\cos\theta \end{bmatrix} \times \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \times \begin{bmatrix} e^{\iota\phi_1}\cos\theta & e^{\iota\phi_2}\sin\theta \\ -e^{-\iota\phi_2}\sin\theta & e^{-\iota\phi_1}\cos\theta \end{bmatrix} \\ &= \begin{bmatrix} \cos^2\theta & \cos\theta\sin\theta e^{-\iota(\phi_1-\phi_2)} \\ \cos\theta\sin\theta e^{\iota(\phi_1-\phi_2)} & \sin^2\theta \end{bmatrix} \end{aligned} \tag{21}$$

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

$$\hat{P_{N\sigma}} = \frac{1}{2}\begin{bmatrix} 1 & \hat{\eta}^{\dagger}_{01} \\ \hat{\eta}_{01} & 1 \end{bmatrix} = \frac{1}{2}\left(\mathbf{I} + \eta_{N\sigma} + \eta^{\dagger}_{N\sigma}\right) \tag{22}$$

$$\mathbf{I} - \hat{P_{N\sigma}} = \frac{1}{2}\begin{bmatrix} 1 & -\hat{\eta}^{\dagger}_{01} \\ -\hat{\eta}_{01} & 1 \end{bmatrix} = \frac{1}{2}\left(\mathbf{I} - \eta_{N\sigma} - \eta^{\dagger}_{N\sigma}\right) \tag{23}$$

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

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

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

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

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

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

Using 18 and the matrix form of $\hat{P_{N\sigma}}$, $\mathcal{H}_{2N}$ and $\mathcal{H}'$ (22, 7 and 15), we get

$$\begin{pmatrix} \hat{H}_{N\sigma,e} & \hat{T}_{N\sigma,e-h} \\ T^{\dagger}_{N\sigma,e-h} & \hat{H}_{N\sigma,h} \end{pmatrix} \begin{pmatrix} 1 & \hat{\eta}^{\dagger}_{01} \\ \hat{\eta}_{01} & 1 \end{pmatrix} = \hat{E}_{N\sigma}\mathbf{I} \begin{pmatrix} 1 & \hat{\eta}^{\dagger}_{01} \\ \hat{\eta}_{01} & 1 \end{pmatrix}$$
$$\implies \begin{pmatrix} \hat{H}_{N\sigma,e} + \hat{T}_{N\sigma,e-h}\hat{\eta}_{01} & \hat{H}_{N\sigma,e}\hat{\eta}^{\dagger}_{01} + \hat{T}_{N\sigma,e-h} \\ \hat{H}_{N\sigma,h}\hat{\eta}_{01} + T^{\dagger}_{N\sigma,e-h} & \hat{H}_{N\sigma,h} + T^{\dagger}_{N\sigma,e-h}\hat{\eta}^{\dagger}_{01} \end{pmatrix} = \begin{pmatrix} \hat{E}_{N\sigma} & \hat{E}_{N\sigma}\hat{\eta}^{\dagger}_{01} \\ \hat{E}_{N\sigma}\hat{\eta}_{01} & \hat{E}_{N\sigma} \end{pmatrix} \tag{24}$$

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

$$\hat{E}_{N\sigma}\hat{\eta}^{\dagger}_{01} = \hat{H}_{N\sigma,e}\hat{\eta}^{\dagger}_{01} + \hat{T}_{N\sigma,e-h} \implies \hat{\eta}^{\dagger}_{01} = \frac{1}{\hat{E}_{N\sigma} - \hat{H}_{N\sigma,e}}\hat{T}_{N\sigma,e-h} = \hat{G}_e(\hat{E}_{N\sigma})\hat{T}_{N\sigma,e-h}$$
$$\implies \hat{\eta}^{\dagger}_{N\sigma} = c^{\dagger}_{N\sigma}\hat{\eta}^{\dagger}_{01} = c^{\dagger}_{N\sigma}\hat{G}_e(\hat{E}_{N\sigma})\hat{T}_{N\sigma,e-h} \tag{25}$$

$$\hat{E}_{N\sigma}\hat{\eta}_{01} = \hat{H}_{N\sigma,h}\hat{\eta}_{01} + T^{\dagger}_{N\sigma,e-h} \implies \hat{\eta}_{01} = \frac{1}{\hat{E}_{N\sigma} - \hat{H}_{N\sigma,h}}T^{\dagger}_{N\sigma,e-h} = \hat{G}_h(\hat{E}_{N\sigma})T^{\dagger}_{N\sigma,e-h}$$
$$\implies \hat{\eta}_{N\sigma} = \hat{\eta}_{01}c_{N\sigma} = \hat{G}_h(\hat{E}_{N\sigma})T^{\dagger}_{N\sigma,e-h}c_{N\sigma} \tag{26}$$

where

$$\hat{G}_e(\hat{E}_{N\sigma}) \equiv \frac{1}{\hat{E}_{N\sigma} - \hat{H}_{N\sigma,e}}.\ \hat{G}_h(\hat{E}_{N\sigma}) \equiv \frac{1}{\hat{E}_{N\sigma} - \hat{H}_{N\sigma,h}} \tag{27}$$

Comparing the definitions of $\hat{\eta}_{N\sigma}$ and $\hat{\eta}^{\dagger}_{N\sigma}$, 25 and 26, gives us a consistency equation:

$$\hat{G}_h(\hat{E}_{N\sigma})T^{\dagger}_{N\sigma,e-h} = T^{\dagger}_{N\sigma,e-h}\hat{G}_e(\hat{E}_{N\sigma}) \tag{28}$$

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

$$\hat{E}_{N\sigma} = \hat{H}_{N\sigma,e} + \hat{T}_{N\sigma,e-h}\hat{\eta}_{01} \tag{29}$$

$$\hat{E}_{N\sigma} = \hat{H}_{N\sigma,h} + T^{\dagger}_{N\sigma,e-h}\hat{\eta}^{\dagger}_{01} \tag{30}$$

These equations provide the commutator and anticommutator of the $\hat{\eta}_{N\sigma}$ and $\hat{\eta}^{\dagger}_{N\sigma}$. From eq 29,

$$\hat{E}_{N\sigma} - \hat{H}_{N\sigma,e} = \hat{T}_{N\sigma,e-h}\hat{\eta}_{01} \implies \hat{G}_e(\hat{E}_{N\sigma})^{-1} = \hat{T}_{N\sigma,e-h}\hat{\eta}_{01}$$
$$\implies \mathbf{1} = \hat{G}_e(\hat{E}_{N\sigma})\hat{T}_{N\sigma,e-h}\hat{\eta}_{01} = \hat{\eta}^{\dagger}_{01}\hat{\eta}_{01} \tag{31}$$

$$\hat{\eta}^\dagger \hat{\eta} = c^\dagger_{N\sigma} \hat{\eta}^\dagger_{01} \hat{\eta}_{01} c_{N\sigma} = c^\dagger_{N\sigma} c_{N\sigma} = \hat{n}_{N\sigma} \tag{32}$$

From 30,

$$\begin{aligned} \hat{E}_{N\sigma} - \hat{H}_{N\sigma,h} = T^\dagger_{N\sigma,e-h} \hat{\eta}^\dagger_{01} &\implies \hat{G}_h(\hat{E}_{N\sigma})^{-1} = T^\dagger_{N\sigma,e-h} \hat{\eta}^\dagger_{01} \\ &\implies \mathbf{1} = \hat{G}_h(\hat{E}_{N\sigma}) T^\dagger_{N\sigma,e-h} \hat{\eta}^\dagger_{01} = \hat{\eta}_{01} \hat{\eta}^\dagger_{01} \end{aligned} \tag{33}$$

$$\hat{\eta} \hat{\eta}^\dagger = c_{N\sigma} \hat{\eta}_{01} \hat{\eta}^\dagger_{01} c^\dagger_{N\sigma} = c_{N\sigma} c^\dagger_{N\sigma} = 1 - \hat{n}_{N\sigma} \tag{34}$$

Combining equations 32 and 34,

$$\begin{aligned} \left[\hat{\eta}, \hat{\eta}^\dagger\right] &= 1 - 2\hat{n}_{N\sigma} \\ \left\{\hat{\eta}, \hat{\eta}^\dagger\right\} &= 1 \end{aligned} \tag{35}$$

Equation 29 provides an expression for the upper block of the diagonalised Hamiltonian,

$$\boxed{\hat{E}_{N\sigma} = \hat{H}_{N\sigma,e} + \hat{T}_{N\sigma,e-h} \hat{\eta}_{01}} \tag{36}$$

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

The lower block can be constructed similarly, starting from 19. We again write the matrices in the basis of $\hat{n}_{N\sigma}$ (using 7, 23, 16) and compare the matrix elements.

$$\begin{aligned} &\begin{pmatrix} \hat{H}_{N\sigma,e} & \hat{T}_{N\sigma,e-h} \\ T^\dagger_{N\sigma,e-h} & \hat{H}_{N\sigma,h} \end{pmatrix} \begin{pmatrix} 1 & -\hat{\eta}^\dagger_{01} \\ -\hat{\eta}_{01} & 1 \end{pmatrix} = \hat{E}'_{N\sigma} \mathbf{I} \begin{pmatrix} 1 & -\hat{\eta}^\dagger_{01} \\ -\hat{\eta}_{01} & 1 \end{pmatrix} \\ \implies &\begin{pmatrix} \hat{H}_{N\sigma,e} - \hat{T}_{N\sigma,e-h} \hat{\eta}_{01} & -\hat{H}_{N\sigma,e} \hat{\eta}^\dagger_{01} + \hat{T}_{N\sigma,e-h} \\ -\hat{H}_{N\sigma,h} \hat{\eta}_{01} + T^\dagger_{N\sigma,e-h} & \hat{H}_{N\sigma,h} - T^\dagger_{N\sigma,e-h} \hat{\eta}^\dagger_{01} \end{pmatrix} = \begin{pmatrix} \hat{E}'_{N\sigma} & -\hat{E}'_{N\sigma} \hat{\eta}^\dagger_{01} \\ -\hat{E}'_{N\sigma} \hat{\eta}_{01} & \hat{E}'_{N\sigma} \end{pmatrix} \end{aligned} \tag{37}$$

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

$$\hat{E}'_{N\sigma} \hat{\eta}^\dagger_{01} = \hat{H}_{N\sigma,e} \hat{\eta}^\dagger_{01} - \hat{T}_{N\sigma,e-h} \implies \hat{\eta}^\dagger_{01} = \frac{-1}{\hat{E}'_{N\sigma} - \hat{H}_{N\sigma,e}} \hat{T}_{N\sigma,e-h} = -\hat{G}_e\left(\hat{E}'_{N\sigma}\right) \hat{T}_{N\sigma,e-h} \tag{38}$$

$$\hat{E}'_{N\sigma} \hat{\eta}_{01} = \hat{H}_{N\sigma,h} \hat{\eta}_{01} - T^\dagger_{N\sigma,e-h} \implies \hat{\eta}_{01} = \frac{-1}{\hat{E}'_{N\sigma} - \hat{H}_{N\sigma,h}} T^\dagger_{N\sigma,e-h} = -\hat{G}_h\left(\hat{E}'_{N\sigma}\right) T^\dagger_{N\sigma,e-h} \tag{39}$$

Comparing equation 38 to equation 25 and equation 39 to equation 26, we get the following consistency equations:

$$
\begin{aligned}
-\hat{G}_e\left(\hat{E}'_{N\sigma}\right)\hat{T}_{N\sigma,e-h} &= \hat{G}_e\left(\hat{E}_{N\sigma}\right)\hat{T}_{N\sigma,e-h} \\
-\hat{G}_h\left(\hat{E}'_{N\sigma}\right)T^\dagger_{N\sigma,e-h} &= \hat{G}_h\left(\hat{E}_{N\sigma}\right)T^\dagger_{N\sigma,e-h}
\end{aligned}
\tag{40}
$$

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

$$
\boxed{\hat{E}'_{N\sigma} = \hat{H}_{N\sigma,e} - \hat{T}_{N\sigma,e-h}\hat{\eta}_{01}} \tag{41}
$$

Looking at equations 36 and 41, we can write down the diagonalised Hamiltonian in the basis of $\hat{n}_{N\sigma}$:

$$
\begin{aligned}
\overline{\mathcal{H}_{2N}} = \hat{U}_{N\sigma}\mathcal{H}_{2N}\hat{U}^\dagger_{N\sigma} &= \begin{pmatrix} \hat{E_{N\sigma}} & 0 \\ 0 & \hat{E'_{N\sigma}} \end{pmatrix} \\
&= \begin{pmatrix} \hat{H}_{N\sigma,e} + \hat{T}_{N\sigma,e-h}\hat{\eta}_{01} & 0 \\ 0 & \hat{H}_{N\sigma,e} - \hat{T}_{N\sigma,e-h}\hat{\eta}_{01} \end{pmatrix}
\end{aligned}
\tag{42}
$$

This concludes the construction of the diagonalised Hamiltonian.

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

The starting equation for the above construction was equation 18. That will also provide an expression for the $\hat{U}_{N\sigma}$. Operating equation 18 to the right of $|1\rangle$ (occupied eigenstate of $\hat{n}_{N\sigma}$) gives

$$
\begin{aligned}
&\mathcal{H}_{2N}\hat{P}_{N\sigma}|1\rangle = \hat{E}_{N\sigma}\otimes\mathbf{I}\;\hat{P}_{N\sigma}\mathcal{H}_{2N}|1\rangle = \hat{E}_{N\sigma}\hat{P}_{N\sigma}|1\rangle \\
&\implies \mathcal{H}_{2N}\hat{U}^\dagger_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma}|1\rangle = \hat{E}_{N\sigma}\hat{U}^\dagger_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma}|1\rangle \qquad \left(\text{substituting expression of } \hat{P}_{N\sigma}\right) \\
&\implies \hat{U}_{N\sigma}\mathcal{H}_{2N}\hat{U}^\dagger_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma}|1\rangle = \hat{U}_{N\sigma}\hat{E}_{N\sigma}\hat{U}^\dagger_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma}|1\rangle \quad \left(\text{operating } \hat{U}_{N\sigma} \text{ from left}\right) \\
&\implies \overline{\mathcal{H}_{2N}}\hat{n}_{N\sigma}\hat{U}_{N\sigma}|1\rangle = \hat{U}_{N\sigma}\hat{E}_{N\sigma}\hat{U}^\dagger_{N\sigma}\hat{n}_{N\sigma}\hat{U}_{N\sigma}|1\rangle
\end{aligned}
\tag{43}
$$

Compare the last equation with 11. In order to satisfy the first equation of 11, we need the following two equations,

$$
\begin{aligned}
\hat{n}_{N\sigma}\hat{U}_{N\sigma}|1\rangle &\propto |1\rangle \\
\hat{U}_{N\sigma}\hat{E}_{N\sigma}\hat{U}^\dagger_{N\sigma} &= E_{N\sigma}
\end{aligned}
\tag{44}
$$

The second equations says

$$
\left[E_{N\sigma}, \hat{U}_{N\sigma}\right] = 0 \tag{45}
$$

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 44,

$$\begin{aligned}\hat{n}_{N\sigma}\hat{U}_{N\sigma}\left|1\right\rangle &= \begin{pmatrix}\mathbf{I} & 0\\ 0 & 0\end{pmatrix}\kappa\begin{pmatrix}\mathbf{I} & \eta^\dagger_{01}\\ -\eta_{01} & \mathbf{I}\end{pmatrix}\begin{pmatrix}\mathbf{I}\\ 0\end{pmatrix}\\ &= \kappa\begin{pmatrix}\mathbf{I}\\ 0\end{pmatrix} \propto \left|1\right\rangle\end{aligned} \tag{46}$$

To find κ,

$$\begin{aligned}\hat{U}_{N\sigma}\hat{U}^\dagger_{N\sigma} = \kappa^2\begin{pmatrix}\mathbf{I} & \eta^\dagger_{01}\\ -\eta_{01} & \mathbf{I}\end{pmatrix}\begin{pmatrix}\mathbf{I} & -\eta^\dagger_{01}\\ \eta_{01} & \mathbf{I}\end{pmatrix} &= \kappa^2\begin{pmatrix}\mathbf{I}+\eta^\dagger_{01}\eta_{01} & 0\\ 0 & \mathbf{I}+\eta^\dagger_{01}\eta_{01}\end{pmatrix}\\ = \kappa^2\begin{pmatrix}\mathbf{I}+\eta^\dagger_{01}\eta_{01} & 0\\ 0 & \mathbf{I}+\eta^\dagger_{01}\eta_{01}\end{pmatrix} &= 2\kappa^2\begin{pmatrix}\mathbf{I} & 0\\ 0 & \mathbf{I}\end{pmatrix}\left(\text{check 31,33 for } \eta^\dagger_{01}\eta_{01},\eta_{01}\eta^\dagger_{01}\right)\\ \implies \kappa = \frac{1}{\sqrt{2}}\end{aligned} \tag{47}$$

$$\boxed{\hat{U}_{N\sigma} = \frac{1}{\sqrt{2}}\left(1 - \hat{\eta} + \hat{\eta}^\dagger\right)} \tag{48}$$

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

First note,

$$\hat{T}^\dagger_{N\sigma,e-h}\left[\hat{E}_{N\sigma}, \hat{G}_e(\hat{E}_{N\sigma})\right] = T^\dagger_{N\sigma,e-h}\hat{E}_{N\sigma}\hat{G}_e(\hat{E}_{N\sigma}) - T^\dagger_{N\sigma,e-h}\hat{G}_e(\hat{E}_{N\sigma})\hat{E}_{N\sigma} \tag{49}$$

Now,

$$T^\dagger_{N\sigma,e-h}\hat{G}_e(\hat{E}_{N\sigma})\hat{E}_{N\sigma} = \hat{\eta}_{01}\hat{E}_{N\sigma} \tag{50}$$

Also,

$$\begin{aligned}T^\dagger_{N\sigma,e-h}\hat{E}_{N\sigma}\hat{G}_e(\hat{E}_{N\sigma}) &= T^\dagger_{N\sigma,e-h}\left[\hat{H}_{N\sigma,e} + \hat{T}_{N\sigma,e-h}\hat{\eta}_{01}\right]\hat{G}_e(\hat{E}_{N\sigma})\\ &= T^\dagger_{N\sigma,e-h}\left[\hat{H}_{N\sigma,e}\hat{G}_e(\hat{E}_{N\sigma}) + \hat{T}_{N\sigma,e-h}\hat{G}_h(\hat{E}_{N\sigma})\hat{T}^\dagger_{N\sigma,e-h}\hat{G}_e(\hat{E}_{N\sigma})\right]\\ &= T^\dagger_{N\sigma,e-h}\hat{H}_{N\sigma,e}\hat{G}_e(\hat{E}_{N\sigma}) + T^\dagger_{N\sigma,e-h}\end{aligned} \tag{51}$$

The last line follows because $\hat{T}_{N\sigma,e-h}\hat{G}_h(\hat{E}_{N\sigma})\hat{T}^\dagger_{N\sigma,e-h}\hat{G}_e(\hat{E}_{N\sigma}) = \mathbf{1}$. From 29, we have

$$\begin{aligned}\hat{E}_{N\sigma} - \hat{H}_{N\sigma,e} = \hat{T}_{N\sigma,e-h}\hat{\eta}_{01} &\implies \hat{G}_e^{-1}(\hat{E}_{N\sigma}) = \hat{T}_{N\sigma,e-h}\hat{G}_h(\hat{E}_{N\sigma})\hat{T}^\dagger_{N\sigma,e-h} \\ &\implies \mathbf{1} = \hat{T}_{N\sigma,e-h}\hat{G}_h(\hat{E}_{N\sigma})\hat{T}^\dagger_{N\sigma,e-h}\hat{G}_e(\hat{E}_{N\sigma})\end{aligned} \tag{52}$$

Continuing from 51,

$$\begin{aligned}T^\dagger_{N\sigma,e-h}\hat{E}_{N\sigma}\hat{G}_e(\hat{E}_{N\sigma}) &= T^\dagger_{N\sigma,e-h}\hat{H}_{N\sigma,e}\hat{G}_e(\hat{E}_{N\sigma}) + T^\dagger_{N\sigma,e-h} \\ &= \hat{H}_{N\sigma,h}T^\dagger_{N\sigma,e-h}\hat{G}_e(\hat{E}_{N\sigma}) + T^\dagger_{N\sigma,e-h}\end{aligned} \tag{53}$$

The last line follows from equation 28:

$$\begin{aligned}&\hat{T}^\dagger_{N\sigma,e-h}\hat{G}_e(\hat{E}_{N\sigma}) = \hat{G}_h(\hat{E}_{N\sigma})\hat{T}^\dagger_{N\sigma,e-h} \\ &\implies (\hat{E}_{N\sigma} - \hat{H}_{N\sigma,h})\hat{T}^\dagger_{N\sigma,e-h} = \hat{T}^\dagger_{N\sigma,e-h}(\hat{E}_{N\sigma} - \hat{H}_{N\sigma,e}) \\ &\implies \hat{E}_{N\sigma}\hat{T}^\dagger_{N\sigma,e-h} - \hat{H}_{N\sigma,h}\hat{T}^\dagger_{N\sigma,e-h} = \hat{T}^\dagger_{N\sigma,e-h}\hat{E}_{N\sigma} - \hat{T}^\dagger_{N\sigma,e-h}\hat{H}_{N\sigma,e} \\ &\implies \hat{H}_{N\sigma,h}\hat{T}^\dagger_{N\sigma,e-h} = \hat{T}^\dagger_{N\sigma,e-h}\hat{H}_{N\sigma,e} \qquad \left(\because \hat{E}_{N\sigma}\hat{T}^\dagger_{N\sigma,e-h} = \hat{T}^\dagger_{N\sigma,e-h}\hat{E}_{N\sigma}\right)\end{aligned} \tag{54}$$

Again continuing from 53,

$$\begin{aligned}&T^\dagger_{N\sigma,e-h}\hat{E}_{N\sigma}\hat{G}_e(\hat{E}_{N\sigma}) = \hat{H}_{N\sigma,h}T^\dagger_{N\sigma,e-h}\hat{G}_e(\hat{E}_{N\sigma}) + T^\dagger_{N\sigma,e-h} \\ &= \hat{H}_{N\sigma,h}\hat{G}_h(\hat{E}_{N\sigma})T^\dagger_{N\sigma,e-h} + T^\dagger_{N\sigma,e-h} && \text{(from eq 28)} \\ &= \hat{H}_{N\sigma,h}\hat{G}_h(\hat{E}_{N\sigma})T^\dagger_{N\sigma,e-h} + T^\dagger_{N\sigma,e-h}G_e(\hat{E}_{N\sigma})T_{N\sigma,e-h}G_h(\hat{E}_{N\sigma})T^\dagger_{N\sigma,e-h} && \text{(from eq 52)} \\ &= \left(\hat{H}_{N\sigma,h} + T^\dagger_{N\sigma,e-h}G_e(\hat{E}_{N\sigma})T_{N\sigma,e-h}\right)\hat{G}_h(\hat{E}_{N\sigma})T^\dagger_{N\sigma,e-h} \\ &= \left(\hat{H}_{N\sigma,h} + T^\dagger_{N\sigma,e-h}\hat{\eta}^\dagger_{01}\right)\hat{G}_h(\hat{E}_{N\sigma})T^\dagger_{N\sigma,e-h} \\ &= \hat{E}_{N\sigma}\hat{G}_h(\hat{E}_{N\sigma})T^\dagger_{N\sigma,e-h} \\ &= \hat{E}_{N\sigma}\hat{\eta}_{01}\end{aligned} \tag{55}$$

Therefore,

$$T^\dagger_{N\sigma,e-h}\hat{E}_{N\sigma}\hat{G}_e(\hat{E}_{N\sigma}) = \hat{E}_{N\sigma}\hat{\eta}_{01} \tag{56}$$

Substituting equations 50 and 56 in equation 49, we have

$$\begin{aligned}\hat{T}^\dagger_{N\sigma,e-h}\left[\hat{E}_{N\sigma}, \hat{G}_e(\hat{E}_{N\sigma})\right] &= \hat{E}_{N\sigma}\hat{\eta}_{01} - \hat{\eta}_{01}\hat{E}_{N\sigma} = \left[\hat{E}_{N\sigma}, \hat{\eta}_{01}\right] \\ &= 0 && \text{(from equation 45)}\end{aligned} \tag{57}$$

Therefore,

$$\boxed{\left[\hat{E}_{N\sigma}, \hat{G}_e(\hat{E}_{N\sigma})\right] = 0} \tag{58}$$

2 A Simple Example

$$\mathcal{H} = -t\left(c_2^\dagger c_1 + c_1^\dagger c_2\right) + V\hat{n}_1\hat{n}_2 - \mu(\hat{n}_1 + \hat{n}_2) \quad \hat{n}_i = c_i^\dagger c_i \tag{59}$$

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 7).

$$\begin{aligned}
\hat{H}_{1,e} &= Tr_1[\mathcal{H}\hat{n}_1] \\
&= Tr_1[V\hat{n}_1\hat{n}_2 - \mu(\hat{n}_1 + \hat{n}_2)] \quad && \left(c \text{ and } c^\dagger \text{ will not conserve the eigenvalue of } \hat{n}\right) \\
&= V\hat{n}_2 - \mu(1 + \hat{n}_2) && (Tr_1[V\hat{n}_1\hat{n}_2] = VTr_1[\hat{n}_1]\hat{n}_2 = V\hat{n}_2)
\end{aligned} \tag{60}$$

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

$$\hat{H}_{1,h} = Tr_1[\mathcal{H}(1 - \hat{n}_1)] = -\mu\hat{n}_2 \tag{61}$$

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

$$\begin{aligned}
T_{1,e-h} &= Tr_1[\mathcal{H}c_1] \\
&= Tr_1[-tc_1^\dagger c_2 c_1] = -tc_2 \quad \text{(the only term that conserves eigenvalue of } \hat{n}\text{)}
\end{aligned} \tag{62}$$

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

$$\mathcal{H} = \begin{pmatrix} V\hat{n}_2 - \mu(1 + \hat{n}_2) & -tc_2 \\ \\ -tc_2^\dagger & -\mu\hat{n}_2 \end{pmatrix} \tag{63}$$

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

From equations 25 and 26, $\hat{\eta}_{01}^\dagger = \hat{G}_e\hat{T}_{1,e-h}$ and $\hat{\eta}_{01} = \hat{G}_h\hat{T}_{1,e-h}^\dagger$. Equation 31 gives

$$\hat{\eta}_{01}^\dagger\hat{\eta}_{01} = 1 \implies \hat{G}_e\hat{T}_{1,e-h}\hat{G}_h\hat{T}_{1,e-h}^\dagger = 1 \tag{64}$$

Again, from equation 28, $\hat{G}_h\hat{T}_{1,e-h}^\dagger = \hat{T}_{1,e-h}^\dagger\hat{G}_e$. With this modification, equation 64 becomes

$$\hat{G}_e\hat{T}_{1,e-h}\hat{T}_{1,e-h}^\dagger\hat{G}_e = 1 \implies \hat{T}_{1,e-h}\hat{T}_{1,e-h}^\dagger = \left(\hat{G}_e^{-1}\right)^2 \tag{65}$$

For this problem,

$$\begin{aligned}
&\hat{T}_{1,e-h}\hat{T}_{1,e-h}^\dagger = t^2 c_2 c_2^\dagger = t^2(1 - \hat{n}_2) = t^2(1 - \hat{n}_2)^2 \\
&\left(\hat{G}_e^{-1}\right)^2 = \left(\hat{E}_1 - \hat{H}_{1,e}\right)^2 = \left(\hat{E}_1 - V\hat{n}_2 + \mu(1 + \hat{n}_2)\right)^2
\end{aligned} \tag{66}$$

Substituting these expressions in equation 65,

$$t^2\left(1 - \hat{n}_2\right)^2 = \left(\hat{E}_1 - V\hat{n}_2 + \mu(1 + \hat{n}_2)\right)^2 \tag{67}$$

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

$$\boxed{\hat{E}_1 = V\hat{n}_2 - \mu(1+\hat{n}_2) + t\,(1-\hat{n}_2) = (V-2\mu)\hat{n}_2 + (t-\mu)(1-\hat{n}_2) \qquad (68)}$$

The lower diagonal block can be determined using the lower diagonal equation of 37:

$$\begin{aligned}
\hat{E}_1' = \hat{H}_{1,h} - \hat{T}^\dagger_{1,e-h}\hat{G}_e\hat{T}_{1,e-h} &= -\mu\hat{n}_2 - t^2 c_2^\dagger \frac{1}{\hat{E}_1 - V\hat{n}_2 + \mu(1+\hat{n}_2)} c_2 \\
&= -\mu\hat{n}_2 - t^2 c_2^\dagger \frac{1}{t(1-\hat{n}_2)} c_2 \qquad \text{(see equation 67)}
\end{aligned} \tag{69}$$

This simplifies when you realise that

$$\begin{aligned}
&(1-\hat{n}_2)c_2\,|\hat{n}_2\rangle = (1-\hat{n}_2)n_2\,|1-n_2\rangle = n_2^2\,|1-n_2\rangle = n_2\,|1-n_2\rangle = c_2\,|1-n_2\rangle \\
&\therefore (1-\hat{n}_2)c_2 = c_2 \implies c_2 = \frac{1}{(1-\hat{n}_2)} c_2
\end{aligned} \tag{70}$$

Substituting this in the expression for $\hat{E}_1'$ gives

$$\boxed{\hat{E}_1' = -\mu\hat{n}_2 - t c_2^\dagger c_2 = -\mu\hat{n}_2 - t\hat{n}_2 = -(\mu+t)\hat{n}_2 \qquad (71)}$$

This gives

$$\begin{aligned}
\overline{\mathcal{H}} &= \begin{array}{c} \begin{array}{cc} |\hat{n}_1 = 1\rangle & |\hat{n}_1 = 0\rangle \end{array} \\ \begin{pmatrix} (V-2\mu)\hat{n}_2 + (t-\mu)(1-\hat{n}_2) & 0 \\ 0 & -(\mu+t)\hat{n}_2 \end{pmatrix} \end{array} \\
&= \begin{array}{c} \begin{array}{cccc} |11\rangle & |10\rangle & |01\rangle & |00\rangle \end{array} \\ \begin{pmatrix} (V-2\mu) & 0 & 0 & 0 \\ 0 & (t-\mu) & 0 & 0 \\ 0 & 0 & -(\mu+t)\hat{n}_2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \end{array}
\end{aligned} \tag{72}$$