Unitary Renormalization Group Approach to Single-Impurity Anderson Model

Abhirup Mukherjee

Supervisor: Dr. Siddhartha Lal

Department of Physics, IISER Kolkata

February 3, 2021

Contents

1 Unitary Renormalization Group Method

1.1 Formalism

This section is adapted from ref.[1]. We are given a Hamiltonian $\mathcal{H}$ which is not completely diagonal in the occupation number basis of the electrons, $\hat{n}_k$: $[\mathcal{H}, n_k] \neq 0$. k labels any set of quantum numbers depending on the system. For spin-less Fermions it can be the momentum of the particle, while for spin-full Fermions it can be the set of momentum and spin. There are terms that scatter electrons from one quantum number k to another quantum number k'.

We take a general Hamiltonian,

$$\mathcal{H} = H_e \hat{n}_{q\beta} + H_h \left(1 - \hat{n}_{q\beta}\right) + c^\dagger_{q\beta} T + T^\dagger c_{q\beta} \tag{1.1}$$

Formally, we can decompose the entire Hamiltonian in the subspace of the electron we want to decouple $(q\beta)$.

$$\mathcal{H} = \begin{array}{c} \begin{array}{cc} |1\rangle & |0\rangle \end{array} \\ \begin{pmatrix} H_1 & T \\ T^\dagger & H_0 \end{pmatrix} \end{array} \tag{1.2}$$

The basis in which this matrix is written is $\{|1\rangle, |0\rangle\}$ where $|i\rangle$ is the set of all states where $\hat{n}_{q\beta} = i$. The aim of one step of the URG is to find a unitary operator U such that the new Hamiltonian $U\mathcal{H}U^\dagger$ is diagonal in this already-chosen basis.

$$\tilde{\mathcal{H}} \equiv U\mathcal{H}U^\dagger = \begin{array}{c} \begin{array}{cc} |1\rangle & |0\rangle \end{array} \\ \begin{pmatrix} \tilde{H}_1 & 0 \\ 0 & \tilde{H}_0 \end{pmatrix} \end{array} \tag{1.3}$$

U_q is defined by

$$\tilde{\mathcal{H}} = U_q \mathcal{H} U_q^\dagger \text{ such that } \left[\tilde{\mathcal{H}}, n_q\right] = 0 \tag{1.4}$$

It is clear that U is the diagonalizing matrix for $\mathcal{H}$. Hence we can frame this problem as an eigenvalue equation as well. Let $|\psi_1\rangle, |\psi_0\rangle$ be the basis in which the original Hamiltonian $\mathcal{H}$ has no off-diagonal terms corresponding to $q\beta$. Hence, we can write

$$\mathcal{H}\left|\psi_i\right\rangle = \tilde{H}_i \left|\psi_i\right\rangle, i \in \{0, 1\} \tag{1.5}$$

Since $|\psi_i\rangle$ is the set of eigenstates of $\mathcal{H}$ and $|i\rangle$ is the set of eigenstates in which $U\mathcal{H}U^\dagger$, we can relate $|\psi_i\rangle$ and $|i\rangle$ by the same transformation : $|\psi_i\rangle = U^\dagger |i\rangle$. We can expand the state $|\psi_i\rangle$ in the subspace of $q\beta$:

$$\left|\psi_i\right\rangle = \sum_{j=0,1} |j\rangle \langle j| \left|\psi_i\right\rangle \equiv |1\rangle \left|\phi^i_1\right\rangle + |0\rangle \left|\phi^i_0\right\rangle \tag{1.6}$$

where $|\phi^i_j\rangle = \langle j| \, |\psi_i\rangle$. If we substitute the expansions 1.6 and 1.2 into the eigenvalue equation 1.5, we get

$$\left[H_e \hat{n}_{q\beta} + H_h \left(1 - \hat{n}_{q\beta}\right) + c^\dagger_{q\beta} T + T^\dagger c_{q\beta}\right] \left[|1\rangle \left|\phi^i_1\right\rangle + |0\rangle \left|\phi^i_0\right\rangle\right] = \tilde{H}_i \left[|1\rangle \left|\phi^i_1\right\rangle + |0\rangle \left|\phi^i_0\right\rangle\right] \tag{1.7}$$

Gathering the terms that result in $\hat{n}_{q\beta} = 1$ gives

$$H_e \left|1\right\rangle \left|\phi_1^i\right\rangle + c^\dagger_{q\beta} T \left|0\right\rangle \left|\phi_0^i\right\rangle = \tilde{H}_i \left|1\right\rangle \left|\phi_1^i\right\rangle \implies \left(\tilde{H}_i - H_e\right) \left|1\right\rangle \left|\phi_1^i\right\rangle = c^\dagger_{q\beta} T \left|0\right\rangle \left|\phi_0^i\right\rangle \tag{1.8}$$

Similarly, gathering the terms that result in $\hat{n}_{q\beta} = 0$ gives

$$H_h \left|0\right\rangle \left|\phi_0^i\right\rangle + T^\dagger c_{q\beta} \left|1\right\rangle \left|\phi_1^i\right\rangle = \tilde{H}_i \left|0\right\rangle \left|\phi_0^i\right\rangle \implies \left(\tilde{H}_i - H_h\right) \left|0\right\rangle \left|\phi_0^i\right\rangle = T^\dagger c_{q\beta} \left|1\right\rangle \left|\phi_1^i\right\rangle \tag{1.9}$$

The diagonal parts $H_e = \text{tr}\left[\mathcal{H}\hat{n}_{q\beta}\right]$ and $H_e = \text{tr}\left[\mathcal{H}\left(1 - \hat{n}_{q\beta}\right)\right]$ can be separated into a purely diagonal part $\mathcal{H}^d$ that contains the single-particle energies and the multi-particle correlation energies or Hartree-like contributions, and an off-diagonal part $\mathcal{H}^i$ that scatters between the remaining degrees of freedom $k\sigma \neq q\beta$. That is,

$$\begin{gathered} H_e\hat{n}_{q\beta} + H_h\left(1 - \hat{n}_{q\beta}\right) = \mathcal{H}^d + \mathcal{H}^i \\ H_e = \text{tr}\left[\mathcal{H}\hat{n}_{q\beta}\right] = \text{tr}\left[\left(\mathcal{H}^d + \mathcal{H}^i\right)\hat{n}_{q\beta}\right] = \mathcal{H}^d_e + \mathcal{H}^i_e \\ H_h = \text{tr}\left[\mathcal{H}\left(1 - \hat{n}_{q\beta}\right)\right] = \text{tr}\left[\left(\mathcal{H}^d + \mathcal{H}^i\right)\left(1 - \hat{n}_{q\beta}\right)\right] = \mathcal{H}^d_h + \mathcal{H}^i_h \end{gathered}$$

Using this separation, we can write eqs. 1.8 and 1.9 as

$$\begin{gathered} \left(\left(\tilde{H}_i - \mathcal{H}^i_e\right) - \mathcal{H}^d_e\right) \left|1\right\rangle \left|\phi_1^i\right\rangle = c^\dagger_{q\beta} T \left|0\right\rangle \left|\phi_0^i\right\rangle \\ \left(\left(\tilde{H}_i - \mathcal{H}^i_h\right) - \mathcal{H}^d_h\right) \left|0\right\rangle \left|\phi_0^i\right\rangle = T^\dagger c_{q\beta} \left|1\right\rangle \left|\phi_1^i\right\rangle \end{gathered} \tag{1.10}$$

We now define a new operator $\hat{\omega}_i = \tilde{H}_i - \mathcal{H}^i$, such that

$$\begin{gathered} \tilde{H}_i - \mathcal{H}^i_e = \text{tr}\left[\left(\tilde{H}_i - \mathcal{H}^i\right)\hat{n}_{q\beta}\right] = \text{tr}\left[\hat{\omega}\hat{n}_{q\beta}\right] \equiv \hat{\omega}_e \\ \tilde{H}_i - \mathcal{H}^i_h = \hat{\omega}_h \end{gathered}$$

We can now write eq. 1.10 in terms of $\hat{\omega}$:

$$\begin{gathered} \left(\hat{\omega}_e - \mathcal{H}^d_e\right) \left|1\right\rangle \left|\phi_1^i\right\rangle = c^\dagger_{q\beta} T \left|0\right\rangle \left|\phi_0^i\right\rangle \\ \left(\hat{\omega}_h - \mathcal{H}^d_h\right) \left|0\right\rangle \left|\phi_0^i\right\rangle = T^\dagger c_{q\beta} \left|1\right\rangle \left|\phi_1^i\right\rangle \end{gathered} \tag{1.11}$$

We now choose the $\left|\phi_j^i\right\rangle$ such that they are eigenstates of $\hat{\omega}_{e,h}$:

$$\begin{gathered} \hat{\omega}_e \left|\phi_1^i\right\rangle = \omega_e \left|\phi_1^i\right\rangle \\ \hat{\omega}_h \left|\phi_0^i\right\rangle = \omega_h \left|\phi_0^i\right\rangle \end{gathered}$$

where $\omega_{e,h}$ are numbers, not operators. The states $\left|\phi_j^i\right\rangle$ are therefore characterized by eigenvalues $\omega_{e,h}$. Eqs. 1.11 simplify to

$$\begin{gathered} \left|1\right\rangle \left|\phi_1^i(\omega_e)\right\rangle = \frac{1}{\omega_e - \mathcal{H}^d_e} c^\dagger_{q\beta} T \left|0\right\rangle \left|\phi_0^i(\omega_h)\right\rangle \\ \left|0\right\rangle \left|\phi_0^i(\omega_h)\right\rangle = \frac{1}{\omega_h - \mathcal{H}^d_h} T^\dagger c_{q\beta} \left|1\right\rangle \left|\phi_1^i(\omega_e)\right\rangle \end{gathered} \tag{1.12}$$

We now define two many-particle transition operators:

$$\begin{gathered} {\eta_e}^\dagger(\omega_e) = \frac{1}{\omega_e - \mathcal{H}^d_e} c^\dagger_{q\beta} T \\ \eta_h(\omega_h) = \frac{1}{\omega_h - \mathcal{H}^d_h} T^\dagger c_{q\beta} \end{gathered} \tag{1.13}$$

In terms of these operators, eqs. 1.12 become

$$\begin{aligned} |1\rangle\,|\phi_1^i\rangle &= {\eta_e}^\dagger\,|0\rangle\,|\phi_0^i\rangle \\ |0\rangle\,|\phi_0^i\rangle &= \eta_h\,|1\rangle\,|\phi_1^i\rangle \end{aligned} \tag{1.14}$$

These allow us to write

$$\begin{aligned} |\psi_1\rangle &= |1\rangle\,|\phi_1^i\rangle + |0\rangle\,|\phi_0^i\rangle = (1+\eta_h)\,|1\rangle\,|\phi_1^i\rangle \\ |\psi_0\rangle &= \left(1+{\eta_e}^\dagger\right)|0\rangle\,|\phi_0^i\rangle \end{aligned} \tag{1.15}$$

Recalling that $|\psi_i\rangle = U^\dagger\,|i\rangle$, we can read off the required transformations:

$$\begin{aligned} U_1 &= 1+\eta_h \\ U_0 &= 1+\eta_e^\dagger \end{aligned} \tag{1.16}$$

The operators η have some important properties. First is the Fermionic nature:

$$\eta_h^2 = {\eta_e^\dagger}^2 = 0 \quad \left[{c^\dagger}^2 = c^2 = 0\right] \tag{1.17}$$

Second is:

$$\begin{aligned} |1\rangle\,|\phi_1^i\rangle = {\eta_e}^\dagger\,|0\rangle\,|\phi_0^i\rangle = \eta_e^\dagger\eta_h\,|1\rangle\,|\phi_1^i\rangle &\implies \eta_e^\dagger\eta_h = \hat{n}_{q\beta} \\ |0\rangle\,|\phi_0^i\rangle = \eta_h\,|1\rangle\,|\phi_1^i\rangle = \eta_h\eta_e^\dagger\,|\phi_0^i\rangle &\implies \eta_h\eta_e^\dagger = 1-\hat{n}_{q\beta} \\ \implies \left\{\eta_h, \eta_e^\dagger\right\} = 1 & \end{aligned} \tag{1.18}$$

Note that the three equations in 1.18 work only when applied on the eigenstate $|\psi_i\rangle$ and not any arbitrary state.

$$\begin{aligned} \eta_e^\dagger\eta_h\,|\psi_i\rangle &= |1\rangle\,|\phi_1^i\rangle = \hat{n}_{q\beta}\,|\psi_i\rangle \\ \eta_h\eta_e^\dagger\,|\psi_i\rangle &= |0\rangle\,|\phi_0^i\rangle = (1-\hat{n}_{q\beta})\,|\psi_i\rangle \\ \left\{\eta_e^\dagger, \eta_h\right\}|\psi_i\rangle &= |\psi_i\rangle \end{aligned}$$

Although we have found the correct similarity transformations U_i (eqs. 1.16), we need to convert them into a unitary transformation. Say we are trying to rotate the eigenstate $|\psi_1\rangle$ into the state $|1\rangle$. We can then work with the transformation

$$U_1 = 1+\eta_h \tag{1.19}$$

In this form, this transformation is not unitary. It can however be written in an exponential form:

$$U_1 = e^{\eta_h} \tag{1.20}$$

using the fact that $\eta_h^2 = 0$. It is shown in ref. [2] that corresponding to a similarity transformation e^ω,there exists a unitary transformation e^G where

$$G = \tanh^{-1}\left(\omega - \omega^\dagger\right) \tag{1.21}$$

Applying that to the problem at hand gives

$$\begin{aligned} U_1^\dagger &= \exp\left(\tanh^{-1}\left(\eta_h - \eta_h^\dagger\right)\right) \\ &= \frac{1+\eta_h-\eta_h^\dagger}{1+\left\{\eta_h, \eta_h^\dagger\right\}} \\ &= \frac{1}{\sqrt{2}}\left(1+\eta_h-\eta_h^\dagger\right) \end{aligned} \tag{1.22}$$

The *unitary* operator that transforms the entangled eigenstate $|\psi_1\rangle$ to the state $|1\rangle$ is thus

$$U_1 = \frac{1}{\sqrt{2}}\left(1+\eta_h^\dagger - \eta_h\right) \tag{1.23}$$

It can also be written as $\exp\left(\frac{\pi}{4}\left(\eta_h^\dagger - \eta_h\right)\right)$ because

$$\begin{aligned}\exp\left(\frac{\pi}{4}\left(\eta_h^\dagger - \eta_h\right)\right) &= 1 + \left(\eta_h^\dagger - \eta_h\right)\frac{\pi}{4} + \frac{1}{2!}\left(\eta_h^\dagger - \eta_h\right)^2\left(\frac{\pi}{4}\right)^2 + \frac{1}{3!}\left(\eta_h^\dagger - \eta_h\right)^3\left(\frac{\pi}{4}\right)^3 + ...\\ &= 1 + \left(\eta_h^\dagger - \eta_h\right)\frac{\pi}{4} - \frac{1}{2!}\left(\frac{\pi}{4}\right)^2 - \frac{1}{3!}\left(\eta_h^\dagger - \eta_h\right)\left(\frac{\pi}{4}\right)^3 + \frac{1}{4!}\left(\frac{\pi}{4}\right)^4 + ...\\ &= \cos\frac{\pi}{4} + \left(\eta_h^\dagger - \eta_h\right)\sin\frac{\pi}{4}\\ &= 1 + \eta_h^\dagger - \eta_h\end{aligned} \tag{1.24}$$

There we used

$$\left(\eta_h^\dagger - \eta_h\right)^2 = {\eta_h^\dagger}^2 + \eta_h^2 - \left\{\eta_h^\dagger, \eta_h\right\} = -1 \quad \left[\because \eta^2 = {\eta^\dagger}^2 = 0\right] \tag{1.25}$$

and hence

$$\left(\eta_h^\dagger - \eta_h\right)^3 = -1\left(\eta_h^\dagger - \eta_h\right) \tag{1.26}$$

and so on. Since U_0 is obtained from U_1 simply by replacing η_h with $\eta_e^\dagger$, we can easily surmise that the unitary transformation that rotates an eigenstate $|\psi_0\rangle$ to the state $|0\rangle$ is

$$U_0 = \frac{1}{\sqrt{2}}\left(1+\eta_e - \eta_e^\dagger\right) = \exp\left(\frac{\pi}{4}\left(\eta_e - \eta_e^\dagger\right)\right) \tag{1.27}$$

The form of the rotated Hamiltonian can now be written down.

$$\begin{aligned}\widetilde{\mathcal{H}} &= U_q \mathcal{H} U_q^\dagger\\ &= \frac{1}{2}\left(1+\eta_q^\dagger - \eta_q\right)\mathcal{H}\left(1+\eta_q - \eta_q^\dagger\right)\\ &= \frac{1}{2}\left(1+\eta_q^\dagger - \eta_q\right)\left(\mathcal{H} + \mathcal{H}\eta - \mathcal{H}\eta_q^\dagger\right)\\ &= \frac{1}{2}\left(\mathcal{H} + \mathcal{H}\eta - \mathcal{H}\eta_q^\dagger + \eta_q^\dagger\mathcal{H} + \eta_q^\dagger\mathcal{H}\eta_q - \eta_q^\dagger\mathcal{H}\eta_q^\dagger - \eta_q\mathcal{H} - \eta_q\mathcal{H}\eta_q + \eta_q\mathcal{H}\eta_q^\dagger\right)\\ &= \frac{1}{2}\left(\mathcal{H}^D + \mathcal{H}^i + \mathcal{H}^I + \mathcal{H}\eta - \mathcal{H}\eta_q^\dagger + \eta_q^\dagger\mathcal{H} + \eta_q^\dagger\mathcal{H}\eta_q - \eta_q^\dagger\mathcal{H}\eta_q^\dagger - \eta_q\mathcal{H} - \eta_q\mathcal{H}\eta_q + \eta_q\mathcal{H}\eta_q^\dagger\right)\\ &= \frac{1}{2}\left(\mathcal{H}^D + \mathcal{H}^i + \mathcal{H}^I + \left[\eta_q^\dagger - \eta, \mathcal{H}\right] + \eta_q^\dagger\mathcal{H}\eta_q - \eta_q^\dagger\mathcal{H}\eta_q^\dagger - \eta_q\mathcal{H}\eta_q + \eta_q\mathcal{H}\eta_q^\dagger\right)\end{aligned} \tag{1.28}$$

In the last step I split $\mathcal{H}$ using eq. 1.29.

$$\mathcal{H} = \mathcal{H}^D + \mathcal{H}^I + \mathcal{H}^i \tag{1.29}$$

$\mathcal{H}^D$ is the diagonal part of the Hamiltonian, something of the form $\sum_k \epsilon_k n_k$. It also has the self energies that might arise from certain interactions. For example, if we have an interaction term of the form $J\sum_{k_1,k_2} c_{k_1}^\dagger c_{k_2}$, the term where both momenta are equal gives a diagonal term $Jc^\dagger_{k_1}c_{k_1}$. Such terms are also included in $\mathcal{H}^D$.

$\mathcal{H}^I$ is the interaction between the current degree of freedom q and the remaining degrees of freedom k. It will consist of terms like $c^\dagger_q c_k$ or $c^\dagger_k c_q$ that scatter between the current degree of freedom and the other degrees of freedom.

The third term $\mathcal{H}^i$ has interactions between the remaining degrees of freedom. This term will also be diagonal in n_k because it doesn't involve scattering either from or into q states. It will involve terms like $c^\dagger_{k_1}c_{k_2}$.

For reasons that will become apparent later, we will split the terms into two groups:

$$\tilde{\mathcal{H}} = \frac{1}{2}\left(\underbrace{\mathcal{H}^D + \mathcal{H}^i + \left[\eta^\dagger_q - \eta, \mathcal{H}\right] + \eta^\dagger_q\mathcal{H}\eta_q + \eta_q\mathcal{H}\eta^\dagger_q}_{\text{group 1}} + \overbrace{\mathcal{H}^I - \eta^\dagger_q\mathcal{H}\eta^\dagger_q - \eta_q\mathcal{H}\eta_q}^{\text{group 2}}\right) \tag{1.30}$$

Group 2 consists of purely off-diagonal terms; they amount to 0. To see how, note that terms that have two η_k or two $\eta^\dagger_q$ can only be nonzero if the intervening $\mathcal{H}$ has a creation or destruction operator. We resolve the Hamiltonian in the basis of q in the following form:

$$\begin{aligned}\mathcal{H} &= \text{Tr}\left[\mathcal{H}\hat{n}_q\right]\hat{n}_q + \text{Tr}\left[\mathcal{H}\left(1-\hat{n}_q\right)\right]\left(1-\hat{n}_q\right) + c^\dagger_q\text{Tr}\left[\mathcal{H}c_q\right] + \text{Tr}\left[c^\dagger_q\mathcal{H}\right]c_q \\ &= H_e\hat{n}_q + H_h(1-\hat{n}_q) + c^\dagger_q T + T^\dagger c_q\end{aligned} \tag{1.31}$$

Using this form, we can write

$$\eta_q\mathcal{H}\eta_q = \eta_q c^\dagger_q T\eta_q \tag{1.32}$$

and

$$\eta^\dagger_q\mathcal{H}\eta^\dagger_q = \eta^\dagger_q T^\dagger c_q\eta^\dagger_q \tag{1.33}$$

We can also write the off-diagonal part as

$$\mathcal{H}^I = c^\dagger_q T + T^\dagger c_q \tag{1.34}$$

Group 2 becomes

$$\text{group 2} = c^\dagger_q T + T^\dagger c_q - \eta^\dagger_q T^\dagger c_q\eta^\dagger_q - \eta_q c^\dagger_q T\eta_q \tag{1.35}$$

To simplify this, we use the definition of $\eta^\dagger_q$, eq. 1.13, to write η_q:

$$\eta_q = \left(\eta^\dagger_q\right)^\dagger = \text{ Tr}\left[c^\dagger_q\mathcal{H}\right]c_q\frac{1}{\hat{\omega} - \text{ Tr}\left[\mathcal{H}^D\hat{n}_q\right]\hat{n}_q} = T^\dagger c_q\frac{1}{\hat{\omega} - H_e\hat{n}_q} \tag{1.36}$$

Using this, we can write

$$\begin{aligned}\eta_q c^\dagger_q T\eta_q &= T^\dagger c_q\frac{1}{\hat{\omega} - H_e\hat{n}_q}c^\dagger_q T\eta_q \\ &= T^\dagger c_q\left(\frac{1}{\hat{\omega} - H_e\hat{n}_q}c^\dagger_q T\right)\eta_q \\ &= T^\dagger c_q\eta^\dagger_q\eta_q && \text{[eq. 1.13]} \\ &= T^\dagger c_q\hat{n}_q && \text{[eq. 1.18]}\end{aligned} \tag{1.37}$$

which gives

$$\eta_q c_q^\dagger T \eta_q = T^\dagger c_q \tag{1.38}$$

Similarly, we can express $\eta_q^\dagger$ by taking Hermitian conjugate of η_q:

$$\eta_q^\dagger = \frac{1}{\hat{\omega} - H_h\left(1 - \hat{n}_q\right)} T^\dagger c_q \tag{1.39}$$

which gives

$$\eta_q^\dagger T^\dagger c_q \eta_q^\dagger = c_q^\dagger T \tag{1.40}$$

Substituting the expressions 1.38 and 1.40, we get group 2 = 0. Substituting this in the rotated Hamiltonian gives

$$\widetilde{\mathcal{H}} = \frac{1}{2}\left(\mathcal{H}^D + \mathcal{H}^i + \mathcal{H}\eta - \mathcal{H}\eta_q^\dagger + \eta_q^\dagger\mathcal{H} + \eta_q^\dagger\mathcal{H}\eta_q - \eta_q\mathcal{H} + \eta_q\mathcal{H}\eta_q^\dagger\right) \tag{1.41}$$

To simplify the last 6 terms, we note the following:

$$\eta_q^\dagger = \frac{1}{\omega - H_e\hat{n}_q} c_q^\dagger T, \qquad \eta_q = \frac{1}{\omega - H_h(1 - \hat{n}_q)} T^\dagger c_q \tag{1.42}$$

Then,

$$\begin{aligned}
&\implies \frac{1}{\omega - H_e\hat{n}_q} c_q^\dagger T = c_q^\dagger T \frac{1}{\omega - H_h(1 - \hat{n}_q)} \\
&\implies c_q^\dagger T H_h(1 - \hat{n}_q) = H_e\hat{n}_q c_q^\dagger T \\
&\implies \frac{1}{\omega - H_e\hat{n}_q} c_q^\dagger T H_h(1 - \hat{n}_q) = \frac{1}{\omega - H_e\hat{n}_q} H_e\hat{n}_q c_q^\dagger T \\
&\implies \eta_q^\dagger H_h(1 - \hat{n}_q) = H_e\hat{n}_q \frac{1}{\omega - H_e\hat{n}_q} c_q^\dagger T \\
&\implies \eta_q^\dagger H_h(1 - \hat{n}_q) = H_e\hat{n}_q\eta_q^\dagger \\
&\implies \eta_q^\dagger H_h = H_e\hat{\eta}_q^\dagger
\end{aligned} \tag{1.43}$$

Using this identity and its conjugate ($\eta_q H_e = H_h\hat{\eta}_q$), the expression for $\eta_q H\eta_q^\dagger$ can be simplified:

$$\begin{aligned}
\eta_q\mathcal{H}\eta_q^\dagger &= \eta_q H_e\hat{n}_q\eta_q^\dagger \\
&= H_h\eta_q\eta_q^\dagger \\
&= H_h(1 - \hat{n}_q)
\end{aligned} \tag{1.44}$$

Similarly,

$$\begin{aligned}
\eta_q^\dagger\mathcal{H}\eta_q &= \eta_q^\dagger H_h\eta_q \\
&= H_e\eta_q^\dagger\eta_q \\
&= H_e\hat{n}_q
\end{aligned} \tag{1.45}$$

Also,

$$\begin{aligned}
\mathcal{H}\eta - \mathcal{H}\eta_q^\dagger + \eta_q^\dagger\mathcal{H} - \eta_q\mathcal{H} = \left(\eta_q^\dagger H_h - H_e\eta_q^\dagger\right) + \left(H_h\eta - \eta H_e\right) + \eta_q^\dagger T^\dagger c_q - \eta_q c_q^\dagger T + \\
c_q^\dagger T\eta_q - T^\dagger c_q\eta_q^\dagger
\end{aligned} \tag{1.46}$$

By virtue of eq. 1.43 and its conjugate, the first two terms will vanish, so we are left with

$$\mathcal{H}\eta - \mathcal{H}\eta_q^\dagger + \eta_q^\dagger\mathcal{H} - \eta_q\mathcal{H} = \eta_q^\dagger T^\dagger c_q - \eta_q c_q^\dagger T + c_q^\dagger T\eta_q - T^\dagger c_q\eta_q^\dagger \tag{1.47}$$

From eqs. 1.38 and 1.40,

$$\eta_q^\dagger T^\dagger c_q = \eta_q^\dagger \eta_q c_q^\dagger T \eta_q = \hat{n}_q c_q^\dagger T \eta_q = c_q^\dagger T \eta_q \tag{1.48}$$

$$T^\dagger c_q \eta_q^\dagger = \eta_q c_q^\dagger T \eta_q \eta_q^\dagger = \eta_q c_q^\dagger T\left(1-\hat{n}_q\right) = \eta_q c_q^\dagger T \tag{1.49}$$

$$\tag{1.50}$$

Eq. 1.47 becomes

$$\mathcal{H}\eta - \mathcal{H}\eta_q^\dagger + \eta_q^\dagger \mathcal{H} - \eta_q \mathcal{H} = c_q^\dagger T \eta_q - \eta_q c_q^\dagger T + c_q^\dagger T \eta_q - \eta_q c_q^\dagger T \quad = 2\left[c_q^\dagger T, \eta_q\right] \tag{1.51}$$

Putting it all together,

$$\begin{aligned}\widetilde{\mathcal{H}} &= \frac{1}{2}\left(\mathcal{H}^D + \mathcal{H}^i + \mathcal{H}\eta - \mathcal{H}\eta_q^\dagger + \eta_q^\dagger\mathcal{H} + \eta_q^\dagger\mathcal{H}\eta_q - \eta_q\mathcal{H} + \eta_q\mathcal{H}\eta_q^\dagger\right) \\ &= \frac{1}{2}\left(\mathcal{H}^D + \mathcal{H}^i\right) + \left[c_q^\dagger T, \eta_q\right] + \frac{1}{2}\left[H_e\hat{n}_q + H_h(1-\hat{n}_q)\right]\end{aligned} \tag{1.52}$$

One further simplification is possible. The last two terms constitute the total diagonal part of the Hamiltonian, but so do the first two terms:

$$\mathcal{H}^D + \mathcal{H}^i = H_e\hat{n}_q + H_h\left(1-\hat{n}_q\right) \tag{1.53}$$

Hence,

$$\begin{aligned}\widetilde{\mathcal{H}} &= \frac{1}{2}\left(\mathcal{H}^D + \mathcal{H}^i + \mathcal{H}\eta - \mathcal{H}\eta_q^\dagger + \eta_q^\dagger\mathcal{H} + \eta_q^\dagger\mathcal{H}\eta_q - \eta_q\mathcal{H} + \eta_q\mathcal{H}\eta_q^\dagger\right) \\ &= H_e\hat{n}_q + H_h(1-\hat{n}_q) + \left[c_q^\dagger T, \eta_q\right] \\ &= \mathrm{Tr}\left[\mathcal{H}\hat{n}_q\right]\hat{n}_q + \mathrm{Tr}\left[\mathcal{H}(\hat{1-n_q})\right]\left(1-\hat{n}_q\right) + \left[c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right), \eta_q\right]\end{aligned} \tag{1.54}$$

The two terms at the front can be written in a slightly different fashion.

$$\begin{aligned}\mathrm{Tr}\left[\mathcal{H}\hat{n}_q\right]\hat{n}_q + \mathrm{Tr}\left[\mathcal{H}(1-\hat{n}_q)\right]\left(1-\hat{n}_q\right) &= \mathrm{Tr}\left[\mathcal{H}\hat{n}_q\right]\hat{n}_q + \mathrm{Tr}\left[\mathcal{H}(\hat{n}_q-1)\right]\left(\hat{n}_q-1\right) \\ &= \mathrm{Tr}\left[\mathcal{H}\hat{n}_q\right]\hat{n}_q + \mathrm{Tr}\left[\mathcal{H}(\hat{n}_q-1)\right]n_q - \mathrm{Tr}\left[\mathcal{H}(\hat{n_q-1})\right] \\ &= \mathrm{Tr}\left[\mathcal{H}\left(2\hat{n}_q-1\right)\right]\hat{n}_q - \mathrm{Tr}\left[\mathcal{H}(\hat{n}_q-1)\right] \\ &= \mathrm{Tr}\left[\mathcal{H}\left(\hat{n}_q-\frac{1}{2}\right)\right]2\hat{n}_q - \mathrm{Tr}\left[\mathcal{H}(\hat{n}_q-\frac{1}{2})\right] + \frac{1}{2}\mathrm{Tr}\left[\mathcal{H}\right] \\ &= \mathrm{Tr}\left[\mathcal{H}\left(\hat{n}_q-\frac{1}{2}\right)\right]\left(2\hat{n}_q-1\right) + \frac{1}{2}\mathrm{Tr}\left[\mathcal{H}\right] \\ &= \mathrm{Tr}\left[\mathcal{H}\tau_q\right]2\tau_q + \frac{1}{2}\mathrm{Tr}\left[\mathcal{H}\right]\end{aligned} \tag{1.55}$$

The last term can be written as:

$$\begin{aligned}\left[c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right), \eta_q\right] &= c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right)\eta_q - \eta_q c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right) \\ &= \left(2\hat{n}_q-1\right)c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right)\eta_q - \left(1-2\hat{n}_q\right)\eta_q c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right)\end{aligned} \tag{1.56}$$

I used $\hat{n}_q c_q^\dagger = c_q^\dagger$ and $\hat{n}_q\eta_q = 0$. Then,

$$\left[c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right), \eta_q\right] = 2\tau_q\left\{c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right), \eta_q\right\} \tag{1.57}$$

The final form of the rotated Hamiltonian is

$$\widetilde{\mathcal{H}} = U_q \mathcal{H} U_q^\dagger = \mathrm{Tr}\left[\mathcal{H}\hat{n}_q\right]\hat{n}_q + \mathrm{Tr}\left[\mathcal{H}(1-\hat{n}_q)\right](1-\hat{n}_q) + 2\tau_q\left\{c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right), \eta_q\right\} \tag{1.58}$$

To check that this indeed commutes with $\hat{n}_q$,

$$\begin{aligned}\left[\widetilde{\mathcal{H}}, \hat{n}_q\right] &= \left[\left[c_q^\dagger T, \eta_q\right], \hat{n}_q\right] \\ &= \left[c_q^\dagger T\eta_q, \hat{n}_q\right] - \left[\eta_q c_q^\dagger T, \hat{n}_q\right] \\ &= c_q^\dagger T\eta_q\hat{n}_q - \hat{n}_q c_q^\dagger T\eta_q \qquad \left[2^{\text{nd}}\ [\ .\ ]\text{ is }0,\ \because c_q^\dagger\hat{n}_q = \hat{n}_q\eta_q = 0\right] \\ &= c_q^\dagger T\eta_q - c_q^\dagger T\eta_q \\ &= 0\end{aligned} \tag{1.59}$$

Within the URG, it is a prescription that the fixed point is reached when the denominator of the RG equation vanishes. This is equivalent to the condition:

$$\begin{aligned}&\hat{\omega} - H_e\hat{n} = 0 \\ \implies &\omega_e = H_e\end{aligned}$$

or

$$\begin{aligned}&\hat{\omega} - H_h\left(1-\hat{n}\right) = 0 \\ \implies &\omega_h = H_h\end{aligned}$$

In either case, we see that the eigenvalue of $\hat{\omega}$ matches the eigenvalue of one of the blocks. This also leads to the vanishing of the off-diagonal block. To see how,

$$\begin{aligned}\eta^\dagger\eta\left|1, \Psi_1\right\rangle &= \left|1, \Psi_1\right\rangle \qquad \left[\eta^\dagger\eta = \hat{n}\right] \\ \implies \frac{1}{\hat{\omega} - \hat{H}_e}c^\dagger T\eta &= \left|1, \Psi_1\right\rangle \\ \implies c^\dagger T\eta &= \left(\hat{\omega} - \hat{H}_e\right)\left|1, \Psi_1\right\rangle \\ &= \left(\omega_e - H_e\right)\left|1, \Psi_1\right\rangle\end{aligned} \tag{1.60}$$

If $\omega_e = H_e$, we will have $c^\dagger T = 0$. This implies $T^\dagger c = 0$ and hence $\mathcal{H}^I = 0$.

1.2 Prescription

Given a Hamiltonian

$$\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_0 + c^\dagger T + T^\dagger c \tag{1.61}$$

the goal is to look at the renormalization of the various couplings in the Hamiltonian as we decouple high energy electron states. Typically we have a shell of electrons at some energy D. During the process, we make one simplification. We assume that there is only one electron on that shell at a time, say with quantum numbers q, σ, and calculate the renormalization of the various couplings due to this electron. We then sum the momentum q over the shell and the spin β, and this gives the total renormalization due to decoupling the entire shell.

From eq. 1.58, the first two terms in the rotated Hamiltonian are just the diagonal parts of the bare Hamiltonian; they are unchanged in that part. The renormalization comes from the third term. For one electron $q\beta$ on the shell, the renormalization is

$$\Delta\mathcal{H}_{q\beta} = 2\tau_{q\beta}\left\{c^{\dagger}_{q\beta}\mathrm{Tr}\left(\mathcal{H}c_{q\beta}\right), \eta_{q\beta}\right\} \tag{1.62}$$

Decoupling the entire shell gives

$$\Delta\mathcal{H} = \sum_{q\beta} 2\tau_{q\beta}\left\{c^{\dagger}_{q\beta}\mathrm{Tr}\left(\mathcal{H}c_{q\beta}\right), \eta_{q\beta}\right\} \tag{1.63}$$

One can look at the particle and hole sectors separately. The particle sector involves those processes which create a particle with high energy in the intermediate state. The hole sector consists of those processes that destroy a deep-lying electron in the intermediate state. It is clear that the first term of the anticommutator, one that starts with $c^{\dagger}$ and ends with η will destroy an electron in the intermediate state. That gives the hole sector contribution:

$$\begin{aligned}\Delta^{-}\mathcal{H} &= \sum_{q\beta} c^{\dagger}_{q\beta}\mathrm{Tr}\left(\mathcal{H}c_{q\beta}\right)\eta_{q\beta} \\ &= \sum_{q\beta} c^{\dagger}_{q\beta}\mathrm{Tr}\left(\mathcal{H}c_{q\beta}\right)\frac{1}{\omega_h - \mathcal{H}^D}\mathrm{Tr}\left(c^{\dagger}_{q\beta}\mathcal{H}\right)c_{q\beta}\end{aligned} \tag{1.64}$$

where we have replaced $\hat{\omega}$ by its eigenvalue ω_h and $H_h = \mathrm{Tr}\left(\mathcal{H}\left(1-\hat{n}_{q\beta}\right)\right)$. The other term in the commutator gives the particle sector contribution:

$$\begin{aligned}\Delta^{+}\mathcal{H} &= \sum_{q\beta} \eta_{q\beta}c^{\dagger}_{q\beta}\mathrm{Tr}\left(\mathcal{H}c_{q\beta}\right) \\ &= \sum_{q\beta} \mathrm{Tr}\left(c^{\dagger}_{q\beta}\mathcal{H}\right)c_{q\beta}\frac{1}{\omega_e - \mathcal{H}^D}c^{\dagger}_{q\beta}\mathrm{Tr}\left(\mathcal{H}c_{q\beta}\right)\end{aligned} \tag{1.65}$$

where we used $2\tau\eta = -\eta$ and $H_e = \mathrm{Tr}\left(\mathcal{H}\hat{n}_{q\beta}\right)$. These equations will now need to be simplified. For example, in the particle sector, we can set $\hat{n}_{q\beta} = 0$ in the numerator, because there is no such excitation in the initial state. Similarly, in the hole sector, we can set $\hat{n}_{q\beta} = 1$ because that state was occupied in the initial state. Another simplification we employ is that H_e and H_h will, in general, have the energies of all the electrons. But we consider only the energy of the on-shell electrons in the denominator. After integrating out these electrons, we can rearrange the remaining operators to determine which term in the Hamiltonian it renormalizes and what is the renormalization.

At first sight, one might think that we must evaluate lots of traces to obtain the terms in $\Delta\mathcal{H}$. A little thought reveals that the terms in the numerator are simply the off-diagonal terms in the Hamiltonian; $\mathrm{Tr}\left(c^{\dagger}_{q\beta}\mathcal{H}\right)c_{q\beta}$ is the off-diagonal term that has $c_{q\beta}$ in it, and $c^{\dagger}_{q\beta}\mathrm{Tr}\left(\mathcal{H}c_{q\beta}\right)$ is the off-diagonal term that has $c^{\dagger}_{q\beta}$ in it. $\mathcal{H}^D$ is just the diagonal part of the Hamiltonian.

References

[1] Anirban Mukherjee and Siddhartha Lal. Holographic unitary renormalization group for correlated electrons - i: A tensor network approach. *Nuclear Physics B*, 960, 2020.

[2] Kenji Suzuki. Construction of Hermitian Effective Interaction in Nuclei: — General Relation between Hermitian and Non-Hermitian Forms —. *Progress of Theoretical Physics*, 68, 1982.