Unitary Renormalization Group Approach to Single-Impurity Anderson Model

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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 transformation 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

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

Since $|\psi_i\rangle$ is the set of eigenstates of $\mathcal{H}$ and $|i\rangle$ is the set of eigenstates in which $U\mathcal{H}U^\dagger$ has no off-diagonal terms corresponding to $q\beta$, 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 $q\beta$:

$$|\psi_i\rangle = \sum_{j=0,1} |j\rangle \langle j| |\psi_i\rangle \equiv |1\rangle |\phi_1^i\rangle + |0\rangle |\phi_0^i\rangle \tag{1.6}$$

where $|\phi_j^i\rangle = \langle j| |\psi_i\rangle$. If we substitute the expansion 1.2 into the eigenvalue equation 1.5, we get

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

The diagonal parts $H_e = \mathrm{tr}\left[\mathcal{H}\hat{n}_{q\beta}\right]$ and $H_e = \mathrm{tr}\left[\mathcal{H}\left(1 - \hat{n}_{q\beta}\right)\right]$ 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,

$$H_e \hat{n}_{q\beta} + H_h \left(1 - \hat{n}_{q\beta}\right) = \mathcal{H}^d + \mathcal{H}^i$$

This gives

$$\left[c_{q\beta}^\dagger T + T^\dagger c_{q\beta}\right] |\psi_i\rangle = \left(\tilde{H}_i - \mathcal{H}^i - \mathcal{H}^d\right) |\psi_i\rangle \tag{1.8}$$

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

$$\left[c_{q\beta}^\dagger T + T^\dagger c_{q\beta}\right] |\psi_i\rangle = \left(\hat{\omega}_i - \mathcal{H}^d\right) |\psi_i\rangle \tag{1.9}$$

Since the only requirement on $|\psi_i\rangle$ is that it diagonalize the Hamiltonian in the subspace of $q\beta$, there is freedom in the choice of this state. We can exploit this freedom and choose the $|\psi_i\rangle$ to be an eigenstate of $\hat{\omega}_i$ corresponding to an eigenvalue ω_i:

$$\left[\mathcal{H}^d + c_{q\beta}^\dagger T + T^\dagger c_{q\beta}\right] |\psi_i(\omega_i)\rangle = \left(\omega_i - \mathcal{H}^d\right) |\psi_i(\omega_i)\rangle \tag{1.10}$$

If we now substitue the expansion 1.6 and gather the terms that result in $\hat{n}_{q\beta} = 1$, we get

$$c_{q\beta}^\dagger T \,|0\rangle\, |\phi_0^i\rangle = \left(\omega_i - \mathcal{H}_e^d\right) |1\rangle\, |\phi_1^i\rangle \tag{1.11}$$

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

$$T^\dagger c_{q\beta} \,|1\rangle\, |\phi_1^i\rangle = \left(\omega_i - \mathcal{H}_h^d\right) |0\rangle\, |\phi_0^i\rangle \tag{1.12}$$

We now define two many-particle transition operators:

$$\begin{aligned} {\eta_e}^\dagger(\omega_i) &= \frac{1}{\omega_i - \mathcal{H}_e^d} c_{q\beta}^\dagger T \\ \eta_h(\omega_i) &= \frac{1}{\omega_i - \mathcal{H}_h^d} T^\dagger c_{q\beta} \end{aligned} \tag{1.13}$$

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:

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

and hence the anticommutator

$$\implies \left\{\eta_h, \eta_e^\dagger\right\} = 1 \tag{1.19}$$

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

$$U_1 = 1 + \eta_h \tag{1.20}$$

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

$$U_1 = e^{\eta_h} \tag{1.21}$$

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

$$G = \tanh^{-1}\left(\omega - \omega^\dagger\right) \tag{1.22}$$

Applying that to the problem at hand gives

$$\begin{aligned} U_1^\dagger &= \exp\left(\tanh^{-1}\left(\eta_h - \eta_h^\dagger\right)\right) \\ &= \frac{1 + \eta_h - \eta_h^\dagger}{1 + \left\{\eta_h, \eta_h^\dagger\right\}} \\ &= \frac{1}{\sqrt{2}}\left(1 + \eta_h - \eta_h^\dagger\right) \end{aligned} \tag{1.23}$$

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

$$U_1 = \frac{1}{\sqrt{2}}\left(1 + \eta_h^\dagger - \eta_h\right) \tag{1.24}$$

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

$$\begin{aligned} \exp\left(\frac{\pi}{4}\left(\eta_h^\dagger - \eta_h\right)\right) &= 1 + \left(\eta_h^\dagger - \eta_h\right)\frac{\pi}{4} + \frac{1}{2!}\left(\eta_h^\dagger - \eta_h\right)^2\left(\frac{\pi}{4}\right)^2 + \frac{1}{3!}\left(\eta_h^\dagger - \eta_h\right)^3\left(\frac{\pi}{4}\right)^3 + ... \\ &= 1 + \left(\eta_h^\dagger - \eta_h\right)\frac{\pi}{4} - \frac{1}{2!}\left(\frac{\pi}{4}\right)^2 - \frac{1}{3!}\left(\eta_h^\dagger - \eta_h\right)\left(\frac{\pi}{4}\right)^3 + \frac{1}{4!}\left(\frac{\pi}{4}\right)^4 + ... \\ &= \cos\frac{\pi}{4} + \left(\eta_h^\dagger - \eta_h\right)\sin\frac{\pi}{4} \\ &= 1 + \eta_h^\dagger - \eta_h \end{aligned} \tag{1.25}$$

There we used

$$\left(\eta_h^\dagger - \eta_h\right)^2 = {\eta_h^\dagger}^2 + \eta_h^2 - \left\{\eta_h^\dagger, \eta_h\right\} = -1 \quad \left[\because \eta^2 = {\eta^\dagger}^2 = 0\right] \tag{1.26}$$

and hence

$$\left(\eta_h^\dagger - \eta_h\right)^3 = -1\left(\eta_h^\dagger - \eta_h\right) \tag{1.27}$$

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

$$U_0 = \frac{1}{\sqrt{2}}\left(1 + \eta_e - \eta_e^\dagger\right) = \exp\left(\frac{\pi}{4}\left(\eta_e - \eta_e^\dagger\right)\right) \tag{1.28}$$

We can now compute the form of the effective Hamiltonian that comes about when we apply U_1 - that is - when we rotate one exact eigenstate $|\psi_1\rangle$ into the occupied Fock space basis $|1\rangle$. From eq. 1.24,

$$\begin{aligned}
U_1\mathcal{H}U_1^\dagger &= \frac{1}{2}\left(1 + \eta_h^\dagger - \eta_h\right)\mathcal{H}\left(1 + \eta_h - \eta_h^\dagger\right) \\
&= \frac{1}{2}\left(1 + \eta_h^\dagger - \eta_h\right)\left(\mathcal{H} + \mathcal{H}\eta_h - \mathcal{H}\eta_h^\dagger\right) \\
&= \frac{1}{2}\left(\mathcal{H} + \mathcal{H}\eta_h - \mathcal{H}\eta_h^\dagger + \eta_h^\dagger\mathcal{H} + \eta_h^\dagger\mathcal{H}\eta_h - \eta_h^\dagger\mathcal{H}\eta_h^\dagger - \eta_h\mathcal{H} - \eta_h\mathcal{H}\eta_h + \eta_h\mathcal{H}\eta_h^\dagger\right) \\
&= \frac{1}{2}\left(\mathcal{H}^D + \mathcal{H}^i + \mathcal{H}^I + \mathcal{H}\eta_h - \mathcal{H}\eta_h^\dagger + \eta_h^\dagger\mathcal{H} + \eta_h^\dagger\mathcal{H}\eta_h - \eta_h^\dagger\mathcal{H}\eta_h^\dagger - \eta_h\mathcal{H} - \eta_h\mathcal{H}\eta_h + \eta_h\mathcal{H}\eta_h^\dagger\right) \\
&= \frac{1}{2}\left(\mathcal{H}^D + \mathcal{H}^i + \mathcal{H}^I + \left[\eta_h^\dagger - \eta_h, \mathcal{H}\right] + \eta_h^\dagger\mathcal{H}\eta_h - \eta_h^\dagger\mathcal{H}\eta_h^\dagger - \eta_h\mathcal{H}\eta_h + \eta_h\mathcal{H}\eta_h^\dagger\right)
\end{aligned} \tag{1.29}$$

In the last two lines, we expanded the Hamiltonian into the three parts $\mathcal{H}^d, \mathcal{H}^i$ and a third piece $\mathcal{H}^I \equiv c_{q\beta}^\dagger T + T^\dagger c_{q\beta}$.

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

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

Group 2 consists of purely off-diagonal terms; they amount to 0. To see how, note that terms that have two η_h or two $\eta_h^\dagger$ can only be nonzero if the intervening $\mathcal{H}$ has an odd number of creation or destruction operators.

$$\eta_h\mathcal{H}\eta_h = \eta_h c_q^\dagger T\eta_h \tag{1.31}$$

and

$$\eta_h^\dagger\mathcal{H}\eta_h^\dagger = \eta_h^\dagger T^\dagger c_q\eta_h^\dagger \tag{1.32}$$

Group 2 becomes

$$\text{group 2} = \mathcal{H}^I - \eta_q^\dagger T^\dagger c_q\eta_q^\dagger - \eta_q c_q^\dagger T\eta_q = c_q^\dagger T + T^\dagger c_q - \eta_q^\dagger T^\dagger c_q\eta_q^\dagger - \eta_q c_q^\dagger T\eta_q \tag{1.33}$$

To simplify this, we use the relation

$$\begin{aligned}\eta_h c_q^\dagger T \eta_h &= T^\dagger c_q \frac{1}{\hat{\omega} - H_e \hat{n}_q} c_q^\dagger T \eta_h \\ &= T^\dagger c_q \left(\frac{1}{\hat{\omega} - H_e \hat{n}_q} c_q^\dagger T \right) \eta_h \\ &= T^\dagger c_q \eta_h^\dagger \eta_h \qquad \text{[eq. 1.13]} \\ &= T^\dagger c_q \hat{n}_q \qquad \text{[eq. 1.18]}\end{aligned} \tag{1.34}$$

which gives

$$\eta_q c_q^\dagger T \eta_q = T^\dagger c_q \tag{1.35}$$

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

$$\eta_q^\dagger = \frac{1}{\hat{\omega} - H_h \left(1 - \hat{n}_q\right)} T^\dagger c_q \tag{1.36}$$

which gives

$$\eta_q^\dagger T^\dagger c_q \eta_q^\dagger = c_q^\dagger T \tag{1.37}$$

Substituting the expressions 1.35 and 1.37, we get group $2 = 0$. Substituting this in the rotated Hamiltonian gives

$$\widetilde{\mathcal{H}} = \frac{1}{2} \left(\mathcal{H}^D + \mathcal{H}^i + \mathcal{H}\eta - \mathcal{H}\eta_q^\dagger + \eta_q^\dagger \mathcal{H} + \eta_q^\dagger \mathcal{H} \eta_q - \eta_q \mathcal{H} + \eta_q \mathcal{H} \eta_q^\dagger \right) \tag{1.38}$$

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

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

Then,

$$\begin{aligned}&\implies \frac{1}{\omega - H_e \hat{n}_q} c_q^\dagger T = c_q^\dagger T \frac{1}{\omega - H_h (1 - \hat{n}_q)} \\ &\implies c_q^\dagger T H_h (1 - \hat{n}_q) = H_e \hat{n}_q c_q^\dagger T \\ &\implies \frac{1}{\omega - H_e \hat{n}_q} c_q^\dagger T H_h (1 - \hat{n}_q) = \frac{1}{\omega - H_e \hat{n}_q} H_e \hat{n}_q c_q^\dagger T \\ &\implies \eta_q^\dagger H_h (1 - \hat{n}_q) = H_e \hat{n}_q \frac{1}{\omega - H_e \hat{n}_q} c_q^\dagger T \\ &\implies \eta_q^\dagger H_h (1 - \hat{n}_q) = H_e \hat{n}_q \eta_q^\dagger \\ &\implies \eta_q^\dagger H_h = H_e \hat{\eta}_q^\dagger\end{aligned} \tag{1.40}$$

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:

$$\begin{aligned}\eta_q \mathcal{H} \eta_q^\dagger &= \eta_q H_e \hat{n}_q \eta_q^\dagger \\ &= H_h \eta_q \eta_q^\dagger \\ &= H_h (1 - \hat{n}_q)\end{aligned} \tag{1.41}$$

Similarly,

$$\begin{aligned}\eta_q^\dagger \mathcal{H} \eta_q &= \eta_q^\dagger H_h \eta_q \\ &= H_e \eta_q^\dagger \eta_q \\ &= H_e \hat{n}_q\end{aligned} \tag{1.42}$$

Also,

$$\mathcal{H}\eta - \mathcal{H}\eta_q^\dagger + \eta_q^\dagger\mathcal{H} - \eta_q\mathcal{H} = \left(\eta_q^\dagger H_h - H_e\eta_q^\dagger\right) + \left(H_h\eta - \eta H_e\right) + \eta_q^\dagger T^\dagger c_q - \eta_q c_q^\dagger T + c_q^\dagger T\eta_q - T^\dagger c_q\eta_q^\dagger \tag{1.43}$$

By virtue of eq. 1.40 and its conjugate, the first two terms will vanish, so we are left with

$$\mathcal{H}\eta - \mathcal{H}\eta_q^\dagger + \eta_q^\dagger\mathcal{H} - \eta_q\mathcal{H} = \eta_q^\dagger T^\dagger c_q - \eta_q c_q^\dagger T + c_q^\dagger T\eta_q - T^\dagger c_q\eta_q^\dagger \tag{1.44}$$

From eqs. 1.35 and 1.37,

$$\eta_q^\dagger T^\dagger c_q = \eta_q^\dagger\eta_q c_q^\dagger T\eta_q = \hat{n}_q c_q^\dagger T\eta_q = c_q^\dagger T\eta_q \tag{1.45}$$

$$T^\dagger c_q\eta_q^\dagger = \eta_q c_q^\dagger T\eta_q\eta_q^\dagger = \eta_q c_q^\dagger T\left(1-\hat{n}_q\right) = \eta_q c_q^\dagger T \tag{1.46}$$

$$\tag{1.47}$$

Eq. 1.44 becomes

$$\mathcal{H}\eta - \mathcal{H}\eta_q^\dagger + \eta_q^\dagger\mathcal{H} - \eta_q\mathcal{H} = c_q^\dagger T\eta_q - \eta_q c_q^\dagger T + c_q^\dagger T\eta_q - \eta_q c_q^\dagger T \quad = 2\left[c_q^\dagger T, \eta_q\right] \tag{1.48}$$

Putting it all together,

$$\begin{aligned}\widetilde{\mathcal{H}} &= \frac{1}{2}\left(\mathcal{H}^D + \mathcal{H}^i + \mathcal{H}\eta - \mathcal{H}\eta_q^\dagger + \eta_q^\dagger\mathcal{H} + \eta_q^\dagger\mathcal{H}\eta_q - \eta_q\mathcal{H} + \eta_q\mathcal{H}\eta_q^\dagger\right) \\ &= \frac{1}{2}\left(\mathcal{H}^D + \mathcal{H}^i\right) + \left[c_q^\dagger T, \eta_q\right] + \frac{1}{2}\left[H_e\hat{n}_q + H_h(1-\hat{n}_q)\right]\end{aligned} \tag{1.49}$$

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

$$\mathcal{H}^D + \mathcal{H}^i = H_e\hat{n}_q + H_h\left(1-\hat{n}_q\right) \tag{1.50}$$

Hence,

$$\begin{aligned}\widetilde{\mathcal{H}} &= \frac{1}{2}\left(\mathcal{H}^D + \mathcal{H}^i + \mathcal{H}\eta - \mathcal{H}\eta_q^\dagger + \eta_q^\dagger\mathcal{H} + \eta_q^\dagger\mathcal{H}\eta_q - \eta_q\mathcal{H} + \eta_q\mathcal{H}\eta_q^\dagger\right) \\ &= H_e\hat{n}_q + H_h(1-\hat{n}_q) + \left[c_q^\dagger T, \eta_q\right] \\ &= \mathrm{Tr}\left[\mathcal{H}\hat{n}_q\right]\hat{n}_q + \mathrm{Tr}\left[\hat{\mathcal{H}(1-n_q)}\right](1-\hat{n}_q) + \left[c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right), \eta_q\right]\end{aligned} \tag{1.51}$$

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

$$\begin{aligned}\mathrm{Tr}\left[\mathcal{H}\hat{n}_q\right]\hat{n}_q + \mathrm{Tr}\left[\mathcal{H}(1-\hat{n}_q)\right](1-\hat{n}_q) &= \mathrm{Tr}\left[\mathcal{H}\hat{n}_q\right]\hat{n}_q + \mathrm{Tr}\left[\mathcal{H}(\hat{n}_q-1)\right](\hat{n}_q-1) \\ &= \mathrm{Tr}\left[\mathcal{H}\hat{n}_q\right]\hat{n}_q + \mathrm{Tr}\left[\mathcal{H}(\hat{n}_q-1)\right]n_q - \mathrm{Tr}\left[\hat{\mathcal{H}(n_q-1)}\right] \\ &= \mathrm{Tr}\left[\mathcal{H}\left(2\hat{n}_q-1\right)\right]\hat{n}_q - \mathrm{Tr}\left[\mathcal{H}(\hat{n}_q-1)\right] \\ &= \mathrm{Tr}\left[\mathcal{H}\left(\hat{n}_q-\frac{1}{2}\right)\right]2\hat{n}_q - \mathrm{Tr}\left[\mathcal{H}(\hat{n}_q-\frac{1}{2})\right] + \frac{1}{2}\mathrm{Tr}\left[\mathcal{H}\right] \\ &= \mathrm{Tr}\left[\mathcal{H}\left(\hat{n}_q-\frac{1}{2}\right)\right]\left(2\hat{n}_q-1\right) + \frac{1}{2}\mathrm{Tr}\left[\mathcal{H}\right] \\ &= \mathrm{Tr}\left[\mathcal{H}\tau_q\right]2\tau_q + \frac{1}{2}\mathrm{Tr}\left[\mathcal{H}\right]\end{aligned} \tag{1.52}$$

The last term can be written as:

$$\begin{aligned}\left[c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right), \eta_q\right] &= c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right)\eta_q - \eta_q c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right) \\ &= \left(2\hat{n}_q - 1\right) c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right)\eta_q - \left(1 - 2\hat{n}_q\right)\eta_q c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right)\end{aligned} \tag{1.53}$$

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

$$\left[c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right), \eta_q\right] = 2\tau_q \left\{c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right), \eta_q\right\} \tag{1.54}$$

The final form of the rotated Hamiltonian is

$$\widetilde{\mathcal{H}} = U_q \mathcal{H} U_q^\dagger = \mathrm{Tr}\left[\mathcal{H}\hat{n}_q\right]\hat{n}_q + \mathrm{Tr}\left[\mathcal{H}(1-\hat{n}_q)\right](1-\hat{n}_q) + 2\tau_q \left\{c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right), \eta_q\right\} \tag{1.55}$$

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

$$\begin{aligned}\left[\widetilde{\mathcal{H}}, \hat{n}_q\right] &= \left[\left[c_q^\dagger T, \eta_q\right], \hat{n}_q\right] \\ &= \left[c_q^\dagger T \eta_q, \hat{n}_q\right] - \left[\eta_q c_q^\dagger T, \hat{n}_q\right] \\ &= c_q^\dagger T \eta_q \hat{n}_q - \hat{n}_q c_q^\dagger T \eta_q \qquad \left[2^{\text{nd}}\ [\ .\ ] \text{ is 0},\ \because c_q^\dagger \hat{n}_q = \hat{n}_q \eta_q = 0\right] \\ &= c_q^\dagger T \eta_q - c_q^\dagger T \eta_q \\ &= 0\end{aligned} \tag{1.56}$$

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,

$$\begin{aligned}&\eta^\dagger \eta \left|1, \Psi_1\right\rangle = \left|1, \Psi_1\right\rangle \qquad \left[\eta^\dagger \eta = \hat{n}\right] \\ \implies\ &\frac{1}{\hat{\omega} - \hat{H}_e} c^\dagger T \eta = \left|1, \Psi_1\right\rangle \\ \implies\ &c^\dagger T \eta = \left(\hat{\omega} - \hat{H}_e\right)\left|1, \Psi_1\right\rangle \\ &\qquad\quad = \left(\omega_e - H_e\right)\left|1, \Psi_1\right\rangle\end{aligned} \tag{1.57}$$

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

$$\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_0 + c^\dagger T + T^\dagger c \tag{1.58}$$

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. 1.55, 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

$$\Delta\mathcal{H}_{q\beta} = 2\tau_{q\beta}\left\{c^\dagger_{q\beta}\mathrm{Tr}\left(\mathcal{H}c_{q\beta}\right), \eta_{q\beta}\right\} \tag{1.59}$$

Decoupling the entire shell gives

$$\Delta\mathcal{H} = \sum_{q\beta} 2\tau_{q\beta}\left\{c^\dagger_{q\beta}\mathrm{Tr}\left(\mathcal{H}c_{q\beta}\right), \eta_{q\beta}\right\} \tag{1.60}$$

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:

$$\begin{aligned}\Delta^-\mathcal{H} &= \sum_{q\beta} c^\dagger_{q\beta}\mathrm{Tr}\left(\mathcal{H}c_{q\beta}\right)\eta_{q\beta} \\ &= \sum_{q\beta} c^\dagger_{q\beta}\mathrm{Tr}\left(\mathcal{H}c_{q\beta}\right)\frac{1}{\omega_h - \mathcal{H}^D}\mathrm{Tr}\left(c^\dagger_{q\beta}\mathcal{H}\right)c_{q\beta}\end{aligned} \tag{1.61}$$

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:

$$\begin{aligned}\Delta^+\mathcal{H} &= \sum_{q\beta} \eta_{q\beta}c^\dagger_{q\beta}\mathrm{Tr}\left(\mathcal{H}c_{q\beta}\right) \\ &= \sum_{q\beta} \mathrm{Tr}\left(c^\dagger_{q\beta}\mathcal{H}\right)c_{q\beta}\frac{1}{\omega_e - \mathcal{H}^D}c^\dagger_{q\beta}\mathrm{Tr}\left(\mathcal{H}c_{q\beta}\right)\end{aligned} \tag{1.62}$$

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; $\mathrm{Tr}\left(c_{q\beta}^{\dagger}\mathcal{H}\right)c_{q\beta}$ is the off-diagonal term that has $c_{q\beta}$ in it, and $c_{q\beta}^{\dagger}\mathrm{Tr}\left(\mathcal{H}c_{q\beta}\right)$ is the off-diagonal term that has $c_{q\beta}^{\dagger}$ in it. $\mathcal{H}^{D}$ is just the diagonal part of the Hamiltonian.

2 Schrieffer-Wolff Transformation in the context of URG and PMS

2.1 Schrieffer-Wolff transformation as a limit of URG

We have a general Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_X \tag{2.1}$$

$\mathcal{H}_0$ is diagonal w.r.t a particular degree of freedom. V is off-diagonal w.r.t that same degree of freedom. Let S be an *anti-Hermitian* and *off-diagonal* operator. $U = e^{S}$ is then a unitary transformation.

$$\begin{aligned} U\mathcal{H}U^{\dagger} &= e^{S}\left(\mathcal{H}_0 + \mathcal{H}_X\right)e^{-S} \\ &= \left(\cosh\left(S\right) + \sinh\left(S\right)\right)\left(\mathcal{H}_0 + \mathcal{H}_X\right)\left(\cosh\left(S\right) + \sinh\left(S\right)\right) \\ &= H_1 + H_2 \end{aligned} \tag{2.2}$$

where H_1 is diagonal and H_2 is off-diagonal.

$$\begin{aligned} H_1 = \cosh\left(S\right)\mathcal{H}_0\cosh\left(S\right) - \sinh\left(S\right)\mathcal{H}_0\sinh\left(S\right) - \cosh\left(S\right)\mathcal{H}_X\sinh\left(S\right) \\ + \sinh\left(S\right)\mathcal{H}_X\cosh\left(S\right) \\ H_2 = -\cosh\left(S\right)\mathcal{H}_0\sinh\left(S\right) + \sinh\left(S\right)\mathcal{H}_0\cosh\left(S\right) + \cosh\left(S\right)\mathcal{H}_X\cosh\left(S\right) \\ - \sinh\left(S\right)\mathcal{H}_X\sinh\left(S\right) \end{aligned} \tag{2.3}$$

The decoupling condition is $H_2 = 0$.

For small S, we have $\sinh S \sim S$ and $\cosh S \sim 1 + \frac{1}{2}S^2$. Therefore, the off-diagonal part, up to second order, is

$$H_2 = -\mathcal{H}_0 S + S\mathcal{H}_0 + \mathcal{H}_X + O(S^3) = [S, \mathcal{H}_0] + \mathcal{H}_X \tag{2.4}$$

The second order decoupling condition is thus

$$[S, \mathcal{H}_0] = -\mathcal{H}_X \tag{2.5}$$

In order to decouple a state $q\beta$ from the SIAM ($\epsilon_q > 0$) , we take an ansatz $S = \left(A + B\hat{n}_{d\bar{\beta}}\right)\left(c_{q\beta}^{\dagger}c_{d\beta} - \text{h.c.}\right)$. Plugging this into the decoupling condition gives

$$-\epsilon_q\left(A + B\hat{n}_{d\bar{\beta}}\right) + \epsilon_d\left(A + B\hat{n}_{d\bar{\beta}}\right) + U\left(A + B\right)\hat{n}_{d\bar{\beta}} = -V \tag{2.6}$$

which gives

$$S = V\left[\frac{1 - \hat{n}_{d\bar{\beta}}}{\epsilon_q - \epsilon_d} + \frac{\hat{n}_{d\bar{\beta}}}{\epsilon_q - \epsilon_d - U}\right] \tag{2.7}$$

The remaining diagonal part constitutes the effective Hamiltonian.

$$\begin{aligned} U\mathcal{H}U^\dagger = H_1 &= \mathcal{H}_0 + \frac{1}{2}\left\{\mathcal{H}_0, S^2\right\} - S\mathcal{H}_0 S + [S, \mathcal{H}_X] \\ &= \mathcal{H}_0 + \frac{1}{2}\left[\left[\mathcal{H}_0, S\right], S\right] + [S, \mathcal{H}_X] \\ &= \mathcal{H}_0 + \frac{1}{2}\left[\mathcal{H}_X, S\right] + [S, \mathcal{H}_X] \\ &= \mathcal{H}_0 + \frac{1}{2}\left[S, \mathcal{H}_X\right] \end{aligned} \tag{2.8}$$

For the SIAM (and noting that we are decoupling $q\beta$), the two parts are

$$\begin{aligned} \mathcal{H}_0 &= \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \epsilon_d \hat{n}_d + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + \sum_{k\sigma \neq q\beta} \left(c^\dagger_{k\sigma} c_{d\sigma} + \text{h.c.}\right) \\ \mathcal{H}_X &= c^\dagger_{q\beta} c_{d\beta} + \text{h.c.} \end{aligned} \tag{2.9}$$

The renormalization in the effective Hamiltonian from decoupling a high energy particle state is thus

$$\begin{aligned} \frac{1}{2}\left[S, \mathcal{H}_X\right] &= |V|^2 \left[\frac{1-\hat{n}_{d\bar{\beta}}}{\epsilon_q - \epsilon_d} + \frac{\hat{n}_{d\bar{\beta}}}{\epsilon_q - \epsilon_d - U}\right] \left[\hat{n}_{q\beta}\left(1-\hat{n}_{d\beta}\right) - \hat{n}_{d\beta}\left(1-\hat{n}_{q\beta}\right)\right] \\ &= -\hat{n}_{d\beta}|V|^2 \left[\frac{1-\hat{n}_{d\bar{\beta}}}{\epsilon_q - \epsilon_d} + \frac{\hat{n}_{d\bar{\beta}}}{\epsilon_q - \epsilon_d - U}\right] \end{aligned} \tag{2.10}$$

In the last step, we put $\hat{n}_{q\beta} = 0$ because previously we assumed $\epsilon_q > 0$ and high energy virtual excitations above the Fermi surface must necessarily be vacant in the initial state. We can obtain the renormalization from decoupling a high energy *hole* state directly from this expression, just by choosing $\hat{n}_{q\beta} = 1$ and setting $\epsilon_q \to -\epsilon_q$.

$$\frac{1}{2}\left[S, \mathcal{H}_X\right] = -\left(1-\hat{n}_{d\beta}\right)|V|^2 \left[\frac{1-\hat{n}_{d\bar{\beta}}}{\epsilon_q + \epsilon_d} + \frac{\hat{n}_{d\bar{\beta}}}{\epsilon_q + \epsilon_d + U}\right] \tag{2.11}$$

These two results - the renormalization in the particle and hole sectors - is *identical to the result obtained from PMS* of the SIAM (see [3]).

Avoiding the perturbative route, we can take $S = \frac{\pi}{4}\left(\eta^\dagger - \eta\right)$, where η and its conjugate are non-perturbative and Fermionic - they satisfy $\eta^2 = \eta^{\dagger 2} = 0$ and $\left\{\eta, \eta^\dagger\right\} = 1$. We can then write

$$\begin{aligned} e^S &= \exp\left(\frac{\pi}{4}\left(\eta^\dagger - \eta\right)\right) \\ &= 1 + \left(\eta^\dagger - \eta\right)\frac{\pi}{4} + \frac{1}{2!}\left(\eta^\dagger - \eta\right)^2\left(\frac{\pi}{4}\right)^2 + \frac{1}{3!}\left(\eta^\dagger - \eta\right)^3\left(\frac{\pi}{4}\right)^3 + ... \\ &= 1 + \left(\eta^\dagger - \eta\right)\frac{\pi}{4} - \frac{1}{2!}\left(\frac{\pi}{4}\right)^2 - \frac{1}{3!}\left(\eta^\dagger - \eta\right)\left(\frac{\pi}{4}\right)^3 + \frac{1}{4!}\left(\frac{\pi}{4}\right)^4 + ... \\ &= \cos\frac{\pi}{4} + \left(\eta^\dagger - \eta\right)\sin\frac{\pi}{4} \\ &= \frac{1}{\sqrt{2}}\left(1 + \eta^\dagger - \eta\right) \end{aligned} \tag{2.12}$$

There we used

$$\left(\eta^\dagger - \eta\right)^2 = {\eta^\dagger}^2 + \eta^2 - \left\{\eta^\dagger, \eta\right\} = -1 \quad \left[\because \eta^2 = {\eta^\dagger}^2 = 0\right] \tag{2.13}$$

and hence

$$\left(\eta^\dagger - \eta\right)^3 = -1\left(\eta^\dagger - \eta\right) \tag{2.14}$$

and so on. This simplification allows us to write

$$\cosh S = \frac{1}{2}\left[e^S + e^{-S}\right] = \frac{1}{2\sqrt{2}}\left(1 + \eta^\dagger - \eta + 1 - \eta^\dagger + \eta\right) = \frac{1}{\sqrt{2}} \tag{2.15}$$

and

$$\sinh S = \frac{1}{2}\left[e^S - e^{-S}\right] = \frac{1}{2\sqrt{2}}\left(1 + \eta^\dagger - \eta - 1 + \eta^\dagger - \eta\right) = \frac{1}{\sqrt{2}}\left(\eta^\dagger - \eta\right) \tag{2.16}$$

The off-diagonal part now becomes

$$H_2 = \frac{1}{2}\left(\mathcal{H}_X - \eta^\dagger \mathcal{H}_X \eta^\dagger - \eta \mathcal{H}_X \eta + \left[\eta^\dagger - \eta, \mathcal{H}_0\right]\right) \tag{2.17}$$

The vanishing of this quantity is now the decoupling condition, and is also given in eq 16 of ref. [1].

To look for a decoupling condition similar to eq. 2.5, we can re-express the cosh and sinh in eq. 2.15 in terms of S, by substituting $\eta^\dagger - \eta = \frac{4}{\pi}S$:

$$\cosh S = \frac{1}{\sqrt{2}}, \text{ and } \sinh S = \frac{4}{\sqrt{2}\pi}S \tag{2.18}$$

That gives

$$H_2 = \frac{1}{2}\left[\frac{4}{\pi}\left[S, \mathcal{H}_0\right] + \mathcal{H}_X - \frac{16}{\pi^2} S \mathcal{H}_X S\right] \tag{2.19}$$

The decoupling condition becomes

$$\left[S, \mathcal{H}_0\right] = -\frac{\pi}{4}\mathcal{H}_X + \frac{4}{\pi} S \mathcal{H}_X S \tag{2.20}$$

This can be compared to the second order condition: $\left[S, \mathcal{H}_0\right] = -\mathcal{H}_X$. We can also write the effective Hamiltonian for this non-perturbative case.

$$U\mathcal{H}U^\dagger = H_1 = \frac{1}{2}\mathcal{H}_0 - \frac{4}{\pi^2} S \mathcal{H}_0 S + \frac{2}{\pi}\left[S, \mathcal{H}_X\right] \tag{2.21}$$

The differences between the perturbative and non-perturbative ways are summarized in table 1. There appear to be two differences between these decoupling conditions: (a) a pre-factor of $\frac{\pi}{4}$ for the first term on the right hand side, and (b) the altogether new second term on the right hand side. Both are outcomes of the non-perturbative nature of URG. This offers evidence that the physics captured by the effective Hamiltonian (and its associated low-energy many-particle Hilbert space) obtained from URG lies well beyond that obtained from SWT. Further, it shows that the SWT can only be justified as an expansion in a small parameter (say, $\frac{1}{U}$) in the Anderson impurity problem), followed by a truncation of the BCH expansion and a projection onto a particular low-energy subspace. The truncation and projection are adopted simultaneously, and appear to impose the limit of $U = \infty$ by hand. The URG flow never attains such a limit, thus suggesting that there exists a lot of interesting physics that could potentially be lost in the SWT procedure. Further, the projection finally applied within SWT means that we can never recover what is thrown away. This is again not the case with URG.

	renormalization	decoupling condition
SWT	$\frac{1}{2}[S, \mathcal{H}_X]$	$[S, \mathcal{H}_0] = -\mathcal{H}_X$
URG	$\frac{2}{\pi}[S, \mathcal{H}_X]$	$[S, \mathcal{H}_0] = -\frac{\pi}{4}\mathcal{H}_X + \frac{4}{\pi}S\mathcal{H}_X S$

Table 1: Comparison of perturbative and non-perturbative canonical transformations

2.2 Kondo model from PMS-type approach

In the previous section, we saw that a step-by-step SWT gives the same effective Hamiltonian as the application of PMS. The converse is also true. That is, decoupling the whole band of mobile electrons using the formalism of PMS gives the same effective Hamiltonian as an SWT.

First note that the goal of PMS here would be to decouple the single-occupied subspace of the impurity from the doublon and holon subspaces. To that end, we write the interaction part of the Hamiltonian as

$$\begin{aligned}\sum_{k\sigma}\left(V_k c^\dagger_{k\sigma} c_{d\sigma} + \text{h.c.}\right) &= \sum_{k\sigma}\left[V_k c^\dagger_{k\sigma} c_{d\sigma}\left\{\hat{n}_{d\bar{\sigma}} + (1-\hat{n}_{d\bar{\sigma}})\right\} + \text{h.c.}\right] \\ &= V_{2\to1} + V_{1\to0} + \text{h.c.}\end{aligned} \tag{2.22}$$

where

$$V_{2\to1} = \sum_{k\sigma} V_k c^\dagger_{k\sigma} c_{d\sigma} \hat{n}_{d\bar{\sigma}} \tag{2.23}$$

takes us from doublon to spinon while

$$V_{1\to0} = \sum_{k\sigma} V_k c^\dagger_{k\sigma} c_{d\sigma} (1-\hat{n}_{d\bar{\sigma}}) \tag{2.24}$$

takes us from spinon to holon. The Hermitian conjugate involves $V_{1\to2} = \sum_{k\sigma} V_k^* c^\dagger_{d\sigma} c_{k\sigma} \hat{n}_{d\bar{\sigma}}$ and $V_{0\to1} = \sum_{k\sigma} V_k^* c^\dagger_{d\sigma} c_{k\sigma} (1-\hat{n}_{d\bar{\sigma}})$. Similarly, the diagonal part can be separated as follows:

$$\mathcal{H}_D = \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \epsilon_d \sum_\sigma \hat{n}_{d\sigma}(1-\hat{n}_{d\bar{\sigma}}) + (2\epsilon_d + U)\,\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} = \mathcal{H}_{\text{bath}} + H_1 + H_2 \tag{2.25}$$

We can now separate the Hamiltonian into the three subspaces:

$$\begin{aligned}E|\psi\rangle &= \mathcal{H}|\psi\rangle \\ &= (\mathcal{H}_0 + V_{0\to1})|\psi_0\rangle + (\mathcal{H}_0 + H_1 + V_{1\to2} + V_{1\to0})|\psi_1\rangle + (\mathcal{H}_0 + H_2 + V_{2\to1})|\psi_2\rangle\end{aligned} \tag{2.26}$$

where $|\psi_i\rangle = |n_d = i\rangle\langle n_d = i||\psi\rangle$. We can separate the entire equation into three individual equations for each of the three subspaces:

$$\begin{aligned}E|\psi_0\rangle &= \mathcal{H}_0|\psi_0\rangle + V_{1\to0}|\psi_1\rangle \\ E|\psi_1\rangle &= (\mathcal{H}_0 + \epsilon_d)|\psi_1\rangle + V_{0\to1}|\psi_0\rangle + V_{2\to1}|\psi_2\rangle \\ E|\psi_2\rangle &= (\mathcal{H}_0 + 2\epsilon_d + U + V_{1\to2})|\psi_1\rangle\end{aligned} \tag{2.27}$$

Eliminating $|\psi_0\rangle$ and $|\psi_2\rangle$ from the equations gives the effective Hamiltonian in the single-occupied subspace.

$$\begin{aligned} E|\psi_1\rangle &= \left[\mathcal{H}_0 + \epsilon_d + V_{0\to1}\frac{1}{E-\mathcal{H}_0}V_{1\to0} + V_{2\to1}\frac{1}{E-\mathcal{H}_0-2\epsilon_d-U}V_{1\to2}\right]|\psi_1\rangle \\ &= \mathcal{H}_{\text{eff}}|\psi_1\rangle \end{aligned} \tag{2.28}$$

We can evaluate the effective Hamiltonian.

$$\mathcal{H}_{\text{eff}} = \mathcal{H}_0 + \epsilon_d + V_{0\to1}\frac{1}{E-\mathcal{H}_0}V_{1\to0} + V_{2\to1}\frac{1}{E-\mathcal{H}_0-2\epsilon_d-U}V_{1\to2} \tag{2.29}$$

The first renormalization term gives

$$V_{0\to1}\frac{1}{E-\mathcal{H}_0}V_{1\to0} = \sum_{kq\sigma\alpha} V_k^* V_q c_{d\sigma}^\dagger c_{k\sigma}\left(1-\hat{n}_{d\bar{\sigma}}\right)\frac{1}{E-\mathcal{H}_0}c_{q\gamma}^\dagger c_{d\gamma}\left(1-\hat{n}_{d\bar{\gamma}}\right) \tag{2.30}$$

We can *approximate* E by replacing it with the bare energy of $|\psi_1\rangle$: $E = \mathcal{H}_0 - \epsilon_q + \epsilon_d$.

$$V_{0\to1}\frac{1}{E-\mathcal{H}_0}V_{1\to0} = \sum_{kq\sigma\gamma} V_k^* V_q c_{d\sigma}^\dagger c_{k\sigma}\left(1-\hat{n}_{d\bar{\sigma}}\right)c_{q\gamma}^\dagger c_{d\gamma}\left(1-\hat{n}_{d\bar{\gamma}}\right)\frac{1}{\epsilon_d-\epsilon_q} \tag{2.31}$$

Similarly, the second term becomes

$$V_{2\to1}\frac{1}{E-\mathcal{H}_0-2\epsilon_d-U}V_{1\to2} = \sum_{kq\sigma\gamma} V_k^* V_q c_{q\gamma}^\dagger c_{d\gamma}\hat{n}_{d\bar{\gamma}}\frac{1}{E-\mathcal{H}_0-2\epsilon_d-U}c_{d\sigma}^\dagger c_{k\sigma}\hat{n}_{d\bar{\sigma}} \tag{2.32}$$

We again approximate E: $E = \mathcal{H}_0 + \epsilon_k - \epsilon_d$:

$$V_{2\to1}\frac{1}{E-\mathcal{H}_0-2\epsilon_d-U}V_{1\to2} = \sum_{kq\sigma\gamma} V_k^* V_q c_{q\gamma}^\dagger c_{d\gamma}\hat{n}_{d\bar{\gamma}}c_{d\sigma}^\dagger c_{k\sigma}\hat{n}_{d\bar{\sigma}}\frac{1}{\epsilon_k-\epsilon_d-U} \tag{2.33}$$

The sum of these two terms give the total renormalization. First we look at those terms where $\gamma = \sigma$. The total renormalization from that part is

$$\begin{aligned} \sum_{kq\sigma} V_k^* V_q\left[\frac{\hat{n}_{d\sigma}\left(1-\hat{n}_{d\bar{\sigma}}\right)c_{k\sigma}c_{q\sigma}^\dagger}{\epsilon_d-\epsilon_q} + \frac{\left(1-\hat{n}_{d\sigma}\right)\hat{n}_{d\bar{\sigma}}c_{q\sigma}^\dagger c_{k\sigma}}{\epsilon_k-\epsilon_d-U}\right] &= \sum_{kq\sigma} V_k^* V_q\left[\frac{\hat{n}_{d\sigma}c_{k\sigma}c_{q\sigma}^\dagger}{\epsilon_d-\epsilon_q} + \frac{\hat{n}_{d\bar{\sigma}}c_{q\sigma}^\dagger c_{k\sigma}}{\epsilon_k-\epsilon_d-U}\right] \\ &= \sum_{kq\sigma} V_k^* V_q\left[\frac{\hat{n}_{d\sigma}c_{q\sigma}^\dagger c_{k\sigma}}{\epsilon_q-\epsilon_d} + \frac{\hat{n}_{d\bar{\sigma}}c_{q\sigma}^\dagger c_{k\sigma}}{\epsilon_k-\epsilon_d-U}\right] \end{aligned} \tag{2.34}$$

In the first step we used $\hat{n}_\sigma\hat{n}_{d\bar{\sigma}} = 0$ because we are in the single-occupied subspace and in the second step we used $c_{k\sigma}c_{q\sigma}^\dagger = \delta_{kq} - c_{q\sigma}^\dagger c_{k\sigma}$ and dropped the constant δ part. We can now write this this thing in terms of spin operator $S_d^z = \frac{1}{2}\sigma\left(\hat{n}_{d\sigma} - \hat{n}_{d\bar{\sigma}}\right)$ and also use $\hat{n}_\sigma + \hat{n}_{\bar{\sigma}} = 1$. They give

$$\begin{aligned} &\sum_{kq\sigma} V_k^* V_q\left[\frac{\left(\frac{1}{2}+\sigma S_d^z\right)c_{q\sigma}^\dagger c_{k\sigma}}{\epsilon_q-\epsilon_d} + \frac{\left(\frac{1}{2}-\sigma S_d^z\right)c_{q\sigma}^\dagger c_{k\sigma}}{\epsilon_k-\epsilon_d-U}\right] \\ &= \sum_{kq\sigma} V_k^* V_q S_d^z\sigma c_{q\sigma}^\dagger c_{k\sigma}\left[\frac{1}{\epsilon_q-\epsilon_d} - \frac{1}{\epsilon_k-\epsilon_d-U}\right] + \frac{1}{2}\sum_{kq\sigma} V_k^* V_q c_{q\sigma}^\dagger c_{k\sigma}\left[\frac{1}{\epsilon_q-\epsilon_d} + \frac{1}{\epsilon_k-\epsilon_d-U}\right] \end{aligned} \tag{2.35}$$

The latter term is a potential scattering term; it vanishes in the particle-hole symmetric case ($\epsilon_d + U = -\epsilon_d$) and we will ignore it from now. The first term is the gives rise to the spin-preserving scattering in the s-d model; we can write $\sum_\sigma \sigma c^\dagger_{q\sigma} c_{k\sigma} = c^\dagger_{q\uparrow} c_{k\uparrow} - c^\dagger_{q\downarrow} c_{k\downarrow} \equiv 2 s^z_{kq}$. Defining $J_{kq} = V_k^* V_q \left[\frac{1}{\epsilon_q - \epsilon_d} - \frac{1}{\epsilon_k - \epsilon_d - U}\right]$, gives us the first term in s-d model

$$2 \sum_{kq} J_{kq} S^z_d s^z_{kq} \tag{2.36}$$

Setting $\gamma = \overline{\sigma}$ in the total renormalization gives the rest of the terms:

$$\sum_{kq\sigma} V_k^* V_q c^\dagger_{d\sigma} c_{d\overline{\sigma}} c^\dagger_{q\overline{\sigma}} c_{k\sigma} \left[\frac{-1}{\epsilon_d - \epsilon_q} + \frac{-1}{\epsilon_k - \epsilon_d - U}\right] = \sum_{kq\sigma} J_{kq} c^\dagger_{d\sigma} c_{d\overline{\sigma}} c^\dagger_{q\overline{\sigma}} c_{k\sigma} \tag{2.37}$$

We can define $S^\sigma_d = c^\dagger_{d\sigma} c_{d\overline{\sigma}}$ where $\sigma \in \{+, -\}$ and $s^{\overline{\sigma}}_{kq} = c^\dagger_{q\overline{\sigma}} c_{k\sigma}$. This gives

$$\sum_{kq\sigma} J_{kq} S^\sigma_d s^{\overline{\sigma}}_{kq} = \sum_{kq} J_{kq} \left(S^+_d s^-_{kq} + S^-_d s^+_{kq}\right) \tag{2.38}$$

The total renormalization, minus the potential scattering and constant terms constitutes the spin-flip scattering part of the Kondo model:

$$\mathcal{H}_{s-d} = 2 \sum_{kq} J_{kq} \left[S^z_d s^z_{kq} + \frac{1}{2}\left(S^+_d s^-_{kq} + S^-_d s^+_{kq}\right)\right] = 2 \sum_{kq} J_{kq} \vec{S}_d \cdot \vec{s}_{kq} \tag{2.39}$$

Note that when we wrote the entire Schrodinger equation in the subspace of $|\psi_1\rangle$, we projected out all contributions of the Hamiltonian in the subspace of the doublon and holon. To recover those parts, we can look at eq. 2.27 by eliminating $|\psi_1\rangle$. That gives

$$\begin{aligned} E|\psi_0\rangle &= \left(\mathcal{H}_0 + V_{1\to 0} \frac{1}{E - \mathcal{H}_0 - \epsilon_d} V_{0\to 1}\right)|\psi_0\rangle + V_{1\to 0} \frac{1}{E - \mathcal{H}_0 - \epsilon_d} V_{2\to 1} \psi_2 \\ E|\psi_2\rangle &= \left(\mathcal{H}_0 + 2\epsilon_d + U + V_{1\to 2} \frac{1}{E - \mathcal{H}_0 - \epsilon_d} V_{2\to 1}\right)|\psi_2\rangle + V_{1\to 2} \frac{1}{E - \mathcal{H}_0 - \epsilon_d} V_{0\to 1} \psi_0 \end{aligned} \tag{2.40}$$

It can be represented in the matrix form:

$$\begin{pmatrix} \mathcal{H}_0 + V_{1\to 0} \frac{1}{E - \mathcal{H}_0 - \epsilon_d} V_{0\to 1} & V_{1\to 0} \frac{1}{E - \mathcal{H}_0 - \epsilon_d} V_{2\to 1} \\ V_{1\to 2} \frac{1}{E - \mathcal{H}_0 - \epsilon_d} V_{0\to 1} & \mathcal{H}_0 + 2\epsilon_d + U + V_{1\to 2} \frac{1}{E - \mathcal{H}_0 - \epsilon_d} V_{2\to 1} \end{pmatrix} \begin{pmatrix} \psi_0 \\ \psi_2 \end{pmatrix} = E \begin{pmatrix} \psi_0 \\ \psi_2 \end{pmatrix} \tag{2.41}$$

There are two scattering terms in each equation. The first scattering term (of the forms $V_{1\to 0} G V_{0\to 1}$ and $V_{1\to 2} G V_{2\to 1}$) involve virtual excitations to the single-occupied subspace. They are diagonal in their respective subspaces. However, *the second scattering term in each equation, of the form $V_{1\to 0} G V_{2\to 1}$ or $V_{1\to 2} G V_{0\to 1}$ scatter between the doublon and holon subspace.* The first one takes you from the doublon to the holon ($2 \to 1 \to 0$), the second one does the oppposte. Let us take a look at these terms. The first term becomes

$$\begin{aligned} V_{1\to 0} \frac{1}{E - \mathcal{H}_0 - \epsilon_d} V_{2\to 1} &= \sum_{kq\sigma\gamma} V_q c^\dagger_{q\gamma} c_{d\gamma} \left(1 - \hat{n}_{d\overline{\gamma}}\right) \frac{1}{E - \mathcal{H}_0 - \epsilon_d} V_k c^\dagger_{k\sigma} c_{d\sigma} \hat{n}_{d\overline{\sigma}} \\ &= \sum_{kq\sigma\gamma} V_q c^\dagger_{q\gamma} c_{d\gamma} \left(1 - \hat{n}_{d\overline{\gamma}}\right) V_k c^\dagger_{k\sigma} c_{d\sigma} \hat{n}_{d\overline{\sigma}} \frac{1}{\epsilon_d + U - \epsilon_k} \end{aligned} \tag{2.42}$$

where I put $E = \mathcal{H}_0 - \epsilon_k + 2\epsilon_d + U$ as the energy of the initial state $|\psi_2\rangle$. Since the expression has $c_{d\gamma}$ followed by $c_{d\sigma}$ with only diagonal terms in between, we must have $\gamma = \overline{\sigma}$. Hence it becomes

$$\begin{aligned}\sum_{kq\sigma} V_q V_k c^\dagger_{q\overline{\sigma}} c_{d\overline{\sigma}} c^\dagger_{k\sigma} c_{d\sigma} \frac{1}{\epsilon_d + U - \epsilon_k} &= \sum_{kq} V_q V_k \frac{1}{\epsilon_d + U - \epsilon_k} \left[c^\dagger_{q\uparrow} c^\dagger_{k\downarrow} c_{d\downarrow} c_{d\uparrow} + c^\dagger_{q\downarrow} c^\dagger_{k\uparrow} c_{d\uparrow} c_{d\downarrow} \right] \\ &= \sum_{kq} V_q V_k \frac{1}{\epsilon_d + U - \epsilon_k} \left[c^\dagger_{q\uparrow} c^\dagger_{k\downarrow} c_{d\downarrow} c_{d\uparrow} + c^\dagger_{k\uparrow} c^\dagger_{q\downarrow} c_{d\downarrow} c_{d\uparrow} \right] \\ &= \sum_{kq} V_q V_k c^\dagger_{q\uparrow} c^\dagger_{k\downarrow} c_{d\downarrow} c_{d\uparrow} \left(\frac{1}{\epsilon_d + U - \epsilon_k} + \frac{1}{\epsilon_d + U - \epsilon_q} \right)\end{aligned} \tag{2.43}$$

In the last step, we relabeled $k \leftrightarrow q$. The second scattering term similarly becomes

$$\begin{aligned}V_{1\to 2} \frac{1}{E - \mathcal{H}_0 - \epsilon_d} V_{0\to 1} &= \sum_{kq\sigma\gamma} V^*_q c^\dagger_{d\gamma} c_{q\gamma} \hat{n}_{d\overline{\gamma}} \frac{1}{E - \mathcal{H}_0 - \epsilon_d} V^*_k c^\dagger_{d\sigma} c_{k\sigma} \left(1 - \hat{n}_{d\overline{\sigma}}\right) \\ &= \sum_{kq\sigma} V^*_q V^*_k c^\dagger_{d\overline{\sigma}} c_{q\overline{\sigma}} c^\dagger_{d\sigma} c_{k\sigma} \frac{1}{\epsilon_k - \epsilon_d} \\ &= \sum_{kq} V^*_q V^*_k \left(\frac{1}{\epsilon_k - \epsilon_d} + \frac{1}{\epsilon_q - \epsilon_d} \right) c^\dagger_{d\uparrow} c^\dagger_{d\downarrow} c_{k\downarrow} c_{q\uparrow}\end{aligned} \tag{2.44}$$

Combining the two terms, we get the total charge-Kondo contribution:

$$\begin{aligned}\mathcal{H}_{ch} = &\sum_{kq} V_q V_k c^\dagger_{q\uparrow} c^\dagger_{k\downarrow} c_{d\downarrow} c_{d\uparrow} \left(\frac{1}{\epsilon_d + U - \epsilon_k} + \frac{1}{\epsilon_d + U - \epsilon_q} \right) \\ &+ \sum_{kq} V^*_q V^*_k c^\dagger_{d\uparrow} c^\dagger_{d\downarrow} c_{k\downarrow} c_{q\uparrow} \left(\frac{1}{\epsilon_k - \epsilon_d} + \frac{1}{\epsilon_q - \epsilon_d} \right)\end{aligned} \tag{2.45}$$

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