Unitary Renormalization Group Approach to Single-Impurity Anderson Model

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1 Unitary Renormalization Group Method

This section is adapted from ref.[1].

1.1 Description of the problem

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 ($q\beta$).

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

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.

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

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 $q\beta$:

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

where $|\phi^i_j\rangle = \langle j| |\psi_i\rangle$. 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 $H_e = \text{tr}\left[\mathcal{H}\hat{n}_{q\beta}\right]$ 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,

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

This gives

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

1.2 Obtaining the decoupling transformation

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

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

From the definition of $\hat{\omega}_i$, we can see that it is Hermitian and has no term that scatters in the subspace of $q\beta$, so it is diagonal in $q\beta$ and we can expand it as $\hat{\omega}_i = \hat{\omega}^1_i\hat{n}_{q\beta} + \hat{\omega}^0_i\left(1-\hat{n}_{q\beta}\right)$. Using the expansion 1.6, we can write

$$\hat{\omega}_i|\psi_i\rangle = \hat{\omega}^1_i|1\rangle|\phi^i_1\rangle + \hat{\omega}^0_i|0\rangle|\phi^i_0\rangle \tag{1.10}$$

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 $|\phi^i_{0,}\rangle$ to be an eigenstates of $\hat{\omega}^{1,0}_i$ corresponding to real eigenvalues $\omega^{1,0}_i$:

$$\left[\mathcal{H}^d + c^\dagger_{q\beta}T + T^\dagger c_{q\beta}\right]|\psi_i(\omega_i)\rangle = \left(\omega^1_i - \mathcal{H}^d\right)|1\rangle|\phi^i_1\rangle + \left(\omega^0_i - \mathcal{H}^d\right)|0\rangle|\phi^i_0\rangle \tag{1.11}$$

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

$$c^\dagger_{q\beta}T|0\rangle|\phi^i_0\rangle = \left(\omega^1_i - \mathcal{H}^d\right)|1\rangle|\phi^i_1\rangle \tag{1.12}$$

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

$$T^\dagger c_{q\beta}|1\rangle|\phi^i_1\rangle = \left(\omega^0_i - \mathcal{H}^d\right)|0\rangle|\phi^i_0\rangle \tag{1.13}$$

We now define two many-particle transition operators:

$$\begin{aligned}\eta^\dagger(\omega^1_i) &= \frac{1}{\omega^1_i - \mathcal{H}^d}c^\dagger_{q\beta}T \\ \eta(\omega^0_i) &= \frac{1}{\omega^0_i - \mathcal{H}^d}T^\dagger c_{q\beta}\end{aligned} \tag{1.14}$$

We can write this compactly as

$$\eta(\hat{\omega}) = \frac{1}{\hat{\omega}_i - \mathcal{H}^d}T^\dagger c_{q\beta} \tag{1.15}$$

where $\hat{\omega}_i = \omega^0_i\left(1-\hat{n}_{q\beta}\right) + \omega^1_i\hat{n}_{q\beta} = \begin{pmatrix}\omega^1_i & \\ & \omega^0_i\end{pmatrix}$ is a 2x2 matrix and $\mathcal{H}^d = \mathcal{H}^d_0\left(1-\hat{n}_{q\beta}\right) + \mathcal{H}^d_1\hat{n}_{q\beta}$. It is easy to check that this reproduces the previous forms of η_0 and $\eta^\dagger_1$. We will

later find that it is important to demand that these two be Hermitian conjugates of each other; that constraint is imposed on the denominators:

$$\eta^\dagger(\omega_i^0) = \eta^\dagger(\omega_i^1) \implies \frac{1}{\omega_i^1 - \mathcal{H}^d} c_{q\beta}^\dagger T = c_{q\beta}^\dagger T \frac{1}{\omega_i^0 - \mathcal{H}^d} \tag{1.16}$$

Henceforth we will assume that this constraint has been imposed.

In terms of these operators, eq. 1.13 becomes

$$\begin{aligned} |1\rangle |\phi_1^i\rangle &= \eta^\dagger |0\rangle |\phi_0^i\rangle \\ |0\rangle |\phi_0^i\rangle &= \eta |1\rangle |\phi_1^i\rangle \end{aligned} \tag{1.17}$$

These allow us to write

$$\begin{aligned} |\psi_1\rangle &= |1\rangle |\phi_1^i\rangle + |0\rangle |\phi_0^i\rangle = (1+\eta) |1\rangle |\phi_1^i\rangle \\ |\psi_0\rangle &= \left(1+\eta^\dagger\right) |0\rangle |\phi_0^i\rangle \end{aligned} \tag{1.18}$$

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

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

1.3 Properties of the many-body transition operator η

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

$$\eta^2 = \eta^{\dagger 2} = 0 \quad \left[c^{\dagger 2} = c^2 = 0\right] \tag{1.20}$$

Second is:

$$\begin{aligned} |1\rangle |\phi_1^i\rangle = \eta^\dagger |0\rangle |\phi_0^i\rangle = \eta^\dagger \eta |1\rangle |\phi_1^i\rangle &\implies \eta^\dagger \eta = \hat{n}_{q\beta} \\ |0\rangle |\phi_0^i\rangle = \eta |1\rangle |\phi_1^i\rangle = \eta\eta^\dagger |\phi_0^i\rangle &\implies \eta\eta^\dagger = 1 - \hat{n}_{q\beta} \end{aligned} \tag{1.21}$$

and hence the anticommutator

$$\implies \left\{\eta, \eta^\dagger\right\} = 1 \tag{1.22}$$

Note that the three equations in 1.21 work only when applied on the eigenstate $|\psi_i\rangle$ and not any arbitrary state.

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

1.4 Form of the unitary operators

Although we have found the correct similarity transformations U_i (eqs. 1.19), 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

$$U_1 = 1 + \eta \tag{1.23}$$

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

$$U_1 = e^{\eta} \tag{1.24}$$

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

$$G = \tanh^{-1}\left(\omega - \omega^{\dagger}\right) \tag{1.25}$$

Applying that to the problem at hand gives

$$\begin{aligned} U_1^{\dagger} &= \exp\left(\tanh^{-1}\left(\eta - \eta^{\dagger}\right)\right) \\ &= \frac{1 + \eta - \eta^{\dagger}}{1 + \{\eta, \eta^{\dagger}\}} \\ &= \frac{1}{\sqrt{2}}\left(1 + \eta - \eta^{\dagger}\right) \end{aligned} \tag{1.26}$$

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

$$U_1 = \frac{1}{\sqrt{2}}\left(1 + \eta^{\dagger} - \eta\right) \tag{1.27}$$

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

$$\begin{aligned} \exp\left(\frac{\pi}{4}\left(\eta^{\dagger} - \eta\right)\right) &= 1 + \left(\eta^{\dagger} - \eta\right)\frac{\pi}{4} + \frac{1}{2!}\left(\eta^{\dagger} - \eta\right)^2\left(\frac{\pi}{4}\right)^2 + \frac{1}{3!}\left(\eta^{\dagger} - \eta\right)^3\left(\frac{\pi}{4}\right)^3 + \ldots \\ &= 1 + \left(\eta^{\dagger} - \eta\right)\frac{\pi}{4} - \frac{1}{2!}\left(\frac{\pi}{4}\right)^2 - \frac{1}{3!}\left(\eta^{\dagger} - \eta\right)\left(\frac{\pi}{4}\right)^3 + \frac{1}{4!}\left(\frac{\pi}{4}\right)^4 + \ldots \\ &= \cos\frac{\pi}{4} + \left(\eta^{\dagger} - \eta\right)\sin\frac{\pi}{4} \\ &= 1 + \eta^{\dagger} - \eta \end{aligned} \tag{1.28}$$

There we used

$$\left(\eta^{\dagger} - \eta\right)^2 = {\eta^{\dagger}}^2 + \eta^2 - \left\{\eta^{\dagger}, \eta\right\} = -1 \quad \left[\because \eta^2 = {\eta^{\dagger}}^2 = 0\right] \tag{1.29}$$

and hence

$$\left(\eta^{\dagger} - \eta\right)^3 = -1\left(\eta^{\dagger} - \eta\right) \tag{1.30}$$

and so on.

1.5 Effective Hamiltonian

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. 1.27,

$$\begin{aligned} U_1\mathcal{H}U_1^\dagger &= \frac{1}{2}\left(1+\eta^\dagger-\eta\right)\mathcal{H}\left(1+\eta-\eta^\dagger\right) \\ &= \frac{1}{2}\left(1+\eta^\dagger-\eta\right)\left(\mathcal{H}+\mathcal{H}\eta-\mathcal{H}\eta^\dagger\right) \\ &= \frac{1}{2}\left(\mathcal{H}+\mathcal{H}\eta-\mathcal{H}\eta^\dagger+\eta^\dagger\mathcal{H}+\eta^\dagger\mathcal{H}\eta-\eta^\dagger\mathcal{H}\eta^\dagger-\eta\mathcal{H}-\eta\mathcal{H}\eta+\eta\mathcal{H}\eta^\dagger\right) \\ &= \frac{1}{2}\left(\mathcal{H}^d+\mathcal{H}^i+\mathcal{H}^I+\mathcal{H}\eta-\mathcal{H}\eta^\dagger+\eta^\dagger\mathcal{H}+\eta^\dagger\mathcal{H}\eta-\eta^\dagger\mathcal{H}\eta^\dagger-\eta\mathcal{H}-\eta\mathcal{H}\eta+\eta\mathcal{H}\eta^\dagger\right) \\ &= \frac{1}{2}\left(\mathcal{H}^d+\mathcal{H}^i+\mathcal{H}^I+\left[\eta^\dagger-\eta,\mathcal{H}\right]+\eta^\dagger\mathcal{H}\eta-\eta^\dagger\mathcal{H}\eta^\dagger-\eta\mathcal{H}\eta+\eta\mathcal{H}\eta^\dagger\right) \end{aligned} \tag{1.31}$$

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, we will split the terms into two groups:

$$\tilde{\mathcal{H}} = \frac{1}{2}\left(\underbrace{\mathcal{H}^d+\mathcal{H}^i+\left[\eta^\dagger-\eta,\mathcal{H}\right]+\eta^\dagger\mathcal{H}\eta+\eta\mathcal{H}\eta^\dagger}_{\text{group 1}}+\overbrace{\mathcal{H}^I-\eta^\dagger\mathcal{H}\eta^\dagger-\eta\mathcal{H}\eta}^{\text{group 2}}\right) \tag{1.32}$$

Group 2 can be easily shown to be 0. Note that terms that have two η or two $\eta^\dagger$ sandwiching a $\mathcal{H}$ can only be nonzero if the intervening $\mathcal{H}$ has an odd number of creation or destruction operators.

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

and

$$\eta^\dagger\mathcal{H}\eta^\dagger = \eta^\dagger T^\dagger c_q\eta^\dagger \tag{1.34}$$

Group 2 becomes

$$\text{group 2} = \mathcal{H}^I-\eta^\dagger T^\dagger c_q\eta^\dagger-\eta c_q^\dagger T\eta = c_q^\dagger T+T^\dagger c_q-\eta^\dagger T^\dagger c_q\eta^\dagger-\eta c_q^\dagger T\eta \tag{1.35}$$

To simplify this, we use the relation

$$\begin{aligned} \eta c_q^\dagger T\eta &= \frac{1}{\omega_i^0-\mathcal{H}^d}T^\dagger c_q c_q^\dagger T\eta \\ &= T^\dagger c_q\frac{1}{\omega_i^1-\mathcal{H}^d}c_q^\dagger T\eta \quad [\text{eq. 1.16}] \\ &= T^\dagger c_q\eta^\dagger\eta \quad [\text{eq. 1.15}] \\ &= T^\dagger c_q\hat{n}_q \quad [\text{eq. 1.21}] \end{aligned} \tag{1.36}$$

which gives

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

Taking the Hermitian conjugate of eq. 1.37 gives

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

Substituting the expressions 1.37 and 1.38 into the expression for group 2, 1.35, shows that is vanishes. This leaves us only with group 1:

$$\widetilde{\mathcal{H}} = \frac{1}{2}\left(\mathcal{H}^d + \mathcal{H}^i + \overbrace{\eta^\dagger \mathcal{H}\eta + \eta\mathcal{H}\eta^\dagger}^{\text{group A}} + \underbrace{\left[\eta^\dagger - \eta, \mathcal{H}\right]}_{groupB}\right) \tag{1.39}$$

Group A simplifies in the following way. First note that $\eta^\dagger \mathcal{H}^I \eta = \eta^\dagger \mathcal{H}^I \eta = 0$ must be 0 because it will involve consecutive $c_{q\beta}$ or consecutive $c^\dagger_{q\beta}$. We are therefore left with the diagonal part of $\mathcal{H}$, which is $H_e \hat{n}_{q\beta} + H_h\left(1 - \hat{n}_{q\beta}\right)$.

$$\eta^\dagger\left[H_e\hat{n}_{q\beta} + H_h\left(1-\hat{n}_{q\beta}\right)\right]\eta + \eta\left[H_e\hat{n}_{q\beta} + H_h\left(1-\hat{n}_{q\beta}\right)\right]\eta^\dagger = \eta^\dagger H_h \eta + \eta H_e \eta^\dagger \tag{1.40}$$

This can be shown (**clear with AM**) to be equal to the diagonal part:

$$\text{group A} = \eta^\dagger H_h \eta + \eta H_e \eta^\dagger = H_e\hat{n}_{q\beta} + H_h\left(1-\hat{n}_{q\beta}\right) = \mathcal{H}^d + \mathcal{H}^i \tag{1.41}$$

It can also be shown (**clear with AM**) that

$$\text{group B} = \left[\eta^\dagger - \eta, \mathcal{H}\right] = 2\left[c^\dagger_{q\beta} T, \eta\right] \tag{1.42}$$

Putting it all together,

$$\tilde{\mathcal{H}} = \mathcal{H}^d + \mathcal{H}^i + \left[c^\dagger_{q\beta} T, \eta\right] \tag{1.43}$$

To check that this indeed commutes with $\hat{n}_{q\beta}$,

$$\begin{aligned}
\left[\widetilde{\mathcal{H}}, \hat{n}_{q\beta}\right] &= \left[\left[c^\dagger_{q\beta}T, \eta\right], \hat{n}_{q\beta}\right] \\
&= \left[c^\dagger_{q\beta}T\eta, \hat{n}_{q\beta}\right] - \left[\eta c^\dagger_{q\beta}T, \hat{n}_{q\beta}\right] \\
&= c^\dagger_{q\beta}T\eta\hat{n}_{q\beta} - \hat{n}_{q\beta}c^\dagger_{q\beta}T\eta \qquad \left[2^{\text{nd}}\ [\ .\ ] \text{ is 0},\ \because c^\dagger_{q\beta}\hat{n}_{q\beta} = \hat{n}_{q\beta}\eta = 0\right] \\
&= c^\dagger_{q\beta}T\eta - c^\dagger_{q\beta}T\eta \\
&= 0
\end{aligned} \tag{1.44}$$

1.6 Fixed point condition

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 either $\omega^1_i = \mathcal{H}^d_1$ or $\omega^0_i = \mathcal{H}^d_0$. This shows that at the fixed point, one of the eigenvalues of $\hat{\omega}_i$ matches the corresponding eigenvalue of the diagonal blocks. This also leads to the vanishing of the off-diagonal block, because eqs. 1.12 and 1.13 gives

$$c^\dagger_{q\beta}T\left|0\right\rangle\left|\phi^i_0\right\rangle = \left(\omega^1_i - \mathcal{H}^d_1\right)\left|1\right\rangle\left|\phi^i_1\right\rangle = 0 \implies c^\dagger_{q\beta}T = 0 \tag{1.45}$$

1.7 Equivalence of the two unitaries

In the subsection 1.4, we determined the form of the operator U_1 that unitarily decouples the node $q\beta$ from the other degrees of freedom. Eq. 1.27 was derived by reading off the

transformation of $|1\rangle$ to $|\psi_1\rangle$, the first equation in 1.18. We could easily have chosen the other equation in the same equation set,

$$|\psi_0\rangle = \left(1+\eta^\dagger\right)|0\rangle\,|\phi_0^i\rangle$$

which gives a similarity transformation $1+\eta^\dagger$ and hence a unitary

$$U_0 = \frac{1}{\sqrt{2}}\left(1+\eta-\eta^\dagger\right) \tag{1.46}$$

This η will however be different from the η in eq. 1.27. The reason is, in order to get U_1, we must start from the eigenvalue equation $\mathcal{H}\,|\psi_1\rangle = \tilde{H}_1\,|\psi_1\rangle$. This means that the corresponding $\hat{\omega}$ will be defined as $\hat{\omega}_1 = \tilde{H}_1 - \mathcal{H}^i$. On the other hand, in order to get U_0 we must start with $\mathcal{H}\,|\psi_0\rangle = \tilde{H}_0\,|\psi_0\rangle$, and hence this $\hat{\omega}$ will be $\hat{\omega}_0 = \tilde{H}_0 - \mathcal{H}^i$. This difference in the $\hat{\omega}$ will define two different sets of η:

$$\begin{aligned}
&\text{Starting from } |\psi_1\rangle\text{: } \eta_1 = \frac{1}{\omega_1^0 - \mathcal{H}^d}T^\dagger c_{q\beta} \quad \text{and } \eta_1^\dagger = \frac{1}{\omega_1^1 - \mathcal{H}^d}T^\dagger c_{q\beta} \\
&\text{Starting from } |\psi_0\rangle\text{: } \eta_0 = \frac{1}{\omega_0^0 - \mathcal{H}^d}T^\dagger c_{q\beta} \quad \text{and } \eta_0^\dagger = \frac{1}{\omega_0^1 - \mathcal{H}^d}T^\dagger c_{q\beta}
\end{aligned} \tag{1.47}$$

The ω_j^i eigenvalues have both upper and lower indices. The upper index i signifies which eigenstate it relates to - $\omega_j\,|i\rangle = \omega_j^i\,|i\rangle$. The lower index refers to the exact eigenstate we started with - starting with $\mathcal{H}\,|\psi_j\rangle = \tilde{H}_j\,|\psi_j\rangle$ leads to ω_j. The two unitaries are

$$\begin{aligned}
U_1 &= \frac{1}{\sqrt{2}}\left(1+\eta_1^\dagger-\eta_1\right) \\
U_0 &= \frac{1}{\sqrt{2}}\left(1+\eta_0-\eta_0^\dagger\right)
\end{aligned} \tag{1.48}$$

Since the two unitaries should give the same effective Hamiltonian, we require $U_1 = U_0$. That requires $\eta_1 = -\eta_0$. Comparing the expressions of the ηs, we get

$$\omega_1^0 - \mathcal{H}_0^d = -\left(\omega_0^0 - \mathcal{H}_0^d\right) \tag{1.49}$$

This is the constraint that ensures that both unitaries give the same effective Hamiltonian. The condition $\eta_1 + \eta_0 = 0$, when expressed without resolving $\hat{\omega}$ into its eigenvalues can also be shown to be a statement of the preservation of the partial trace under the RG flow.

$$\begin{aligned}
\eta_1 &= \frac{1}{\tilde{H}_1 - \mathcal{H}^i - \mathcal{H}^d}T^\dagger c_{q\beta} \\
\eta_0 &= \frac{1}{\tilde{H}_0 - \mathcal{H}^i - \mathcal{H}^d}T^\dagger c_{q\beta} \\
\implies \eta_1 + \eta_0 &= \left[\frac{1}{\tilde{H}_1 - \mathcal{H}^i - \mathcal{H}^d} + \frac{1}{\tilde{H}_0 - \mathcal{H}^i - \mathcal{H}^d}\right]T^\dagger c_{q\beta} = 0 \\
\implies \tilde{H}_1 - \mathcal{H}^i - \mathcal{H}^d &= -\left[\tilde{H}_0 - \mathcal{H}^i - \mathcal{H}^d\right] \\
\implies \tilde{H}_1 + \tilde{H}_0 &= 2\mathcal{H}_0
\end{aligned} \tag{1.50}$$

$\mathcal{H}_0 = \mathcal{H}^i + \mathcal{H}^d$ is the total diagonal part of the bare model. To match the dimensions, we must take $\tilde{H}_1 = E_1 \otimes I$ and similarly $\tilde{H}_0 = E_0 \otimes I$, where the rotated Hamiltonian is

$$\tilde{H} = \begin{pmatrix} E_1 & 0 \\ 0 & E_0 \end{pmatrix} \tag{1.51}$$

Therefore, the trace of the rotated Hamiltonian is $t_{\text{new}} = E_1 + E_0$. The trace of the LHS in the final equation of 1.50 is $\text{tr}\left(\tilde{H}_1 + \tilde{H}_0\right) = \text{tr}\left(E_1 \otimes I + E_0 \otimes I\right) = 2\left(E_1 + E_0\right) = 2t_{\text{new}}$. The trace of the RHS in final equation of 1.50 is $2 \times \text{tr}\left(\mathcal{H}_0\right) = 2t_{\text{old}}$ where $t_{\text{old}} = \text{tr}\left(\mathcal{H}_0\right)$ is the trace of the old Hamiltonian. Equating the LHS and RHS gives $t_{\text{new}} = t_{\text{old}}$.

1.8 Prescription

Given a Hamiltonian

$$\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_0 + c^\dagger T + T^\dagger c \tag{1.52}$$

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. 1.43, 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

$$\Delta\mathcal{H} = \left[c^\dagger_{q\beta}\text{Tr}\left(\mathcal{H}c_{q\beta}\right), \eta\right] = c^\dagger_{q\beta}\text{Tr}\left(\mathcal{H}c_{q\beta}\right)\eta - \eta c^\dagger_{q\beta}\text{Tr}\left(\mathcal{H}c_{q\beta}\right) \tag{1.53}$$

It is clear that the first term takes into account virtual excitations that start from a filled state ($\hat{n}_{q\beta} = 1$ initially) - such a term is said to be a part of the *particle sector*.

$$\Delta_1\mathcal{H} = c^\dagger_{q\beta}\text{Tr}\left(\mathcal{H}c_{q\beta}\right)\eta \tag{1.54}$$

The second term, on the other hand, considers excitations that start from an empty state. They constitute the *hole sector*.

$$\Delta_0\mathcal{H} = -\eta c^\dagger_{q\beta}\text{Tr}\left(\mathcal{H}c_{q\beta}\right) \tag{1.55}$$

Since the effective Hamiltonian eq. 1.43 was derived with the aim of obtaining the particle sector diagonal part, it makes sense to repeat the calculation but now obtain the unitary from the other equation:

$$|\psi_0\rangle = \left(1 + \eta^\dagger\right)|0\rangle\,|\phi^i_0\rangle \implies U_0 = 1 - \eta^\dagger + \eta \tag{1.56}$$

We can similarly obtain a renormalised Hamiltonian for this unitary; it comes out to be

$$\Delta\mathcal{H} = \eta c^\dagger_{q\beta}\text{Tr}\left(\mathcal{H}c_{q\beta}\right) - c^\dagger_{q\beta}\text{Tr}\left(\mathcal{H}c_{q\beta}\right)\eta \tag{1.57}$$

The hole sector renormalization then comes out to be

$$\Delta_0\mathcal{H} = \eta c^\dagger_{q\beta}\text{Tr}\left(\mathcal{H}c_{q\beta}\right) \tag{1.58}$$

The renormalization due to the entire shell is obtained by summing over all states on the shell. Written out explicitly, they take the forms.

$$\Delta_0\mathcal{H} = \sum_{q\beta} c^\dagger_{q\beta}\text{Tr}\left(\mathcal{H}c_{q\beta}\right)\frac{1}{\omega_1 - \mathcal{H}_1^d}\text{Tr}\left(c^\dagger_{q\beta}\mathcal{H}\right)c_{q\beta} \tag{1.59}$$

$$\Delta_1\mathcal{H} = \sum_{q\beta} \text{Tr}\left(c^\dagger_{q\beta}\mathcal{H}\right)c_{q\beta}\frac{1}{\omega_0 - \mathcal{H}_0^d}c^\dagger_{q\beta}\text{Tr}\left(\mathcal{H}c_{q\beta}\right) \tag{1.60}$$

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 typically employ is that $\mathcal{H}^d_{0,1}$ 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; $\text{Tr}\left(c^\dagger_{q\beta}\mathcal{H}\right)c_{q\beta}$ is the off-diagonal term that has $c_{q\beta}$ in it, and $c^\dagger_{q\beta}\text{Tr}\left(\mathcal{H}c_{q\beta}\right)$ is the off-diagonal term that has $c^\dagger_{q\beta}$ in it. $\mathcal{H}^D$ is just the diagonal part of the Hamiltonian.

2 Schrieffer-Wolff Transformation in context of URG

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 $S = \left(A + B\hat{n}_{d\bar{\beta}}\right)\left(c^\dagger_{q\beta}c_{d\beta} - \text{h.c.}\right)$ 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

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

	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

The decoupling condition becomes

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

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

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

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.

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

$$\begin{aligned}\sum_{k\sigma}\left(V_k c^\dagger_{k\sigma} c_{d\sigma} + \text{h.c.}\right) &= \sum_{k\sigma}\left[V_k c^\dagger_{k\sigma} c_{d\sigma}\left\{\hat{n}_{d\bar{\sigma}} + (1 - \hat{n}_{d\bar{\sigma}})\right\} + \text{h.c.}\right] \\ &= V_{2\to 1} + V_{1\to 0} + \text{h.c.}\end{aligned} \tag{2.22}$$

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

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

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 $V_{0\to1} = \sum_{k\sigma} V_k^* c^\dagger_{d\sigma} c_{k\sigma} \left(1 - \hat{n}_{d\bar{\sigma}}\right)$. Similarly, the diagonal part can be separated as follows:

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

We can now separate the Hamiltonian into the three subspaces:

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

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

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

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

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

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

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

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

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

Similarly, the second term becomes

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

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

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

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

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

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 $c_{k\sigma}c^\dagger_{q\sigma} = \delta_{kq} - c^\dagger_{q\sigma}c_{k\sigma}$ and dropped the constant δ part. We can now write this this thing in terms of spin operator $S^z_d = \frac{1}{2}\sigma\left(\hat{n}_{d\sigma}-\hat{n}_{d\bar{\sigma}}\right)$ and also use $\hat{n}_\sigma + \hat{n}_{\bar{\sigma}} = 1$. They give

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

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 $\sum_\sigma \sigma c^\dagger_{q\sigma}c_{k\sigma} = c^\dagger_{q\uparrow}c_{k\uparrow} - c^\dagger_{q\downarrow}c_{k\downarrow} \equiv 2s^z_{kq}$. 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 $\gamma = \bar{\sigma}$ in the total renormalization gives the rest of the terms:

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

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

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

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 $V_{1\to 0}GV_{0\to 1}$ and $V_{1\to 2}GV_{2\to 1}$) 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 $V_{1\to 0}GV_{2\to 1}$ or $V_{1\to 2}GV_{0\to 1}$ 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

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

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 $\gamma=\bar{\sigma}$. Hence it becomes

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

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

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

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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