1 URG 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'.

To begin, we choose an electron with a particular value of quantum numbers, which we label q. It might be the electron with the highest momentum or that at the first lattice site. The goal is to obtain a unitary transformation U_q that diagonalizes this Hamiltonian in this particular electron's basis. Once this is done, we can choose another electron (the next highest momentum or the second lattice site) and diagonalize the Hamiltonian in this electron's basis.

U_q is defined by

$$\tilde{\mathcal{H}} = U_q \mathcal{H} U_q^\dagger \text{ such that } \left[\tilde{\mathcal{H}}, n_q\right] = 0 \tag{1.1}$$

Another way to express the above problem is that, with the original Hamiltonian $\mathcal{H}$, the diagonal terms are not zero:

$$n_q \mathcal{H} (1 - n_q) \neq 0 \tag{1.2}$$

so we want to find a rotated Hamiltonian $\tilde{\mathcal{H}} = U_q \mathcal{H} U_q^\dagger$ such that the off-diagonal term is zero:

$$n_q \tilde{\mathcal{H}} (1 - n_q) = 0 \tag{1.3}$$

To make progress, we write the Hamiltonian $\mathcal{H}$ as

$$\mathcal{H} = \mathcal{H}^D + \mathcal{H}^I + \mathcal{H}^i \tag{1.4}$$

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

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

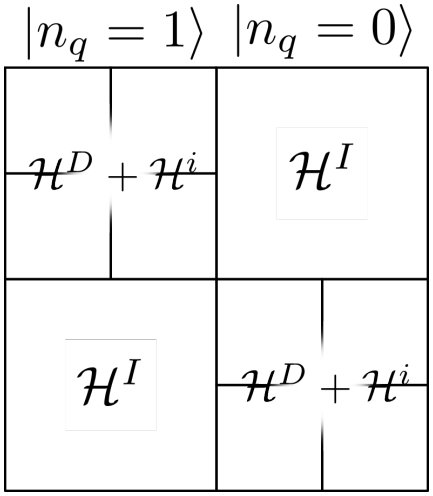

Figure 1: Decomposition of Hamiltonian

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

Let $\left\{|\Psi\rangle_q\right\}$ be the set of states in which $\mathcal{H}$ assumes a diagonal form in the space of q. This diagonal form is of course also what we get when we apply the unitary transformation U_q on the Hamiltonian.

$$\mathcal{H}\,|\Psi\rangle_q = \tilde{\mathcal{H}}\,|\Psi\rangle_q \tag{1.5}$$

This is the equation we will use to find U_q. But first we will write ψ in the following fashion:

$$|\Psi\rangle = a_1\,|1,\Psi_1\rangle + a_0\,|0,\Psi_0\rangle \tag{1.6}$$

In the kets $|1,\Psi_1\rangle$ and $|0,\Psi_0\rangle$, the first entry (0/1) signifies whether the degree of freedom q is occupied or not, and the second entry is the wavefunction of the remaining degrees of freedom. This is just a resolution of the total wavefunction in the two-dimensional Hilbert space of q. Substituting the decomposition of $|\Psi\rangle$ and $\mathcal{H}$ into eq. 1.5 gives

$$\tilde{\mathcal{H}}\left(a_1\,|1,\Psi_1\rangle + a_0\,|0,\Psi_0\rangle\right) = \left[\mathcal{H}^D + \mathcal{H}^I + \mathcal{H}^i\right]\left(a_1\,|1,\Psi_1\rangle + a_0\,|0,\Psi_0\rangle\right) \tag{1.7}$$

To get expressions from this, note that on the left hand side, $\tilde{\mathcal{H}}$ does not scatter q, so it will not change the left entry in the kets; it can only change the right entries. Similarly, on the right hand side, $\mathcal{H}^D$ and $\mathcal{H}^i$ will not change the occupation of the k degree of freedom. $\mathcal{H}^I$ however *will* change it. Matching the states with $|0\rangle$ gives

$$\tilde{\mathcal{H}} a_0\,|0,\Psi_0\rangle = \left(\mathcal{H}^D + \mathcal{H}^i\right) a_0\,|0,\Psi_0\rangle + \mathcal{H}^I a_1\,|1,\Psi_1\rangle \tag{1.8}$$

We can simplify this equation by noting that

$$\mathcal{H}^D = \mathrm{Tr}\left[\mathcal{H}^D \hat{n}_q\right]\hat{n}_q + \mathrm{Tr}\left[\mathcal{H}^D(1-\hat{n}_q)\right](1-\hat{n}_q) \tag{1.9}$$

$$\implies \mathcal{H}^D\,|0,\psi_0\rangle = \mathrm{Tr}\left[\mathcal{H}^D(1-\hat{n}_q)\right](1-\hat{n}_q)\,|0,\psi_0\rangle \tag{1.10}$$

and

$$\mathcal{H}^I = \text{ Tr}\left[c_q^\dagger \mathcal{H}\right] c_q + c_q^\dagger \text{ Tr}\left[\mathcal{H} c_q\right] \implies \mathcal{H}^I \left|1, \psi_1\right\rangle = \text{ Tr}\left[c_q^\dagger \mathcal{H}\right] c_q \left|1, \psi_1\right\rangle \tag{1.11}$$

Substituting these in the equation gives

$$\tilde{\mathcal{H}} a_0 \left|0, \Psi_0\right\rangle = \left\{ \text{ Tr}\left[\mathcal{H}^D (1 - \hat{n}_q)\right] (1 - \hat{n}_q) + \mathcal{H}^i \right\} a_0 \left|0, \Psi_0\right\rangle + \text{ Tr}\left[c_q^\dagger \mathcal{H}\right] c_q a_1 \left|1, \Psi_1\right\rangle \tag{1.12}$$

$$\implies \left\{ \tilde{\mathcal{H}} - \mathcal{H}^i - \text{ Tr}\left[\mathcal{H}^D (1 - \hat{n}_q)\right] (1 - \hat{n}_q) \right\} a_0 \left|0, \Psi_0\right\rangle = \text{ Tr}\left[c_q^\dagger \mathcal{H}\right] c_q a_1 \left|1, \Psi_1\right\rangle \tag{1.13}$$

Defining $\hat{\omega} = \tilde{\mathcal{H}} - \mathcal{H}^i$, we get the result

$$a_0 \left|0, \Psi_0\right\rangle = \left[\hat{\omega} - \text{ Tr}\left[\mathcal{H}^D (1 - \hat{n}_q)\right] (1 - \hat{n}_q)\right]^{-1} \text{ Tr}\left[c_q^\dagger \mathcal{H}\right] c_q a_1 \left|1, \Psi_1\right\rangle \tag{1.14}$$

We define

$$\eta_q \equiv \frac{1}{\hat{\omega} - \text{ Tr}\left[\mathcal{H}^D (1 - \hat{n}_q)\right] (1 - \hat{n}_q)} \text{ Tr}\left[c_q^\dagger \mathcal{H}\right] c_q \tag{1.15}$$

which gives the equation a compact form

$$a_0 \left|0, \Psi_0\right\rangle = \eta_q a_1 \left|1, \Psi_1\right\rangle \tag{1.16}$$

The equation obtained by matching the states $|1\rangle$ is

$$\begin{aligned} a_1 \overline{\mathcal{H}} \left|1, \Psi_1\right\rangle &= \left(\mathcal{H}^D + \mathcal{H}^i\right) a_1 \left|1, \Psi_1\right\rangle + \mathcal{H}^I a_0 \left|0, \Psi_0\right\rangle \\ &= \left(\text{ Tr } \left[\mathcal{H}^D \hat{n}_q\right] \hat{n}_q + \mathcal{H}^i \right) a_1 \left|1, \Psi_1\right\rangle + c_q^\dagger \text{ Tr } \left[\mathcal{H} c_q\right] a_0 \left|0, \Psi_0\right\rangle \\ \implies a_1 \left|\Psi_1\right\rangle &= \left(\overline{\mathcal{H}} - \mathcal{H}^i - \text{ Tr } \left[\mathcal{H}^D \hat{n}_q\right] \hat{n}_q\right)^{-1} c_q^\dagger \text{ Tr } \left[\mathcal{H} c_q\right] a_0 \left|0, \Psi_0\right\rangle \\ &= \mu_q a_0 \left|0, \Psi_0\right\rangle \end{aligned} \tag{1.17}$$

where

$$\mu_q = \frac{1}{\hat{\omega} - \text{ Tr}\left[\mathcal{H}^D \hat{n}_q\right] \hat{n}_q} c_q^\dagger \text{ Tr}\left[\mathcal{H} c_q\right] \tag{1.18}$$

We thus get the following two equations:

$$a_0 \left|0, \Psi_0\right\rangle = \eta_q a_1 \left|1, \Psi_1\right\rangle \tag{1.19}$$

$$a_1 \left|1, \Psi_1\right\rangle = \mu_q a_0 \left|0, \Psi_0\right\rangle \tag{1.20}$$

Combining eqs. 1.19 and 1.20, we get

$$a_0 \left|0, \Psi_0\right\rangle = \eta_q a_1 \left|1, \Psi_1\right\rangle = \eta_q \mu_q a_0 \left|0, \Psi_0\right\rangle \tag{1.21}$$

Combining this with the fact that μ_q should have a $c_q^\dagger$ and hence should give $\mu_q \left|1, \Psi_1\right\rangle$, we get

$$\eta_q \mu_q = 1 - \hat{n}_q \tag{1.22}$$

Similarly, combining the equations the other way round gives

$$\mu_q \eta_q = \hat{n}_q \tag{1.23}$$

As a consequence,

$$\begin{aligned} \{\eta_q, \mu_q\} &= 1 \\ [\eta_q, \mu_q] &= 1 - 2\hat{n}_q \end{aligned} \tag{1.24}$$

Other properties include

$$\eta_q^2 = (\mu_q)^2 = 0 \tag{1.25}$$

$$\hat{n}_q \eta_q = (1 - \hat{n}_q)\mu_q = 0 \tag{1.26}$$

$$\eta_q \hat{n}_q = \eta_q \tag{1.27}$$

$$\mu_q (1 - \hat{n}_q) = \mu_q \tag{1.28}$$

We now need to find the unitary operation U_q that disentangles the state $|1, \Psi_1\rangle$ from the state $|\Psi\rangle$. For the sake of unitarity, we restrict $\mu_q = \eta_q^\dagger$. This restriction is transferred to the values of $\hat{\omega}$. Using eq. 1.19,

$$|\Psi\rangle = a_1 |1, \Psi_1\rangle + a_0 |0, \Psi_0\rangle = a_1 |1, \Psi_1\rangle + \eta_q a_1 |1, \Psi_1\rangle = (1 + \eta_q) |1, \Psi_1\rangle \tag{1.29}$$

Since $\eta^2 = 0$, we can write $1 + \eta_q = e^{\eta_q}$. $S \equiv e^{\eta_q}$ constitutes a similarity transformation. It is shown in ref. [2] that corresponding to a similarity transformation e^{ω},there exists a unitary transformation e^G where

$$G = \tanh^{-1}\left(\omega - \omega^\dagger\right) \tag{1.30}$$

Applying that to the problem at hand gives

$$\begin{aligned} U^\dagger &= \exp\left(\tanh^{-1}\left(\eta - \eta^\dagger\right)\right) \\ &= \frac{1 + \eta - \eta^\dagger}{1 + \{\eta, \eta^\dagger\}} \\ &= \frac{1}{\sqrt{2}}\left(1 + \eta - \eta^\dagger\right) \end{aligned} \tag{1.31}$$

The unitary operator that transforms the entangled eigenstate $|\Psi\rangle$ to the eigenstate with good quantum number n_q, $|1, \Psi_1\rangle$ is thus

$$U_q = \frac{1}{\sqrt{2}}\left(1 + \eta_q^\dagger - \eta_q\right) \tag{1.32}$$

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

$$\begin{aligned}
\exp\left(\frac{\pi}{4}\left(\eta_q^\dagger - \eta_q\right)\right) &= 1 + \left(\eta_q^\dagger - \eta_q\right)\frac{\pi}{4} + \frac{1}{2!}\left(\eta_q^\dagger - \eta_q\right)^2\left(\frac{\pi}{4}\right)^2 + \frac{1}{3!}\left(\eta_q^\dagger - \eta_q\right)^3\left(\frac{\pi}{4}\right)^3 + ... \\
&= 1 + \left(\eta_q^\dagger - \eta_q\right)\frac{\pi}{4} - \frac{1}{2!}\left(\frac{\pi}{4}\right)^2 - \frac{1}{3!}\left(\eta_q^\dagger - \eta_q\right)\left(\frac{\pi}{4}\right)^3 + \frac{1}{4!}\left(\frac{\pi}{4}\right)^4 + ... \\
&= \cos\frac{\pi}{4} + \left(\eta_q^\dagger - \eta_q\right)\sin\frac{\pi}{4} \\
&= 1 + \eta_q^\dagger - \eta_q
\end{aligned} \tag{1.33}$$

There we used

$$\left(\eta_q^\dagger - \eta_q\right)^2 = {\eta_q^\dagger}^2 + \eta_q^2 - \left\{\eta_q^\dagger, \eta_q\right\} = -1 \quad \left[\because \eta^2 = {\eta^\dagger}^2 = 0\right] \tag{1.34}$$

and so

$$\left(\eta_q^\dagger - \eta_q\right)^3 = -1\left(\eta_q^\dagger - \eta_q\right) \tag{1.35}$$

and so on.

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

$$\begin{aligned}
\widetilde{\mathcal{H}} &= U_q \mathcal{H} U_q^\dagger \\
&= \frac{1}{2}\left(1 + \eta_q^\dagger - \eta_q\right)\mathcal{H}\left(1 + \eta_q - \eta_q^\dagger\right) \\
&= \frac{1}{2}\left(1 + \eta_q^\dagger - \eta_q\right)\left(\mathcal{H} + \mathcal{H}\eta - \mathcal{H}\eta_q^\dagger\right) \\
&= \frac{1}{2}\left(\mathcal{H} + \mathcal{H}\eta - \mathcal{H}\eta_q^\dagger + \eta_q^\dagger\mathcal{H} + \eta_q^\dagger\mathcal{H}\eta_q - \eta_q^\dagger\mathcal{H}\eta_q^\dagger - \eta_q\mathcal{H} - \eta_q\mathcal{H}\eta_q + \eta_q\mathcal{H}\eta_q^\dagger\right) \\
&= \frac{1}{2}\left(\mathcal{H}^D + \mathcal{H}^i + \mathcal{H}^I + \mathcal{H}\eta - \mathcal{H}\eta_q^\dagger + \eta_q^\dagger\mathcal{H} + \eta_q^\dagger\mathcal{H}\eta_q - \eta_q^\dagger\mathcal{H}\eta_q^\dagger - \eta_q\mathcal{H} - \eta_q\mathcal{H}\eta_q + \eta_q\mathcal{H}\eta_q^\dagger\right) \\
&= \frac{1}{2}\left(\mathcal{H}^D + \mathcal{H}^i + \mathcal{H}^I + \left[\eta_q^\dagger - \eta, \mathcal{H}\right] + \eta_q^\dagger\mathcal{H}\eta_q - \eta_q^\dagger\mathcal{H}\eta_q^\dagger - \eta_q\mathcal{H}\eta_q + \eta_q\mathcal{H}\eta_q^\dagger\right)
\end{aligned} \tag{1.36}$$

In the last step I split $\mathcal{H}$ using eq. 1.4. For reasons that will become apparent later, we will split the terms into two groups:

$$\tilde{\mathcal{H}} = \frac{1}{2}\left(\underbrace{\mathcal{H}^D + \mathcal{H}^i + \left[\eta_q^\dagger - \eta, \mathcal{H}\right] + \eta_q^\dagger\mathcal{H}\eta_q + \eta_q\mathcal{H}\eta_q^\dagger}_{\text{group 1}} + \overbrace{\mathcal{H}^I - \eta_q^\dagger\mathcal{H}\eta_q^\dagger - \eta_q\mathcal{H}\eta_q}^{\text{group 2}}\right) \tag{1.37}$$

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

$$\begin{aligned}
\mathcal{H} &= \mathrm{Tr}\left[\mathcal{H}\hat{n}_q\right]\hat{n}_q + \mathrm{Tr}\left[\mathcal{H}\left(1 - \hat{n}_q\right)\right]\left(1 - \hat{n}_q\right) + c_q^\dagger \mathrm{Tr}\left[\mathcal{H}c_q\right] + \mathrm{Tr}\left[c_q^\dagger\mathcal{H}\right]c_q \\
&= H_e\hat{n}_q + H_h(1 - \hat{n}_q) + c_q^\dagger T + T^\dagger c_q
\end{aligned} \tag{1.38}$$

Using this form, we can write

$$\eta_q \mathcal{H} \eta_q = \eta_q c_q^\dagger T \eta_q \tag{1.39}$$

and

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

We can also write the off-diagonal part as

$$\mathcal{H}^I = c_q^\dagger T + T^\dagger c_q \tag{1.41}$$

Group 2 becomes

$$\text{group 2} = c_q^\dagger T + T^\dagger c_q - \eta_q^\dagger T^\dagger c_q \eta_q^\dagger - \eta_q c_q^\dagger T \eta_q \tag{1.42}$$

To simplify this, we use the definition of $\eta_q^\dagger$, eq. 1.18, to write η_q:

$$\eta_q = \left(\eta_q^\dagger\right)^\dagger = \ \text{Tr}\left[c_q^\dagger \mathcal{H}\right] c_q \frac{1}{\hat{\omega} - \ \text{Tr}\left[\mathcal{H}^D \hat{n}_q\right] \hat{n}_q} = T^\dagger c_q \frac{1}{\hat{\omega} - H_e \hat{n}_q} \tag{1.43}$$

Using this, we can write

$$\begin{aligned} \eta_q c_q^\dagger T \eta_q &= T^\dagger c_q \frac{1}{\hat{\omega} - H_e \hat{n}_q} c_q^\dagger T \eta_q \\ &= T^\dagger c_q \left(\frac{1}{\hat{\omega} - H_e \hat{n}_q} c_q^\dagger T \right) \eta_q \\ &= T^\dagger c_q \eta_q^\dagger \eta_q \qquad \text{[eq. 1.18]} \\ &= T^\dagger c_q \hat{n}_q \qquad \text{[eq. 1.23]} \end{aligned} \tag{1.44}$$

which gives

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

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

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

which gives

$$\eta_q^\dagger T^\dagger c_q \eta_q^\dagger = c_q^\dagger T \tag{1.47}$$

Substituting the expressions 1.45 and 1.47, we get group 2 = 0. Substituting this in the rotated Hamiltonian gives

$$\widetilde{\mathcal{H}} = \frac{1}{2} \left(\mathcal{H}^D + \mathcal{H}^i + \mathcal{H}\eta - \mathcal{H}\eta_q^\dagger + \eta_q^\dagger \mathcal{H} + \eta_q^\dagger \mathcal{H} \eta_q - \eta_q \mathcal{H} + \eta_q \mathcal{H} \eta_q^\dagger \right) \tag{1.48}$$

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

$$\eta_q^\dagger = \frac{1}{\omega - H_e \hat{n}_q} c_q^\dagger T, \qquad \eta_q = \frac{1}{\omega - H_h (1 - \hat{n}_q)} T^\dagger c_q \tag{1.49}$$

Then,

$$\begin{aligned}
&\implies \frac{1}{\omega - H_e\hat{n}_q} c_q^\dagger T = c_q^\dagger T \frac{1}{\omega - H_h(1-\hat{n}_q)} \\
&\implies c_q^\dagger T H_h(1-\hat{n}_q) = H_e \hat{n}_q c_q^\dagger T \\
&\implies \frac{1}{\omega - H_e\hat{n}_q} c_q^\dagger T H_h(1-\hat{n}_q) = \frac{1}{\omega - H_e\hat{n}_q} H_e \hat{n}_q c_q^\dagger T \\
&\implies \eta_q^\dagger H_h(1-\hat{n}_q) = H_e \hat{n}_q \frac{1}{\omega - H_e\hat{n}_q} c_q^\dagger T \\
&\implies \eta_q^\dagger H_h(1-\hat{n}_q) = H_e \hat{n}_q \eta_q^\dagger \\
&\implies \eta_q^\dagger H_h = H_e \hat{\eta}_q^\dagger
\end{aligned} \tag{1.50}$$

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:

$$\begin{aligned}
\eta_q \mathcal{H} \eta_q^\dagger &= \eta_q H_e \hat{n}_q \eta_q^\dagger \\
&= H_h \eta_q \eta_q^\dagger \\
&= H_h(1-\hat{n}_q)
\end{aligned} \tag{1.51}$$

Similarly,

$$\begin{aligned}
\eta_q^\dagger \mathcal{H} \eta_q &= \eta_q^\dagger H_h \eta_q \\
&= H_e \eta_q^\dagger \eta_q \\
&= H_e \hat{n}_q
\end{aligned} \tag{1.52}$$

Also,

$$\begin{aligned}
\mathcal{H}\eta - \mathcal{H}\eta_q^\dagger + \eta_q^\dagger \mathcal{H} - \eta_q \mathcal{H} = \left(\eta_q^\dagger H_h - H_e \eta_q^\dagger\right) + (H_h \eta - \eta H_e) + \eta_q^\dagger T^\dagger c_q - \eta_q c_q^\dagger T + \\
c_q^\dagger T \eta_q - T^\dagger c_q \eta_q^\dagger
\end{aligned} \tag{1.53}$$

By virtue of eq. 1.50 and its conjugate, the first two terms will vanish.

$$\mathcal{H}\eta - \mathcal{H}\eta_q^\dagger + \eta_q^\dagger \mathcal{H} - \eta_q \mathcal{H} = \eta_q^\dagger T^\dagger c_q - \eta_q c_q^\dagger T + c_q^\dagger T \eta_q - T^\dagger c_q \eta_q^\dagger \tag{1.54}$$

From eqs. 1.45 and 1.47,

$$\eta_q^\dagger T^\dagger c_q = \eta_q^\dagger \eta_q c_q^\dagger T \eta_q = \hat{n}_q c_q^\dagger T \eta_q = c_q^\dagger T \eta_q \tag{1.55}$$

$$T^\dagger c_q \eta_q^\dagger = \eta_q c_q^\dagger T \eta_q \eta_q^\dagger = \eta_q c_q^\dagger T \left(1 - \hat{n}_q\right) = \eta_q c_q^\dagger T \tag{1.56}$$

$$\tag{1.57}$$

Eq. 1.54 becomes

$$\mathcal{H}\eta - \mathcal{H}\eta_q^\dagger + \eta_q^\dagger \mathcal{H} - \eta_q \mathcal{H} = c_q^\dagger T \eta_q - \eta_q c_q^\dagger T + c_q^\dagger T \eta_q - \eta_q c_q^\dagger T \ = 2\left[c_q^\dagger T, \eta_q\right] \tag{1.58}$$

Putting it all together,

$$\begin{aligned}
\widetilde{\mathcal{H}} &= \frac{1}{2}\left(\mathcal{H}^D + \mathcal{H}^i + \mathcal{H}\eta - \mathcal{H}\eta_q^\dagger + \eta_q^\dagger \mathcal{H} + \eta_q^\dagger \mathcal{H} \eta_q - \eta_q \mathcal{H} + \eta_q \mathcal{H} \eta_q^\dagger\right) \\
&= \frac{1}{2}\left(\mathcal{H}^D + \mathcal{H}^i\right) + \left[c_q^\dagger T, \eta_q\right] + \frac{1}{2}\left[H_e \hat{n}_q + H_h(1-\hat{n}_q)\right]
\end{aligned} \tag{1.59}$$

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

$$\mathcal{H}^D + \mathcal{H}^i = H_e \hat{n}_q + H_h \left(1 - \hat{n}_q\right) \tag{1.60}$$

Hence,

$$\begin{aligned}
\widetilde{\mathcal{H}} &= \frac{1}{2}\left(\mathcal{H}^D + \mathcal{H}^i + \mathcal{H}\eta - \mathcal{H}\eta_q^\dagger + \eta_q^\dagger \mathcal{H} + \eta_q^\dagger \mathcal{H}\eta_q - \eta_q \mathcal{H} + \eta_q \mathcal{H}\eta_q^\dagger\right) \\
&= H_e \hat{n}_q + H_h(1 - \hat{n}_q) + \left[c_q^\dagger T, \eta_q\right] \\
&= \mathrm{Tr}\left[\mathcal{H}\hat{n}_q\right]\hat{n}_q + \mathrm{Tr}\left[\mathcal{H}\hat{(}1 - n_q)\right](1 - \hat{n}_q) + \left[c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right), \eta_q\right]
\end{aligned} \tag{1.61}$$

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

$$\begin{aligned}
\mathrm{Tr}\left[\mathcal{H}\hat{n}_q\right]\hat{n}_q + \mathrm{Tr}\left[\mathcal{H}(1 - \hat{n}_q)\right](1 - \hat{n}_q) &= \mathrm{Tr}\left[\mathcal{H}\hat{n}_q\right]\hat{n}_q + \mathrm{Tr}\left[\mathcal{H}(\hat{n}_q - 1)\right](\hat{n}_q - 1) \\
&= \mathrm{Tr}\left[\mathcal{H}\hat{n}_q\right]\hat{n}_q + \mathrm{Tr}\left[\mathcal{H}(\hat{n}_q - 1)\right] n_q - \mathrm{Tr}\left[\mathcal{H}\hat{(}n_q - 1)\right] \\
&= \mathrm{Tr}\left[\mathcal{H}\left(2\hat{n}_q - 1\right)\right]\hat{n}_q - \mathrm{Tr}\left[\mathcal{H}(\hat{n}_q - 1)\right] \\
&= \mathrm{Tr}\left[\mathcal{H}\left(\hat{n}_q - \frac{1}{2}\right)\right] 2\hat{n}_q - \mathrm{Tr}\left[\mathcal{H}(\hat{n}_q - \frac{1}{2})\right] + \frac{1}{2}\mathrm{Tr}\left[\mathcal{H}\right] \\
&= \mathrm{Tr}\left[\mathcal{H}\left(\hat{n}_q - \frac{1}{2}\right)\right](2\hat{n}_q - 1) + \frac{1}{2}\mathrm{Tr}\left[\mathcal{H}\right] \\
&= \mathrm{Tr}\left[\mathcal{H}\tau_q\right] 2\tau_q + \frac{1}{2}\mathrm{Tr}\left[\mathcal{H}\right]
\end{aligned} \tag{1.62}$$

The last term can be written as:

$$\begin{aligned}
\left[c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right), \eta_q\right] &= c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right)\eta_q - \eta_q c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right) \\
&= \left(2\hat{n}_q - 1\right) c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right)\eta_q - \left(1 - 2\hat{n}_q\right)\eta_q c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right)
\end{aligned} \tag{1.63}$$

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

$$\left[c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right), \eta_q\right] = 2\tau_q \left\{c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right), \eta_q\right\} \tag{1.64}$$

The final form of the rotated Hamiltonian is

$$\widetilde{\mathcal{H}} = U_q \mathcal{H} U_q^\dagger = \mathrm{Tr}\left[\mathcal{H}\hat{n}_q\right]\hat{n}_q + \mathrm{Tr}\left[\mathcal{H}(1 - \hat{n}_q)\right](1 - \hat{n}_q) + 2\tau_q \left\{c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right), \eta_q\right\} \tag{1.65}$$

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

$$\begin{aligned}
\left[\widetilde{\mathcal{H}}, \hat{n}_q\right] &= \left[\left[c_q^\dagger T, \eta_q\right], \hat{n}_q\right] \\
&= \left[c_q^\dagger T\eta_q, \hat{n}_q\right] - \left[\eta_q c_q^\dagger T, \hat{n}_q\right] \\
&= c_q^\dagger T\eta_q\hat{n}_q - \hat{n}_q c_q^\dagger T\eta_q \qquad \left[2^{\text{nd}}\ [\ .\ ] \text{ is 0},\ \because c_q^\dagger \hat{n}_q = \hat{n}_q\eta_q = 0\right] \\
&= c_q^\dagger T\eta_q - c_q^\dagger T\eta_q \\
&= 0
\end{aligned} \tag{1.66}$$

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,

$$\begin{aligned} &\eta^\dagger \eta \left|1, \Psi_1\right\rangle = \left|1, \Psi_1\right\rangle \qquad\qquad \left[\eta^\dagger \eta = \hat{n}\right] \\ \implies &\frac{1}{\hat{\omega} - \hat{H}_e} c^\dagger T \eta = \left|1, \Psi_1\right\rangle \\ \implies &c^\dagger T \eta = \left(\hat{\omega} - \hat{H}_e\right) \left|1, \Psi_1\right\rangle \\ &\qquad\quad = \left(\omega_e - H_e\right) \left|1, \Psi_1\right\rangle \end{aligned} \tag{1.67}$$

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

$$\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_0 + c^\dagger T + T^\dagger c \tag{1.68}$$

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. 1.65, 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

$$\Delta\mathcal{H}_{q\beta} = 2\tau_{q\beta} \left\{ c_{q\beta}^\dagger \mathrm{Tr}\left(\mathcal{H} c_{q\beta}\right), \eta_{q\beta} \right\} \tag{1.69}$$

Decoupling the entire shell gives

$$\Delta\mathcal{H} = \sum_{q\beta} 2\tau_{q\beta} \left\{ c_{q\beta}^\dagger \mathrm{Tr}\left(\mathcal{H} c_{q\beta}\right), \eta_{q\beta} \right\} \tag{1.70}$$

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:

$$\begin{aligned}\Delta^-\mathcal{H} &= \sum_{q\beta} c^\dagger_{q\beta}\mathrm{Tr}\left(\mathcal{H}c_{q\beta}\right)\eta_{q\beta} \\ &= \sum_{q\beta} c^\dagger_{q\beta}\mathrm{Tr}\left(\mathcal{H}c_{q\beta}\right)\frac{1}{\omega_h-\mathcal{H}^D}\mathrm{Tr}\left(c^\dagger_{q\beta}\mathcal{H}\right)c_{q\beta}\end{aligned} \tag{1.71}$$

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:

$$\begin{aligned}\Delta^+\mathcal{H} &= \sum_{q\beta}\eta_{q\beta}c^\dagger_{q\beta}\mathrm{Tr}\left(\mathcal{H}c_{q\beta}\right) \\ &= \sum_{q\beta}\mathrm{Tr}\left(c^\dagger_{q\beta}\mathcal{H}\right)c_{q\beta}\frac{1}{\omega_e-\mathcal{H}^D}c^\dagger_{q\beta}\mathrm{Tr}\left(\mathcal{H}c_{q\beta}\right)\end{aligned} \tag{1.72}$$

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

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

2 Kondo Model URG

$$\mathcal{H} = \sum_{k\alpha}\epsilon_k\hat{n}_{k\alpha} + \frac{J_z}{2}\sum_{k,k'}S^z_d\left(c^\dagger_{k\uparrow}c_{k'\uparrow} - c^\dagger_{k\downarrow}c_{k'\downarrow}\right) + \frac{J_t}{2}\sum_{k,k'}\left(S^+_d c^\dagger_{k\downarrow}c_{k'\uparrow} + S^-_d c^\dagger_{k\uparrow}c_{k'\downarrow}\right) \tag{2.1}$$

We take an electron $q\uparrow$ on the shell. The diagonal part of the Hamiltonian is

$$\mathcal{H}^D = \epsilon_q\hat{n}_{q\uparrow} + \frac{1}{2}J_z S^z_d\hat{n}_{q\uparrow} \tag{2.2}$$

This is the piece that comes in the denominator. Note that in this form, the hole energy comes out to be zero, because the Hamiltonian is written only in terms of $\hat{n}_{q\beta}$. To remedy this, we write the Hamiltonian in terms of $\tau_{q\beta} = \hat{n}_{q\beta} - \frac{1}{2}$.

$$\mathcal{H}^D = \epsilon_q \tau_{q\uparrow} + \frac{1}{2} J_z S_d^z \tau_{q\uparrow} \tag{2.3}$$

A constant $\frac{1}{2}\epsilon_q$ has been dropped while transforming the first term. The second term transforms exactly because we can just the bare Hamiltonian term $S_d^z\,(\hat{n}_{q\uparrow} - \hat{n}_{q\downarrow})$ as $S_d^z\,(\tau_{q\uparrow} - \tau_{q\downarrow})$.

The off-diagonal part involving the electron on the shell is

$$\mathcal{H}^I = \frac{1}{2} J_z \sum_{kq} S_d^z \left(c_{k\uparrow}^\dagger c_{q\uparrow} + c_{q\uparrow}^\dagger c_{k\uparrow} \right) + \frac{1}{2} J_t \sum_{kq} \left(S_d^+ c_{k\downarrow}^\dagger c_{q\uparrow} + S_d^- c_{q\uparrow}^\dagger c_{k\downarrow} \right) \tag{2.4}$$

These are the terms that come in the numerator.

2.1 Particle sector

The renormalization in the particle sector is

$$\Delta^+ \mathcal{H} = \sum_{kk'q} \frac{1}{2} \left(J_z S_d^z c_{k\uparrow}^\dagger c_{q\uparrow} + J_t S_d^+ c_{k\downarrow}^\dagger c_{q\uparrow} \right) \frac{1}{\omega^+ - \mathcal{H}^D} \frac{1}{2} \left(J_z S_d^z c_{q\uparrow}^\dagger c_{k'\uparrow} + J_t S_d^- c_{q\uparrow}^\dagger c_{k'\downarrow} \right) \tag{2.5}$$

ω^+ represents the quantum fluctuation scale for the particle sector. Notice that all the operators on the left of the propagator have a $c_{q\uparrow}$ and those on the right have a $c_{q\uparrow}^\dagger$. This combination produces a particle in the intermediate state. In this intermediate state, since we have $\tau_{q\uparrow} = \frac{1}{2}$, we can evaluate the diagonal part from eq. 2.3:

$$\mathcal{H}^D = \frac{1}{2}\epsilon_q + \frac{1}{4} J_z S_d^z \tag{2.6}$$

There are two terms in each bracket, so in total there are four terms. The first term has two S^z.

$$\begin{aligned}
\Delta_1^+\mathcal{H} &= \sum_{kk'q}\frac{1}{4}J_z^2 S_d^z c_{k\uparrow}^\dagger c_{q\uparrow}\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{4}J_z S_d^z}S_d^z c_{q\uparrow}^\dagger c_{k'\uparrow} \\
&= \sum_{kk'q}\frac{1}{4}J_z^2 c_{k\uparrow}^\dagger c_{q\uparrow}\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{4}J_z S_d^z}S_d^z S_d^z c_{q\uparrow}^\dagger c_{k'\uparrow} \\
&= \sum_{kk'q}\frac{1}{16}J_z^2 c_{k\uparrow}^\dagger c_{q\uparrow}\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{4}J_z S_d^z}c_{q\uparrow}^\dagger c_{k'\uparrow} \\
&= \frac{1}{16}J_z^2\sum_{kk'q} c_{k\uparrow}^\dagger c_{q\uparrow}c_{q\uparrow}^\dagger c_{k'\uparrow}\left[\frac{\frac{1}{2}+S_d^z}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{8}J_z} + \frac{\frac{1}{2}-S_d^z}{\omega^+ - \frac{1}{2}\epsilon_q + \frac{1}{8}J_z}\right] \\
&= \frac{1}{32}J_z^2\sum_{kk'q} c_{k\uparrow}^\dagger c_{k'\uparrow}\left[\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{8}J_z} + \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q + \frac{1}{8}J_z}\right] \\
&+ \frac{1}{16}J_z^2\sum_{kk'q} S_d^z c_{k\uparrow}^\dagger c_{k'\uparrow}\left[\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{8}J_z} - \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q + \frac{1}{8}J_z}\right]
\end{aligned} \tag{2.7}$$

The first term is a potential scattering term; the second term renormalizes the up spin part of the S_d^z term, that is, J_z.

The second term gives

$$\Delta_2^+\mathcal{H} = \sum_{kk'q}\frac{1}{4}J_z J_t S_d^z c_{k\uparrow}^\dagger c_{q\uparrow}\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{8}J_z S_d^z}S_d^- c_{q\uparrow}^\dagger c_{k'\downarrow} \tag{2.8}$$

The S_d^- in the numerator on the right means we must have $S_d^z = -\frac{1}{2}$ in the denominator.

$$\begin{aligned}
\Delta_2^+\mathcal{H} &= \frac{1}{4}J_z J_t\sum_{kk'q} S_d^z c_{k\uparrow}^\dagger c_{q\uparrow}\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q + \frac{1}{8}J_z}S_d^- c_{q\uparrow}^\dagger c_{k'\downarrow} \\
&= \frac{1}{4}J_z J_t\sum_{kk'q} S_d^z S_d^- c_{k\uparrow}^\dagger c_{q\uparrow}c_{q\uparrow}^\dagger c_{k'\downarrow}\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q + \frac{1}{8}J_z} \\
&= -\frac{1}{8}J_z J_t\sum_{kk'q} S_d^- c_{k\uparrow}^\dagger c_{k'\downarrow}\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q + \frac{1}{8}J_z}
\end{aligned} \tag{2.9}$$

There we used $S_d^z S_d^- = -\frac{1}{2}S_d^-$. This renormalizes J_t.

The third term gives

$$\Delta_3^+\mathcal{H} = \sum_{kk'q}\frac{1}{4}J_z J_t S_d^+ c_{k\downarrow}^\dagger c_{q\uparrow}\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{4}J_z S_d^z}S_d^z c_{q\uparrow}^\dagger c_{k'\uparrow} \tag{2.10}$$

The S_d^+ in the numerator on the left means we must have $S_d^z = -\frac{1}{2}$ in the denominator.

$$\begin{aligned}\Delta_3^+\mathcal{H} &= \frac{1}{4}J_zJ_t\sum_{kk'q} S_d^+ c_{k\downarrow}^\dagger c_{q\uparrow}\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q + \frac{1}{8}J_z}S_d^z c_{q\uparrow}^\dagger c_{k'\uparrow} \\ &= \frac{1}{4}J_zJ_t\sum_{kk'q} S_d^+ S_d^z c_{k\downarrow}^\dagger c_{q\uparrow} c_{q\uparrow}^\dagger c_{k'\uparrow}\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q + \frac{1}{8}J_z} \\ &= -\frac{1}{8}J_zJ_t\sum_{kk'q} S_d^+ c_{k\downarrow}^\dagger c_{k'\uparrow}\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q + \frac{1}{8}J_z}\end{aligned} \tag{2.11}$$

There we used $S_d^+S_d^z = -\frac{1}{2}S_d^+$. This renormalizes J_t.

The fourth term gives

$$\Delta_4^+\mathcal{H} = \sum_{kk'q}\frac{1}{4}J_t^2 S_d^+ c_{k\downarrow}^\dagger c_{q\uparrow}\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{4}J_zS_d^z}S_d^- c_{q\uparrow}^\dagger c_{k'\downarrow} \tag{2.12}$$

The S_d^+ in the numerator on the left means we must have $S_d^z = -\frac{1}{2}$ in the denominator.

$$\begin{aligned}\Delta_4^+\mathcal{H} &= \frac{1}{4}J_t^2\sum_{kk'q} S_d^+ c_{k\downarrow}^\dagger c_{q\uparrow}\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q + \frac{1}{8}J_z}S_d^- c_{q\uparrow}^\dagger c_{k'\downarrow} \\ &= \frac{1}{4}J_t^2\sum_{kk'q} S_d^+ S_d^- c_{k\downarrow}^\dagger c_{q\uparrow} c_{q\uparrow}^\dagger c_{k'\downarrow}\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q + \frac{1}{8}J_z} \\ &= \frac{1}{4}J_t^2\sum_{kk'q}\left(\frac{1}{2} + S_d^z\right) c_{k\downarrow}^\dagger c_{k'\downarrow}\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q + \frac{1}{8}J_z}\end{aligned} \tag{2.13}$$

There we used $S_d^+S_d^- = \left(\frac{1}{2} + S_d^z\right)$. The first term produces a potential scattering and the second term renormalizes J_z.

2.2 Hole sector

The renormalization in the hole sector is

$$\Delta^-\mathcal{H} = \sum_{kk'q}\frac{1}{2}\left(J_zS_d^z c_{q\uparrow}^\dagger c_{k'\uparrow} + J_tS_d^- c_{q\uparrow}^\dagger c_{k'\downarrow}\right)\frac{1}{\omega^- - \mathcal{H}^D}\frac{1}{2}\left(J_zS_d^z c_{k\uparrow}^\dagger c_{q\uparrow} + J_tS_d^+ c_{k\downarrow}^\dagger c_{q\uparrow}\right) \tag{2.14}$$

The ω^- represents the quantum fluctuation energy scale for the hole sector. In this intermediate state, since we have $\tau_{q\uparrow} = -\frac{1}{2}$, we can evaluate the diagonal part from eq. 2.3:

$$\mathcal{H}^D = -\frac{1}{2}\epsilon_q^- - \frac{1}{4}J_zS_d^z \tag{2.15}$$

The energy ϵ_q^- has to be opposite to ϵ_q, because the state was initially occupied, so this energy has to be inside the Fermi surface: $\epsilon_q^- = -\epsilon_q$.

$$\mathcal{H}^D = \frac{1}{2}\epsilon_q - \frac{1}{4}J_z S_d^z \tag{2.16}$$

The first term has two S^z.

$$\begin{aligned}
\Delta_1^-\mathcal{H} &= \sum_{kk'q} S_d^z c_{q\uparrow}^\dagger c_{k'\uparrow}\frac{1}{4}J_z^2\frac{1}{\omega^- - \mathcal{H}^D}S_d^z c_{k\uparrow}^\dagger c_{q\uparrow} \\
&= \frac{1}{16}J_z^2\sum_{kk'q} c_{k'\uparrow}c_{k\uparrow}^\dagger\frac{1}{\omega^- - \frac{1}{2}\epsilon_q + \frac{1}{4}J_z S_d^z} \\
&= \frac{1}{16}J_z^2\sum_{kk'q} c_{k'\uparrow}c_{k\uparrow}^\dagger\left[\frac{\frac{1}{2}+S_d^z}{\omega^- - \frac{1}{2}\epsilon_q + \frac{1}{8}J_z} + \frac{\frac{1}{2}-S_d^z}{\omega^- - \frac{1}{2}\epsilon_q - \frac{1}{8}J_z}\right] \\
&= -\frac{1}{32}J_z^2\sum_{kk'q} c_{k\uparrow}^\dagger c_{k'\uparrow}\left[\frac{1}{\omega^- - \frac{1}{2}\epsilon_q + \frac{1}{8}J_z} + \frac{1}{\omega^- - \frac{1}{2}\epsilon_q - \frac{1}{8}J_z}\right] \\
&- \frac{1}{16}J_z^2\sum_{kk'q} c_{k\uparrow}^\dagger c_{k'\uparrow}S_d^z\left[\frac{1}{\omega^- - \frac{1}{2}\epsilon_q + \frac{1}{8}J_z} - \frac{1}{\omega^- - \frac{1}{2}\epsilon_q - \frac{1}{8}J_z}\right]
\end{aligned} \tag{2.17}$$

In the last step, we dropped a constant term which came from the commutator of $c_k^\dagger$ and $c_{k'}$. Note that this term exactly cancels the first term in the particle sector.

The second term gives

$$\Delta_2^-\mathcal{H} = \sum_{kk'q}\frac{1}{4}J_z J_t S_d^- c_{q\uparrow}^\dagger c_{k'\downarrow}\frac{1}{\omega^- - \frac{1}{2}\epsilon_q + \frac{1}{4}J_z S_d^z}S_d^z c_{k\uparrow}^\dagger c_{q\uparrow} \tag{2.18}$$

The S_d^- in the numerator on the left means we must have $S_d^z = \frac{1}{2}$ in the denominator.

$$\begin{aligned}
\Delta_2^-\mathcal{H} &= \frac{1}{4}J_z J_t\sum_{kk'q} S_d^- S_d^z c_{q\uparrow}^\dagger c_{k'\downarrow}c_{k\uparrow}^\dagger c_{q\uparrow}\frac{1}{\omega^- - \frac{1}{2}\epsilon_q + \frac{1}{8}J_z} \\
&= \frac{1}{8}J_z J_t\sum_{kk'q} S_d^- c_{k'\downarrow}c_{k\uparrow}^\dagger\frac{1}{\omega^- - \frac{1}{2}\epsilon_q + \frac{1}{8}J_z} \\
&= -\frac{1}{8}J_z J_t\sum_{kk'q} S_d^- c_{k\uparrow}^\dagger c_{k'\downarrow}\frac{1}{\omega^- - \frac{1}{2}\epsilon_q + \frac{1}{8}J_z}
\end{aligned} \tag{2.19}$$

There we used $S_d^- S_d^z = \frac{1}{2}S_d^-$. This renormalizes J_t.

The third term gives

$$\Delta_3^-\mathcal{H} = \sum_{kk'q}\frac{1}{4}J_z J_t S_d^z c_{q\uparrow}^\dagger c_{k'\uparrow}\frac{1}{\omega^- - \frac{1}{2}\epsilon_q + \frac{1}{4}J_z S_d^z}S_d^+ c_{k\downarrow}^\dagger c_{q\uparrow} \tag{2.20}$$

The S_d^+ in the numerator on the right means we must have $S_d^z = \frac{1}{2}$ in the denominator.

$$\begin{aligned}\Delta_3^- \mathcal{H} &= \frac{1}{4} J_z J_t \sum_{kk'q} S_d^z S_d^+ c_{q\uparrow}^\dagger c_{k'\uparrow} c_{k\downarrow}^\dagger c_{q\uparrow} \frac{1}{\omega^- - \frac{1}{2}\epsilon_q + \frac{1}{8} J_z} \\ &= \frac{1}{4} J_z J_t \sum_{kk'q} S_d^+ c_{k\downarrow}^\dagger c_{k'\uparrow} \frac{1}{\omega^- - \frac{1}{2}\epsilon_q + \frac{1}{8} J_z} \\ &= -\frac{1}{8} J_z J_t \sum_{kk'q} S_d^+ c_{k\downarrow}^\dagger c_{k'\uparrow} \frac{1}{\omega^- - \frac{1}{2}\epsilon_q + \frac{1}{8} J_z}\end{aligned} \tag{2.21}$$

There we used $S_d^z S_d^+ = \frac{1}{2} S_d^+$. This renormalizes J_t.

The fourth term gives

$$\Delta_4^- \mathcal{H} = \sum_{kk'q} \frac{1}{4} J_t^2 S_d^- c_{q\uparrow}^\dagger c_{k'\downarrow} \frac{1}{\omega^- - \frac{1}{2}\epsilon_q + \frac{1}{4} J_z S_d^z} S_d^+ c_{k\downarrow}^\dagger c_{q\uparrow} \tag{2.22}$$

The S_d^+ in the numerator on the right means we must have $S_d^z = \frac{1}{2}$ in the denominator.

$$\begin{aligned}\Delta_4^- \mathcal{H} &= \frac{1}{4} J_t^2 \sum_{kk'q} S_d^- S_d^+ c_{q\uparrow}^\dagger c_{k'\downarrow} c_{k\downarrow}^\dagger c_{q\uparrow} \frac{1}{\omega^- - \frac{1}{2}\epsilon_q + \frac{1}{8} J_z} \\ &= \frac{1}{4} J_t^2 \sum_{kk'q} \left(\frac{1}{2} - S_d^z \right) c_{k'\downarrow} c_{k\downarrow}^\dagger \frac{1}{\omega^- - \frac{1}{2}\epsilon_q + \frac{1}{8} J_z} \\ &= -\frac{1}{4} J_t^2 \sum_{kk'q} \left(\frac{1}{2} - S_d^z \right) c_{k\downarrow}^\dagger c_{k'\downarrow} \frac{1}{\omega^- - \frac{1}{2}\epsilon_q + \frac{1}{8} J_z}\end{aligned} \tag{2.23}$$

There we used $S_d^- S_d^+ = \left(\frac{1}{2} - S_d^z\right)$.

2.3 Scaling equations

Focusing on the first terms of each sector, we can see that

$$\begin{aligned}\Delta_1^+ \mathcal{H} &= \frac{1}{16} J_z^2 \sum_{kk'q} c_{k\uparrow}^\dagger c_{k'\uparrow} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{4} J_z S_d^z} \\ \Delta_1^- \mathcal{H} &= -\frac{1}{16} J_z^2 \sum_{kk'q} c_{k\uparrow}^\dagger c_{k'\uparrow} \frac{1}{\omega^- - \frac{1}{2}\epsilon_q + \frac{1}{4} J_z S_d^z}\end{aligned} \tag{2.24}$$

To connect the two ω, we can use $\eta = \eta^{\dagger\dagger}$. If we choose the scattering term $c^\dagger T = \sum_k S_d^z c_{q\uparrow}^\dagger c_{k\uparrow}$, then

$$\eta = \frac{1}{\omega^- - \frac{1}{2}\epsilon_q + \frac{1}{4} J_z S_d^z} \sum_k S_d^z c_{k\uparrow}^\dagger c_{q\uparrow} \tag{2.25}$$

and

$$\begin{aligned}\eta^\dagger &= \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{4}J_z S_d^z}\sum_k S_d^z c_{q\uparrow}^\dagger c_{k\uparrow} \\ \implies \left(\eta^\dagger\right)^\dagger &= \sum_k S_d^z c_{k\uparrow}^\dagger c_{q\uparrow}\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{4}J_z S_d^z} \\ &= \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{4}J_z S_d^z}\sum_k S_d^z c_{k\uparrow}^\dagger c_{q\uparrow}\end{aligned} \tag{2.26}$$

Comparing η and $\left(\eta^\dagger\right)^\dagger$, we can write

$$\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{4}J_z S_d^z} = \frac{1}{\omega^- - \frac{1}{2}\epsilon_q + \frac{1}{4}J_z S_d^z} \tag{2.27}$$

Using this on eq. 2.24 gives

$$\Delta_1\mathcal{H} \equiv \Delta_1^+\mathcal{H} + \Delta_1^-\mathcal{H} = 0 \tag{2.28}$$

This means there is no net renormalization from the first terms in each sector. Doing similar things for the other terms gives

$$\begin{aligned}\Delta_2^+ + \Delta_3^+ &= \Delta_2^- + \Delta_3^- \\ \implies \Delta_2\mathcal{H} + \Delta_3\mathcal{H} &= 2\Delta_2^+ + 2\Delta_3^+\end{aligned} \tag{2.29}$$

Adding the terms that renormalize S_d^+ from both sectors gives the renormalization

$$-\frac{1}{2}J_z J_t \sum_q \frac{1}{\omega - \epsilon_q + \frac{1}{4}J_z} \tag{2.30}$$

Note that the term is actually $\frac{1}{2}S_d^+$ and not just S_d^+, so that has to be taken into account while reading off the renormalization. Performing the calculation with the spin down term gives an equal renormalization, so

$$\Delta J_t = -J_z J_t \sum_q \frac{1}{\omega - \epsilon_q + \frac{1}{4}J_z} \tag{2.31}$$

Similarly, adding the term 4 from both sectors gives a renormalization in $-\frac{1}{2}S_d^z c_{k\downarrow}^\dagger c_{k'\downarrow}^\dagger$:

$$-\frac{1}{2}J_t^2 \sum_q \frac{1}{\omega - \epsilon_q + \frac{1}{4}J_z} \tag{2.32}$$

Doing the calculation with the down spin should produce the other term, $\frac{1}{2}S_d^z c_{k\uparrow}^\dagger c_{k'\uparrow}$, but that does not add to the previous renormalization, so there is no multiplication by 2 here:

$$\Delta J_z = -J_t^2 \sum_q \frac{1}{\omega - \epsilon_q + \frac{1}{4}J_z} \tag{2.33}$$

For the symmetric model ($J_z = J_t = J$, we get the equation

$$\Delta J = -J^2 \sum_q \frac{1}{\omega - \epsilon_q + \frac{1}{4}J} \tag{2.34}$$

To obtain the familiar Kondo model one-loop form, we need to take low energy excitations ($\omega \ll \epsilon_q$, expand the denominator and take only $O(J^0)$ and assume isotropic dispersion $\epsilon_q = D$.

$$\delta J = J^2 \rho |\delta D| \frac{1}{D} \tag{2.35}$$

2.4 Renormalized Hamiltonian

The renormalized Hamiltonian after disentangling the shell at Λ_N is

$$\mathcal{H}_{N-1} = \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{k,k'<\Lambda_N} \left[\frac{J_z^{N-1}}{2} S_d^z \left(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow} \right) + \frac{J_t^{N-1}}{2} \left(S_d^+ c_{k\downarrow}^\dagger c_{k'\uparrow} + S_d^- c_{k\uparrow}^\dagger c_{k'\downarrow} \right) \right] + \frac{J_z^N}{2} \sum_{q=\Lambda_N} S_d^z \left(\hat{n}_{q\uparrow} - \hat{n}_{q\downarrow} \right) \tag{2.36}$$

where $J^i = J^{i+1} + \Delta J^{i+1}$.

3 Anderson Model URG

3.1 Without spin-spin interaction

The model is the usual single-impurity Anderson model Hamiltonian.

$$\mathcal{H} = \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{k\sigma} \left(V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right) + \epsilon_d \sum_\sigma \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \tag{3.1}$$

At first order, the rotated Hamiltonian is

$$\mathcal{H}_{j-1} = 2^{-n_j} \mathrm{Tr}_{1,2,\ldots,n_j} \mathcal{H}_j + \sum_{q\beta} \tau_{q\beta} \left\{ c_{q\beta}^\dagger \mathrm{Tr}_{q\beta} \left(\mathcal{H} c_{q\beta} \right), \eta_{q\beta} \right\} \tag{3.2}$$

n_j is the number of states on the shell Λ_j. We take the full Hamiltonian as our $\mathcal{H}_j$. Since this is the first step of the RG, the shell being decoupled is the highest one, which we call Λ_N.

Particle Sector

The particle sector involves only particle excitations. The state $q\beta$ is occupied in the intermediate (excited) state. This contribution will be given by the first term in the anti-commutator of eq. 3.2.

Calculation of first term The first term, the initial trace, is a sequential trace over all the states on the shell being disentangled. At each trace, we consider only electrons on the current degree of freedom and on shells below the current shell:

$$\begin{aligned}
\frac{1}{2}\mathrm{Tr}_{q\uparrow}\mathcal{H}_j &= \sum_{k<\Lambda_N,\sigma} \epsilon_k \hat{n}_{k\sigma} + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + \frac{1}{2}\mathrm{Tr}_{q\uparrow}\left\{\epsilon_k \hat{n}_{q\uparrow}\right\} \\
&= \sum_{k<\Lambda_N,\sigma} \epsilon_k \hat{n}_{k\sigma} + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + \frac{1}{2}\epsilon_q \qquad (3.3) \\
\frac{1}{2}\mathrm{Tr}_{q\downarrow}\frac{1}{2}\mathrm{Tr}_{q\uparrow}\mathcal{H}_j &= \sum_{k<\Lambda_N,\sigma} \epsilon_k \hat{n}_{k\sigma} + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + \epsilon_q \\
\implies 2^{-n_j}\mathrm{Tr}_{1,2,\ldots,n_j}\mathcal{H}_j &= \sum_{k<\Lambda_N,\sigma} \epsilon_k \hat{n}_{k\sigma} + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + \sum_{|q|=\Lambda_N} \epsilon_q \qquad (3.4)
\end{aligned}$$

Calculation of second term The second term involves some other traces:

$$\begin{aligned}
\mathrm{Tr}_{q\beta}\left(\mathcal{H}c_{q\beta}\right) &= \sum_{k\sigma} V_k \mathrm{Tr}_{q\beta}\left(c^\dagger_{k\sigma}c_{d\sigma}c_{q\beta}\right) \\
&= \sum_{k\sigma} V_k c_{d\sigma}\delta_{\sigma\beta}\delta_{kq} \\
&= V_q c_{d\beta} \qquad (3.5) \\
\mathrm{Tr}_{q\beta}\left(c^\dagger_{q\beta}\mathcal{H}\right) &= V^*_q c^\dagger_{d\beta}
\end{aligned}$$

$$\begin{aligned}
\mathcal{H}^D &= \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} \\
\mathrm{Tr}_{q\beta}\left(\mathcal{H}^D\hat{n}_{q\beta}\right) &= \sum_{k<\Lambda_N,\sigma} \epsilon_k \hat{n}_{k\sigma} + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + \epsilon_q \qquad (3.6)
\end{aligned}$$

There is a more straightforward way of getting these expressions. Some thought reveals that $c^\dagger_{q\beta}\mathrm{Tr}_{q\beta}\left(\mathcal{H}c_{q\beta}\right)$ is, by definition, the part of the Hamiltonian that scatters from electrons *not at* $q\beta$ to $q\beta$. In other words, **it is that off-diagonal part of the Hamiltonian that involves a** $c^\dagger_{q\beta}$. That part is, of course, $V_q c^\dagger_{q\beta}c_{d\beta}$. Similarly, $\mathrm{Tr}_{q\beta}\left(c^\dagger_{q\beta}\mathcal{H}\right)c_{q\beta}$ is the off-diagonal part that has a $c_{q\beta}$, $V^*_q c^\dagger_{d\beta}c_{q\beta}$. Finally, the term in the denominator of η is simply the diagonal part of the Hamiltonian, which in our case is the kinetic energies of all the electrons and the impurity diagonal part. The point of this paragraph is that one can write down these terms simply by looking at the Hamiltonian and without carrying out any

trace.

$$\begin{aligned}\eta_{q\beta} &= \mathrm{Tr}_{q\beta}\left(c_{q\beta}^{\dagger}\mathcal{H}\right)c_{q\beta}\frac{1}{\hat{\omega}-\mathrm{Tr}_{q\beta}\left(\mathcal{H}^{D}\hat{n}_{q\beta}\right)\hat{n}_{q\beta}} \\ &= V_q^{*}c_{d\beta}^{\dagger}c_{q\beta}\frac{1}{\hat{\omega}-\left(\sum_{k<\Lambda_N,\sigma}\epsilon_k\hat{n}_{k\sigma}+\epsilon_d\sum_{\sigma}\hat{n}_{d\sigma}+U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}-\epsilon_q\right)\hat{n}_{q\beta}} \\ &= V_q^{*}c_{d\beta}^{\dagger}c_{q\beta}\frac{1}{\omega\tau_{q\beta}-\left(\epsilon_d\sum_{\sigma}\hat{n}_{d\sigma}+U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}+\epsilon_q\right)\tau_{q\beta}}\end{aligned} \tag{3.7}$$

At the last step, I replaced $\hat{\omega}-\sum_{k<\Lambda_N,\sigma}\epsilon_k\hat{n}_{k\sigma}\hat{n}_{q\beta}-\frac{1}{2}\left(\epsilon_d\sum_{\sigma}\hat{n}_{d\sigma}+U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}+\epsilon_q\right)$ with $\omega\tau_{q\beta}$. Note that since this term has a $c_{d\beta}^{\dagger}$, it will not vanish only when acting on a state with $\hat{n}_{d\beta}=0$. Hence we can drop the terms $\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}$ and $\epsilon_{d\beta}\hat{n}_{d\beta}$ in the denominator. Also, since it has a $c_{q\beta}$, we can set the $\tau_{q\beta}$ in the denominator to $\frac{1}{2}$. Putting together the individual pieces, we can now write the second term:

$$\begin{aligned}\sum_{q\beta}\tau_{q\beta}\left\{c_{q\beta}^{\dagger}\mathrm{Tr}_{q\beta}\left(\mathcal{H}c_{q\beta}\right),\eta_{q\beta}\right\} &= \sum_{q\beta}\tau_{q\beta}\left\{V_q c_{q\beta}^{\dagger}c_{d\beta},V_q^{*}c_{d\beta}^{\dagger}c_{q\beta}\frac{1}{\frac{1}{2}\left(\omega-\epsilon_q-\epsilon_d\hat{n}_{d\overline{\beta}}\right)}\right\} \\ &= \sum_{q\beta}2\tau_{q\beta}\left\{V_q c_{q\beta}^{\dagger}c_{d\beta},V_q^{*}c_{d\beta}^{\dagger}c_{q\beta}\frac{1}{\omega-\epsilon_q-\epsilon_d\hat{n}_{d\overline{\beta}}}\right\}\end{aligned} \tag{3.8}$$

We now note that the factor with ω can be written as follows:

$$\begin{aligned}\frac{1}{\omega-\epsilon_q-\epsilon_d\hat{n}_{d\overline{\beta}}} &= \frac{\hat{n}_{d\overline{\beta}}}{\omega-\epsilon_q-\epsilon_d}+\frac{1-\hat{n}_{d\overline{\beta}}}{\omega-\epsilon_q} \\ &= \hat{n}_{d\overline{\beta}}\frac{\epsilon_d}{\left(\omega-\epsilon_q-\epsilon_d\right)\left(\omega-\epsilon_q\right)}+\frac{1}{\omega-\epsilon_q}\end{aligned} \tag{3.9}$$

Since these terms commute with the other terms, they can be taken out of the anticommutator; what's left is

$$\left\{V_q c_{q\beta}^{\dagger}c_{d\beta},V_q^{*}c_{d\beta}^{\dagger}c_{q\beta}\right\} = |V_q|^2\left[\hat{n}_{q\beta}\left(1-\hat{n}_{d\beta}\right)+\hat{n}_{d\beta}\left(1-\hat{n}_{q\beta}\right)\right] \tag{3.10}$$

The τ and the $\hat{n}$ can be multiplied:

$$2\tau_{q\beta}\left(1-\hat{n}_{q\beta}\right) = \left(\hat{n}_{q\beta}-1\right) \tag{3.11}$$

$$2\tau_{q\beta}\hat{n}_{q\beta} = \hat{n}_{q\beta} \tag{3.12}$$

The total thing becomes

$$\begin{aligned}&\sum_{q\beta}|V_q|^2\left[\hat{n}_{d\beta}\left(\hat{n}_{q\beta}-1\right)+\hat{n}_{q\beta}\left(1-\hat{n}_{d\beta}\right)\right]\left[\hat{n}_{d\overline{\beta}}\frac{\epsilon_d}{\left(\omega-\epsilon_q-\epsilon_d\right)\left(\omega-\epsilon_q\right)}+\frac{1}{\omega-\epsilon_q}\right] \\ &\quad = \sum_{q\beta}|V_q|^2\left[\hat{n}_{q\beta}-\hat{n}_{d\beta}\right]\left[\hat{n}_{d\overline{\beta}}\frac{\epsilon_d}{\left(\omega-\epsilon_q-\epsilon_d\right)\left(\omega-\epsilon_q\right)}+\frac{1}{\omega-\epsilon_q}\right]\end{aligned} \tag{3.13}$$

Putting $\hat{n}_{q\beta} = 1$, and dropping the non-operator terms, we get

$$\sum_{\beta} \hat{n}_{d\beta} \sum_{q} |V_q|^2 \frac{\epsilon_q - \omega + 2\epsilon_d}{(\omega - \epsilon_q)(\omega - \epsilon_q - \epsilon_d)} - \hat{n}_{d\uparrow}\hat{n}_{d\downarrow} \sum_{q\beta} |V_q|^2 \frac{\epsilon_d}{(\omega - \epsilon_q)(\omega - \epsilon_q - \epsilon_d)} \tag{3.14}$$

The first term is the renormalization in on-site energy, $\sum_\beta \hat{n}_{d\beta}\Delta\epsilon_{d\beta}$, and the second term is the renormalization in the onsite repulsion, $\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\Delta U$.

Renormalized Hamiltonian Combining eqs. 3.4 and 3.14, we get

$$\mathcal{H}_{N-1} = \sum_{k<\Lambda_N,\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{|q|=\Lambda_N} \epsilon_q + \sum_{\sigma} (\epsilon_{d\sigma} + \Delta\epsilon_{d\sigma})\hat{n}_{d\sigma} + (U + \Delta U)\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} \tag{3.15}$$

The second term is the renormalization in the kinetic energy of the disentangled electrons, the third term is the renormalized impurity site energy and the fourth term is the renormalized onsite repulsion.

$$\Delta\epsilon_d^N \equiv \epsilon_d\big|_{N-1} - \epsilon_d\big|_N = \sum_q |V_q|^2 \frac{\epsilon_q - \omega + 2\epsilon_d}{(\omega - \epsilon_q)(\omega - \epsilon_q - \epsilon_d)} \tag{3.16}$$

According to Hewson eq. 3.62 (page 68),

$$\frac{\mathrm{d}\epsilon_d}{\mathrm{d}\ln D} = -\frac{\Delta}{\pi} + O(V^3) = -\rho_0|V|^2 + O(V^3) \tag{3.17}$$

in the limit of $U + \epsilon_d \gg D$ and $|\epsilon_d| \ll D$, under the assumptions that V_k is independent of k and the conduction band is flat ($\rho(\epsilon) = \rho_0$ for $\epsilon \in [-D, D]$).

Assuming that we integrate out a ring at energy D and of thickness $-|\delta D|$, such that $\epsilon_q = D$ everywhere on the ring, the number of available states is

$$\delta n = \frac{\mathrm{d}n}{\mathrm{d}E} \times \delta E = \rho(D) \times |\delta D| \tag{3.18}$$

We can then replace the summation in eq. 3.16 by δn:

$$\delta\epsilon_d(D) = |V|^2\rho(D)|\delta D| \frac{D - \omega + 2\epsilon_d}{(\omega - D)(\omega - D - \epsilon_d)} \tag{3.19}$$

where $\rho(D)$ is the number of single-spin states on the shell D. This can be compared to eq. 3.17. In two dimensions, the energy density of states is independent of energy. Setting $\omega = 0$, we get

$$\begin{aligned} \delta\epsilon_d(D) &= |V|^2\rho(D)|\delta D| \frac{D + 2\epsilon_d}{D(D + \epsilon_d)} \\ &= |V|^2\rho(D)\frac{|\delta D|}{D}\frac{D + 2\epsilon_d}{D + \epsilon_d} \end{aligned} \tag{3.20}$$

I used $\delta D = -|\delta D|$. Changing to continuum equation,

$$\frac{\mathrm{d}\epsilon_d}{\mathrm{d}\ln D} = -\frac{\Delta}{\pi}\frac{D+2\epsilon_d}{D+\epsilon_d} \tag{3.21}$$

In the regime where the single-occupied impurity level is comfortably inside the conduction band ($D \gg |\epsilon_d|$), we can approximate both the numerator and denominator as simply D. Then,

$$\frac{\mathrm{d}\epsilon_d}{\mathrm{d}\ln D} = -\frac{\Delta}{\pi} \tag{3.22}$$

$$\implies \epsilon_d + \frac{\Delta}{\pi}\log D = \text{constant} \tag{3.23}$$

Turning to the general equation 3.16, under the assumption of momentum-independent scattering, the continuum equation is

$$\begin{aligned}\frac{\mathrm{d}\epsilon_d}{\mathrm{d}\ln D} &= |V|^2 n(D)\frac{\omega - D - 2\epsilon_d}{(\omega - D)(\omega - D - \epsilon_d)} \\ &= |V|^2 n(D)\left(\frac{2}{\omega - D} - \frac{1}{\omega - D - \epsilon_d}\right)\end{aligned} \tag{3.24}$$

$n(D)$ is not the density of states, but the total number of states on the shell at energy D. Similarly, the renormalization in U is

$$\begin{aligned}\delta U &= -\sum_{q\beta}|V_q|^2\frac{\epsilon_d}{(\omega - \epsilon_q)(\omega - \epsilon_q - \epsilon_d)} \\ &= -|V|^2 n(D)\sum_{\beta}\frac{\epsilon_d}{(\omega - D)(\omega - D - \epsilon_d)} \\ &= -2|V|^2 n(D)\frac{\epsilon_d}{(\omega - D)(\omega - D - \epsilon_d)} \\ \implies \frac{\mathrm{d}U}{\mathrm{d}\ln D} &= 2|V|^2 n(D)\frac{\epsilon_d}{(\omega - D)(\omega - D - \epsilon_d)} \\ &= 2|V|^2 n(D)\left(\frac{1}{\omega - D - \epsilon_d} - \frac{1}{\omega - D}\right)\end{aligned} \tag{3.25}$$

In the penultimate step, I used the fact that since the onsite energy for either spin is same, the summation just returns a factor of 2. Putting $\omega = 0$,

$$\begin{aligned}\frac{\mathrm{d}\epsilon_d}{\mathrm{d}\ln D} &= |V|^2 n(D)\left(\frac{1}{D + \epsilon_d} - \frac{2}{D}\right) \\ \frac{\mathrm{d}U}{\mathrm{d}\ln D} &= 2|V|^2 n(D)\left(\frac{1}{D} - \frac{1}{D + \epsilon_d}\right)\end{aligned} \tag{3.26}$$

3.2 With Kondo-like interaction

The four-Fermi interaction we are considering is of the form

$$\mathcal{H}_I = \sum_{k,k',\sigma_i} u c^\dagger_{d\sigma_2} c_{d\sigma_4} c_{k'\sigma_3} c^\dagger_{k\sigma_1} \delta_{(\sigma_1+\sigma_2=\sigma_3+\sigma_4)} \tag{3.27}$$

The u in general depends on the spin and the momenta. Expanding the summation by using the delta gives

$$\mathcal{H}_I = \underbrace{\sum_{k,k',\sigma,\sigma'} u_1 \hat{n}_{d\sigma'} c^\dagger_{k\sigma} c_{k'\sigma}}_{\text{spin-preserving scattering}} + \overbrace{\sum_{k,k',\sigma} u_2 c^\dagger_{d\overline{\sigma}} c_{d\sigma} c^\dagger_{k\sigma} c_{k'\overline{\sigma}}}^{\text{spin-flip scattering}} \tag{3.28}$$

At this point, we drop the dependence of u on the momenta and assume it depends only on the spin transfer. The first term (attached with u_1) involves no spin-flip between the scattering momenta or the scattering impurity electrons ($k\sigma \to k'\sigma, d\sigma' \to d\sigma'$). We label this coupling as u_P. The other coupling involves a spin-flip scattering, so we label that as u_A.

$$\mathcal{H}_{I,N} = \sum_{k,k',\sigma,\sigma'} u_P \hat{n}_{d\sigma'} c^\dagger_{k\sigma} c_{k'\sigma} + \sum_{k,k',\sigma} u_A c^\dagger_{d\overline{\sigma}} c_{d\sigma} c^\dagger_{k\sigma} c_{k'\overline{\sigma}} \tag{3.29}$$

where the N in the denominator means the sum is over all momenta up to $|k| = \Lambda_N$. The parallel scattering has two components, when expanded, is of the form

$$u_{\uparrow\uparrow} \hat{n}_{d\uparrow} c^\dagger_{k\uparrow} c_{k'\uparrow} + u_{\downarrow\downarrow} \hat{n}_{d\downarrow} c^\dagger_{k\downarrow} c_{k'\uparrow} + u_{\uparrow\downarrow} \hat{n}_{d\uparrow} c^\dagger_{k\downarrow} c_{k'\downarrow} + u_{\downarrow\uparrow} \hat{n}_{d\downarrow} c^\dagger_{k\uparrow} c_{k'\uparrow} \tag{3.30}$$

We define J_z and J_t such that this term can be written as

$$\begin{aligned} \mathcal{H}_I &= J_z \frac{\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow}}{2} \sum_{kk'} \left(c^\dagger_{k\uparrow} c_{k'\uparrow} - c^\dagger_{k\downarrow} c_{k'\downarrow} \right) + J_t \sum_{kk'} \left[c^\dagger_{d\uparrow} c_{d\downarrow} c^\dagger_{k\downarrow} c_{k'\uparrow} + c^\dagger_{d\downarrow} c_{d\uparrow} c^\dagger_{k\uparrow} c_{k'\downarrow} \right] \\ &= 2 J_z S^z_d s^z + J_t \left(S^+_d s^- + S^-_d s^+ \right) \end{aligned} \tag{3.31}$$

The spin-like operators are defined as

$$\begin{aligned} S^z_d &\equiv \frac{1}{2} \left(\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow} \right) & S^+_d &\equiv c^\dagger_{d\uparrow} c_{d\downarrow} & S^-_d &\equiv c^\dagger_{d\downarrow} c_{d\uparrow} \\ s^z_{kk'} &\equiv \frac{1}{2} \left(c^\dagger_{k\uparrow} c_{k'\uparrow} - c^\dagger_{k\downarrow} c_{k'\downarrow} \right) & s^+_{kk'} &\equiv c^\dagger_{k\uparrow} c_{k'\downarrow} & s^-_{kk'} &\equiv c^\dagger_{k\downarrow} c_{k'\uparrow} \\ & & s^a &\equiv \sum_{kk'} s^a_{kk'} \end{aligned} \tag{3.32}$$

This is the same interaction that constitutes the Kondo model and gives rise to the quenching of the local moment at low energies. The total Hamiltonian for this *Anderson-Kondo*

model is thus

$$\mathcal{H} = \sum_{k\sigma}\left(\epsilon_k \hat{n}_{k\sigma} + V_k c^\dagger_{k\sigma} c_{d\sigma} + h.c.\right) + \epsilon_d \sum_\sigma \hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + 2J_z S^z_d s^z + J_t\left(S^+_d s^- + S^-_d s^+\right) \tag{3.33}$$

For the special case of $2J_z = 2J_t = J$, we get the SU(2) symmetric Heisenberg-like interaction

$$\mathcal{H}_I = J\left[S^z_d s^z + \frac{1}{2}\left(S^+_d s^- + S^-_d s^+\right)\right] = J\mathbf{S_d}\cdot\mathbf{s} \tag{3.34}$$

For the URG, we take two electrons on the shell Λ_N, $q\beta$ and $q\overline{\beta}$, then decouple the electron $q\beta$. The reason for taking two electrons is to allow the symmetries to be preserved. For simplicity, we will only consider those diagonal terms in the denominator that either have both $q\beta$ and $q\overline{\beta}$or both $q\beta$ and d or both $q\overline{\beta}$ and d. Terms that have purely $q\overline{\beta}$ will not be considered. Also, the scattering between just d and $q\overline{\beta}$ can be ignored since it is diagonal in $q\beta$. The Hamiltonian for such a system is

$$\begin{aligned}\mathcal{H}_N = {} & H_{N-1} + H_{\text{imp}} + \epsilon_q \hat{n}_{q\beta} + 2J_z S^z_d s^z_q + V_q c^\dagger_{q\beta} c_{d\beta} + \text{h.c.} + \\ & \sum_{k<\Lambda_N}\left[J_z S^z_d \beta\left(c^\dagger_{k\beta} c_{q\beta} + c^\dagger_{q\beta} c_{k\beta}\right) + J_t\left(c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{q\beta} + c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k\overline{\beta}}\right)\right] \\ & + J_t\left(c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{q\overline{\beta}} c_{q\beta} + c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{q\overline{\beta}}\right)\end{aligned} \tag{3.35}$$

where $s^z_q = \frac{1}{2}\left(\hat{n}_{q\uparrow} - \hat{n}_{q\downarrow}\right)$ and H_{imp} is the impurity-diagonal part of the Hamiltonian $(\epsilon_d \hat{n}_d + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow})$ and

$$H_{N-1} = \sum_{k<\Lambda_N,\sigma}\left[\left(\epsilon_k + \sigma J_z S^z_d\right)\hat{n}_{k\sigma} + V_k c^\dagger_{k\sigma} c_{d\sigma} + \text{h.c.}\right] + H_{I,N-1} \tag{3.36}$$

The diagonal (number-preserving) part is

$$\mathcal{H}_D = H^D_{N-1} + \epsilon_q\left(\hat{n}_{q\beta} + \hat{n}_{q\overline{\beta}}\right) + 2J_z S^z_d s^z_q + H_{imp} \tag{3.37}$$

In line with the simplifications mentioned above, we will work with the following terms:

$$\mathcal{H}_D = \epsilon_q \hat{n}_{q\beta} + 2J_z S^z_d s^z_q + H_{imp} \tag{3.38}$$

To allow the calculation of hole and particle energies on an equal footing, we will make a transformation at the bare model itself:

$$\sum_{k\sigma}\epsilon_k \hat{n}_{k\sigma} = \sum_{k\sigma}\epsilon_k \hat{\tau}_{k\sigma} + \mathcal{C} \tag{3.39}$$

where $\tau \equiv \hat{n} - \frac{1}{2}$ and $\mathcal{C}$ is non-dynamic and will hence be dropped. This transforms the diagonal part $\mathcal{H}^D$. Eq. 3.38 becomes

$$\mathcal{H}_D = \epsilon_q \tau_{q\beta} + 2J_z S^z_d s^z_q + H_{imp} \tag{3.40}$$

3.2.1 Particle sector

The renormalization in the Hamiltonian in the particle sector is

$$\begin{aligned}\Delta^{+}\mathcal{H}_N = \sum_{q\beta}\left[V_q^* c_{d\beta}^\dagger c_{q\beta} + J_z\beta S_d^z \sum_k c_{k\beta}^\dagger c_{q\beta} + J_t \sum_k c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{q\beta}\right] \times \frac{1}{\hat{\omega}^+ - \mathcal{H}_D} \\ \times \left[V_q c_{q\beta}^\dagger c_{d\beta} + J_z\beta S_d^z \sum_k c_{q\beta}^\dagger c_{k\beta} + J_t \sum_k c_{d\overline{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\overline{\beta}}\right]\end{aligned} \tag{3.41}$$

The entire renormalization expression has nine terms- one of order $|V_q|^2$, four of order $V_q J$ and four of order J^2. The particle sector intermediate state has a partcle excitation, so the state will be occupied. Hence $\tau_{q\beta} = \frac{1}{2}$ in the intermediate state. We make this substitution in eq. 3.38:

$$\mathcal{H}_D^+ = \frac{1}{2}\epsilon_q + 2J_z S_d^z s_q^z + H_{imp} \tag{3.42}$$

1.

$$\Delta_1^+\mathcal{H}_N = \sum_{q\beta} |V_q|^2 c_{d\beta}^\dagger c_{q\beta} \frac{1}{\hat{\omega}^+ - \mathcal{H}_D^+} c_{q\beta}^\dagger c_{d\beta} \tag{3.43}$$

The intermediate state is characterized by $\hat{n}_{d\beta} = 0, \hat{n}_{q\beta} = 1 - \hat{n}_{q\overline{\beta}} = 1$. Therefore, at the propagator, we have

$$\begin{aligned}H_1 = \mathcal{H}_D^+ &= \epsilon_q \frac{1}{2} + \beta J_z S_d^z \left(\hat{n}_{q\beta} - \hat{n}_{q\overline{\beta}}\right) + H_{imp} \\ &= \epsilon_q \frac{1}{2} - \frac{1}{2} J_z \hat{n}_{d\overline{\beta}} + \epsilon_d \hat{n}_{d\overline{\beta}}\end{aligned} \tag{3.44}$$

H_1 is the intermediate state Hamiltonian. As a simplification, we replace $\hat{\omega}^+$ with its eigenvalue ω^+.

$$\begin{aligned}\Delta_1^+\mathcal{H}_N &= \sum_{q\beta} |V_q|^2 c_{d\beta}^\dagger c_{q\beta} \frac{1}{\hat{\omega}^+ - H_1} c_{q\beta}^\dagger c_{d\beta} \\ &= \sum_{q\beta} |V_q|^2 c_{d\beta}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{d\beta} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d \hat{n}_{d\overline{\beta}} + \frac{1}{2} J_z \hat{n}_{d\overline{\beta}}}\end{aligned} \tag{3.45}$$

Since $q\beta$ is on the upper band edge, we can assume it is unoccupied in the initial state, and set $c_{q\beta}c_{q\beta}^\dagger = 1$. Then,

$$\begin{aligned}
\Delta_1^+\mathcal{H}_N &= \sum_{q\beta} |V_q|^2 \hat{n}_{d\beta} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q + \left(\frac{J_z}{2} - \epsilon_d\right)\hat{n}_{d\overline{\beta}}} \\
&= \sum_{q\beta} |V(q)|^2 \hat{n}_{d\beta} \left[\frac{\hat{n}_{d\overline{\beta}}}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} + \frac{\left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega^+ - \frac{1}{2}\epsilon_q}\right] \\
&= \sum_{q\beta} |V(q)|^2 \hat{n}_{d\beta} \left[\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q} + \hat{n}_{d\overline{\beta}} \left(\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} - \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q}\right)\right]
\end{aligned} \tag{3.46}$$

2.

$$\Delta_2^+\mathcal{H}_N = \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_z \beta S_d^z c_{q\beta}^\dagger c_{k\beta} \tag{3.47}$$

This can be simplified by noting that since the propagator is diagonal, the only operator that changes $\hat{n}_d$ and S_d^z is the $c_{d\beta}^\dagger$, and therefore

$$c_{d\beta}^\dagger J_z \beta S_d^z = c_{d\beta}^\dagger \frac{1}{2}\left(-J_z\right)\hat{n}_{d\overline{\beta}} \tag{3.48}$$

The expression simplifies to

$$\Delta_2^+\mathcal{H}_N = \frac{1}{2}\left(-J_z\right)\sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{q\beta} \hat{n}_{d\overline{\beta}} \frac{1}{\omega^+ - \mathcal{H}_D^+} c_{q\beta}^\dagger c_{k\beta} \tag{3.49}$$

Intermediate ($\hat{n}_{q\beta} = 1 - \hat{n}_{q\overline{\beta}} = 1, \hat{n}_{d\overline{\beta}} = 1, \hat{n}_{d\beta} = 0$) energy is

$$H_1 = \mathcal{H}_D^+ = \frac{1}{2}\epsilon_q + J_z\beta S_d^z + \epsilon_d = \frac{1}{2}\epsilon_q - \frac{1}{2}J_z + \epsilon_d \tag{3.50}$$

The first term $\frac{1}{2}\epsilon_q + J_z\beta S_d^z$ is the total dispersion of the electron $q\beta$. The ϵ_d is the impurity energy and the third term is the total background energy.

$$\begin{aligned}
\Delta_2^+\mathcal{H}_N &= -\frac{1}{2}J_z \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{q\beta} \hat{n}_{d\overline{\beta}} c_{q\beta}^\dagger c_{k\beta} \frac{1}{\omega^+ - H_1} \\
&= -\frac{1}{2}J_z \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{k\beta} \frac{\hat{n}_{d\overline{\beta}}}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z}
\end{aligned} \tag{3.51}$$

3.

$$\Delta_3^+\mathcal{H}_N = \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_t c_{d\overline{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\overline{\beta}} \tag{3.52}$$

Intermediate ($\hat{n}_{d\beta}=0, \hat{n}_{q\beta}=1-\hat{n}_{q\overline{\beta}}=\hat{n}_{d\overline{\beta}}=1$) energy is

$$H_1 = \frac{1}{2}\epsilon_q - \frac{1}{2}J_z + \epsilon_d \tag{3.53}$$

$$\begin{aligned}
\Delta_3^+\mathcal{H}_N &= \sum_{q\beta k} J_t V_q^* c_{d\beta}^\dagger c_{q\beta} c_{d\overline{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\overline{\beta}} \frac{1}{\omega^+ - H_1} \\
&= -J_t \sum_{q\beta k} V_q^* \hat{n}_{d\beta}\left(1-\hat{n}_{q\beta}\right) c_{d\overline{\beta}}^\dagger c_{k\overline{\beta}} \frac{1}{\omega^+ - H_1} \\
&= -J_t \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{k\beta} \frac{\hat{n}_{d\overline{\beta}}}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z}
\end{aligned} \tag{3.54}$$

4.

$$\Delta_4^+\mathcal{H}_N = \sum_{q\beta k\sigma} J_z \beta S_d^z c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} V_q c_{q\beta}^\dagger c_{d\beta} \tag{3.55}$$

The first step is a simplification:

$$J_z \beta S_d^z c_{d\beta} = \frac{1}{2}\left(-J_z\right)\hat{n}_{d\overline{\beta}} c_{d\beta} \tag{3.56}$$

Intermediate ($\hat{n}_{d\beta}=0, \hat{n}_{q\beta}=1-\hat{n}_{q\overline{\beta}}=\hat{n}_{d\overline{\beta}}=1$) energy is

$$H_1 = \frac{1}{2}\epsilon_q - \frac{1}{2}J_z + \epsilon_d \tag{3.57}$$

$$\begin{aligned}
\Delta_4^+\mathcal{H}_N &= -\frac{1}{2}J_z \sum_{q\beta k} V_q \hat{n}_{d\overline{\beta}} c_{k\beta}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{d\beta} \frac{1}{\omega^+ - H_1} \\
&= \sum_{q\beta k} -\frac{1}{2}J_z V_q \hat{n}_{d\overline{\beta}}\left(1-\hat{n}_{q\beta}\right) c_{k\beta}^\dagger c_{d\beta} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} \\
&= -\frac{1}{2}J_z \sum_{q\beta k} V_q c_{k\beta}^\dagger c_{d\beta} \frac{\hat{n}_{d\overline{\beta}}}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z}
\end{aligned} \tag{3.58}$$

5.

$$\Delta_5^+\mathcal{H}_N = \sum_{q\beta k\sigma} J_t c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} V_q c_{q\beta}^\dagger c_{d\beta} \tag{3.59}$$

Intermediate ($\hat{n}_{d\beta}=0, \hat{n}_{q\beta}=1-\hat{n}_{q\overline{\beta}}=\hat{n}_{d\overline{\beta}}=1$) energy is

$$H_1 = \frac{1}{2}\epsilon_q - \frac{1}{2}J_z + \epsilon_d \tag{3.60}$$

$$\begin{aligned}\Delta_5^+\mathcal{H}_N &= \sum_{q\beta k} J_t V_q c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{d\beta} \frac{1}{\omega^+ - H_1} \\ &= -\sum_{q\beta k} J_t V_q \left(1-\hat{n}_{q\beta}\right)\hat{n}_{d\beta} c_{k\overline{\beta}}^\dagger c_{d\overline{\beta}} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} \\ &= -J_t \sum_{q\beta k} V_q c_{k\beta}^\dagger c_{d\beta} \frac{\hat{n}_{d\overline{\beta}}}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z}\end{aligned} \tag{3.61}$$

6.

$$\Delta_6^+\mathcal{H}_N = \sum_{k'q\beta k} J_z S_d^z \beta c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_z S_d^z \beta c_{q\beta}^\dagger c_{k'\beta} \tag{3.62}$$

The first step is a simplification:

$$(\beta S_d^z)^2 = \frac{1}{4}\left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right)^2 = \frac{1}{4}\left(\hat{n}_{d\beta} + \hat{n}_{d\beta} - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right) = \frac{1}{4}\left(\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right) \tag{3.63}$$

Note that this term projects onto the singly-occupied subspace; both the doubly- and zero-occupied states will give zero for this term. Intermediate ($\hat{n}_{q\beta} = 1 - \hat{n}_{q\overline{\beta}} = 1$) energy is

$$H_1 = \frac{1}{2}\epsilon_q + \beta J_z S_d^z + H_{imp} \tag{3.64}$$

Since the $(S^z)^2$ term filters out only the single-occupied subspace, we can write $H_{imp} = \epsilon_d$.

$$\begin{aligned}\Delta_6^+\mathcal{H}_N &= \frac{1}{4}J_z^2 \sum_{k'q\beta k} \left(\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right) c_{k\beta}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{k'\beta} \frac{1}{\omega^+ - H_1} \\ &= \frac{1}{4}J_z^2 \sum_{k'q\beta k} \left(\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right)\left(1-\hat{n}_{q\beta}\right) c_{k\beta}^\dagger c_{k'\beta} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - H_{imp} - \beta J_z S_d^z} \\ &= \frac{1}{4}J_z^2 \sum_{k'q\beta k} c_{k\beta}^\dagger c_{k'\beta} \frac{\left(\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right)}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d - \beta J_z S_d^z} \\ &= \frac{1}{4}J_z^2 \sum_{k'q\beta k} c_{k\beta}^\dagger c_{k'\beta} \left[\frac{\hat{n}_{d\beta}\left(1-\hat{n}_{d\overline{\beta}}\right)}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d - \frac{1}{2}J_z} + \frac{\hat{n}_{d\overline{\beta}}\left(1-\hat{n}_{d\beta}\right)}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z}\right]\end{aligned} \tag{3.65}$$

In the last step, we used the fact that $\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}$ is not zero only in the singly occupied subspace, hence we can expand it into $\hat{n}_\uparrow\left(1-\hat{n}_\downarrow\right) + \hat{n}_\downarrow\left(1-\hat{n}_\uparrow\right)$.

7.

$$\Delta_7^+\mathcal{H}_N = \sum_{q\beta kk'} \beta J_z S_d^z c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_t c_{d\overline{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\overline{\beta}} \tag{3.66}$$

The first step is a simplification:

$$\beta S_d^z c_{d\overline{\beta}}^\dagger c_{d\beta} = \beta S_d^z S_{d\overline{\beta}}^+ = \beta \frac{1}{2}\overline{\beta} S_{d\overline{\beta}}^+ = -\frac{1}{2} c_{d\overline{\beta}}^\dagger c_{d\beta} \tag{3.67}$$

Intermediate ($\hat{n}_{d\beta} = 0, \hat{n}_{q\beta} = 1 - \hat{n}_{q\overline{\beta}} = \hat{n}_{d\overline{\beta}} = 1$) energy is

$$H_1 = \frac{1}{2}\epsilon_q + \beta J_z S_d^z + \epsilon_d = \frac{1}{2}\epsilon_q - \frac{1}{2}J_z + \epsilon_d \tag{3.68}$$

$$\begin{aligned}
\Delta_7^+ \mathcal{H}_N &= \sum_{q\beta kk'} \frac{1}{2} J_z J_t c_{k\beta}^\dagger c_{q\beta} c_{d\overline{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\overline{\beta}} \frac{-1}{\omega^+ - H_1} \\
&= -\frac{1}{2} J_z J_t \sum_{q\beta kk'} (1 - \hat{n}_{q\beta})\, c_{d\overline{\beta}}^\dagger c_{d\beta} c_{k\beta}^\dagger c_{k'\overline{\beta}} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} \\
&= -\frac{1}{2} J_z J_t \sum_{q\beta kk'} c_{d\overline{\beta}}^\dagger c_{d\beta} c_{k\beta}^\dagger c_{k'\overline{\beta}} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z}
\end{aligned} \tag{3.69}$$

8.

$$\Delta_8^+ \mathcal{H}_N = \sum_{q\beta kk'} J_t c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_z \beta S_d^z c_{q\beta}^\dagger c_{k'\beta} \tag{3.70}$$

The first step is a simplification:

$$c_{d\beta}^\dagger c_{d\overline{\beta}} \beta S_d^z = S_{d\beta}^+ \beta S_d^z = \beta \frac{1}{2}\overline{\beta} S_{d\overline{\beta}}^+ = -\frac{1}{2} c_{d\beta}^\dagger c_{d\overline{\beta}} \tag{3.71}$$

Intermediate ($\hat{n}_{d\beta} = 0, \hat{n}_{q\beta} = 1 - \hat{n}_{q\overline{\beta}} = \hat{n}_{d\overline{\beta}} = 1$) energy is

$$H_1 = \frac{1}{2}\epsilon_q + \beta J_z S_d^z + \epsilon_d = \frac{1}{2}\epsilon_q - \frac{1}{2}J_z + \epsilon_d \tag{3.72}$$

$$\begin{aligned}
\Delta_8^+ \mathcal{H}_N &= -\sum_{q\beta kk'} \frac{1}{2} J_z J_t c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{k'\beta} \frac{1}{\omega^+ - H_1} \\
&= -\frac{1}{2} J_z J_t \sum_{q\beta kk'} (1 - \hat{n}_{q\beta})\, c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{k'\beta} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} \\
&= -\frac{1}{2} J_z J_t \sum_{q\beta kk'} c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{k'\beta} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z}
\end{aligned} \tag{3.73}$$

9.

$$\Delta_9^+ \mathcal{H}_N = \sum_{q\beta kk\prime} J_t c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_t c_{d\overline{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\overline{\beta}} \tag{3.74}$$

Intermediate ($\hat{n}_{d\beta}=0, \hat{n}_{q\beta}=1-\hat{n}_{q\overline{\beta}}=\hat{n}_{d\overline{\beta}}=1$) energy is

$$H_1 = \frac{1}{2}\epsilon_q - \frac{1}{2}J_z + \epsilon_d \tag{3.75}$$

$$\begin{aligned}
\Delta_9^+ \mathcal{H}_N &= \sum_{q\beta kk\prime} J_t^2 c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{q\beta} c_{d\overline{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\overline{\beta}} \frac{1}{\omega^+ - H_1} \\
&= J_t^2 \sum_{q\beta kk\prime} \left(1-\hat{n}_{q\beta}\right) \hat{n}_{d\beta} \left(1-\hat{n}_{d\overline{\beta}}\right) c_{k\overline{\beta}}^\dagger c_{k'\overline{\beta}} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} \\
&= J_t^2 \sum_{q\beta kk\prime} c_{k\beta}^\dagger c_{k'\beta} \frac{\hat{n}_{d\overline{\beta}}\left(1-\hat{n}_{d\beta}\right)}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z}
\end{aligned} \tag{3.76}$$

Scaling equations for particle sector

The scaling equations are obtained as follows. The first term gives the renormalization in ϵ_d and U. The renormalization in U will come with a factor of 2 because $\sum_\beta \hat{n}_{d\beta}\hat{n}_{d\overline{\beta}} = 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}$. Terms 2 and 3 renormalize V^*. Terms 4 and 5 renormalize V. Since these renormalizations are same, we write just one them. Also, in the terms 2 through 5, the renormalization is actually that of $V\hat{n}_{d\overline{\beta}}$, not strictly of V. In other words, if we split V as $V = V\left[\hat{n}_{d\overline{\beta}} + \left(1-\hat{n}_{d\overline{\beta}}\right)\right] = V^1\hat{n}_{d\overline{\beta}} + V^0\left(1-\hat{n}_{d\overline{\beta}}\right)$, then these terms will renormalize V^1. However, we do not make this distinction here because in the particle sector, we will get a renormalization in V^0, and that will turn out to be the same, so we can just talk about the renormalization in V instead of splitting it. Terms 7 and * renormalize J_t and 9 renormalizes the anti-parallel part of J_z, that is, the part in which the conduction electron has spin $\overline{\beta}$. The other term, with spin β will renormalize in the hole sector. Term 6 can be ignored for now because it will get canceled by an opposite term in the hole sector, see 3.5. Otherwise it will renormalize J_z.

$$\Delta^+\epsilon_d = \sum_q |V(q)|^2 \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q} \tag{3.77}$$

$$\Delta^+ U = \sum_q 2|V(q)|^2 \left(\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} - \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q}\right) \tag{3.78}$$

$$\Delta^+ V = -\left(\frac{1}{2}J_z + J_t\right) \sum_q V_q \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} \tag{3.79}$$

$$\Delta^+ J_t = -J_z J_t \sum_q \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} \tag{3.80}$$

$$\Delta^+ J_z = -J_t^2 \sum_q \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} \tag{3.81}$$

3.2.2 Hole sector

The renormalization in the Hamiltonian in the hole sector is

$$\begin{aligned}\Delta^{-}\mathcal{H}_N = \sum_{q\beta}\left[V_q c^{\dagger}_{q\beta}c_{d\beta} + J_z\beta S^z_d\sum_{k\sigma}\hat{n}_{d\sigma}c_{k\beta}c^{\dagger}_{q\beta} + J_t\sum_{k\sigma}c^{\dagger}_{d\bar{\beta}}c^{\dagger}_{q\beta}c_{d\beta}c_{k\bar{\beta}}\right]\times\frac{1}{\hat{\omega}^{-}-\mathcal{H}^{-}_D}\\ \times\left[V^{*}_q c^{\dagger}_{d\beta}c_{q\beta} + J_z\beta S^z_d\sum_{k\sigma}\hat{n}_{d\sigma}c_{q\beta}c^{\dagger}_{k\beta} + J_t\sum_{k\sigma}c^{\dagger}_{d\beta}c^{\dagger}_{k\bar{\beta}}c_{d\bar{\beta}}c_{q\beta}\right]\end{aligned} \tag{3.82}$$

$\mathcal{H}^{-}_D$ is the energy of the hole state. Since the hole state consists of a missing electron, the diagonal part can be evaluated by substituting $\tau_{q\beta} = -\frac{1}{2}$ and $\epsilon_q = -\epsilon_q$ in eq. 3.38.

$$\mathcal{H}^{-}_D = \frac{1}{2}\epsilon_q + J_z S^z_d s^z_q + H_{\text{imp}} \tag{3.83}$$

1.

$$\Delta^{-}_1\mathcal{H}_N = \sum_{q\beta}|V_q|^2 c^{\dagger}_{q\beta}c_{d\beta}\frac{1}{\hat{\omega}^{-}-\mathcal{H}^{-}_D}c^{\dagger}_{d\beta}c_{q\beta} \tag{3.84}$$

The intermediate ($\hat{n}_{q\beta}=0, \hat{n}_{d\beta}=1$) energy is

$$H_1 = \epsilon_d + (\epsilon_d+U)\,\hat{n}_{d\bar{\beta}} + \frac{1}{2}\epsilon_q - \beta J_z S^z_d = \frac{1}{2}\epsilon_q - \frac{1}{2}J_z\left(1-\hat{n}_{d\bar{\beta}}\right) + \epsilon_d + (\epsilon_d+U)\,\hat{n}_{d\bar{\beta}} \tag{3.85}$$

$$\Delta^{-}_1\mathcal{H}_N = \sum_{q\beta}|V_q|^2\hat{n}_{q\beta}\left(1-\hat{n}_{d\beta}\right)\frac{1}{\omega^{-}-H_1} \tag{3.86}$$

For hole excitations, the initial state must be filled, so we can set $\hat{n}_{q\beta}=1$.

$$\begin{aligned}\Delta^{-}_1\mathcal{H}_N &= \sum_{q\beta}|V_q|^2\hat{n}_{q\beta}\left(1-\hat{n}_{d\beta}\right)\frac{1}{\omega^{-}-\frac{1}{2}\epsilon_q+\frac{1}{2}J_z\left(1-\hat{n}_{d\bar{\beta}}\right)-\epsilon_d-(\epsilon_d+U)\,\hat{n}_{d\bar{\beta}}}\\ &= \sum_{q\beta}|V_q|^2\left(1-\hat{n}_{d\beta}\right)\left[\frac{\hat{n}_{d\bar{\beta}}}{\omega^{-}-\frac{1}{2}\epsilon_q-2\epsilon_d-U}+\frac{1-\hat{n}_{d\bar{\beta}}}{\omega^{-}-\frac{1}{2}\epsilon_q-\epsilon_d+\frac{1}{2}J_z}\right]\\ &= \sum_{q\beta}|V(q)|^2\left[\hat{n}_{d\bar{\beta}}\left(\frac{1}{\omega^{-}-\frac{1}{2}\epsilon_q-2\epsilon_d-U}-\frac{2}{\omega^{-}-\frac{1}{2}\epsilon_q-\epsilon_d+\frac{1}{2}J_z}\right)\right.\\ &\qquad\left.+\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\left(\frac{1}{\omega^{-}-\frac{1}{2}\epsilon_q-\epsilon_d+\frac{1}{2}J_z}-\frac{1}{\omega^{-}-\frac{1}{2}\epsilon_q-2\epsilon_d-U}\right)\right]\end{aligned} \tag{3.87}$$

2.

$$\Delta^{-}_2\mathcal{H}_N = \sum_{q\beta k}V_q c^{\dagger}_{q\beta}c_{d\beta}\frac{1}{\hat{\omega}^{-}-\mathcal{H}^{-}_D}J_z\beta S^z_d c^{\dagger}_{k\beta}c_{q\beta} \tag{3.88}$$

The first step is a simplification:

$$c_{d\beta}J_z\beta S_d^z = c_{d\beta}\frac{1}{2}J_z\left(1-\hat{n}_{d\overline{\beta}}\right) \tag{3.89}$$

The intermediate ($\hat{n}_{q\beta}=0,\hat{n}_{d\beta}=1$) energy is

$$H_1 = -\frac{1}{2}\epsilon_q+\epsilon_d+\left(\epsilon_d+U\right)\hat{n}_{d\overline{\beta}}-\frac{1}{2}J_z\left(1-\hat{n}_{d\overline{\beta}}\right) \tag{3.90}$$

$$\begin{aligned}\Delta_2^-\mathcal{H}_N &= \sum_{q\beta k}\frac{1}{2}J_z\left(1-\hat{n}_{d\overline{\beta}}\right)V_q c_{q\beta}^\dagger c_{d\beta}\left(1-\hat{n}_{d\overline{\beta}}\right)c_{k\beta}^\dagger c_{q\beta}\frac{1}{\omega^- - H_1}\\ &= -\sum_{q\beta k}\hat{n}_{q\beta}c_{k\beta}^\dagger c_{d\beta}\frac{V_q\frac{1}{2}J_z\left(1-\hat{n}_{d\overline{\beta}}\right)}{\omega^- -\frac{1}{2}\epsilon_q-\epsilon_d-\left(\epsilon_d+U\right)\hat{n}_{d\overline{\beta}}+\frac{1}{2}J_z\left(1-\hat{n}_{d\overline{\beta}}\right)} \\ &= -\frac{1}{2}J_z\sum_{q\beta k}V_q\hat{n}_{q\beta}c_{k\beta}^\dagger c_{d\beta}\frac{\left(1-\hat{n}_{d\overline{\beta}}\right)}{\omega^- -\frac{1}{2}\epsilon_q-\epsilon_d+\frac{1}{2}J_z}\end{aligned} \tag{3.91}$$

3.

$$\Delta_3^-\mathcal{H}_N = \sum_{q\beta k}V_q c_{q\beta}^\dagger c_{d\beta}\frac{1}{\hat{\omega}^- - \mathcal{H}_D^-}J_t c_{d\beta}^\dagger c_{d\overline{\beta}}c_{k\overline{\beta}}^\dagger c_{q\beta} \tag{3.92}$$

The intermediate ($\hat{n}_{q\beta}=\hat{n}_{d\overline{\beta}}=0,\hat{n}_{d\beta}=1$) energy is

$$H_1 = \epsilon_d-\frac{1}{2}\epsilon_q-\frac{1}{2}J_z\beta S_d^z = \epsilon_d-\frac{1}{2}\epsilon_q-\frac{1}{2}J_z \tag{3.93}$$

$$\begin{aligned}\Delta_3^-\mathcal{H}_N &= \sum_{q\beta k}J_t V_q c_{q\beta}^\dagger c_{d\beta}c_{d\beta}^\dagger c_{d\overline{\beta}}c_{k\overline{\beta}}^\dagger c_{q\beta}\frac{1}{\omega^- - H_1}\\ &= \sum_{q\beta k}J_t V_q\hat{n}_{q\beta}\left(1-\hat{n}_{d\beta}\right)c_{k\overline{\beta}}^\dagger c_{d\overline{\beta}}\frac{-1}{\omega^- -\frac{1}{2}\epsilon_q-\epsilon_d+\frac{1}{2}J_z} \\ &= -J_t\sum_{q\beta k}V_q c_{k\beta}^\dagger c_{d\beta}\frac{1-\hat{n}_{d\overline{\beta}}}{\omega^- -\frac{1}{2}\epsilon_q-\epsilon_d+\frac{1}{2}J_z}\end{aligned} \tag{3.94}$$

4.

$$\Delta_4^-\mathcal{H}_N = \sum_{q\beta k}\frac{1}{2}J_z\beta S_d^z c_{q\beta}^\dagger c_{k\beta}\frac{1}{\hat{\omega}^- - \mathcal{H}_D^-}V_q^* c_{d\beta}^\dagger c_{q\beta} \tag{3.95}$$

There is a simplification:

$$\frac{1}{2}J_z\beta S_d^z c_{d\beta}^\dagger = \frac{1}{2}J_z\left(1-\hat{n}_{d\overline{\beta}}\right)c_{d\beta}^\dagger \tag{3.96}$$

The intermediate ($\hat{n}_{q\beta}=0,\hat{n}_{d\beta}=1$) energy is

$$H_1 = -\frac{1}{2}\epsilon_q+\epsilon_d+\left(\epsilon_d+U\right)\hat{n}_{d\overline{\beta}}-\frac{1}{2}J_z\left(1-\hat{n}_{d\overline{\beta}}\right) \tag{3.97}$$

$$\begin{aligned}\Delta_4^- \mathcal{H}_N &= \sum_{q\beta k} V_q^* c_{q\beta}^\dagger c_{k\beta} c_{d\beta}^\dagger c_{q\beta} \frac{\frac{1}{2}J_z\left(1-\hat{n}_{d\overline{\beta}}\right)}{\omega^- - H_1} \\ &= \sum_{q\beta k} \hat{n}_{q\beta} V_q^* c_{k\beta} c_{d\beta}^\dagger \frac{\frac{1}{2}J_z\left(1-\hat{n}_{d\overline{\beta}}\right)}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d - (\epsilon_d + U)\,\hat{n}_{d\overline{\beta}} + \frac{1}{2}J_z\left(1-\hat{n}_{d\overline{\beta}}\right)} \\ &= -\frac{1}{2}J_z \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{k\beta} \frac{1-\hat{n}_{d\overline{\beta}}}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z}\end{aligned} \tag{3.98}$$

5.

$$\Delta_5^- \mathcal{H}_N = \sum_{q\beta k} J_t c_{d\overline{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\overline{\beta}} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} V_q^* c_{d\beta}^\dagger c_{q\beta} \tag{3.99}$$

The intermediate ($\hat{n}_{q\beta} = \hat{n}_{d\overline{\beta}} = 0, \hat{n}_{d\beta} = 1$) energy is

$$H_1 = -\frac{1}{2}\epsilon_q + \epsilon_d - \frac{1}{2}J_z \tag{3.100}$$

$$\begin{aligned}\Delta_5^- \mathcal{H}_N &= \sum_{q\beta k} J_t V_q^* c_{d\overline{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\overline{\beta}} c_{d\beta}^\dagger c_{q\beta} \frac{1}{\hat{\omega}^- - H_1} \\ &= -J_t \sum_{q\beta k} V_q^* \hat{n}_{q\beta}\left(1-\hat{n}_{d\beta}\right) c_{d\overline{\beta}}^\dagger c_{k\overline{\beta}} \frac{1}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} \\ &= -J_t \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{k\beta} \frac{1-\hat{n}_{d\overline{\beta}}}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z}\end{aligned} \tag{3.101}$$

6.

$$\Delta_6^- \mathcal{H}_N = \sum_{q\beta k k'} J_z \beta S_d^z c_{q\beta}^\dagger c_{k'\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_z \beta S_d^z c_{k\beta}^\dagger c_{q\beta} \tag{3.102}$$

From eq. 3.63,

$$(\beta S_d^z)^2 = \frac{1}{4}\left(\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right) \tag{3.103}$$

The intermediate ($\hat{n}_{q\beta} = 0$) energy is

$$H_1 = H_{\text{imp}} - \frac{1}{2}\epsilon_q - \beta J_z S_d^z \tag{3.104}$$

$$
\begin{aligned}
\Delta_6^- \mathcal{H}_N &= \sum_{q\beta kk'} \frac{J_z^2}{4} \left(\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right) c_{q\beta}^\dagger c_{k'\beta} c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega^- - H_1} \\
&= \frac{J_z^2}{4} \sum_{q\beta kk'} \hat{n}_{q\beta} \left(\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right) c_{k'\beta} c_{k\beta}^\dagger \frac{1}{\omega^- - \frac{1}{2}\epsilon_q - H_{\text{imp}} + \beta J_z S_d^z} \\
&= -\frac{J_z^2}{4} \sum_{q\beta kk'} c_{k\beta}^\dagger c_{k'\beta} \left[\frac{\hat{n}_{d\beta}\left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} + \frac{\hat{n}_{d\overline{\beta}}\left(1 - \hat{n}_{d\beta}\right)}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d - \frac{1}{2}J_z} \right] \\
&\quad + \frac{J_z^2}{4} \sum_{q\beta k} \left[\frac{\hat{n}_{d\beta}\left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} + \frac{\hat{n}_{d\overline{\beta}}\left(1 - \hat{n}_{d\beta}\right)}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d - \frac{1}{2}J_z} \right]
\end{aligned}
\tag{3.105}
$$

7.

$$
\Delta_7^- \mathcal{H}_N = \sum_{q\beta kk'} J_z \beta S_d^z c_{q\beta}^\dagger c_{k'\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_t c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{q\beta} \tag{3.106}
$$

Simplification:

$$
\beta S_d^z c_{d\beta}^\dagger c_{d\overline{\beta}} = \beta S_d^z S_{d\beta}^+ = \beta \frac{1}{2} \beta S_{d\beta}^+ = \frac{1}{2} c_{d\beta}^\dagger c_{d\overline{\beta}} \tag{3.107}
$$

The intermediate ($\hat{n}_{q\beta} = \hat{n}_{d\overline{\beta}} = 0, \hat{n}_{d\beta} = 1$) energy is

$$
H_1 = \epsilon_d - \frac{1}{2}\epsilon_q - \frac{1}{2}J_z \tag{3.108}
$$

$$
\begin{aligned}
\Delta_7^- \mathcal{H}_N &= \sum_{q\beta kk'} \frac{1}{2} J_z J_t c_{q\beta}^\dagger c_{k'\beta} c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{q\beta} \frac{1}{\omega^- - H_1} \\
&= \sum_{q\beta kk'} \frac{1}{2} J_z J_t \hat{n}_{q\beta} c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{k'\beta} \frac{-1}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} \\
&= -\frac{1}{2} J_z J_t \sum_{q\beta kk'} c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{k'\beta} \frac{1}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} \\
&= -\frac{1}{2} J_z J_t \sum_{q\beta kk'} c_{d\overline{\beta}}^\dagger c_{d\beta} c_{k\beta}^\dagger c_{k'\overline{\beta}} \frac{1}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z}
\end{aligned}
\tag{3.109}
$$

8.

$$
\Delta_8^- \mathcal{H}_N = \sum_{q\beta kk'} J_t c_{d\overline{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\overline{\beta}} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_z \beta S_d^z c_{k\beta}^\dagger c_{q\beta} \tag{3.110}
$$

Simplification:

$$
c_{d\overline{\beta}}^\dagger c_{d\beta} \beta S_d^z = S_{d\overline{\beta}}^+ S_d^z \beta = \beta \frac{1}{2} S_{d\overline{\beta}}^+ \beta = \frac{1}{2} c_{d\overline{\beta}}^\dagger c_{d\beta} \tag{3.111}
$$

The intermediate ($\hat{n}_{q\beta} = \hat{n}_{d\overline{\beta}} = 0, \hat{n}_{d\beta} = 1$) energy is

$$
H_1 = -\frac{1}{2}\epsilon_q - \frac{1}{2}J_z + \epsilon_d \tag{3.112}
$$

$$\begin{aligned}\Delta_8^-\mathcal{H}_N &= \sum_{q\beta kk'}\frac{1}{2}J_zJ_tc^\dagger_{d\overline{\beta}}c_{d\beta}c^\dagger_{q\beta}c_{k'\overline{\beta}}c^\dagger_{k\beta}c_{q\beta}\frac{1}{\omega^- - H_1}\\ &= \sum_{q\beta kk'}\frac{1}{2}J_zJ_t\hat{n}_{q\beta}c^\dagger_{d\overline{\beta}}c_{d\beta}c^\dagger_{k\beta}c_{k'\overline{\beta}}\frac{-1}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d - \frac{1}{2}J_z}\\ &= -\frac{1}{2}J_zJ_t\sum_{q\beta kk'}c^\dagger_{d\overline{\beta}}c_{d\beta}c^\dagger_{k\beta}c_{k'\overline{\beta}}\frac{1}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z}\end{aligned} \tag{3.113}$$

9.

$$\Delta_9^-\mathcal{H}_N = \sum_{q\beta kk'}J_tc^\dagger_{d\overline{\beta}}c_{d\beta}c^\dagger_{q\beta}c_{k'\overline{\beta}}\frac{1}{\hat{\omega}^- - \mathcal{H}_D^-}J_tc^\dagger_{d\beta}c_{d\overline{\beta}}c^\dagger_{k\overline{\beta}}c_{q\beta} \tag{3.114}$$

The intermediate ($\hat{n}_{q\beta} = \hat{n}_{d\overline{\beta}} = 0, \hat{n}_{d\beta} = 1$) energy is

$$H_1 = -\frac{1}{2}\epsilon_q - \frac{1}{2}J_z + \epsilon_d \tag{3.115}$$

$$\begin{aligned}\Delta_9^-\mathcal{H}_N &= \sum_{q\beta kk'}J_t^2c^\dagger_{d\overline{\beta}}c_{d\beta}c^\dagger_{q\beta}c_{k'\overline{\beta}}c^\dagger_{d\beta}c_{d\overline{\beta}}c^\dagger_{k\overline{\beta}}c_{q\beta}\frac{1}{\omega^- - H_1}\\ &= \sum_{q\beta kk'}J_t^2\hat{n}_{q\beta}c^\dagger_{d\overline{\beta}}c_{d\beta}c_{k'\overline{\beta}}c^\dagger_{d\beta}c_{d\overline{\beta}}c^\dagger_{k\overline{\beta}}\frac{1}{\omega^- - H_1}\\ &= -\sum_{q\beta kk'}J_t^2\hat{n}_{q\beta}\hat{n}_{d\overline{\beta}}c_{d\beta}c_{k'\overline{\beta}}c^\dagger_{d\beta}c^\dagger_{k\overline{\beta}}\frac{1}{\omega^- - H_1}\\ &= \sum_{q\beta kk'}J_t^2\hat{n}_{q\beta}\hat{n}_{d\overline{\beta}}\left(1-\hat{n}_{d\beta}\right)c_{k'\overline{\beta}}c^\dagger_{k\overline{\beta}}\frac{1}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z}\\ &= -J_t^2\sum_{q\beta kk'}c^\dagger_{k\beta}c_{k'\beta}\frac{\hat{n}_{d\beta}\left(1-\hat{n}_{d\overline{\beta}}\right)}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} + J_t^2\sum_{qk\beta}\frac{\hat{n}_{d\overline{\beta}}\left(1-\hat{n}_{d\beta}\right)}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z}\end{aligned} \tag{3.116}$$

Scaling equations for hole sector

The scaling equations are obtained similarly as in the particle sector. The important things to note are the following. The first two terms in term 6 here cancel the term 6 of the particle sector. The last two terms in term 6 and the last term in term 9 renormalize U and ϵ_d.

$$\begin{aligned}\Delta^-\epsilon_d &= \sum_q|V(q)|^2\left(\frac{1}{\omega^- - \frac{1}{2}\epsilon_q - 2\epsilon_d - U} - \frac{2}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z}\right) +\\ &\qquad \sum_{qk}\left[\frac{\frac{1}{4}J_z^2 + J_t^2}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} + \frac{\frac{1}{4}J_z^2}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d - \frac{1}{2}J_z}\right]\\ \Delta^-U &= 2\sum_q|V(q)|^2\left(\frac{1}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} - \frac{1}{\omega^- - \frac{1}{2}\epsilon_q - 2\epsilon_d - U}\right) -\end{aligned}$$

$$2\sum_{qk}\left[\frac{\frac{1}{4}J_z^2+J_t^2}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} + \frac{\frac{1}{4}J_z^2}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d - \frac{1}{2}J_z}\right]$$

$$\Delta^- V = -\left(\frac{1}{2}J_z + J_t\right)\sum_q V_q \frac{1}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z}$$

$$\Delta^- J_t = -J_z J_t \sum_q \frac{1}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z}$$

$$\Delta^- J_z = -J_t^2 \sum_q \frac{1}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z}$$

3.3 Particle-Hole symmetry

The Anderson model Hamiltonian, eq. 3.33, has an impurity particle-hole symmetry for a certain condition of the couplings. To see this, we apply the particle-hole transformation $c_k \to c_k^\dagger, c_d \to -c_d^\dagger$ to the Hamiltonian. Since we are looking at the impurity symmetry, we will only look at the terms involving the impurity. The particle-hole symmetry of the conduction bath is a separate thing and that requires a specific lattice. Hence we will not consider kinetic energy term in this discussion. The rest of the terms transform as

$$\epsilon_d \sum_\sigma \hat{n}_{d\sigma} \to 2\epsilon_d - \epsilon_d \sum_\sigma \hat{n}_{d\sigma} \tag{3.117}$$

$$U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} \to U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} - U\sum_\sigma \hat{n}_{d\sigma} + U \tag{3.118}$$

$$\sum_{k\sigma} V(k)c_{k\sigma}^\dagger c_{d\sigma} + hc \to \sum_{k\sigma} -V(k)c_{k\sigma}c_{d\sigma}^\dagger + hc = \sum_{k\sigma} V^*(k)c_{k\sigma}^\dagger c_{d\sigma} + hc \tag{3.119}$$

$$S^z \sum_{kq} s_{kq}^z \to (-S^z)\sum_{kq}\left(-s_{kq}^z\right) = S^z \sum_{kq} s_{kq}^z \tag{3.120}$$

$$S^\pm \sum_{kq} s_{kq}^\mp \to \left(-S^\pm\right)\sum_{kq}\left(-s_{kq}^\mp\right) = S^\pm \sum_{kq} s_{kq}^\mp \tag{3.121}$$

The transformation of the spin terms, eqs. 3.120 and 3.121, can be understood from the fact that since a spin degree of freedom can be written in terms of the number operator as $\hat{S} = \hat{n} - \frac{1}{2}$, it must transform by flipping its sign: $\hat{S} = \hat{n} - \frac{1}{2} \to \frac{1}{2} - \hat{n} = -\hat{S}$. The spin terms are thus invariant under the particle-hole transformation. The impurity-bath hopping term can be made symmetric by making $V(k)$ real; then we would have, from eq. 3.119,

$$V(k)\left(c_{k\sigma}^\dagger c_{d\sigma} + c_{d\sigma}^\dagger c_{k\sigma}\right) \to V(k)\left(c_{d\sigma}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger c_{d\sigma}\right) \tag{3.122}$$

The impurity diagonal terms, ϵ_d and U, require a specific condition. Combining eqs. 3.117 and 3.118,

$$\epsilon_d \hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} \to (-\epsilon_d - U)\,\hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} \tag{3.123}$$

We dropped some constant terms in the transformed Hamiltonian. For particle-hole symmetry, the left and right hand sides must be same. The required condition is thus

$$\epsilon_d = -\epsilon_d - U \implies \epsilon_d + \frac{1}{2}U = 0 \tag{3.124}$$

This same condition can be obtained in a more physical way. If we consider the singly-occupied state of the impurity as the reference state, the doubly-occupied state is the particle-excitation and the vacant state is the hole excitation. If we measure the energies with w.r.t this singly occupied state, the energy of the particle state is $E_p = 2\epsilon_d + U - \epsilon_d = \epsilon_d + U$ and that of the hole state is $E_h = 0 - \epsilon_d = -\epsilon_d$. Particle-hole symmetry then requires the particle and hole levels to be degenerate, which means $E_p = E_h$, and we recover the condition eq. 3.124.

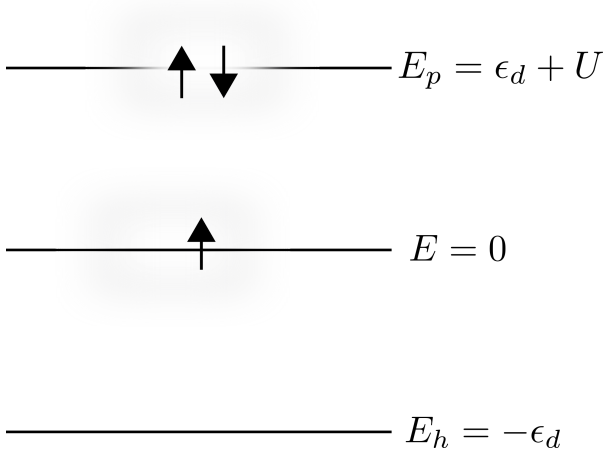

Figure 2: Particle and hole excitations of the impurity

Since the URG is unitary, if we start from a model that is particle-hole symmetric, the RG equations should uphold that symmetry. What this means is that if we have $\epsilon_d + \frac{1}{2}U = 0$ in the bare model, the new couplings should also satisfy $\epsilon_d' + \frac{1}{2}U' = 0$. This means we must have

$$\Delta\left(\epsilon_d + \frac{1}{2}U\right) = 0 \tag{3.125}$$

The quantity $\gamma = \epsilon_d + \frac{1}{2}U$ is thus an RG-invariant for the particle-hole symmetric model; it does not change under the RG flow. It is often referred to as the asymmetry parameter; it quantifies the asymmetry in the model. We need to check if our equations satisfy this. Looking at both the particle and hole equations, we can find the RG equation for the asymmetry parameter

$$\begin{aligned}
\Delta^+\gamma \equiv \Delta^+\left(\epsilon_d + \frac{1}{2}U\right) &= \sum_q |V(q)|^2 \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} \\
\Delta^-\gamma \equiv \Delta^-\left(\epsilon_d + \frac{1}{2}U\right) &= -\sum_q |V(q)|^2 \frac{1}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z}
\end{aligned} \tag{3.126}$$

For a particle-hole symmetric bare model, we can set $\omega^+ = \omega^-$. That gives $\Delta\gamma = 0$.

3.4 "Poor Man's" one-loop form for asymmetric Anderson model

In the limit of $\epsilon_d, J \ll D \ll U$, the equation for ϵ_d becomes, up to lowest order in J,

$$\delta\epsilon_d = -\sum_q \frac{|V_q|^2}{\omega^+ - \epsilon_q} \tag{3.127}$$

If we assume an isotropic dispersion ($\epsilon_q = D$), where D is the current(running) bandwidth and a momentum-independent hopping potential V,

$$\delta\epsilon_d = -\frac{1}{\omega^+ - D}\sum_q |V_q|^2 = -\frac{1}{\omega^+ - D}\rho(D)|\delta D||V|^2$$

There we used

$$\sum_q = \sum_{\epsilon_q \in [D-|\delta D|, D]} = \rho(D)|\delta D| \tag{3.128}$$

where $\rho(D)$ is the single-spin density of states at the energy D and $|\Delta D|$ is the thickness of the band that we disentangled at this step. In the literature, we usually define a quantity that denotes the amount of hybridisation between the impurity and the bath: $\Delta \equiv \pi\rho(D)|V|^2$. In terms of this Δ, we get

$$\delta\epsilon_d = -\frac{\Delta|\delta D|}{\omega^+ - D} \tag{3.129}$$

For low energy excitations, we can use $\omega^+ \ll D$. Further, since we have defined $\delta\epsilon_d = \epsilon_d(D - |\delta D|) - \epsilon_d(D)$, we must have $\delta D = D - |\delta D| - D = -|\delta D|$.

$$\frac{\mathrm{d}\epsilon_d}{\mathrm{d}D} = -\frac{\Delta}{D} \tag{3.130}$$

This is the form obtained from Poor Man's scaling of the asymmetric Anderson model.

3.5 Vanishing of $\Delta^6\mathcal{H}$

If take the scattering term $J_z\beta S_d^z c_{q\beta}^\dagger c_{k'\beta}$ and construct the η and $\eta^\dagger$ operators from them,

$$\begin{aligned}\eta &= \frac{1}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \beta J_z S_d^z} J_z\beta S_d^z c_{k'\beta}^\dagger c_{q\beta} \\ \eta^\dagger &= \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - H_{\mathrm{imp}} - \beta J_z S_d^z} J_z\beta S_d^z c_{q\beta}^\dagger c_{k'\beta}\end{aligned} \tag{3.131}$$

From the expression of η, we can take its Hermitian conjugate to get another expression for $\eta^\dagger$:

$$\eta^\dagger = J_z\beta S_d^z c_{q\beta}^\dagger c_{k'\beta}\frac{1}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \beta J_z S_d^z} \tag{3.132}$$

Comparing the two expressions gives

$$\frac{1}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \beta J_z S_d^z} = \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - H_{\mathrm{imp}} - \beta J_z S_d^z} \tag{3.133}$$

Substituting this equation into either Δ_6^+ or Δ_6^- gives $\Delta_6^+\mathcal{H} = -\Delta_6^-\mathcal{H}$, so $\Delta_6\mathcal{H} = 0$.

3.6 SU(2) invariance and Kondo model one-loop form

Setting $J_z = J_t = \frac{1}{2}J$ makes the interaction $SU(2)$ symmetric; the last two RG equations can then be written in the common form:

$$2\Delta J_z = 2\Delta J_t = \Delta J = -J^2 \sum_q \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J} \tag{3.134}$$

In order to reach the Kondo RG equations, we need to make the appropriate physical change; the difference between the Anderson model and the Kondo model is that the impurity charge fluctuations are frozen at single occupation in the latter. This means that the ground state of the impurity is now at ϵ_d. We can take account of this change by now measuring ω^+ from the single occupation energy itself, ϵ_d. Hence we should redefine $\omega^+ - \epsilon_d \to \tilde{\omega}^+$.

$$2\Delta J_z = 2\Delta J_t = \Delta J = -J^2 \sum_q \frac{1}{\tilde{\omega}^+ - \frac{1}{2}\epsilon_q + \frac{1}{4}J} \tag{3.135}$$

If we now consider low energy excitations ($\tilde{\omega}^+ - \epsilon_q \approx -\epsilon_q$) and expand the denominator in powers of J and keep only the lowest order, we get

$$\Delta J = -J^2 \sum_q \frac{1}{-\frac{1}{2}\epsilon_q} \tag{3.136}$$

For an isotropic dispersion, we can use $\epsilon_q = D$. The sum can then be evaluated as

$$\sum_q = \rho(D)\Delta D \tag{3.137}$$

The flow equation of J becomes

$$\Delta J = 2J^2\rho(D)\frac{|\Delta D|}{D} \tag{3.138}$$

This is the familiar one-loop Kondo flow equation obtained from Poor man's scaling. To get the continuum version, we must note that since we are decreasing the bandwidth, we have to set $\Delta D = -|\Delta D|$. Therefore,

$$\frac{\mathrm{d}J}{\mathrm{d}\ln D} = -2J^2\rho(D) \tag{3.139}$$

3.7 Connection with Kondo URG result

Recall eq. 3.135.

$$\Delta J = -J^2 \sum_q \frac{1}{\tilde{\omega}^+ - \frac{1}{2}\epsilon_q + \frac{1}{4}J} \tag{3.140}$$

For $\tilde{\omega}^+ = 0$ and $\epsilon_q = D$, we get

$$\Delta J = 2J^2 \sum_q \frac{1}{D - \frac{1}{2}J} \tag{3.141}$$

This has the same fixed point structure as the Kondo URG scaling equation.

4 Connection between Unitary Renormalization Group and Poor Man's Scaling

We first motivate the formalism of PMS method. The problem is defined as

$$\mathcal{H} |\Psi\rangle = E |\Psi\rangle \tag{4.1}$$

$\mathcal{H}$ is the total Hamiltonian and $|\Psi\rangle$ and E are the exact eigenstate and eigenvalue of $\mathcal{H}$. The problems we deal with typically have a bath of mobile electrons, with energies spanning from $-D$ to D. We are interested in finding effective Hamiltonians after "removing" the highest shell in the conduction bath. This will give us a Hamiltonian to which we can again apply the same procedure.

We want to decouple one electron at momentum q. We can split the exact wavefunction as

$$|\Psi\rangle = |\Psi_0\rangle + |\Psi_1\rangle \tag{4.2}$$

where $|\Psi_0\rangle = (1 - \hat{n}_q) |\Psi^N\rangle$ is that part of the wavefunction where the state q is occupied. $|\Psi_1^N\rangle = \hat{n}_q |\Psi\rangle$ is that part of the wavefunction where the state q is occupied. We can also split the Hamiltonian as

$$\mathcal{H} = \mathcal{H}^d + V_0 + V_+ + V_- \tag{4.3}$$

$\mathcal{H}^d$ is the diagonal part; it has the purely energy terms as well as self-energies that may arise from the diagonal parts of interactions; V_0 is the purely off-diagonal term that does not change $\hat{n}_q$; it is the scattering *inside* the low energy subspace. V_+ and V_- are the purely off-diagonal terms that *do* change $\hat{n}_q$; V_+ takes you from $\hat{n}_q = 0$ to $\hat{n}_q = 1$ and V_- does the opposite.

Substituting eqs. 4.3 and 4.2 in eq. 4.1 gives

$$\left(\mathcal{H}^d + V_0 + V_+ + V_-\right) \left(|\Psi_0\rangle + |\Psi_1\rangle\right) = E \left(|\Psi_0\rangle + |\Psi_1\rangle\right) \tag{4.4}$$

Gathering the kets with $\hat{n}_q = 0, 1$ gives

$$\begin{aligned} \left(\mathcal{H}_0^d + V_0\right) |\Psi_0\rangle + V_- |\Psi_1\rangle &= E |\Psi_0\rangle \\ \left(\mathcal{H}_1^d + V_0\right) |\Psi_1\rangle + V_+ |\Psi_0\rangle &= E |\Psi_1\rangle \end{aligned} \tag{4.5}$$

The second equation can be written as

$$|\Psi_1\rangle = \eta^\dagger |\Psi_0\rangle \tag{4.6}$$

where

$$\left(\eta^\dagger\right)_{\text{PMS}} = \frac{1}{E - \mathcal{H}_1^d - V_0} V_+ \tag{4.7}$$

Substituting this in the second equation gives

$$\left(\mathcal{H}_0^d + V_0 + V_- \eta^\dagger\right) |\Psi_0\rangle = E |\Psi_0\rangle \tag{4.8}$$

This new Hamiltonian,

$$\tilde{\mathcal{H}}_0 = \mathcal{H}_0^d + V_0 + V_- \eta^\dagger \tag{4.9}$$

has the high energy mode removed; the scattering terms start from the low energy subspace and end at the low energy subspace as well. The renormalization in the low energy subspace scatterings is

$$\Delta V_0 = V_- \eta^\dagger \tag{4.10}$$

If we eliminate $|\Psi_0\rangle$ instead of $|\Psi_1\rangle$, we get the renormalized equation in the high energy subspace:

$$|\Psi_0\rangle = \eta |\Psi_1\rangle \tag{4.11}$$

where

$$(\eta)_{\text{PMS}} = \frac{1}{E - \mathcal{H}_0^d - V_0} V_- \tag{4.12}$$

,so

$$\left(\mathcal{H}_1^d + V_0 + V_+ \eta\right) |\Psi_1\rangle = E |\Psi_1\rangle \tag{4.13}$$

The renormalized Hamiltonian in the high energy subspace is thus

$$\tilde{\mathcal{H}}_1 = \mathcal{H}_1^d + V_0 + V_+ \eta \tag{4.14}$$

If we want to keep both the high energy and low energy parts of the Hamiltonian, the new Hamiltonian is

$$\begin{aligned} \tilde{\mathcal{H}} &= \tilde{\mathcal{H}}_1 \hat{n} + \tilde{\mathcal{H}}_0 (1 - \hat{n}) \\ &= \mathcal{H}_0^d + \mathcal{H}_1^d + V_0 + V_+ \eta + V_- \eta^\dagger \end{aligned} \tag{4.15}$$

The total renormalization is

$$(\Delta\mathcal{H})_{\text{PMS}} = V_+ (\eta)_{\text{PMS}} + V_- \left(\eta^\dagger\right)_{\text{PMS}} \tag{4.16}$$

It can be shown that if we define a unitary operator $U = 1 - \eta + \eta^\dagger$, the transformed Hamiltonian $U\mathcal{H}U^\dagger$ is the same as eq. 4.15. This, along with the properties of η, have been shown in section 1.1. The important feature of eq. 4.15 is that there is no term in the transformed Hamiltonian which scatters between $|\Psi_0\rangle$ and $|\Psi_0\rangle$- the two subspaces have been truly decoupled.

$$\left[U\mathcal{H}U^\dagger, n_q\right] = 0 \tag{4.17}$$

We can write down the renormalized Schrodinger equation in the low energy subspace, from eq. 4.8,

$$\tilde{\mathcal{H}}_0 |\Psi_0\rangle = E |\Psi_0\rangle \tag{4.18}$$

and again repeat the entire process. $\tilde{\mathcal{H}}_0$ now takes the place of $\mathcal{H}$ and $|\Psi_0\rangle$ takes the place of $|\Psi\rangle$ in eq. 4.1.

The expression for URG is obtained in an almost identical way. The only difference is that instead of starting with the exact eigenpair $(E, |\Psi\rangle)$, we start with a more general pair $(\tilde{\mathcal{H}}, |\Phi\rangle)$ where $|\Phi\rangle$ is not necessarily an exact eigenstate of $\mathcal{H}$. It is defined by $\mathcal{H}'$, which is in turn defined as $\hat{n}_q \mathcal{H}' (1 - \hat{n}_q) = 0$. $|\Phi\rangle$ is then defined by

$$\mathcal{H} |\Phi\rangle = \mathcal{H}' |\Phi\rangle \tag{4.19}$$

This definition of $\mathcal{H}'$ is the very minimum that we must have in order to fulfill our goal (decouple q).

The operators η and its conjugate change accordingly:

$$\begin{aligned} (\eta)_{\text{URG}} &= \frac{1}{\tilde{\mathcal{H}} - \mathcal{H}_0^d - V_0} V_- \\ &= \frac{1}{\hat{\omega} - \mathcal{H}_0^d} V_- \end{aligned} \tag{4.20}$$

where $\hat{\omega} \equiv \mathcal{H}' - V_0$ now embodies the quantum fluctuations inherent in the Hamiltonian through the scattering term V_0. Similarly,

$$\left(\eta^\dagger\right)_{\text{URG}} = \frac{1}{\hat{\omega} - \mathcal{H}_1^d} V_+ \tag{4.21}$$

The renormalization is again

$$(\Delta\mathcal{H})_{\text{URG}} = V_+ (\eta)_{\text{URG}} + V_- \left(\eta^\dagger\right)_{\text{URG}} \tag{4.22}$$

This again allows us to write down a unitary operator that decouples the entangled state:

$$U = 1 - \eta + \eta^\dagger, \left[\hat{n}_q, U\mathcal{H}U^\dagger\right] = 0 \tag{4.23}$$

where $\tilde{\mathcal{H}} = U^\dagger \mathcal{H} U$. We can now write down a new problem in this decoupled space with the rotated items and attempt to decouple another electron q'. We will again choose some general eigenpair $(\mathcal{H}', |\Phi\rangle)$ such that $\tilde{\mathcal{H}} |\Phi\rangle = \mathcal{H}' |\Phi\rangle$ and $[\mathcal{H}', \hat{n}_{q'}] = 0$.

Summarizing, the general Hamiltonian is not diagonal in the Fock space basis. URG, in order to proceed, selects one non-Fock basis of states $|\Phi\rangle$ such that q is decoupled in that Hamiltonian. Since there can be lots of such basis, there is a freedom in this choice.

With this basis in mind, URG then finds a unitary operator which when operated on the Hamiltonian takes me to the form in which it is diagonal in the Fock space basis. Note that this form is a function of the chosen $|\Phi\rangle$. We then select the second degree of freedom and repeat the process. What PMS does is, it exploits the freedom of choice and selects the exact eigenstate $|\Psi\rangle$ of the Hamiltonian as the non-Fock basis $|\Phi\rangle$. Doing that returns a rotated Hamiltonian which is diagonal in q, and is a function of the chosen state, same as URG. The conclusion is that depending on which state we choose as our diagonal non-Fock basis, URG and PMS will cause flows along different lines in general.

As the couplings flow, V_0 will also flow, leading to a flow of $\hat{\omega}$. Just at the fixed point, the denominator of URG vanishes, giving the equation

$$\left(\hat{\omega} - \mathcal{H}_1^d\right) V_+ |\Psi_0\rangle \text{ or } \left(\hat{\omega} - \mathcal{H}_1^d\right) V_- |\Psi_1\rangle \tag{4.24}$$

This means that one of the eigenvalues of $\hat{\omega}$ matches with the eigenvalue of the diagonal part $\mathcal{H}^d$, either in the occupied sector ($\mathcal{H}_1^d$) or unoccupied sector ($\mathcal{H}_1^d$). Since the eigenvalues are unchanged during the unitary renormalization, this implies that ω takes up one of the eigenvalues of the whole Hamiltonian $\mathcal{H}$. This will correspond to the fixed point obtained from PMS if we had started PMS with that eigenvalue.

In short, while the PMS flow is parametrised by one of the exact energy eigenvalues E, the URG flow is parametrised by a non-trivial operator $\hat{\omega}$ which incorporates both a diagonal part and an off-diagonal part and itself flows under the URG. At the fixed point, the off-diagonal part cancels out and the $\hat{\omega}$ finally flows to one of the energy eigenvalues and the URG fixed point matches with one of the PMS fixed points.

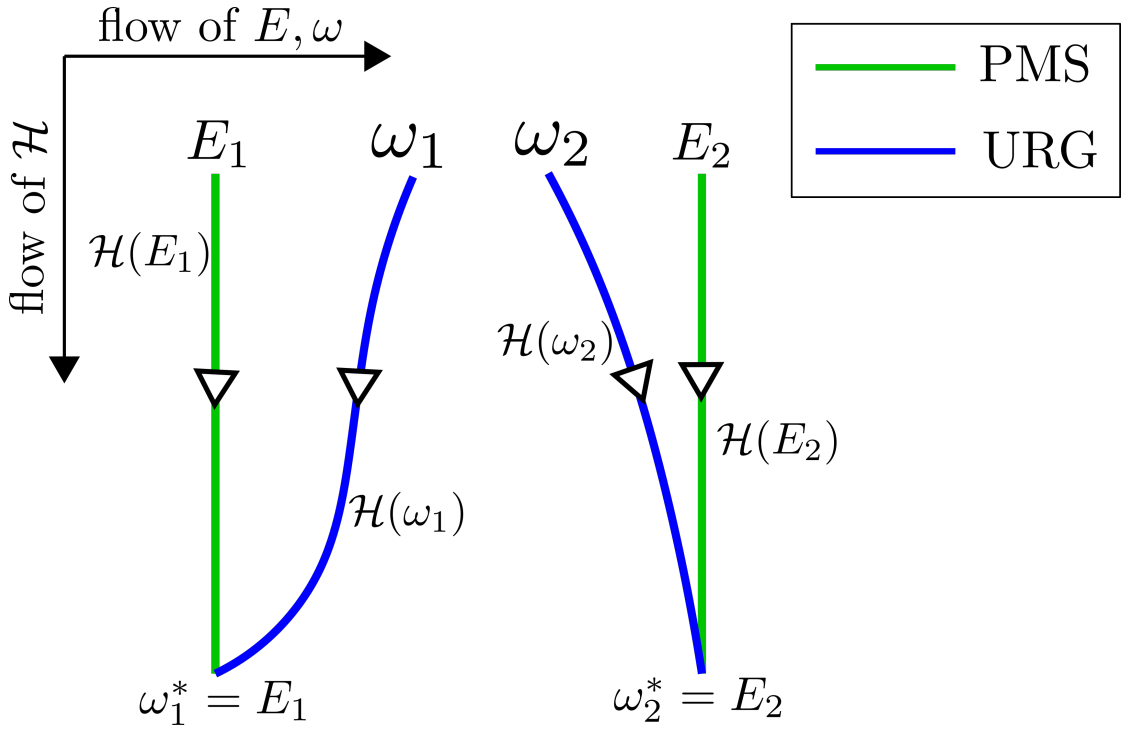

Figure 3: Flows of PMS(green) and URG(blue)

To demonstrate the implementation, we can look at a specific model. For the SIAM,

$$\mathcal{H} = \sum_{k\sigma} \left(\epsilon_k \tau_{k\sigma} + V c^\dagger_{k\sigma} c_{d\sigma} + \text{h.c.} \right) \tag{4.25}$$

We want to decouple the state $q\beta$ from the rest of the electrons. We have $\hat{\mathcal{H}}_0 = \epsilon_d \hat{n}_d + U\hat{n}_{d\uparrow} n_{d\downarrow} + \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma}$, $V_0 = \sum_{k<q,\sigma} c^\dagger_{k\sigma} c_{d\sigma} + \text{h.c.}$, $V_+ = V c^\dagger_{q\beta} c_{d\beta}$ and $V_- = V c^\dagger_{d\beta} c_{q\beta}$. The renormalization in particle sector

$$\Delta V_0 = c^\dagger_{d\beta} c_{q\beta} \frac{1}{(E - V_0) - \hat{\mathcal{H}}^d_0} c^\dagger_{q\beta} c_{d\beta} \tag{4.26}$$

The intermediate energy (at the propagator) is

$$\hat{\mathcal{H}}^d_0 = \sum_{k,\sigma} \epsilon_k \tau_{k\sigma} + \epsilon_d \hat{n}_{d\overline{\beta}} \tag{4.27}$$

This is because the $c_{d\beta}$ at the right of the propagator ensures that we must have $\hat{n}_{d\beta} = 0$ at the propagator.

$$\Delta V_0 = c^\dagger_{d\beta} c_{q\beta} \frac{1}{(E - V_0) - \sum_{k,\sigma} \epsilon_k \tau_{k\sigma} - \epsilon_d \hat{n}_{d\overline{\beta}}} c^\dagger_{q\beta} c_{d\beta} \tag{4.28}$$

Since E is the exact eigenvalue, we do not have an expression for it. Instead, we approximate $E - V_0$ by substituting it with the current diagonal part corresponding to the initial state on which this entire term will act. The intial state is characterized by $\hat{n}_{q\beta} = 0$ and $\hat{n}_{d\beta} = 1$, so

$$E - V_0 = \sum_{k<q,\sigma} \epsilon_k \tau_{k\sigma} - \frac{1}{2}\epsilon_q + \epsilon_d + (\epsilon_d + U)\, \hat{n}_{d\overline{\beta}} \tag{4.29}$$

The $-\frac{1}{2}\epsilon_q$ comes from substituting $\hat{n}_{q\beta} = 0$ in $\epsilon_q \tau_{q\beta}$.

Substituting this in ΔV_0 gives

$$\begin{aligned}
\Delta V_0 &= c^\dagger_{d\beta} c_{q\beta} \frac{1}{-\frac{1}{2}\epsilon_q - \epsilon_q \tau_{q\beta} + \epsilon_d + U\hat{n}_{d\overline{\beta}}} c^\dagger_{q\beta} c_{d\beta} \\
&= c^\dagger_{d\beta} c_{q\beta} \frac{1}{-\epsilon_q + \epsilon_d + U\hat{n}_{d\overline{\beta}}} c^\dagger_{q\beta} c_{d\beta} \\
&= c^\dagger_{d\beta} c_{q\beta} c^\dagger_{q\beta} c_{d\beta} \frac{1}{-\epsilon_q + \epsilon_d + U\hat{n}_{d\overline{\beta}}} \\
&= -c^\dagger_{d\beta} c_{q\beta} c^\dagger_{q\beta} c_{d\beta} \frac{1}{\epsilon_q - \epsilon_d - U\hat{n}_{d\overline{\beta}}} \\
&= (1 - \hat{n}_{q\beta}) \left(\frac{-\hat{n}_{d\beta}\hat{n}_{d\overline{\beta}}}{\epsilon_q - \epsilon_d - U} + \frac{-\hat{n}_{d\beta}\left(1 - \hat{n}_{d\overline{\beta}}\right)}{\epsilon_q - \epsilon_d} \right)
\end{aligned} \tag{4.30}$$

On the second line, we substituted $\tau_{q\beta} = \frac{1}{2}$ in the denominator, which is ensured by the $c^\dagger_{q\beta}$ to the right of the propagator. The first term renormalizes the energy of the doublon state and the second term renormalizes that of the singly-occupied state:

$$\begin{aligned} \Delta E_2 &= \frac{-1}{\epsilon_q - \epsilon_d - U} \\ \Delta E_1 &= \frac{-1}{\epsilon_q - \epsilon_d} \end{aligned} \tag{4.31}$$

The renormalization in the hole sector is

$$\begin{aligned} \Delta V_0 &= c^\dagger_{q\beta} c_{d\beta} \frac{1}{(E - V_0) - \hat{\mathcal{H}}^d_0} c^\dagger_{d\beta} c_{q\beta} \\ &= c^\dagger_{q\beta} c_{d\beta} \frac{1}{(E - V_0) - \sum_{k,\sigma} \epsilon_k \tau_{k\sigma} - \epsilon_d - (\epsilon_d + U)\, \hat{n}_{d\overline{\beta}}} c^\dagger_{d\beta} c_{q\beta} \end{aligned} \tag{4.32}$$

This time we substitute

$$\begin{aligned} E - V_0 &= \sum_{k<q,\sigma} \epsilon_k \tau_{k\sigma} + \tau_{q\beta} \epsilon^-_q + \epsilon_d \hat{n}_{d\overline{\beta}} \\ &= \sum_{k<q,\sigma} \epsilon_k \tau_{k\sigma} + \frac{1}{2} \epsilon^-_q + \epsilon_d \hat{n}_{d\overline{\beta}} \end{aligned} \tag{4.33}$$

In the last step we put $\tau_{q\beta} = \frac{1}{2}$ because the state is occupied in the initial configuratin. Note that since the electron $q\beta$ was occupied in the intial state, the energy ϵ^-_q in this sector must be opposite to that of the particle sector, ϵ_q. Hence $\epsilon^-_q = -\epsilon_q$, which gives

$$\begin{aligned} \Delta V_0 &= c^\dagger_{q\beta} c_{d\beta} \frac{1}{-\frac{1}{2}\epsilon_q - \epsilon^-_q \tau_{q\beta} - \epsilon_d - U \hat{n}_{d\overline{\beta}}} c^\dagger_{d\beta} c_{q\beta} \\ &= c^\dagger_{q\beta} c_{d\beta} c^\dagger_{d\beta} c_{q\beta} \frac{1}{-\epsilon_q - \epsilon_d - U \hat{n}_{d\overline{\beta}}} \\ &= \hat{n}_{q\beta} \left(\frac{-\left(1 - \hat{n}_{d\beta}\right) \hat{n}_{d\overline{\beta}}}{\epsilon_q + \epsilon_d + U} + \frac{-\left(1 - \hat{n}_{d\beta}\right) \left(1 - \hat{n}_{d\overline{\beta}}\right)}{\epsilon_q + \epsilon_d} \right) \end{aligned} \tag{4.34}$$

In the second line, we put $\epsilon^-_q = -\epsilon_q$ and $\tau_{q\beta} = -\frac{1}{2}$. The first term renormalizes the singly-occupied state while the second term renormalizes the holon state. Combining with the particle sector results, the total renormalization in all the three impurity states (holon, single and doublon) are

$$\begin{aligned} \Delta E_0 &= -\frac{1}{\epsilon_q + \epsilon_d} \\ \Delta E_1 &= -\frac{1}{\epsilon_q + \epsilon_d + U} - \frac{1}{\epsilon_q - \epsilon_d} \\ \Delta E_2 &= -\frac{1}{\epsilon_q - \epsilon_d - U} \end{aligned} \tag{4.35}$$

These results are also obtained in ref. [3]. The complete process is depicted in fig. 4.

Some conclusions:

- The *only* difference in the formalism of PMS and URG is that while PMS uses the exact energy eigenvalue E to parameterise the flow, URG uses a general intermediate decoupled Hamiltonian to do the same. Since the E is also, technically, an intermediate decoupled Hamiltonian (it is the final Hamiltonian), PMS can be seen as an URG but with a specific choice for the paramter.

- In practise, PMS replaces $E - V_0$ with the diagonal part of the initial state at the current step of the RG. We are talking about the energy of the initial state, not the intermediate state. This is because, from eq. 4.1, E is the energy of the initial state on which $V_\pm$ act.

- The ideal solution would have been to substitute the exact energy and the total scattering term V, but since we do not know E and keeping the V would make the thing untractable, we use our current best guess (renormalised diagonal part). As the RG flows, both E_j and V flow, such that at the fixed point, V becomes zero (scattering terms get removed) and E_j morphs into the exact E.

- In practise, URG replaces the $\hat{\omega}$ with a guess for the final energy E. This however ignores the renormalization of $\hat{\omega}$. A better approach would be to replace it with E_j, following PMS. That would act like the one-particle renormalization of $\hat{\omega}$.

- PMS mostly drops any diagonal component of the scattering from the denominator. For example, in the PMS of the Kondo model by Anderson [4] or that of the anisotropic power law Kondo model by Chenge et.al [5], they do not keep the term $J_z S_d^z s^z$ in the denominator although it is number(spin) conserving. Such terms are kept in the denominator of the URG though. It must be mentioned however that ref. [6] *does* bring a diagonal charge-charge interaction in the denominator in the PMS of the extended Anderson model.

5 Schrieffer-Wolff Transformation as a limit of URG

We have a general Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_X \tag{5.1}$$

$\mathcal{H}_0$ 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.

$$\begin{aligned} U\mathcal{H}U^\dagger &= e^S \left(\mathcal{H}_0 + \mathcal{H}_X\right) e^{-S} \\ &= \left(\cosh\left(S\right) + \sinh\left(S\right)\right) \left(\mathcal{H}_0 + \mathcal{H}_X\right) \left(\cosh\left(S\right) + \sinh\left(S\right)\right) \\ &= H_1 + H_2 \end{aligned} \tag{5.2}$$

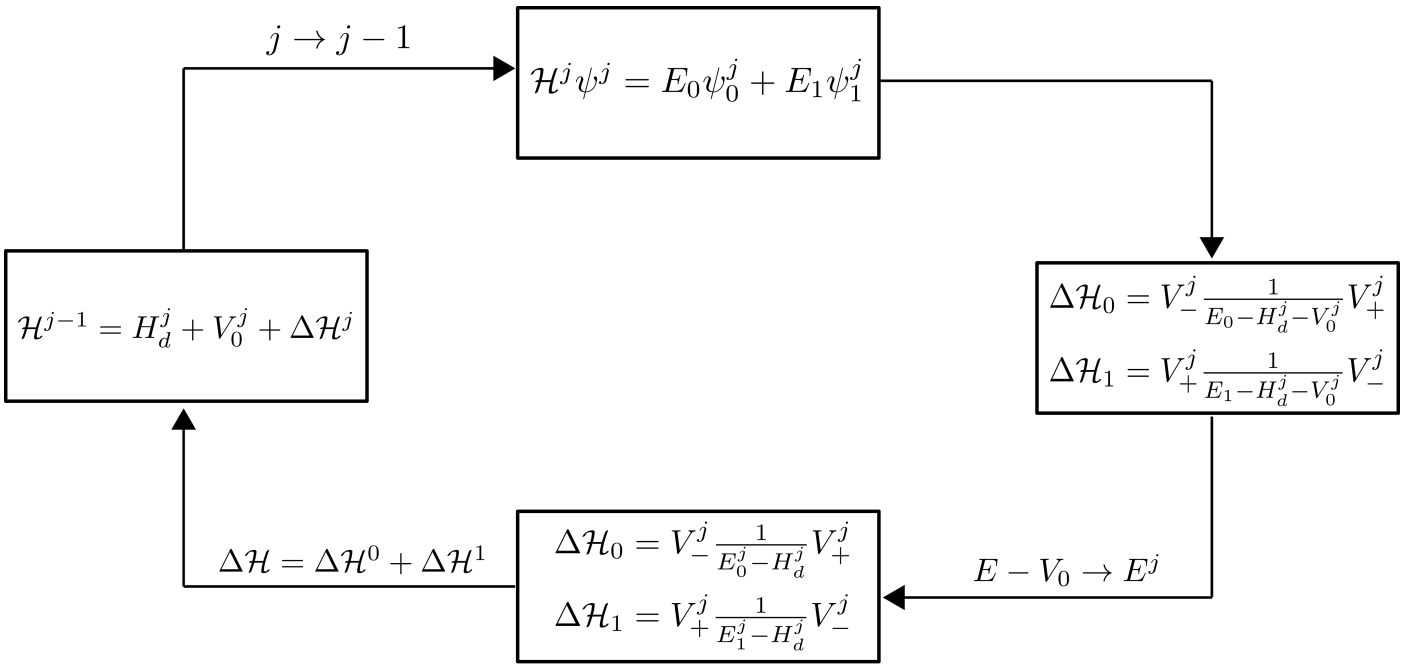

Figure 4: Flow chart of "Poor Man's" scaling algorithm

where H_1 is diagonal and H_2 is off-diagonal.

$$\begin{aligned} H_1 = \cosh(S)\,\mathcal{H}_0\cosh(S) - \sinh(S)\,\mathcal{H}_0\sinh(S) - \cosh(S)\,\mathcal{H}_X\sinh(S) \\ + \sinh(S)\,\mathcal{H}_X\cosh(S) \\ H_2 = -\cosh(S)\,\mathcal{H}_0\sinh(S) + \sinh(S)\,\mathcal{H}_0\cosh(S) + \cosh(S)\,\mathcal{H}_X\cosh(S) \\ - \sinh(S)\,\mathcal{H}_X\sinh(S) \end{aligned} \tag{5.3}$$

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

$$H_2 = -\mathcal{H}_0 S + S\mathcal{H}_0 + \mathcal{H}_X + O(S^3) = [S, \mathcal{H}_0] + \mathcal{H}_X \tag{5.4}$$

The second order decoupling condition is thus

$$[S, \mathcal{H}_0] = -\mathcal{H}_X \tag{5.5}$$

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

$$-\epsilon_q\left(A + B\hat{n}_{d\bar{\beta}}\right) + \epsilon_d\left(A + B\hat{n}_{d\bar{\beta}}\right) + U(A+B)\,\hat{n}_{d\bar{\beta}} = -V \tag{5.6}$$

which gives

$$S = V\left[\frac{1-\hat{n}_{d\overline{\beta}}}{\epsilon_q - \epsilon_d} + \frac{\hat{n}_{d\overline{\beta}}}{\epsilon_q - \epsilon_d - U}\right] \tag{5.7}$$

The remaining diagonal part constitutes the effective Hamiltonian.

$$\begin{aligned} H_1 &= \mathcal{H}_0 + \frac{1}{2}\left\{\mathcal{H}_0, S^2\right\} - S\mathcal{H}_0 S + [S, \mathcal{H}_X] \\ &= \mathcal{H}_0 + \frac{1}{2}\left[[\mathcal{H}_0, S], S\right] + [S, \mathcal{H}_X] \\ &= \mathcal{H}_0 + \frac{1}{2}\left[\mathcal{H}_X, S\right] + [S, \mathcal{H}_X] \\ &= \mathcal{H}_0 + \frac{1}{2}\left[S, \mathcal{H}_X\right] \end{aligned} \tag{5.8}$$

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

$$\begin{aligned} \mathcal{H}_0 &= \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \epsilon_d \hat{n}_d + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + \sum_{k\sigma \neq q\beta}\left(c^\dagger_{k\sigma} c_{d\sigma} + \text{h.c.}\right) \\ \mathcal{H}_X &= c^\dagger_{q\beta} c_{d\beta} + \text{h.c.} \end{aligned} \tag{5.9}$$

The renormalization in the effective Hamiltonian is thus

$$\frac{1}{2}\left[S, \mathcal{H}_X\right] = -\hat{n}_{d\beta}|V|^2\left[\frac{1-\hat{n}_{d\overline{\beta}}}{\epsilon_q - \epsilon_d} + \frac{\hat{n}_{d\overline{\beta}}}{\epsilon_q - \epsilon_d - U}\right] \tag{5.10}$$

This is *identical to the result obtained from PMS* of the SIAM (see [3]). This shows that the extra terms that are generated in SWT (the s-d term) appear *only because the connection between the impurity subspaces are integrated out in one shot.*

Avoiding the perturbative route, we can take $S = \frac{\pi}{4}\left(\eta^\dagger - \eta\right)$. The η and its conjugate satisfy the properties laid out in the formalism of URG, and are in general non-perturbative since they encode the whole scattering term inside the $\hat{\omega}$. From the properties of η ($\eta^2 = {\eta^\dagger}^2 = 0$), we can write

$$\cosh S = \frac{1}{\sqrt{2}}, \text{ and } \sinh S = \frac{1}{\sqrt{2}}\left(\eta^\dagger - \eta\right) \tag{5.11}$$

The off-diagonal part now becomes

$$H_2 = \frac{1}{2}\left(\mathcal{H}_X - \eta^\dagger \mathcal{H}_X \eta^\dagger - \eta\mathcal{H}_X\eta + \left[\eta^\dagger - \eta, \mathcal{H}_0\right]\right) \tag{5.12}$$

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. 5.5, we can re-express the cosh and sinh in eq. 5.11 in terms of S, by substituting $\eta^\dagger - \eta = \frac{4}{\pi}S$:

$$\cosh S = \frac{1}{\sqrt{2}}, \text{ and } \sinh S = \frac{4}{\sqrt{2}\pi}S \tag{5.13}$$

That gives

$$H_2 = \frac{1}{2}\left[\frac{4}{\pi}[S, \mathcal{H}_0] + \mathcal{H}_X - \frac{16}{\pi^2}S\mathcal{H}_X S\right] \tag{5.14}$$

The decoupling condition becomes

$$[S, \mathcal{H}_0] = -\frac{\pi}{4}\mathcal{H}_X + \frac{4}{\pi}S\mathcal{H}_X S \tag{5.15}$$

This can be compared to the second order condition: $[S, \mathcal{H}_0] = -\mathcal{H}_X$.

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