# Unitary Renormalization Group Approach to Single-Impurity Anderson Model

Abhirup Mukherjee

Supervisor: Dr. Siddhartha Lal

*Department of Physics, IISER Kolkata*

January 17, 2021

# Contents

# 1 Star Graph URG

The star graph problem consists of $N$ spin-like degrees of freedom (lablled 1 through N) individually talking to a spin at the center (labelled 0). Each spin $i$ ($\in [0, N]$) has an on-site energy $\epsilon_i$. The coupling strength between 0 and $i$ ($\in [1, N]$) is $J_i$. We choose the on-site energies such that $\epsilon_{i+1} > \epsilon_i, i \in [N-1, 1]$. In this way, $\epsilon_1$ is the infrared limit and $\epsilon_N$ is the ultraviolet limit.

$$\mathcal{H} = \sum_{i=0}^{N} \epsilon_i S_i^z + \sum_{i=1}^{N} J_i \vec{S}_0 \cdot \vec{S}_i \tag{1.1}$$

By converting the last term into $S^z$ and $S^{\pm}$, we can write the Hamiltonian as

$$\mathcal{H} = \sum_{i=0}^{N} \epsilon_i S_i^z + \sum_{i=1}^{N} J_i \left[ S_0^z S_i^z + \frac{1}{2}\left( S_0^+ S_i^- + S_0^- S_i^+ \right) \right] \tag{1.2}$$

The diagonal terms are the ones that preserve the number or (in this case) spin.

$$\mathcal{H}^D = \sum_{i=0}^{N} \epsilon_i S_i^z + \sum_{i=1}^{N} J_i S_0^z S_i^z \tag{1.3}$$

This is the piece that comes in the denominator. The off-diagonal terms are the ones that change the number or spin. For this problem, they are the last two terms, $S_0^+ S_i^-$ and $S_0^- S_i^+$.

The RG involves decoupling the nodes $N$ through 1, and looking at the resultant renormalization in $\epsilon_i$ and $J_i$. As a simplification, we will ignore the lower nodes in the denominator and keep only the node currently being decoupled, ie node $N$. Since node 0 is connected to node $N$, we will keep node 0 in the denominator as well. Making this simplification gives

$$\mathcal{H}^D = \epsilon_0 S_0^z + \epsilon_N S_N^z + J_N S_0^z S_N^z \tag{1.4}$$

## 1.1 Particle sector

This sector consists of the renormalization caused due to particle excitations in the intermediate state. In the spin language, this translates to looking at those terms where the node that is being decoupled, $N$, is upwards in the excited state.

$$\Delta^+ \mathcal{H} = \frac{1}{2} J_N S_0^+ S_N^- \frac{1}{\hat{\omega} - \mathcal{H}^D} \frac{1}{2} J_N S_0^- S_N^+ \tag{1.5}$$

Note that we have chosen those particle scattering term because the $S_N^+$ on the right will create an up spin in the intermediate state, hence justifying the particle sector. The next order of business is to evaluate the $\mathcal{H}^D$ in the propagator. Since the propagator has an

$S_0^- S_N^+$ in front, we can substitute $S_0^z = -\frac{1}{2}$ and $S_N^z = \frac{1}{2}$ in $\mathcal{H}^D$. Any other value would be annihilated by the operator at the front ($S^+ \left|\frac{1}{2}\right\rangle = S^- \left|-\frac{1}{2}\right\rangle = 0$). Therefore, from eq. 1.4.

$$\mathcal{H}^D = -\frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N - \frac{1}{4}J_N \tag{1.6}$$

Substituting this in $\Delta^+\mathcal{H}$ gives

$$\Delta^+\mathcal{H} = \frac{1}{2}J_N S_0^+ S_N^- \frac{1}{\hat{\omega} + \frac{1}{2}\epsilon_0 - \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \frac{1}{2} J_N S_0^- S_N^+ \tag{1.7}$$

At this point we make another simplification, we replace $\hat{\omega}$ by its eigenvalue $\omega^+$. The + in the superscript indicates that it is from hte particle sector.

$$\begin{aligned}
\Delta^+\mathcal{H} &= \frac{1}{2}J_N S_0^+ S_N^- \frac{1}{\omega^+ + \frac{1}{2}\epsilon_0 - \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \frac{1}{2} J_N S_0^- S_N^+ \\
&= \frac{1}{4}J_N^2 S_0^+ S_N^- S_0^- S_N^+ \frac{1}{\omega^+ + \frac{1}{2}\epsilon_0 - \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \\
&= \frac{1}{4}J_N^2 S_0^+ S_0^- S_N^- S_N^+ \frac{1}{\omega^+ + \frac{1}{2}\epsilon_0 - \frac{1}{2}\epsilon_N + \frac{1}{4}J_N}
\end{aligned} \tag{1.8}$$

Here we used the fact that the spins commute. We can now use the identities $S^+ S^- = \left(\frac{1}{2} + S^z\right)$ and $S^- S^+ = \left(\frac{1}{2} - S^z\right)$ to write

$$S_0^+ S_0^- S_N^- S_N^+ = \left(\frac{1}{2} + S_0^z\right)\left(\frac{1}{2} - S_N^z\right) \tag{1.9}$$

Since we want a particle in the intermediate state, we must have a hole in the initial state. Hence, we can substitute $S_N^z = -\frac{1}{2}$ in the last equation:

$$S_0^+ S_0^- S_N^- S_N^+ = \left(\frac{1}{2} + S_0^z\right) \tag{1.10}$$

This gives

$$\Delta^+\mathcal{H} = \frac{1}{4}J_N^2 \left(\frac{1}{2} + S_0^z\right) \frac{1}{\omega^+ + \frac{1}{2}\epsilon_0 - \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \tag{1.11}$$

This is the final form and we can now read off the renormalizations. The term with $S_0^z$ will renormalize the term in the Hamiltonian that comes with $S_0^z$, which is the term with $\epsilon_0$.

$$\Delta^+\epsilon_0 = \frac{1}{4}J_N^2 \frac{1}{\omega^+ + \frac{1}{2}\epsilon_0 - \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \tag{1.12}$$

The remaining part is operator less and will hence renormalize the on-site energy of the term that was just decoupled, that is $N$:

$$\Delta^+\epsilon_N = \frac{1}{8}J_N^2 \frac{1}{\omega^+ + \frac{1}{2}\epsilon_0 - \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \tag{1.13}$$

## 1.2 Hole sector

This sector consists of the renormalization caused due to hole excitations in the intermediate state. In the spin language, this translates to looking at those terms where the node that is being decoupled, $N$, is downwards in the excited state.

$$\Delta^{-}\mathcal{H} = \frac{1}{2} J_N S_0^- S_N^+ \frac{1}{\hat{\omega} - \mathcal{H}^D} \frac{1}{2} J_N S_0^+ S_N^- \tag{1.14}$$

Note that we have chosen those particle scattering term because the $S_N^-$ on the right will create a down spin in the intermediate state, hence justifying the hole sector. The next order of business is to evaluate the $\mathcal{H}^D$ in the propagator. Since the propagator has an $S_0^+ S_N^-$ in front, we can substitute $S_0^z = \frac{1}{2}$ and $S_N^z = -\frac{1}{2}$ in $\mathcal{H}^D$. Any other value would be annihilated by the operator at the front $(S^+ |\frac{1}{2}\rangle = S^- |-\frac{1}{2}\rangle = 0)$. Therefore, from eq. 1.4.

$$\mathcal{H}^D = \frac{1}{2}\epsilon_0 - \frac{1}{2}\epsilon_N - \frac{1}{4} J_N \tag{1.15}$$

Substituting this in $\Delta^{-}\mathcal{H}$ gives

$$\Delta^{-}\mathcal{H} = \frac{1}{2} J_N S_0^- S_N^+ \frac{1}{\hat{\omega} - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \frac{1}{2} J_N S_0^+ S_N^- \tag{1.16}$$

At this point we make another simplification, we replace $\hat{\omega}$ by its eigenvalue $\omega^-$.

$$\begin{aligned}
\Delta^{-}\mathcal{H} &= \frac{1}{2} J_N S_0^- S_N^+ \frac{1}{\omega^- - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \frac{1}{2} J_N S_0^+ S_N^- \\
&= \frac{1}{4} J_N^2 S_0^- S_N^+ S_0^+ S_N^- \frac{1}{\omega^- - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \\
&= \frac{1}{4} J_N^2 S_0^- S_0^+ S_N^+ S_N^- \frac{1}{\omega^- - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N}
\end{aligned} \tag{1.17}$$

Here we used the fact that the spins commute. We can now use the identities $S^+S^- = \left(\frac{1}{2} + S^z\right)$ and $S^-S^+ = \left(\frac{1}{2} - S^z\right)$ to write

$$S_0^- S_0^+ S_N^+ S_N^- = \left(\frac{1}{2} - S_0^z\right)\left(\frac{1}{2} + S_N^z\right) \tag{1.18}$$

Since we want a hole in the intermediate state, we must have a particle in the initial state. Hence, we can substitute $S_N^z = \frac{1}{2}$ in the last equation:

$$S_0^- S_0^+ S_N^+ S_N^- = \left(\frac{1}{2} - S_0^z\right) \tag{1.19}$$

This gives

$$\Delta^{-}\mathcal{H} = \frac{1}{4} J_N^2 \left(\frac{1}{2} - S_0^z\right) \frac{1}{\omega^- - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \tag{1.20}$$

This is the final form and we can now read off the renormalizations. The term with $S_0^z$ will renormalize the term in the Hamiltonian that comes with $S_0^z$, which is the term with $\epsilon_0$.

$$\Delta^- \epsilon_0 = -\frac{1}{4} J_N^2 \frac{1}{\omega^- - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \tag{1.21}$$

The remaining part is operator less and will hence renormalize the on-site energy of the term that was just decoupled, that is $N$:

$$\Delta^- \epsilon_N = \frac{1}{8} J_N^2 \frac{1}{\omega^- - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \tag{1.22}$$

## 1.3 Summary

These are the scaling equations for the couplings $\epsilon_0$ and $\epsilon_N$ on decoupling the $N^{\text{th}}$ node. Further calculations will involve checking where the couplings are relevant, what fixed point conditions exist and form of the effective Hamiltonians at the fixed points. If we consider the RG equations for $\epsilon_0$ for the time being,

$$\begin{aligned} \Delta^+ \epsilon_0 &= \frac{1}{4} J_N^2 \frac{1}{\omega^+ + \frac{1}{2}\epsilon_0 - \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \\ \Delta^- \epsilon_0 &= -\frac{1}{4} J_N^2 \frac{1}{\omega^- - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \end{aligned} \tag{1.23}$$

Since $J_N$ does not renormalize and $\epsilon_N$ is the unrenormalized guy, we can abosrb them into the $\omega$ to make matters simpler: $\omega_N^+ = \omega^+ + \frac{1}{4}J_N - \frac{1}{2}\epsilon_N$, $\omega_N^- = \omega^- + \frac{1}{4}J_N + \frac{1}{2}\epsilon_N$.

$$\begin{aligned} \Delta^+ \epsilon_0 &= \frac{1}{4} J_N^2 \frac{1}{\omega_N^+ + \frac{1}{2}\epsilon_0} \\ \Delta^- \epsilon_0 &= -\frac{1}{4} J_N^2 \frac{1}{\omega_N^- - \frac{1}{2}\epsilon_0} \end{aligned} \tag{1.24}$$

$\omega^\pm$ are numbers that remain fixed during renormalization. In general they also renormalize, but we haven't kept track of that in this simplified calculation. Note the property of $\omega_N^+$ that it grows as we go on decoupling the nodes, because $\epsilon_N > \epsilon_{N-1}$. In contrast, $\omega_N^-$ shrinks as we go on decoupling nodes, for the same reason.

We can now look for nature of flow ((ir)relevance) and fixed points. From the URG prescription, we know that **a fixed point is reached when the denominator vanishes**.

For the hole sector, $\Delta^-\epsilon_0$ is positive when $\omega_N^- - \frac{1}{2}\epsilon_0 < 0$ and negative otherwise.

- For $\omega_N^- - \frac{1}{2}\epsilon_0 > 0$, $\epsilon_0$ is irrelevant. This will lead to a runaway denominator, where $\epsilon_0$ goes on decreasing and $\omega_N^-$ goes on increasing such that the denominator goes on increasing and there is no way of making it 0.

- For $\omega_N^- - \frac{1}{2}\epsilon_0 < 0$, $\epsilon_0$ is relevant, so $\epsilon_0$ will increase and $\omega_N^-$ will decrease, so the denominator will go on decreasing and never be zero.

For the particle sector, $\Delta^+\epsilon_0$ is positive when $\omega_N^+ + \frac{1}{2}\epsilon_0 > 0$ and negative otherwise. Hence, $\epsilon_0$ will grow in the former regime and shrink in the latter. Lets consider the two cases separately:

- When $\omega_N^+ + \frac{1}{2}\epsilon_0 > 0$, $\epsilon_0$ will grow. Since $\omega_N^+$ also grows, the expression $\omega_N^+ + \frac{1}{2}\epsilon_0$ will become more and more positive as the RG progresses and there is no possibility of the denominator becoming zero. We cannot reach a fixed point in this regime, so ignore this regime.

- When $\omega_N^+ + \frac{1}{2}\epsilon_0 < 0$, $\epsilon_0$ will shrink. Here it is possible to reach a fixed point, but in this case, both $\epsilon_i$ as well as $\epsilon_0$ are decreasing, so this is like an overall scaling of the Hamiltonian. It is unlikely that it contains interesting physics, so we ignore this case as well and move on to the hole sector.

# 2 Kondo Model URG

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

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

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

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 $S_d^z \left(\hat{n}_{q\uparrow} - \hat{n}_{q\downarrow}\right)$ as $S_d^z \left(\tau_{q\uparrow} - \tau_{q\downarrow}\right)$.

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

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

$\omega^+$ 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 $c^\dagger_{q\uparrow}$. 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 $S^z$.

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

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

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

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.

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

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

The fourth term gives

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

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

$$\Delta^{-}\mathcal{H} = \sum_{kk'q} \frac{1}{2}\left(J_z S_d^z c^\dagger_{q\uparrow}c_{k'\uparrow} + J_t S_d^- c^\dagger_{q\uparrow}c_{k'\downarrow}\right)\frac{1}{\omega^- - \mathcal{H}^D}\frac{1}{2}\left(J_z S_d^z c^\dagger_{k\uparrow}c_{q\uparrow} + J_t S_d^+ c^\dagger_{k\downarrow}c_{q\uparrow}\right) \quad (2.14)$$

The $\omega^-$ 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:

$$\mathcal{H}^D = -\frac{1}{2}\epsilon_q - \frac{1}{4}J_z S_d^z \quad (2.15)$$

The first term has two $S^z$.

$$\begin{aligned}
\Delta_1^-\mathcal{H} &= \sum_{kk'q} S_d^z c^\dagger_{q\uparrow}c_{k'\uparrow}\frac{1}{4}J_z^2\frac{1}{\omega^- - \mathcal{H}^D}S_d^z c^\dagger_{k\uparrow}c_{q\uparrow} \\
&= \frac{1}{16}J_z^2\sum_{kk'q} c_{k'\uparrow}c^\dagger_{k\uparrow}\frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{4}J_z S_d^z} \\
&= \frac{1}{16}J_z^2\sum_{kk'q} c_{k'\uparrow}c^\dagger_{k\uparrow}\left[\frac{\frac{1}{2}+S_d^z}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{8}J_z} + \frac{\frac{1}{2}-S_d^z}{\omega^- + \frac{1}{2}\epsilon_q - \frac{1}{8}J_z}\right] \\
&= -\frac{1}{32}J_z^2\sum_{kk'q} c^\dagger_{k\uparrow}c_{k'\uparrow}\left[\frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{8}J_z} + \frac{1}{\omega^- + \frac{1}{2}\epsilon_q - \frac{1}{8}J_z}\right] \\
&\quad - \frac{1}{16}J_z^2\sum_{kk'q} c^\dagger_{k\uparrow}c_{k'\uparrow}S_d^z\left[\frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{8}J_z} - \frac{1}{\omega^- + \frac{1}{2}\epsilon_q - \frac{1}{8}J_z}\right]
\end{aligned} \quad (2.16)$$

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

The second term gives

$$\Delta_2^-\mathcal{H} = \sum_{kk'q}\frac{1}{4}J_z J_t S_d^- c^\dagger_{q\uparrow}c_{k'\downarrow}\frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{4}J_z S_d^z}S_d^z c^\dagger_{k\uparrow}c_{q\uparrow} \quad (2.17)$$

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

$$\begin{aligned}
\Delta_2^-\mathcal{H} &= \frac{1}{4}J_z J_t\sum_{kk'q} S_d^- S_d^z c^\dagger_{q\uparrow}c_{k'\downarrow}c^\dagger_{k\uparrow}c_{q\uparrow}\frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{8}J_z} \\
&= \frac{1}{8}J_z J_t\sum_{kk'q} S_d^- c_{k'\downarrow}c^\dagger_{k\uparrow}\frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{8}J_z} \\
&= -\frac{1}{8}J_z J_t\sum_{kk'q} S_d^- c^\dagger_{k\uparrow}c_{k'\downarrow}\frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{8}J_z}
\end{aligned} \quad (2.18)$$

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

The third term gives

$$\Delta_3^- \mathcal{H} = \sum_{kk'q} \frac{1}{4} J_z J_t S_d^z c_{q\uparrow}^\dagger c_{k'\uparrow} \frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{4} J_z S_d^z} S_d^+ c_{k\downarrow}^\dagger c_{q\uparrow} \tag{2.19}$$

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

$$\begin{aligned}
\Delta_3^- \mathcal{H} &= \frac{1}{4} J_z J_t \sum_{kk'q} S_d^z S_d^+ c_{q\uparrow}^\dagger c_{k'\uparrow} c_{k\downarrow}^\dagger c_{q\uparrow} \frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{8} J_z} \\
&= \frac{1}{4} J_z J_t \sum_{kk'q} S_d^+ c_{k\downarrow}^\dagger c_{k'\uparrow} \frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{8} J_z} \\
&= -\frac{1}{8} J_z J_t \sum_{kk'q} S_d^+ c_{k\downarrow}^\dagger c_{k'\uparrow} \frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{8} J_z}
\end{aligned} \tag{2.20}$$

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

The fourth term gives

$$\Delta_4^- \mathcal{H} = \sum_{kk'q} \frac{1}{4} J_t^2 S_d^- c_{q\uparrow}^\dagger c_{k'\downarrow} \frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{4} J_z S_d^z} S_d^+ c_{k\downarrow}^\dagger c_{q\uparrow} \tag{2.21}$$

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

$$\begin{aligned}
\Delta_4^- \mathcal{H} &= \frac{1}{4} J_t^2 \sum_{kk'q} S_d^- S_d^+ c_{q\uparrow}^\dagger c_{k'\downarrow} c_{k\downarrow}^\dagger c_{q\uparrow} \frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{8} J_z} \\
&= \frac{1}{4} J_t^2 \sum_{kk'q} \left( \frac{1}{2} - S_d^z \right) c_{k'\downarrow} c_{k\downarrow}^\dagger \frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{8} J_z} \\
&= -\frac{1}{4} J_t^2 \sum_{kk'q} \left( \frac{1}{2} - S_d^z \right) c_{k\downarrow}^\dagger c_{k'\downarrow} \frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{8} J_z}
\end{aligned} \tag{2.22}$$

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

$$\begin{aligned}
\Delta_1^+ \mathcal{H} &= \frac{1}{16} J_z^2 \sum_{kk'q} c_{k\uparrow}^\dagger c_{k'\uparrow} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{4} J_z S_d^z} \\
\Delta_1^- \mathcal{H} &= -\frac{1}{16} J_z^2 \sum_{kk'q} c_{k\uparrow}^\dagger c_{k'\uparrow} \frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{4} J_z S_d^z}
\end{aligned} \tag{2.23}$$

To connect the two $\omega$, 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

$$\eta = \frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{4}J_z S_d^z} \sum_k S_d^z c_{k\uparrow}^\dagger c_{q\uparrow} \tag{2.24}$$

and

$$\begin{aligned}
\eta^\dagger &= \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{4}J_z S_d^z} \sum_k S_d^z c_{q\uparrow}^\dagger c_{k\uparrow} \\
\implies \left(\eta^\dagger\right)^\dagger &= \sum_k S_d^z c_{k\uparrow}^\dagger c_{q\uparrow} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{4}J_z S_d^z} \\
&= \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{4}J_z S_d^z} \sum_k S_d^z c_{k\uparrow}^\dagger c_{q\uparrow}
\end{aligned} \tag{2.25}$$

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

$$\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{4}J_z S_d^z} = \frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{4}J_z S_d^z} \tag{2.26}$$

Using this on eq. 2.23 gives

$$\Delta_1 \mathcal{H} \equiv \Delta_1^+ \mathcal{H} + \Delta_1^- \mathcal{H} = 0 \tag{2.27}$$

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

$$\begin{aligned}
\Delta_2^+ + \Delta_3^+ &= \Delta_2^- + \Delta_3^- \\
\implies \Delta_2 \mathcal{H} + \Delta_3 \mathcal{H} &= 2\Delta_2^+ + 2\Delta_3^+
\end{aligned} \tag{2.28}$$

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

$$-\frac{1}{2} J_z J_t \sum_q \frac{1}{\omega - \epsilon_q + \frac{1}{4}J_z} \tag{2.29}$$

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

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

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

$$-\frac{1}{2} J_t^2 \sum_q \frac{1}{\omega - \epsilon_q + \frac{1}{4}J_z} \tag{2.31}$$

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

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

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

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

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 $\epsilon_q = D$.

$$\delta J = J^2 \rho |\delta D| \frac{1}{D} \tag{2.34}$$

## 2.4 Renormalized Hamiltonian

The renormalized Hamiltonian after disentangling the shell at $\Lambda_N$ is

$$\begin{aligned}\mathcal{H}_{N-1} = \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{k,k'<\Lambda_N} \left[ \frac{J_z^{N-1}}{2} S_d^z \left( c^\dagger_{k\uparrow}c_{k'\uparrow} - c^\dagger_{k\downarrow}c_{k'\downarrow} \right) + \frac{J_t^{N-1}}{2} \left( S_d^+ c^\dagger_{k\downarrow}c_{k'\uparrow} + S_d^- c^\dagger_{k\uparrow}c_{k'\downarrow} \right) \right] \\ + \frac{J_z^N}{2} \sum_{q=\Lambda_N} S_d^z \left( \hat{n}_{q\uparrow} - \hat{n}_{q\downarrow} \right)\end{aligned} \tag{2.35}$$

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.

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

At first order, the rotated Hamiltonian is

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

$n_j$ is the number of states on the shell $\Lambda_j$. 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 $\Lambda_N$.

**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:

$$\begin{aligned}
\frac{1}{2}\mathrm{Tr}_{q\uparrow}\mathcal{H}_j &= \sum_{k<\Lambda_N,\sigma}\epsilon_k\hat{n}_{k\sigma} + \epsilon_d\sum_\sigma \hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + \frac{1}{2}\mathrm{Tr}_{q\uparrow}\left\{\epsilon_k\hat{n}_{q\uparrow}\right\} \\
&= \sum_{k<\Lambda_N,\sigma}\epsilon_k\hat{n}_{k\sigma} + \epsilon_d\sum_\sigma \hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + \frac{1}{2}\epsilon_q \\
\frac{1}{2}\mathrm{Tr}_{q\downarrow}\frac{1}{2}\mathrm{Tr}_{q\uparrow}\mathcal{H}_j &= \sum_{k<\Lambda_N,\sigma}\epsilon_k\hat{n}_{k\sigma} + \epsilon_d\sum_\sigma \hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + \epsilon_q
\end{aligned} \tag{3.3}$$

$$\implies 2^{-n_j}\mathrm{Tr}_{1,2,\ldots,n_j}\mathcal{H}_j = \sum_{k<\Lambda_N,\sigma}\epsilon_k\hat{n}_{k\sigma} + \epsilon_d\sum_\sigma \hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + \sum_{|q|=\Lambda_N}\epsilon_q \tag{3.4}$$

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

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

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

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 $\eta$ 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.

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

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 $c^\dagger_{d\beta}$, 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:

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

We now note that the factor with $\omega$ 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

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

The $\tau$ 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

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

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 $\delta n$:

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

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

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

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

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

The Hamiltonian for a single electron $q\beta$ on the $N^{th}$ shell is

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

where $H_{imp}$ 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 part (the part that appears in the denominator of the URG equations) is

$$\mathcal{H}_D = \sum_{k<\Lambda_N,\sigma}\left(\epsilon_k + \sigma J_z S^z_d\right)\hat{n}_{k\sigma} + \epsilon_q\hat{n}_{q\beta} + \beta J_z S^z_d\hat{n}_{q\beta} + H_{imp} \tag{3.37}$$

As a simplification, we will ignore the terms that pertain to the lower electrons ($k < q$) in $\mathcal{H}_D$.

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

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

$$\begin{gathered}\sum_{k\sigma}\epsilon_k\hat{n}_{k\sigma} = \sum_{k\sigma}\epsilon_k\hat{\tau}_{k\sigma} + \mathcal{C}\\ J_z S^z_d\sum_k\left(\hat{n}_{k\uparrow} - \hat{n}_{k\downarrow}\right) = J_z S^z_d\sum_k\left(\hat{\tau}_{k\uparrow} - \hat{\tau}_{k\downarrow}\right)\end{gathered} \tag{3.39}$$

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

$$\mathcal{H}^+_D = \epsilon_q\hat{\tau}_{q\beta} + \beta J_z S^z_d\hat{\tau}_{q\beta} + H_{imp} \tag{3.40}$$

### 3.2.1 Particle sector

The renormalization in the Hamiltonian in the particle sector is

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

The entire renormalization expression has nine terms- one of order $|V_q|^2$, four of order $V_qJ$ and four of order $J^2$. Since this state is characterized by a particle in the intermediate state, the diagonal part can be evaluated by substituting $\tau_{q\beta} = \frac{1}{2}$ in eq. 3.38:

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

**1.**

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

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

$$\begin{aligned}H_1 = \mathcal{H}_D^+ &= \epsilon_q\frac{1}{2} + \frac{1}{2}\beta J_z S_d^z + H_{imp}\\ &= \epsilon_q\frac{1}{2} - \frac{1}{4}J_z\hat{n}_{d\overline{\beta}} + \epsilon_d\hat{n}_{d\overline{\beta}}\end{aligned} \tag{3.44}$$

$H_1$ is the intermediate state Hamiltonian. As a simplification, we replace $\hat{\omega}^+$ with its eigenvalue $2\omega^+\tau^+ = \omega^+$.

$$\begin{aligned}\Delta_1^+\mathcal{H}_N &= \sum_{q\beta}|V_q|^2 c^\dagger_{d\beta}c_{q\beta}\frac{1}{\hat{\omega}^+ - H_1}c^\dagger_{q\beta}c_{d\beta}\\ &= \sum_{q\beta}|V_q|^2 c^\dagger_{d\beta}c_{q\beta}c^\dagger_{q\beta}c_{d\beta}\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d\hat{n}_{d\overline{\beta}} + \frac{1}{4}J_z\hat{n}_{d\overline{\beta}}}\end{aligned} \tag{3.45}$$

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

$$\begin{aligned}\Delta_1^+\mathcal{H}_N &= \sum_{q\beta}|V_q|^2\hat{n}_{d\beta}\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q + \left(\frac{J_z}{2} - \epsilon_d\right)\hat{n}_{d\overline{\beta}}}\\ &= \sum_{q\beta}|V(q)|^2\hat{n}_{d\beta}\left[\frac{\hat{n}_{d\overline{\beta}}}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} + \frac{\left(1-\hat{n}_{d\overline{\beta}}\right)}{\omega^+ - \frac{1}{2}\epsilon_q}\right]\\ &= \sum_{q\beta}|V(q)|^2\hat{n}_{d\beta}\left[\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q} + \hat{n}_{d\overline{\beta}}\left(\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} - \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q}\right)\right]\end{aligned} \tag{3.46}$$

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

$$H_1 = \mathcal{H}_D^+ = \frac{1}{2}\epsilon_q + \frac{1}{4} J_z \beta S_d^z + \epsilon_d = \frac{1}{2}\epsilon_q - \frac{1}{4} J_z + \epsilon_d \tag{3.50}$$

The first term $\frac{1}{2}\epsilon_q + \frac{1}{4} J_z \beta S_d^z$ is the total dispersion of the electron $q\beta$. The $\epsilon_d$ is the impurity energy and the third term is the total background energy.

$$\begin{aligned}\Delta_2^+\mathcal{H}_N &= -\frac{1}{2} J_z \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{q\beta} \hat{n}_{d\overline{\beta}} c_{q\beta}^\dagger c_{k\beta} \frac{1}{\omega^+ - H_1} \\ &= -\frac{1}{2} J_z \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{k\beta} \frac{\hat{n}_{d\overline{\beta}}}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4} J_z}\end{aligned} \tag{3.51}$$

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

$$H_1 = \frac{1}{2}\epsilon_q - \frac{1}{4} J_z + \epsilon_d \tag{3.53}$$

$$\begin{aligned}\Delta_3^+\mathcal{H}_N &= \sum_{q\beta k} J_t V_q^* c_{d\beta}^\dagger c_{q\beta} c_{d\overline{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\overline{\beta}} \frac{1}{\omega^+ - H_1} \\ &= -J_t \sum_{q\beta k} V_q^* \hat{n}_{d\beta} \left(1 - \hat{n}_{q\beta}\right) c_{d\overline{\beta}}^\dagger c_{k\overline{\beta}} \frac{1}{\omega^+ - H_1} \\ &= -J_t \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{k\beta} \frac{\hat{n}_{d\overline{\beta}}}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4} J_z}\end{aligned} \tag{3.54}$$

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

$$H_1 = \frac{1}{2}\epsilon_q - \frac{1}{4}J_z + \epsilon_d \tag{3.57}$$

$$\begin{aligned}
\Delta_4^+ \mathcal{H}_N &= -\frac{1}{2}J_z \sum_{q\beta k} V_q \hat{n}_{d\overline{\beta}} c_{k\beta}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{d\beta} \frac{1}{\omega^+ - H_1} \\
&= \sum_{q\beta k} -\frac{1}{2} J_z V_q \hat{n}_{d\overline{\beta}} \left(1 - \hat{n}_{q\beta}\right) c_{k\beta}^\dagger c_{d\beta} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \\
&= -\frac{1}{2}J_z \sum_{q\beta k} V_q c_{k\beta}^\dagger c_{d\beta} \frac{\hat{n}_{d\overline{\beta}}}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}
\end{aligned} \tag{3.58}$$

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

$$H_1 = \frac{1}{2}\epsilon_q - \frac{1}{4}J_z + \epsilon_d \tag{3.60}$$

$$\begin{aligned}
\Delta_5^+ \mathcal{H}_N &= \sum_{q\beta k} J_t V_q c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{d\beta} \frac{1}{\omega^+ - H_1} \\
&= -\sum_{q\beta k} J_t V_q \left(1 - \hat{n}_{q\beta}\right) \hat{n}_{d\beta} c_{k\overline{\beta}}^\dagger c_{d\overline{\beta}} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \\
&= -J_t \sum_{q\beta k} V_q c_{k\beta}^\dagger c_{d\beta} \frac{\hat{n}_{d\overline{\beta}}}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}
\end{aligned} \tag{3.61}$$

**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:

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

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

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

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

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

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.**

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

The first step is a simplification:

$$\beta S_d^z c^\dagger_{d\overline{\beta}} c_{d\beta} = \beta S_d^z S^+_{d\overline{\beta}} = \beta \frac{1}{2}\overline{\beta} S^+_{d\overline{\beta}} = -\frac{1}{2} c^\dagger_{d\overline{\beta}} c_{d\beta} \tag{3.67}$$

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

$$H_1 = \frac{1}{2}\epsilon_q + \beta J_z S_d^z + \epsilon_d = \frac{1}{2}\epsilon_q - \frac{1}{4}J_z + \epsilon_d \tag{3.68}$$

$$\begin{aligned}
\Delta_7^+ \mathcal{H}_N &= \sum_{q\beta kk'} \frac{1}{2} J_z J_t c^\dagger_{k\beta} c_{q\beta} c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k'\overline{\beta}} \frac{-1}{\omega^+ - H_1} \\
&= -\frac{1}{2} J_z J_t \sum_{q\beta kk'} \left(1 - \hat{n}_{q\beta}\right) c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{k\beta} c_{k'\overline{\beta}} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \\
&= -\frac{1}{2} J_z J_t \sum_{q\beta kk'} c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{k\beta} c_{k'\overline{\beta}} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}
\end{aligned} \tag{3.69}$$

**8.**

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

The first step is a simplification:

$$c^\dagger_{d\beta} c_{d\overline{\beta}} \beta S_d^z = S^+_{d\beta} \beta S_d^z = \beta \frac{1}{2} \overline{\beta} S^+_{d\beta} = -\frac{1}{2} c^\dagger_{d\beta} c_{d\overline{\beta}} \tag{3.71}$$

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

$$H_1 = \frac{1}{2}\epsilon_q + \beta J_z S_d^z + \epsilon_d = \frac{1}{2}\epsilon_q - \frac{1}{4} J_z + \epsilon_d \tag{3.72}$$

$$\begin{aligned}
\Delta_8^+\mathcal{H}_N &= -\sum_{q\beta kk'} \frac{1}{2} J_z J_t c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{q\beta} c^\dagger_{q\beta} c_{k'\beta} \frac{1}{\omega^+ - H_1} \\
&= -\frac{1}{2} J_z J_t \sum_{q\beta kk'} \left(1 - \hat{n}_{q\beta}\right) c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{k'\beta} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4} J_z} \\
&= -\frac{1}{2} J_z J_t \sum_{q\beta kk'} c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{k'\beta} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4} J_z}
\end{aligned} \tag{3.73}$$

**9.**

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

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

$$H_1 = \frac{1}{2}\epsilon_q - \frac{1}{4} J_z + \epsilon_d \tag{3.75}$$

$$\begin{aligned}
\Delta_9^+\mathcal{H}_N &= \sum_{q\beta kk'} J_t^2 c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{q\beta} c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k'\overline{\beta}} \frac{1}{\omega^+ - H_1} \\
&= J_t^2 \sum_{q\beta kk'} \left(1 - \hat{n}_{q\beta}\right) \hat{n}_{d\beta} \left(1 - \hat{n}_{d\overline{\beta}}\right) c^\dagger_{k\overline{\beta}} c_{k'\overline{\beta}} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4} J_z} \\
&= J_t^2 \sum_{q\beta kk'} c^\dagger_{k\beta} c_{k'\beta} \frac{\hat{n}_{d\overline{\beta}} \left(1 - \hat{n}_{d\beta}\right)}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4} J_z}
\end{aligned} \tag{3.76}$$

**Scaling equations for particle sector**

The scaling equations are obtained as follows. The first term gives the renormalization in $\epsilon_d$ 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 the renormalization in $V^0$, and they 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 $\beta$ 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 3.3 just under eq. 3.127. Otherwise it will renormalize $J_z$.

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

$$\Delta^+U = \sum_q 2|V(q)|^2 \left(\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} - \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q}\right) \tag{3.78}$$

$$\Delta^+V = -\left(\frac{1}{2}J_z + J_t\right)\sum_q V_q \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \tag{3.79}$$

$$\Delta^+J_t = -J_zJ_t\sum_q \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \tag{3.80}$$

$$\Delta^+J_z = -J_t^2\sum_q \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \tag{3.81}$$

### 3.2.2 Hole sector

The renormalization in the Hamiltonian in the hole sector is

$$\begin{aligned}\Delta^-\mathcal{H}_N = \sum_{q\beta}&\left[V_q c^\dagger_{q\beta}c_{d\beta} + J_z\beta S_d^z\sum_{k\sigma}\hat{n}_{d\sigma}c_{k\beta}c^\dagger_{q\beta} + J_t\sum_{k\sigma}c^\dagger_{d\overline{\beta}}c^\dagger_{q\beta}c_{d\beta}c_{k\overline{\beta}}\right]\times\frac{1}{\hat{\omega}^- - \mathcal{H}_D^-}\\ &\times\left[V_q^* c^\dagger_{d\beta}c_{q\beta} + J_z\beta S_d^z\sum_{k\sigma}\hat{n}_{d\sigma}c_{q\beta}c^\dagger_{k\beta} + J_t\sum_{k\sigma}c^\dagger_{d\beta}c^\dagger_{k\overline{\beta}}c_{d\overline{\beta}}c_{q\beta}\right]\end{aligned} \tag{3.82}$$

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

$$\mathcal{H}_D^- = -\frac{1}{2}\epsilon_q - \frac{1}{2}\beta J_z S_d^z + H_{\text{imp}} \tag{3.83}$$

**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

$$H_1 = \epsilon_d + (\epsilon_d + U)\,\hat{n}_{d\bar{\beta}} - \frac{1}{2}\epsilon_q - \frac{1}{2}\beta J_z S_d^z = -\frac{1}{2}\epsilon_q - \frac{1}{4}J_z\left(1 - \hat{n}_{d\bar{\beta}}\right) + \epsilon_d + (\epsilon_d + U)\,\hat{n}_{d\bar{\beta}} \tag{3.85}$$

$$\Delta_1^- \mathcal{H}_N = \sum_{q\beta} |V_q|^2 \hat{n}_{q\beta}\,(1 - \hat{n}_{d\beta})\,\frac{1}{\omega^- - H_1} \tag{3.86}$$

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

$$\begin{aligned}
\Delta_1^- \mathcal{H}_N &= \sum_{q\beta} |V_q|^2 \hat{n}_{q\beta}\,(1 - \hat{n}_{d\beta})\,\frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{4}J_z\left(1 - \hat{n}_{d\bar{\beta}}\right) - \epsilon_d - (\epsilon_d + U)\,\hat{n}_{d\bar{\beta}}} \\
&= \sum_{q\beta} |V_q|^2\,(1 - \hat{n}_{d\beta})\left[\frac{\hat{n}_{d\bar{\beta}}}{\omega^- + \frac{1}{2}\epsilon_q - 2\epsilon_d - U} + \frac{1 - \hat{n}_{d\bar{\beta}}}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}\right] \\
&= \sum_{q\beta} |V(q)|^2 \left[\hat{n}_{d\bar{\beta}}\left(\frac{1}{\omega^- + \frac{1}{2}\epsilon_q - 2\epsilon_d - U} - \frac{2}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}\right)\right. \\
&\qquad \left. + \hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\left(\frac{1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} - \frac{1}{\omega^- + \frac{1}{2}\epsilon_q - 2\epsilon_d - U}\right)\right]
\end{aligned} \tag{3.87}$$

**2.**

$$\Delta_2^- \mathcal{H}_N = \sum_{q\beta k} V_q c_{q\beta}^\dagger c_{d\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_z \beta S_d^z c_{k\beta}^\dagger c_{q\beta} \tag{3.88}$$

The first step is a simplification:

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

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

$$H_1 = -\frac{1}{2}\epsilon_q + \epsilon_d + (\epsilon_d + U)\,\hat{n}_{d\bar{\beta}} - \frac{1}{4}J_z\left(1 - \hat{n}_{d\bar{\beta}}\right) \tag{3.90}$$

$$\begin{aligned}
\Delta_2^- \mathcal{H}_N &= \sum_{q\beta k} \frac{1}{2} J_z \left(1 - \hat{n}_{d\bar{\beta}}\right) V_q c_{q\beta}^\dagger c_{d\beta} \left(1 - \hat{n}_{d\bar{\beta}}\right) c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega^- - H_1} \\
&= -\sum_{q\beta k} \hat{n}_{q\beta} c_{k\beta}^\dagger c_{d\beta} \frac{V_q \frac{1}{2} J_z \left(1 - \hat{n}_{d\bar{\beta}}\right)}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d - (\epsilon_d + U)\,\hat{n}_{d\bar{\beta}} + \frac{1}{4}J_z\left(1 - \hat{n}_{d\bar{\beta}}\right)} \\
&= -\frac{1}{2} J_z \sum_{q\beta k} V_q \hat{n}_{q\beta} c_{k\beta}^\dagger c_{d\beta} \frac{\left(1 - \hat{n}_{d\bar{\beta}}\right)}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}
\end{aligned} \tag{3.91}$$

**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

$$H_1 = \epsilon_d - \frac{1}{2}\epsilon_q - \frac{1}{2} J_z \beta S_d^z = \epsilon_d - \frac{1}{2}\epsilon_q - \frac{1}{4} J_z \tag{3.93}$$

$$\begin{aligned} \Delta_3^- \mathcal{H}_N &= \sum_{q\beta k} J_t V_q c_{q\beta}^\dagger c_{d\beta} c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{q\beta} \frac{1}{\omega^- - H_1} \\ &= \sum_{q\beta k} J_t V_q \hat{n}_{q\beta} \left(1 - \hat{n}_{d\beta}\right) c_{k\overline{\beta}}^\dagger c_{d\overline{\beta}} \frac{-1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4} J_z} \\ &= -J_t \sum_{q\beta k} V_q c_{k\beta}^\dagger c_{d\beta} \frac{1 - \hat{n}_{d\overline{\beta}}}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4} J_z} \end{aligned} \tag{3.94}$$

**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

$$H_1 = -\frac{1}{2}\epsilon_q + \epsilon_d + \left(\epsilon_d + U\right) \hat{n}_{d\overline{\beta}} - \frac{1}{4} J_z \left(1 - \hat{n}_{d\overline{\beta}}\right) \tag{3.97}$$

$$\begin{aligned} \Delta_4^- \mathcal{H}_N &= \sum_{q\beta k} V_q^* c_{q\beta}^\dagger c_{k\beta} c_{d\beta}^\dagger c_{q\beta} \frac{\frac{1}{2} J_z \left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega^- - H_1} \\ &= \sum_{q\beta k} \hat{n}_{q\beta} V_q^* c_{k\beta} c_{d\beta}^\dagger \frac{\frac{1}{2} J_z \left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d - \left(\epsilon_d + U\right) \hat{n}_{d\overline{\beta}} + \frac{1}{4} J_z \left(1 - \hat{n}_{d\overline{\beta}}\right)} \\ &= -\frac{1}{2} J_z \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{k\beta} \frac{1 - \hat{n}_{d\overline{\beta}}}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4} J_z} \end{aligned} \tag{3.98}$$

**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

$$H_1 = -\frac{1}{2}\epsilon_q + \epsilon_d - \frac{1}{4} J_z \tag{3.100}$$

$$\begin{aligned}\Delta_5^- \mathcal{H}_N &= \sum_{q\beta k} J_t V_q^* c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k\overline{\beta}} c^\dagger_{d\beta} c_{q\beta} \frac{1}{\hat{\omega}^- - H_1} \\ &= -J_t \sum_{q\beta k} V_q^* \hat{n}_{q\beta} \left(1 - \hat{n}_{d\beta}\right) c^\dagger_{d\overline{\beta}} c_{k\overline{\beta}} \frac{1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \\ &= -J_t \sum_{q\beta k} V_q^* c^\dagger_{d\beta} c_{k\beta} \frac{1 - \hat{n}_{d\overline{\beta}}}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}\end{aligned} \tag{3.101}$$

**6.**

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

From eq. 3.63,

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

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

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

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

**7.**

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

Simplification:

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

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

$$H_1 = \epsilon_d - \frac{1}{2}\epsilon_q - \frac{1}{4}J_z \tag{3.108}$$

$$
\begin{aligned}
\Delta_7^-\mathcal{H}_N &= \sum_{q\beta kk'} \frac{1}{2} J_z J_t c^\dagger_{q\beta} c_{k'\beta} c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{q\beta} \frac{1}{\omega^- - H_1} \\
&= \sum_{q\beta kk'} \frac{1}{2} J_z J_t \hat{n}_{q\beta} c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{k'\beta} \frac{-1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \\
&= -\frac{1}{2} J_z J_t \sum_{q\beta kk'} c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{k'\beta} \frac{1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \\
&= -\frac{1}{2} J_z J_t \sum_{q\beta kk'} c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{k\beta} c_{k'\overline{\beta}} \frac{1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}
\end{aligned} \tag{3.109}
$$

**8.**

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

Simplification:

$$
c^\dagger_{d\overline{\beta}} c_{d\beta} \beta S_d^z = S^+_{d\overline{\beta}} S_d^z \beta = \beta \frac{1}{2} S^+_{d\overline{\beta}} \beta = \frac{1}{2} c^\dagger_{d\overline{\beta}} c_{d\beta} \tag{3.111}
$$

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

$$
H_1 = -\frac{1}{2}\epsilon_q - \frac{1}{4}J_z + \epsilon_d \tag{3.112}
$$

$$
\begin{aligned}
\Delta_8^-\mathcal{H}_N &= \sum_{q\beta kk'} \frac{1}{2} J_z J_t c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k'\overline{\beta}} c^\dagger_{k\beta} c_{q\beta} \frac{1}{\omega^- - H_1} \\
&= \sum_{q\beta kk'} \frac{1}{2} J_z J_t \hat{n}_{q\beta} c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{k\beta} c_{k'\overline{\beta}} \frac{-1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d - \frac{1}{4}J_z} \\
&= -\frac{1}{2} J_z J_t \sum_{q\beta kk'} c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{k\beta} c_{k'\overline{\beta}} \frac{1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}
\end{aligned} \tag{3.113}
$$

**9.**

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

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

$$
H_1 = -\frac{1}{2}\epsilon_q - \frac{1}{4}J_z + \epsilon_d \tag{3.115}
$$

$$
\begin{aligned}
\Delta_9^-\mathcal{H}_N &= \sum_{q\beta kk'} J_t^2 c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k'\overline{\beta}} c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{q\beta} \frac{1}{\omega^- - H_1} \\
&= \sum_{q\beta kk'} J_t^2 \hat{n}_{q\beta} c^\dagger_{d\overline{\beta}} c_{d\beta} c_{k'\overline{\beta}} c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} \frac{1}{\omega^- - H_1} \\
&= -\sum_{q\beta kk'} J_t^2 \hat{n}_{q\beta} \hat{n}_{d\overline{\beta}} c_{d\beta} c_{k'\overline{\beta}} c^\dagger_{d\beta} c^\dagger_{k\overline{\beta}} \frac{1}{\omega^- - H_1} \\
&= \sum_{q\beta kk'} J_t^2 \hat{n}_{q\beta} \hat{n}_{d\overline{\beta}} \left(1 - \hat{n}_{d\beta}\right) c_{k'\overline{\beta}} c^\dagger_{k\overline{\beta}} \frac{1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \\
&= -J_t^2 \sum_{q\beta kk'} c^\dagger_{k\beta} c_{k'\beta} \frac{\hat{n}_{d\beta}\left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} + J_t^2 \sum_{qk\beta} \frac{\hat{n}_{d\overline{\beta}}\left(1 - \hat{n}_{d\beta}\right)}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}
\end{aligned}
\tag{3.116}
$$

#### 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 $\epsilon_d$.

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

## 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, $\epsilon_d$ and $U$, require a specific condition. Combining eqs. 3.117 and 3.118,

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

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.

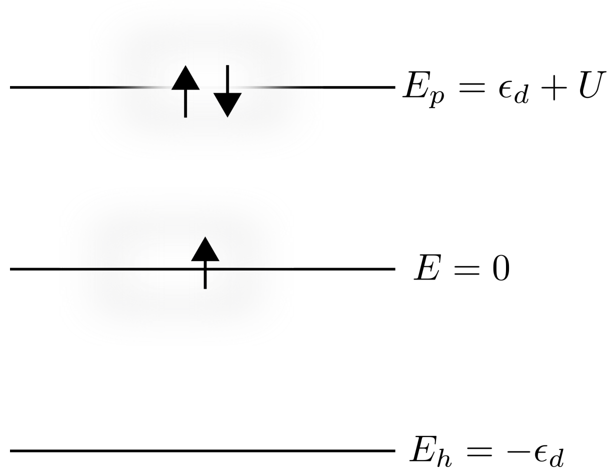


Figure 1: Particle and hole excitations of the impurity

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

$$\begin{aligned}\Delta^+\gamma \equiv \Delta^+\left(\epsilon_d + \frac{1}{2}U\right) &= \sum_q |V(q)|^2 \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \\ \Delta^-\gamma \equiv \Delta^-\left(\epsilon_d + \frac{1}{2}U\right) &= -\sum_q |V(q)|^2 \frac{1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}\end{aligned} \tag{3.126}$$

At this point, we must note that $\omega^+$ and $\omega^-$, the quantum fluctuation energy scales, for the particle and hole sectors are not entirely independent. Recall that if we require the RG to be unitary, we must have $\eta(\omega^-) = \left(\eta^\dagger(\omega^+)\right)^\dagger$. This condition constrains the relation between $\omega^\pm$. To see what the relation is, we can demand $\Delta\gamma \equiv \Delta^+\gamma + \Delta^-\gamma = 0$. That gives

$$\omega^+ - \frac{1}{2}\epsilon_q = \omega^- + \frac{1}{2}\epsilon_q \tag{3.127}$$

If we apply this condition to the term 6 in hole sector, we see that it cancels the term 6 in particle sector.

## 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 $\epsilon_d$ becomes, up to lowest order in $J$,

$$\delta\epsilon_d = -\sum_q \frac{|V_q|^2}{\omega^+ - \epsilon_q} \tag{3.128}$$

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

$$\sum_q = \sum_{\epsilon_q \in [D-|\delta D|, D]} = \rho(D)|\delta D| \tag{3.129}$$

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 $\Delta$, we get

$$\delta\epsilon_d = -\frac{\Delta|\delta D|}{\omega^+ - D} \tag{3.130}$$

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 $\delta D = D - |\delta D| - D = -|\delta D|$.

$$\frac{\mathrm{d}\epsilon_d}{\mathrm{d}D} = -\frac{\Delta}{D} \tag{3.131}$$

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

## 3.5 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:

$$2\Delta J_z = 2\Delta J_t = \Delta J = -J^2 \sum_q \frac{1}{\omega^+ - \epsilon_q - \epsilon_d + \frac{1}{4}J} \tag{3.132}$$

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 $\epsilon_d$. We can take account of this change by now measuring $\omega^+$ from the single occupation energy itself, $\epsilon_d$. Hence we should redefine $\omega^+ - \epsilon_d \to \tilde{\omega}^+$.

$$2\Delta J_z = 2\Delta J_t = \Delta J = -J^2 \sum_q \frac{1}{\tilde{\omega}^+ - \epsilon_q + \frac{1}{4}J} \tag{3.133}$$

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

$$\Delta J = -J^2 \sum_q \frac{1}{-\epsilon_q} \tag{3.134}$$

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

$$\sum_q = \rho(D)\Delta D \tag{3.135}$$

The flow equation of $J$ becomes

$$\Delta J = J^2 \rho(D) \frac{|\Delta D|}{D} \tag{3.136}$$

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,

$$\frac{\mathrm{d}J}{\mathrm{d}\ln D} = -J^2 \rho(D) \tag{3.137}$$

## 3.6 Connection with Kondo URG result

Recall eq. 3.133.

$$\Delta J = -J^2 \sum_q \frac{1}{\tilde{\omega}^+ - \epsilon_q + \frac{1}{4}J} \tag{3.138}$$

For $\tilde{\omega}^+ = \frac{1}{2}D$, we get

$$\Delta J = 2J^2 \sum_q \frac{1}{D - \frac{1}{2}J} \tag{3.139}$$

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

## 3.7 Fixed points for the symmetric Anderson model with $J_z = J_t$

We first consider the simpler case where $\epsilon_d + \frac{1}{2}U = 0$ and $J_z = J_t = \frac{1}{2}J$. We also assume an isotropic dispersion $\epsilon_q = D$ and momentum independent potential $V(q) \equiv V$. For convenience, we define $n(D) = \sum_{\epsilon_q = D}$ and $\mathcal{V}(D) = \sum_{\epsilon_k < D}$. The former is the number of states on the energy shell at $D$, while the latter is the number of states inside the energy shell $D$. The scaling equations for the hole sector become:

$$\begin{aligned}
\Delta U &= \frac{|V|^2\left(U+\frac{1}{2}J\right)n(D)}{\left(\omega^- - D\right)\left(\omega^- - D - \frac{1}{2}U - \frac{1}{4}J\right)} - \frac{1}{8}\frac{J^2 n(D)\mathcal{V}(D)\left[6\left(\omega^- - D\right) - 3U - J\right]}{\left(\omega^- - \epsilon_q - \frac{1}{2}U\right)^2 - \frac{1}{16}J^2} \\
\Delta V &= -\frac{3}{4}JVn(D)\frac{1}{\omega^- - D - \frac{1}{2}U - \frac{1}{4}J} \\
\Delta J &= -\frac{1}{2}J^2 n(D)\frac{1}{\omega^- - D - \frac{1}{2}U - \frac{1}{4}J}
\end{aligned}$$

**In absence of Kondo-type interaction ($J = 0$)**

We first consider the case where $J = 0$. The only relevant equation is then that of $U$, because $V$ and $J$ will then not flow.

$$\Delta U = \frac{|V|^2 U n(D)}{\left(\omega^- - D\right)\left(\omega^- - D - \frac{1}{2}U\right)} \tag{3.140}$$

To get a feel for this equation, we look at a specific value of $\omega^- = \frac{1}{2}U$. For this value,

$$\Delta U = \frac{|V|^2 U n(D)}{D\left(D - \frac{1}{2}U\right)} \tag{3.141}$$

If we start with bare values $U$ and $D$ such that $U < 2D$, then $U$ is relevant, and it will increase. Meanwhile, the bandwidth will decrease as we go to lower energies. The fixed point is achieved when the denominator becomes zero.

$$U^* = 2D^* \tag{3.142}$$

The opposite thing happens if we start with bare values such that $U > 2D$. Then, $U$ is irrelevant and it will decrease until it reaches the same fixed point condition. This fixed point, characterized by $U^* = 2D^*$ and $J = 0$, is the *local moment fixed point*. It is stable along both directions in the $U-$axis. It is however unstable to perturbations in $J$, as we will see later.

There is another fixed point in this picture, the free orbital fixed point at $U = V = 0$. It is unstable in all directions. The two fixed points and the flows are schematically shown in fig. 2. One specific flow line for $J = 0$ is shown in fig. 3.

**With the Kondo-type interaction ($J > 0$)**

In this case, all three equations will come into play. Using the value $\omega^- = \frac{1}{2}U + \frac{1}{2}J$, the equations become

$$\Delta U = \frac{|V|^2\left(U+\frac{1}{2}J\right)n(D)}{\left(D - \frac{1}{4}J\right)\left(D - \frac{1}{2}U - \frac{1}{2}J\right)} + \frac{1}{8}\frac{J^2 n(D)\mathcal{V}(D)\left[6D - 2J\right]}{\left(D - \frac{1}{4}J\right)\left(D - \frac{3}{4}J\right)}$$

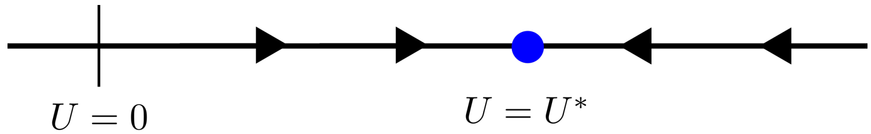


Figure 2: Flows towards local moment for $J = 0$

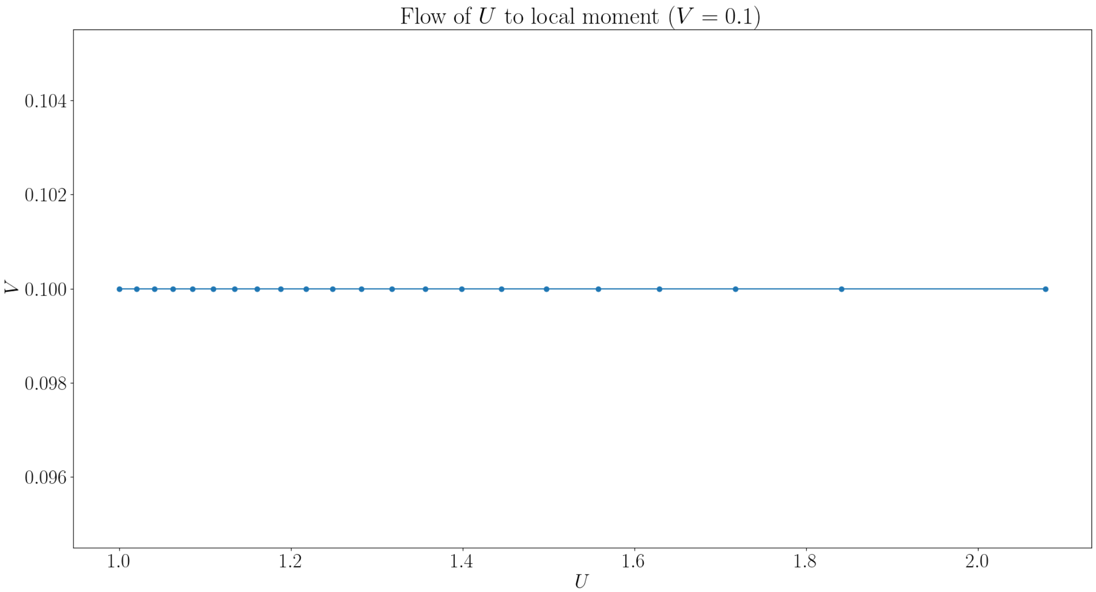


Figure 3: Plot of a particular flow from free orbital (leftmost) to local moment (rightmost) for $J = 0$

$$\Delta V = \frac{3}{4} J n(D) V \frac{1}{D - \frac{1}{4}J}$$
$$\Delta J = \frac{1}{2} J^2 n(D) \frac{1}{D - \frac{1}{4}J}$$

We can now see how the couplings will flow if we start at the local moment fixed point and add a small perturbation $J$. Because of the condition for the local moment fixed point, we know that $D^* - \frac{1}{2}U^* = 0$. Also, close to the local moment, $J$ is small so we can ignore the $J^2$ term. The equations thus become

$$\Delta U = -2 \frac{|V|^2 \left(U^* + \frac{1}{2}J\right) n(D)}{\left(D^* - \frac{1}{4}J\right) J} < 0$$
$$\Delta V = \frac{3}{4} J n(D) V \frac{1}{D^* - \frac{1}{4}J} > 0$$
$$\Delta J = \frac{1}{2} J^2 n(D) \frac{1}{D^* - \frac{1}{4}J} > 0$$

The $U$ is irrelevant and will flow down. The $J$ on the other hand is relevant and will flow to some large value. This fixed point, characterized by a large positive $J$ is the strong-coupling fixed point.

A similar flow happens if we start from the free orbital fixed point. There, $U$ is 0, and the equations look like

$$\Delta U = \frac{1}{2}\frac{|V|^2 Jn(D)}{\left(D - \frac{1}{4}J\right)\left(D - \frac{1}{2}J\right)} > 0$$

$$\Delta V = \frac{3}{4}Jn(D)V\frac{1}{D - \frac{1}{4}J} > 0$$

$$\Delta J = \frac{1}{2}J^2 n(D)\frac{1}{D - \frac{1}{4}J} > 0$$

Here both $U$ and $J$ are relevant and they flow up to the strong-coupling fixed point. A schematic flow diagram is shown in fig. 4.

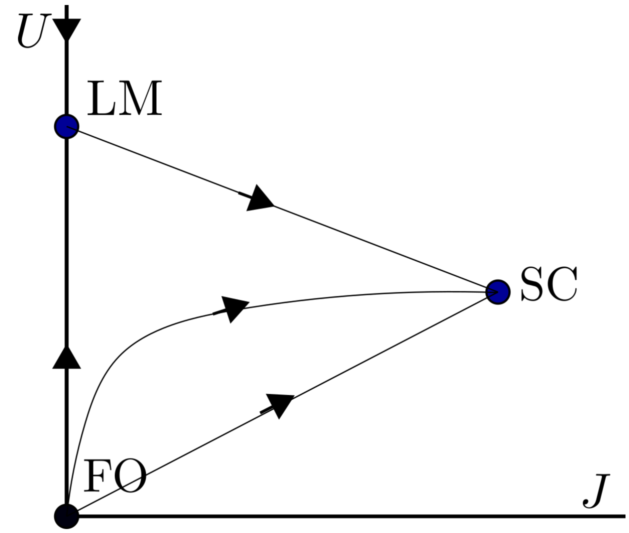


Figure 4: Schematic flows from local moment and free orbital to strong-coupling

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

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

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

$\mathcal{H}$ is the total Hamiltonian and $\left|\Psi\right\rangle$ 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

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

where $\left|\Psi_0\right\rangle = (1-\hat{n}_q)\left|\Psi^N\right\rangle$ is that part of the wavefunction where the state $q$ is occupied. $\left|\Psi_1^N\right\rangle = \hat{n}_q\left|\Psi\right\rangle$ 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

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

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

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

Eliminating $\left|\Psi_1\right\rangle$ from the two equations gives

$$\left(\mathcal{H}_0^d + V_0 + V_-\frac{1}{E - \mathcal{H}_1^d - V_0}V_+\right)\left|\Psi_0\right\rangle = E\left|\Psi_0\right\rangle \tag{4.6}$$

This new Hamiltonian,

$$\tilde{\mathcal{H}}_0 = \mathcal{H}_0^d + V_0 + V_-\frac{1}{E - \mathcal{H}_1^d - V_0}V_+ \tag{4.7}$$

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

$$\Delta V_0\Big|_{PMS} = V_- \frac{1}{E - \mathcal{H}_1^d - V_0} V_+ \tag{4.8}$$

We can write down the renormalized Schrodinger equation in the low energy subspace, from eq. 4.6,

$$\tilde{\mathcal{H}}_0 \left|\Psi_0\right\rangle = E \left|\Psi_0\right\rangle \tag{4.9}$$

and again repeat the entire process. $\tilde{\mathcal{H}}_0$ now takes the place of $\mathcal{H}$ and $\left|\Psi_0\right\rangle$ takes the place of $\left|\Psi\right\rangle$ 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 $(E, \left|\Psi\right\rangle)$, we start with a more general pair $(\tilde{\mathcal{H}}, \left|\Phi\right\rangle)$ where $\left|\Phi\right\rangle$ is not necessarily an exact eigenstate of $\mathcal{H}$. It is defined by $\mathcal{H}'$, which is in turn defined as $\hat{n}_q \mathcal{H}' \left(1 - \hat{n}_q\right) = 0$. $\left|\Phi\right\rangle$ is then defined by

$$\mathcal{H} \left|\Phi\right\rangle = \mathcal{H}' \left|\Phi\right\rangle \tag{4.10}$$

This definition of $\mathcal{H}'$ is the very minimum that we must have in order to fulfill our goal (decouple $q$). The final expression for the renormalization can be written directly from the PMS expression simply by replacing $E$ with $\mathcal{H}'$.

$$\Delta V_0\Big|_{URG} = V_- \frac{1}{\mathcal{H}_1' - \mathcal{H}_1^d - V_0} V_+ \tag{4.11}$$

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

$$U \left|\Phi\right\rangle = \left|\Phi_0\right\rangle \text{ and } \left[\hat{n}_q, \tilde{\mathcal{H}}\right] = 0 \tag{4.12}$$

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 $(\mathcal{H}', \left|\Phi\right\rangle)$ such that $\tilde{\mathcal{H}} \left|\Phi\right\rangle = \mathcal{H}' \left|\Phi\right\rangle$ 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 $\left|\Phi\right\rangle$ 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 $\left|\Phi\right\rangle$. 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 $\left|\Psi\right\rangle$ of the Hamiltonian as the non-Fock basis $\left|\Phi\right\rangle$. 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.

In the context of URG, we define a quantum fluctuation energy scale $\hat{\omega}$:

$$\hat{\omega} = \mathcal{H}'_1 - V_0 \tag{4.13}$$

This allows us to write

$$\Delta V_0\big|_{URG} = V_- \frac{1}{\hat{\omega} - \mathcal{H}^d_1} V_+ \tag{4.14}$$

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

$$\left(\hat{\omega} - \mathcal{H}^d_1\right) V_+ \left|\Psi_0\right\rangle \text{ or } \left(\hat{\omega} - \mathcal{H}^d_1\right) V_- \left|\Psi_1\right\rangle \tag{4.15}$$

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 $(\mathcal{H}^d_1)$ or unoccupied sector $(\mathcal{H}^d_1)$. Since the eigenvalues are unchanged during the unitary renormalization, this implies that $\omega$ 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.

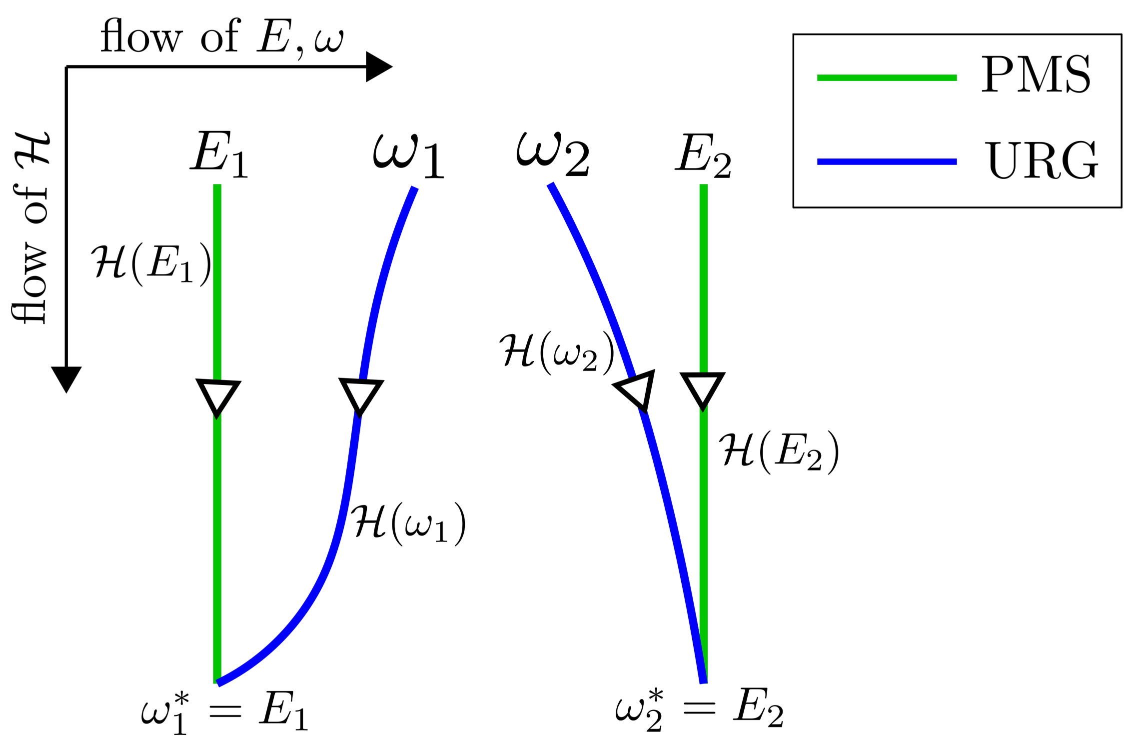


Figure 5: Flows of PMS(green) and URG(blue)

To make matters more clear, we can look at a specific term. For the SIAM, we will consider the scattering $V = c^\dagger_{q\uparrow} c_{d\uparrow}$. $q\uparrow$ is a state in the high energy subspace.

$$\Delta V_P = c^\dagger_{d\uparrow} c_{q\uparrow} \frac{1}{E - \hat{\mathcal{H}}_0} c^\dagger_{q\uparrow} c_{d\uparrow} \tag{4.16}$$

The intermediate energy (at the propagator) is

$$E_1 = \epsilon_d \hat{n}_{d\overline{\beta}} + \epsilon_q \tag{4.17}$$

which gives

$$\begin{aligned}
\Delta V_P &= c^\dagger_{d\uparrow} c_{q\uparrow} \frac{1}{E - \epsilon_q - \epsilon_d \hat{n}_{d\overline{\beta}}} c^\dagger_{q\uparrow} c_{d\uparrow} \\
&= \frac{1}{E - \epsilon_q - \epsilon_d \hat{n}_{d\overline{\beta}}} c^\dagger_{d\uparrow} c_{q\uparrow} c^\dagger_{q\uparrow} c_{d\uparrow} \\
&= \left( \frac{\hat{n}_{d\overline{\beta}}}{E^a - \epsilon_q - \epsilon_d} + \frac{1 - \hat{n}_{d\overline{\beta}}}{E^b - \epsilon_q} \right) c^\dagger_{d\uparrow} c_{q\uparrow} c^\dagger_{q\uparrow} c_{d\uparrow}
\end{aligned} \tag{4.18}$$

There are two terms. The two terms differ in their initial states; one starts from $n_{d\overline{\beta}} = 1$ (corresponding to $E^a$) and the other starts from $n_{d\overline{\beta}} = 0$ (corresponding to $E^b$). From the definition of the $T-$matrix we can see that different initial states will give rise to different final eigenstates. To treat the various energies $E^a$ and $E^b$ on an equal footing, we need to subtract off the initial energies:

$$\begin{aligned}
&E_0 = \epsilon_d + (\epsilon_d + U)\, \hat{n}_{d\overline{\beta}} \\
\implies &E_0^a = 2\epsilon_d + U \\
&E_0^b = \epsilon_d
\end{aligned} \tag{4.19}$$

Defining $\xi = E - E_0$, We can then write

$$\begin{aligned}
\Delta V_P &= \left( \frac{\hat{n}_{d\overline{\beta}}}{\xi + E_0^a - \epsilon_q - \epsilon_d} + \frac{1 - \hat{n}_{d\overline{\beta}}}{\xi + E_0^b - \epsilon_q} \right) c^\dagger_{d\uparrow} c_{q\uparrow} c^\dagger_{q\uparrow} c_{d\uparrow} \\
&= \left( \frac{\hat{n}_{d\overline{\beta}}}{\xi - \epsilon_q + \epsilon_d + U} + \frac{1 - \hat{n}_{d\overline{\beta}}}{\xi - \epsilon_q + \epsilon_d} \right) c^\dagger_{d\uparrow} c_{q\uparrow} c^\dagger_{q\uparrow} c_{d\uparrow}
\end{aligned} \tag{4.20}$$

The quantity $\xi$ now represents the energy of the many-body eigenstate above the non-interacting state. We typically take that to be very small and ignore it w.r.t the bandwidth $\epsilon_q$. This gives the ground state of the total Hamiltonian.

$$\Delta V_P = - \left( \frac{\hat{n}_{d\overline{\beta}}}{\epsilon_q - \epsilon_d - U} + \frac{1 - \hat{n}_{d\overline{\beta}}}{\epsilon_q - \epsilon_d} \right) c^\dagger_{d\uparrow} c_{q\uparrow} c^\dagger_{q\uparrow} c_{d\uparrow} \tag{4.21}$$

The URG calculation proceeds similarly with the $\omega$ replacing the $E$.

$$\Delta V_U = \left( \frac{\hat{n}_{d\overline{\beta}}}{\omega - \epsilon_q + \epsilon_d + U} + \frac{1 - \hat{n}_{d\overline{\beta}}}{\omega - \epsilon_q + \epsilon_d} \right) c^\dagger_{d\uparrow} c_{q\uparrow} c^\dagger_{q\uparrow} c_{d\uparrow} \tag{4.22}$$

Setting $\omega = 0$ gives us the lowest energy scale renormalization and reproduces the PMS result, while tuning the value of $\omega$ allows us to access high energy states as well. The $\eta$ in URG can be written for PMS as well:

$$\eta_p = \frac{1}{E - \hat{\mathcal{H}}_0} V, \eta_p^\dagger = \frac{1}{E - \hat{\mathcal{H}}_0} V^\dagger \tag{4.23}$$

Here $V$ destroys a high energy electron and $V^\dagger$ creates one.[1]

# References

[1] Jun Kondo. *Prog. Theor. Phys.*, 32, 1964.