

Unitary Renormalization Group Approach to Single-Impurity Anderson Model

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0.1 With Kondo-like interaction

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

$$\mathcal{H}_I = \sum_{k,k',\sigma_i} u c_{d\sigma_2}^\dagger c_{d\sigma_4} c_{k'\sigma_3} c_{k\sigma_1}^\dagger \delta_{(\sigma_1+\sigma_2=\sigma_3+\sigma_4)} \quad (0.1)$$

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

$$\mathcal{H}_I = \underbrace{\sum_{k,k',\sigma,\sigma'} u_1 \hat{n}_{d\sigma'} c_{k\sigma}^\dagger c_{k'\sigma}}_{\text{spin-preserving scattering}} + \overbrace{\sum_{k,k',\sigma} u_2 c_{d\bar{\sigma}}^\dagger c_{d\sigma} c_{k\sigma}^\dagger c_{k'\bar{\sigma}}}^{\text{spin-flip scattering}} \quad (0.2)$$

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 ($k\sigma \rightarrow k'\sigma, d\sigma' \rightarrow d\sigma'$). We label this coupling as u_P . The other coupling involves a spin-flip scattering, so we label that as u_A .

$$\mathcal{H}_{I,N} = \sum_{k,k',\sigma,\sigma'} u_P \hat{n}_{d\sigma'} c_{k\sigma}^\dagger c_{k'\sigma} + \sum_{k,k',\sigma} u_A c_{d\bar{\sigma}}^\dagger c_{d\sigma} c_{k\sigma}^\dagger c_{k'\bar{\sigma}} \quad (0.3)$$

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

$$u_{\uparrow\uparrow} \hat{n}_{d\uparrow} c_{k\uparrow}^\dagger c_{k'\uparrow} + u_{\downarrow\downarrow} \hat{n}_{d\downarrow} c_{k\downarrow}^\dagger c_{k'\downarrow} + u_{\uparrow\downarrow} \hat{n}_{d\uparrow} c_{k\downarrow}^\dagger c_{k'\downarrow} + u_{\downarrow\uparrow} \hat{n}_{d\downarrow} c_{k\uparrow}^\dagger c_{k'\uparrow} \quad (0.4)$$

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

$$\begin{aligned} \mathcal{H}_I &= J_z \frac{\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow}}{2} \sum_{kk'} \left(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow} \right) + J_t \sum_{kk'} \left[c_{d\uparrow}^\dagger c_{d\downarrow} c_{k\downarrow}^\dagger c_{k'\uparrow} + c_{d\downarrow}^\dagger c_{d\uparrow} c_{k\uparrow}^\dagger c_{k'\downarrow} \right] \\ &= 2J_z S_d^z s^z + J_t (S_d^+ s^- + S_d^- s^+) \end{aligned} \quad (0.5)$$

The spin-like operators are defined as

$$\begin{aligned} S_d^z &\equiv \frac{1}{2} (\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow}) & S_d^+ &\equiv c_{d\uparrow}^\dagger c_{d\downarrow} & S_d^- &\equiv c_{d\downarrow}^\dagger c_{d\uparrow} \\ s_{kk'}^z &\equiv \frac{1}{2} (c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow}) & s_{kk'}^+ &\equiv c_{k\uparrow}^\dagger c_{k'\downarrow} & s_{kk'}^- &\equiv c_{k\downarrow}^\dagger c_{k'\uparrow} \\ s^a &\equiv \sum_{kk'} s_{kk'}^a \end{aligned} \quad (0.6)$$

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

$$\mathcal{H} = \sum_{k\sigma} \left(\epsilon_k \hat{n}_{k\sigma} + V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right) + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + 2J_z S_d^z s^z + J_t (S_d^+ s^- + S_d^- s^+) \quad (0.7)$$

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

$$\mathcal{H}_I = J \left[S_d^z s^z + \frac{1}{2} (S_d^+ s^- + S_d^- s^+) \right] = J \mathbf{S}_d \cdot \mathbf{s} \quad (0.8)$$

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

$$\begin{aligned} \mathcal{H}_N = H_{N-1} + H_{\text{imp}} + (\epsilon_q + \beta J_z S_d^z) \hat{n}_{q\beta} + V_q c_{q\beta}^\dagger c_{d\beta} + h.c. + \sum_{k < \Lambda_N} \left[J_z S_d^z \beta \left(c_{k\beta}^\dagger c_{q\beta} + c_{q\beta}^\dagger c_{k\beta} \right) \right. \\ \left. + J_t \left(c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} + c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\bar{\beta}} \right) \right] \end{aligned} \quad (0.9)$$

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

$$H_{N-1} = \sum_{k < \Lambda_N, \sigma} \left[(\epsilon_k + \sigma J_z S_d^z) \hat{n}_{k\sigma} + V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right] + H_{I, N-1} \quad (0.10)$$

The diagonal part (the part that appears in the denominator of the URG equations) is

$$\mathcal{H}_D = \sum_{k < \Lambda_N, \sigma} (\epsilon_k + \sigma J_z S_d^z) \hat{n}_{k\sigma} + \epsilon_q \hat{n}_{q\beta} + \beta J_z S_d^z \hat{n}_{q\beta} + H_{\text{imp}} \quad (0.11)$$

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

$$\mathcal{H}_D^+ = \epsilon_q \hat{n}_{q\beta} + \beta J_z S_d^z \hat{n}_{q\beta} + H_{\text{imp}} \quad (0.12)$$

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

$$\begin{aligned} \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} &= \sum_{k\sigma} \epsilon_k \hat{\tau}_{k\sigma} + \mathcal{C} \\ J_z S_d^z \sum_k (\hat{n}_{k\uparrow} - \hat{n}_{k\downarrow}) &= J_z S_d^z \sum_k (\hat{\tau}_{k\uparrow} - \hat{\tau}_{k\downarrow}) \end{aligned} \quad (0.13)$$

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. 0.12 becomes

$$\mathcal{H}_D^+ = \epsilon_q \hat{\tau}_{q\beta} + \beta J_z S_d^z \hat{\tau}_{q\beta} + H_{\text{imp}} \quad (0.14)$$

0.2 Particle sector

The renormalization in the Hamiltonian in the particle sector is

$$\begin{aligned} \Delta^+ \mathcal{H}_N = \sum_{q\beta} \left[V_q^* c_{d\beta}^\dagger c_{q\beta} + J_z \beta S_d^z \sum_k c_{k\beta}^\dagger c_{q\beta} + J_t \sum_k c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \right] \times \frac{1}{\hat{\omega}^+ - \mathcal{H}_D} \\ \times \left[V_q c_{q\beta}^\dagger c_{d\beta} + J_z \beta S_d^z \sum_k c_{q\beta}^\dagger c_{k\beta} + J_t \sum_k c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\bar{\beta}} \right] \end{aligned} \quad (0.15)$$

The entire renormalization expression has nine terms- one of order $|V_q|^2$, four of order $V_q J$ and four of order J^2 . 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. 0.12:

$$\mathcal{H}_D^+ = \epsilon_q \frac{1}{2} + \frac{1}{2} \beta J_z S_d^z + H_{imp} \quad (0.16)$$

1.

$$\Delta_1^+ \mathcal{H}_N = \sum_{q\beta} |V_q|^2 c_{d\beta}^\dagger c_{q\beta} \frac{1}{\hat{\omega}^+ - \mathcal{H}_D^+} c_{q\beta}^\dagger c_{d\beta} \quad (0.17)$$

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

$$\begin{aligned} H_1 = \mathcal{H}_D^+ &= \epsilon_q \frac{1}{2} + \frac{1}{2} \beta J_z S_d^z + H_{imp} \\ &= \epsilon_q \frac{1}{2} - \frac{1}{4} J_z \hat{n}_{d\bar{\beta}} + \epsilon_d \hat{n}_{d\bar{\beta}} \end{aligned} \quad (0.18)$$

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

$$\begin{aligned} \Delta_1^+ \mathcal{H}_N &= \sum_{q\beta} |V_q|^2 c_{d\beta}^\dagger c_{q\beta} \frac{1}{\hat{\omega}^+ - H_1} c_{q\beta}^\dagger c_{d\beta} \\ &= \sum_{q\beta} |V_q|^2 c_{d\beta}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{d\beta} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d \hat{n}_{d\bar{\beta}} + \frac{1}{4} J_z \hat{n}_{d\bar{\beta}}} \end{aligned} \quad (0.19)$$

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

$$\begin{aligned} \Delta_1^+ \mathcal{H}_N &= \sum_{q\beta} |V_q|^2 \hat{n}_{d\beta} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q + \left(\frac{J_z}{2} - \epsilon_d\right) \hat{n}_{d\bar{\beta}}} \\ &= \sum_{q\beta} |V(q)|^2 \hat{n}_{d\beta} \left[\frac{\hat{n}_{d\bar{\beta}}}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4} J_z} + \frac{(1 - \hat{n}_{d\bar{\beta}})}{\omega^+ - \frac{1}{2}\epsilon_q} \right] \\ &= \sum_{q\beta} |V(q)|^2 \hat{n}_{d\beta} \left[\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q} + \hat{n}_{d\bar{\beta}} \left(\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4} J_z} - \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q} \right) \right] \end{aligned} \quad (0.20)$$

2.

$$\Delta_2^+ \mathcal{H}_N = \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_z \beta S_d^z c_{q\beta}^\dagger c_{k\beta} \quad (0.21)$$

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

$$c_{d\beta}^\dagger J_z \beta S_d^z = c_{d\beta}^\dagger \frac{1}{2} (-J_z) \hat{n}_{d\bar{\beta}} \quad (0.22)$$

The expression simplifies to

$$\Delta_2^+ \mathcal{H}_N = \frac{1}{2} (-J_z) \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{q\beta} \hat{n}_{d\bar{\beta}} \frac{1}{\omega^+ - \mathcal{H}_D^+} c_{q\beta}^\dagger c_{k\beta} \quad (0.23)$$

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

$$H_1 = \mathcal{H}_D^+ = \frac{1}{2} \epsilon_q + \frac{1}{4} J_z \beta S_d^z + \epsilon_d = \frac{1}{2} \epsilon_q - \frac{1}{4} J_z + \epsilon_d \quad (0.24)$$

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 ϵ_d is the impurity energy and the third term is the total background energy.

$$\begin{aligned} \Delta_2^+ \mathcal{H}_N &= -\frac{1}{2} J_z \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{q\beta} \hat{n}_{d\bar{\beta}} c_{q\beta}^\dagger c_{k\beta} \frac{1}{\omega^+ - H_1} \\ &= -\frac{1}{2} J_z \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{k\beta} \frac{\hat{n}_{d\bar{\beta}}}{\omega^+ - \frac{1}{2} \epsilon_q - \epsilon_d + \frac{1}{4} J_z} \end{aligned} \quad (0.25)$$

3.

$$\Delta_3^+ \mathcal{H}_N = \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_t c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\bar{\beta}} \quad (0.26)$$

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

$$H_1 = \frac{1}{2} \epsilon_q - \frac{1}{4} J_z + \epsilon_d \quad (0.27)$$

$$\begin{aligned} \Delta_3^+ \mathcal{H}_N &= \sum_{q\beta k} J_t V_q^* c_{d\beta}^\dagger c_{q\beta} c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\bar{\beta}} \frac{1}{\omega^+ - H_1} \\ &= -J_t \sum_{q\beta k} V_q^* \hat{n}_{d\beta} (1 - \hat{n}_{q\beta}) c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}} \frac{1}{\omega^+ - H_1} \\ &= -J_t \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{k\beta} \frac{\hat{n}_{d\bar{\beta}}}{\omega^+ - \frac{1}{2} \epsilon_q - \epsilon_d + \frac{1}{4} J_z} \end{aligned} \quad (0.28)$$

4.

$$\Delta_4^+ \mathcal{H}_N = \sum_{q\beta k\sigma} J_z \beta S_d^z c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} V_q c_{q\beta}^\dagger c_{d\beta} \quad (0.29)$$

The first step is a simplification:

$$J_z \beta S_d^z c_{d\beta} = \frac{1}{2} (-J_z) \hat{n}_{d\bar{\beta}} c_{d\beta} \quad (0.30)$$

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

$$H_1 = \frac{1}{2} \epsilon_q - \frac{1}{4} J_z + \epsilon_d \quad (0.31)$$

$$\begin{aligned} \Delta_4^+ \mathcal{H}_N &= -\frac{1}{2} J_z \sum_{q\beta k} V_q \hat{n}_{d\bar{\beta}} c_{k\beta}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{d\beta} \frac{1}{\omega^+ - H_1} \\ &= \sum_{q\beta k} -\frac{1}{2} J_z V_q \hat{n}_{d\bar{\beta}} (1 - \hat{n}_{q\beta}) c_{k\beta}^\dagger c_{d\beta} \frac{1}{\omega^+ - \frac{1}{2} \epsilon_q - \epsilon_d + \frac{1}{4} J_z} \\ &= -\frac{1}{2} J_z \sum_{q\beta k} V_q c_{k\beta}^\dagger c_{d\beta} \frac{\hat{n}_{d\bar{\beta}}}{\omega^+ - \frac{1}{2} \epsilon_q - \epsilon_d + \frac{1}{4} J_z} \end{aligned} \quad (0.32)$$

5.

$$\Delta_5^+ \mathcal{H}_N = \sum_{q\beta k\sigma} J_t c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} V_q c_{q\beta}^\dagger c_{d\beta} \quad (0.33)$$

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

$$H_1 = \frac{1}{2} \epsilon_q - \frac{1}{4} J_z + \epsilon_d \quad (0.34)$$

$$\begin{aligned} \Delta_5^+ \mathcal{H}_N &= \sum_{q\beta k} J_t V_q c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{d\beta} \frac{1}{\omega^+ - H_1} \\ &= -\sum_{q\beta k} J_t V_q (1 - \hat{n}_{q\beta}) \hat{n}_{d\beta} c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} \frac{1}{\omega^+ - \frac{1}{2} \epsilon_q - \epsilon_d + \frac{1}{4} J_z} \\ &= -J_t \sum_{q\beta k} V_q c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} \frac{\hat{n}_{d\bar{\beta}}}{\omega^+ - \frac{1}{2} \epsilon_q - \epsilon_d + \frac{1}{4} J_z} \end{aligned} \quad (0.35)$$

6.

$$\Delta_6^+ \mathcal{H}_N = \sum_{k'q\beta k} J_z S_d^z \beta c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_z S_d^z \beta c_{q\beta}^\dagger c_{k'\beta} \quad (0.36)$$

The first step is a simplification:

$$(\beta S_d^z)^2 = \frac{1}{4} (\hat{n}_{d\beta} - \hat{n}_{d\bar{\beta}})^2 = \frac{1}{4} (\hat{n}_{d\beta} + \hat{n}_{d\beta} - 2\hat{n}_{d\uparrow} \hat{n}_{d\downarrow}) = \frac{1}{4} (\hat{n}_d - 2\hat{n}_{d\uparrow} \hat{n}_{d\downarrow}) \quad (0.37)$$

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

$$H_1 = \frac{1}{2}\epsilon_q + \frac{1}{2}\beta J_z S_d^z + H_{imp} \quad (0.38)$$

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

$$\begin{aligned} \Delta_6^+ \mathcal{H}_N &= \frac{1}{4} J_z^2 \sum_{k'q\beta k} (\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}) c_{k\beta}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{k'\beta} \frac{1}{\omega^+ - H_1} \\ &= \frac{1}{4} J_z^2 \sum_{k'q\beta k} (\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}) (1 - \hat{n}_{q\beta}) c_{k\beta}^\dagger c_{k'\beta} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - H_{imp} - \frac{1}{2}\beta J_z S_d^z} \\ &= \frac{1}{4} J_z^2 \sum_{k'q\beta k} c_{k\beta}^\dagger c_{k'\beta} \frac{(\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow})}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d - \frac{1}{2}\beta J_z S_d^z} \\ &= \frac{1}{4} J_z^2 \sum_{k'q\beta k} c_{k\beta}^\dagger c_{k'\beta} \left[\frac{\hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}})}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d - \frac{1}{4}J_z} + \frac{\hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta})}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \right] \end{aligned} \quad (0.39)$$

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 $\hat{n}_\uparrow(1 - \hat{n}_\downarrow) + \hat{n}_\downarrow(1 - \hat{n}_\uparrow)$.

7.

$$\Delta_7^+ \mathcal{H}_N = \sum_{q\beta k k'} \beta J_z S_d^z c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_t c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\bar{\beta}} \quad (0.40)$$

The first step is a simplification:

$$\beta S_d^z c_{d\bar{\beta}}^\dagger c_{d\beta} = \beta S_d^z S_{d\bar{\beta}}^+ = \beta \frac{1}{2} \bar{\beta} S_{d\bar{\beta}}^+ = -\frac{1}{2} c_{d\bar{\beta}}^\dagger c_{d\beta} \quad (0.41)$$

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

$$H_1 = \frac{1}{2}\epsilon_q + \beta J_z S_d^z + \epsilon_d = \frac{1}{2}\epsilon_q - \frac{1}{4}J_z + \epsilon_d \quad (0.42)$$

$$\begin{aligned} \Delta_7^+ \mathcal{H}_N &= \sum_{q\beta k k'} \frac{1}{2} J_z J_t c_{k\beta}^\dagger c_{q\beta} c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\bar{\beta}} \frac{-1}{\omega^+ - H_1} \\ &= -\frac{1}{2} J_z J_t \sum_{q\beta k k'} (1 - \hat{n}_{q\beta}) c_{d\bar{\beta}}^\dagger c_{d\beta} c_{k\beta}^\dagger c_{k'\bar{\beta}} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \\ &= -\frac{1}{2} J_z J_t \sum_{q\beta k k'} c_{d\bar{\beta}}^\dagger c_{d\beta} c_{k\beta}^\dagger c_{k'\bar{\beta}} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \end{aligned} \quad (0.43)$$

8.

$$\Delta_8^+ \mathcal{H}_N = \sum_{q\beta k k'} J_t c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_z \beta S_d^z c_{q\beta}^\dagger c_{k'\beta} \quad (0.44)$$

The first step is a simplification:

$$c_{d\beta}^\dagger c_{d\bar{\beta}} \beta S_d^z = S_{d\beta}^+ \beta S_d^z = \beta \frac{1}{2} \bar{\beta} S_{d\bar{\beta}}^+ = -\frac{1}{2} c_{d\beta}^\dagger c_{d\bar{\beta}} \quad (0.45)$$

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

$$H_1 = \frac{1}{2} \epsilon_q + \beta J_z S_d^z + \epsilon_d = \frac{1}{2} \epsilon_q - \frac{1}{4} J_z + \epsilon_d \quad (0.46)$$

$$\begin{aligned} \Delta_8^+ \mathcal{H}_N &= - \sum_{q\beta k k'} \frac{1}{2} J_z J_t c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{k'\beta} \frac{1}{\omega^+ - H_1} \\ &= -\frac{1}{2} J_z J_t \sum_{q\beta k k'} (1 - \hat{n}_{q\beta}) c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{k'\beta} \frac{1}{\omega^+ - \frac{1}{2} \epsilon_q - \epsilon_d + \frac{1}{4} J_z} \\ &= -\frac{1}{2} J_z J_t \sum_{q\beta k k'} c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{k'\beta} \frac{1}{\omega^+ - \frac{1}{2} \epsilon_q - \epsilon_d + \frac{1}{4} J_z} \end{aligned} \quad (0.47)$$

9.

$$\Delta_9^+ \mathcal{H}_N = \sum_{q\beta k k'} J_t c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_t c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\bar{\beta}} \quad (0.48)$$

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

$$H_1 = \frac{1}{2} \epsilon_q - \frac{1}{4} J_z + \epsilon_d \quad (0.49)$$

$$\begin{aligned} \Delta_9^+ \mathcal{H}_N &= \sum_{q\beta k k'} J_t^2 c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\bar{\beta}} \frac{1}{\omega^+ - H_1} \\ &= J_t^2 \sum_{q\beta k k'} (1 - \hat{n}_{q\beta}) \hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}}) c_{k\bar{\beta}}^\dagger c_{k'\bar{\beta}} \frac{1}{\omega^+ - \frac{1}{2} \epsilon_q - \epsilon_d + \frac{1}{4} J_z} \\ &= J_t^2 \sum_{q\beta k k'} c_{k\bar{\beta}}^\dagger c_{k'\bar{\beta}} \frac{\hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta})}{\omega^+ - \frac{1}{2} \epsilon_q - \epsilon_d + \frac{1}{4} J_z} \end{aligned} \quad (0.50)$$

Scaling equations for particle sector

The scaling equations are obtained as follows. The first term gives the renormalization in ϵ_d and U . The renormalization in U will come with a factor of 2 because $\sum_\beta \hat{n}_{d\beta} \hat{n}_{d\bar{\beta}} = 2\hat{n}_{d\uparrow} \hat{n}_{d\downarrow}$. 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 $V\hat{n}_{d\bar{\beta}}$, not strictly of V . In other words, if we split V as $V = V[\hat{n}_{d\bar{\beta}} + (1 - \hat{n}_{d\bar{\beta}})] = V^1\hat{n}_{d\bar{\beta}} + V^0(1 - \hat{n}_{d\bar{\beta}})$, 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 $\bar{\beta}$. The other term, with spin β will renormalize in the hole sector. Term 6 can be ignored for now because it will get canceled by an opposite term in the hole sector, see 0.4 just under eq. 0.101. Otherwise it will renormalize J_z .

$$\Delta^+\epsilon_d = \sum_q |V(q)|^2 \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q} \quad (0.51)$$

$$\Delta^+U = \sum_q 2|V(q)|^2 \left(\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} - \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q} \right) \quad (0.52)$$

$$\Delta^+V = - \left(\frac{1}{2}J_z + J_t \right) \sum_q V_q \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \quad (0.53)$$

$$\Delta^+J_t = -J_zJ_t \sum_q \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \quad (0.54)$$

$$\Delta^+J_z = -J_t^2 \sum_q \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \quad (0.55)$$

0.3 Hole sector

The renormalization in the Hamiltonian in the hole sector is

$$\begin{aligned} \Delta^-\mathcal{H}_N = \sum_{q\beta} \left[V_q c_{q\beta}^\dagger c_{d\beta} + J_z \beta S_d^z \sum_{k\sigma} \hat{n}_{d\sigma} c_{k\beta} c_{q\beta}^\dagger + J_t \sum_{k\sigma} c_{d\bar{\beta}}^\dagger c_{q\beta}^\dagger c_{d\beta} c_{k\bar{\beta}} \right] \times \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} \\ \times \left[V_q^* c_{d\beta}^\dagger c_{q\beta} + J_z \beta S_d^z \sum_{k\sigma} \hat{n}_{d\sigma} c_{q\beta} c_{k\beta}^\dagger + J_t \sum_{k\sigma} c_{d\beta}^\dagger c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} c_{q\beta} \right] \end{aligned} \quad (0.56)$$

\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. 0.12.

$$\mathcal{H}_D^- = -\frac{1}{2}\epsilon_q - \frac{1}{2}\beta J_z S_d^z + H_{\text{imp}} \quad (0.57)$$

1.

$$\Delta_1^-\mathcal{H}_N = \sum_{q\beta} |V_q|^2 c_{q\beta}^\dagger c_{d\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} c_{d\beta}^\dagger c_{q\beta} \quad (0.58)$$

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

$$H_1 = \epsilon_d + (\epsilon_d + U) \hat{n}_{d\bar{\beta}} - \frac{1}{2}\epsilon_q - \frac{1}{2}\beta J_z S_d^z = -\frac{1}{2}\epsilon_q - \frac{1}{4}J_z (1 - \hat{n}_{d\bar{\beta}}) + \epsilon_d + (\epsilon_d + U) \hat{n}_{d\bar{\beta}} \quad (0.59)$$

$$\Delta_1^- \mathcal{H}_N = \sum_{q\beta} |V_q|^2 \hat{n}_{q\beta} (1 - \hat{n}_{d\beta}) \frac{1}{\omega^- - H_1} \quad (0.60)$$

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

$$\begin{aligned} \Delta_1^- \mathcal{H}_N &= \sum_{q\beta} |V_q|^2 \hat{n}_{q\beta} (1 - \hat{n}_{d\beta}) \frac{1}{\omega^- + \frac{1}{2}\epsilon_q - \frac{1}{4}J_z (1 - \hat{n}_{d\bar{\beta}}) - \epsilon_d - (\epsilon_d + U) \hat{n}_{d\bar{\beta}}} \\ &= \sum_{q\beta} (1 - \hat{n}_{d\beta}) \left[\frac{|V_q^1|^2 \hat{n}_{d\bar{\beta}}}{\omega^- + \frac{1}{2}\epsilon_q - 2\epsilon_d - U} + \frac{|V_q^0|^2 (1 - \hat{n}_{d\bar{\beta}})}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \right] \\ &= \sum_{q\beta} |V(q)|^2 \left[\hat{n}_{d\bar{\beta}} \left(\frac{1}{\omega^- + \frac{1}{2}\epsilon_q - 2\epsilon_d - U} - \frac{2}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \right) \right. \\ &\quad \left. + \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \left(\frac{1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} - \frac{1}{\omega^- + \frac{1}{2}\epsilon_q - 2\epsilon_d - U} \right) \right] \end{aligned} \quad (0.61)$$

2.

$$\Delta_2^- \mathcal{H}_N = \sum_{q\beta k} V_q c_{q\beta}^\dagger c_{d\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D} J_z \beta S_d^z c_{k\beta}^\dagger c_{q\beta} \quad (0.62)$$

The first step is a simplification:

$$c_{d\beta} J_z \beta S_d^z = c_{d\beta} \frac{1}{2} J_z (1 - \hat{n}_{d\bar{\beta}}) \quad (0.63)$$

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

$$H_1 = -\frac{1}{2}\epsilon_q + \epsilon_d + (\epsilon_d + U) \hat{n}_{d\bar{\beta}} - \frac{1}{4}J_z (1 - \hat{n}_{d\bar{\beta}}) \quad (0.64)$$

$$\begin{aligned} \Delta_2^- \mathcal{H}_N &= \sum_{q\beta k} \frac{1}{2} J_z (1 - \hat{n}_{d\bar{\beta}}) V_q c_{q\beta}^\dagger c_{d\beta} (1 - \hat{n}_{d\bar{\beta}}) c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega^- - H_1} \\ &= - \sum_{q\beta k} \hat{n}_{q\beta} c_{k\beta}^\dagger c_{d\beta} \frac{V_q \frac{1}{2} J_z (1 - \hat{n}_{d\bar{\beta}})}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d - (\epsilon_d + U) \hat{n}_{d\bar{\beta}} + \frac{1}{4}J_z (1 - \hat{n}_{d\bar{\beta}})} \\ &= -\frac{1}{2} J_z \sum_{q\beta k} V_q \hat{n}_{q\beta} c_{k\beta}^\dagger c_{d\beta} \frac{(1 - \hat{n}_{d\bar{\beta}})}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \end{aligned} \quad (0.65)$$

3.

$$\Delta_3^- \mathcal{H}_N = \sum_{q\beta k} V_q c_{q\beta}^\dagger c_{d\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_t c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \quad (0.66)$$

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

$$H_1 = \epsilon_d - \frac{1}{2}\epsilon_q - \frac{1}{2}J_z\beta S_d^z = \epsilon_d - \frac{1}{2}\epsilon_q - \frac{1}{4}J_z \quad (0.67)$$

$$\begin{aligned} \Delta_3^- \mathcal{H}_N &= \sum_{q\beta k} J_t V_q c_{q\beta}^\dagger c_{d\beta} c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}}^\dagger c_{q\beta} \frac{1}{\omega^- - H_1} \\ &= \sum_{q\beta k} J_t V_q \hat{n}_{q\beta} (1 - \hat{n}_{d\beta}) c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} \frac{-1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \\ &= -J_t \sum_{q\beta k} V_q c_{k\bar{\beta}}^\dagger c_{d\beta} \frac{1 - \hat{n}_{d\bar{\beta}}}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \end{aligned} \quad (0.68)$$

4.

$$\Delta_4^- \mathcal{H}_N = \sum_{q\beta k} \frac{1}{2} J_z \beta S_d^z c_{q\beta}^\dagger c_{k\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} V_q^* c_{d\beta}^\dagger c_{q\beta} \quad (0.69)$$

There is a simplification:

$$\frac{1}{2} J_z \beta S_d^z c_{d\beta}^\dagger = \frac{1}{2} J_z (1 - \hat{n}_{d\bar{\beta}}) c_{d\beta}^\dagger \quad (0.70)$$

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

$$H_1 = -\frac{1}{2}\epsilon_q + \epsilon_d + (\epsilon_d + U) \hat{n}_{d\bar{\beta}} - \frac{1}{4}J_z (1 - \hat{n}_{d\bar{\beta}}) \quad (0.71)$$

$$\begin{aligned} \Delta_4^- \mathcal{H}_N &= \sum_{q\beta k} V_q^* c_{q\beta}^\dagger c_{k\beta} c_{d\beta}^\dagger c_{q\beta} \frac{\frac{1}{2}J_z (1 - \hat{n}_{d\bar{\beta}})}{\omega^- - H_1} \\ &= \sum_{q\beta k} \hat{n}_{q\beta} V_q^* c_{k\beta} c_{d\beta}^\dagger \frac{\frac{1}{2}J_z (1 - \hat{n}_{d\bar{\beta}})}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d - (\epsilon_d + U) \hat{n}_{d\bar{\beta}} + \frac{1}{4}J_z (1 - \hat{n}_{d\bar{\beta}})} \\ &= -\frac{1}{2}J_z \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{k\beta} \frac{1 - \hat{n}_{d\bar{\beta}}}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \end{aligned} \quad (0.72)$$

5.

$$\Delta_5^- \mathcal{H}_N = \sum_{q\beta k} J_t c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\bar{\beta}} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} V_q^* c_{d\beta}^\dagger c_{q\beta} \quad (0.73)$$

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

$$H_1 = -\frac{1}{2}\epsilon_q + \epsilon_d - \frac{1}{4}J_z \quad (0.74)$$

$$\begin{aligned}
\Delta_5^- \mathcal{H}_N &= \sum_{q\beta k} J_t V_q^* c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\bar{\beta}} c_{d\beta}^\dagger c_{q\beta} \frac{1}{\hat{\omega}^- - H_1} \\
&= -J_t \sum_{q\beta k} V_q^* \hat{n}_{q\beta} (1 - \hat{n}_{d\beta}) c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}} \frac{1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \\
&= -J_t \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{k\beta} \frac{1 - \hat{n}_{d\bar{\beta}}}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}
\end{aligned} \tag{0.75}$$

6.

$$\Delta_6^- \mathcal{H}_N = \sum_{q\beta k k'} J_z \beta S_d^z c_{q\beta}^\dagger c_{k'\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_z \beta S_d^z c_{k\beta}^\dagger c_{q\beta} \tag{0.76}$$

From eq. 0.37,

$$(\beta S_d^z)^2 = \frac{1}{4} (\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}) \tag{0.77}$$

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

$$H_1 = H_{\text{imp}} - \frac{1}{2}\epsilon_q - \frac{1}{2}\beta J_z S_d^z \tag{0.78}$$

$$\begin{aligned}
\Delta_6^- \mathcal{H}_N &= \sum_{q\beta k k'} \frac{J_z^2}{4} (\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}) c_{q\beta}^\dagger c_{k'\beta} c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega^- - H_1} \\
&= \frac{J_z^2}{4} \sum_{q\beta k k'} \hat{n}_{q\beta} (\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}) c_{k'\beta} c_{k\beta}^\dagger \frac{1}{\omega^- + \frac{1}{2}\epsilon_q - H_{\text{imp}} + \frac{1}{2}\beta J_z S_d^z} \\
&= -\frac{J_z^2}{4} \sum_{q\beta k k'} c_{k\beta}^\dagger c_{k'\beta} \left[\frac{\hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}})}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} + \frac{\hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta})}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d - \frac{1}{4}J_z} \right] \\
&\quad + \frac{J_z^2}{4} \sum_{q\beta k} \left[\frac{\hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}})}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} + \frac{\hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta})}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d - \frac{1}{4}J_z} \right]
\end{aligned} \tag{0.79}$$

7.

$$\Delta_7^- \mathcal{H}_N = \sum_{q\beta k k'} J_z \beta S_d^z c_{q\beta}^\dagger c_{k'\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_t c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \tag{0.80}$$

Simplification:

$$\beta S_d^z c_{d\beta}^\dagger c_{d\bar{\beta}} = \beta S_d^z S_{d\beta}^+ = \beta \frac{1}{2} \beta S_{d\beta}^+ = \frac{1}{2} c_{d\beta}^\dagger c_{d\bar{\beta}} \tag{0.81}$$

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

$$H_1 = \epsilon_d - \frac{1}{2}\epsilon_q - \frac{1}{4}J_z \tag{0.82}$$

$$\begin{aligned}
\Delta_7^- \mathcal{H}_N &= \sum_{q\beta k k'} \frac{1}{2} J_z J_t c_{q\beta}^\dagger c_{k'\beta} c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \frac{1}{\omega^- - H_1} \\
&= \sum_{q\beta k k'} \frac{1}{2} J_z J_t \hat{n}_{q\beta} c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{k'\beta} \frac{-1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \\
&= -\frac{1}{2} J_z J_t \sum_{q\beta k k'} c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{k'\beta} \frac{1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \\
&= -\frac{1}{2} J_z J_t \sum_{q\beta k k'} c_{d\bar{\beta}}^\dagger c_{d\beta} c_{k\beta}^\dagger c_{k'\bar{\beta}} \frac{1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}
\end{aligned} \tag{0.83}$$

8.

$$\Delta_8^- \mathcal{H}_N = \sum_{q\beta k k'} J_t c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\bar{\beta}} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_z \beta S_d^z c_{k\beta}^\dagger c_{q\beta} \tag{0.84}$$

Simplification:

$$c_{d\bar{\beta}}^\dagger c_{d\beta} \beta S_d^z = S_{d\bar{\beta}}^+ S_d^z \beta = \beta \frac{1}{2} S_{d\bar{\beta}}^+ \beta = \frac{1}{2} c_{d\bar{\beta}}^\dagger c_{d\beta} \tag{0.85}$$

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

$$H_1 = -\frac{1}{2}\epsilon_q - \frac{1}{4}J_z + \epsilon_d \tag{0.86}$$

$$\begin{aligned}
\Delta_8^- \mathcal{H}_N &= \sum_{q\beta k k'} \frac{1}{2} J_z J_t c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \frac{1}{\omega^- - H_1} \\
&= \sum_{q\beta k k'} \frac{1}{2} J_z J_t \hat{n}_{q\beta} c_{d\bar{\beta}}^\dagger c_{d\beta} c_{k\bar{\beta}}^\dagger c_{k'\beta} \frac{-1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d - \frac{1}{4}J_z} \\
&= -\frac{1}{2} J_z J_t \sum_{q\beta k k'} c_{d\bar{\beta}}^\dagger c_{d\beta} c_{k\beta}^\dagger c_{k'\bar{\beta}} \frac{1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}
\end{aligned} \tag{0.87}$$

9.

$$\Delta_9^- \mathcal{H}_N = \sum_{q\beta k k'} J_t c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\bar{\beta}} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_t c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \tag{0.88}$$

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

$$H_1 = -\frac{1}{2}\epsilon_q - \frac{1}{4}J_z + \epsilon_d \tag{0.89}$$

$$\begin{aligned}
\Delta_9^- \mathcal{H}_N &= \sum_{q\beta k k'} J_t^2 c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\bar{\beta}} c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \frac{1}{\omega^- - H_1} \\
&= \sum_{q\beta k k'} J_t^2 \hat{n}_{q\beta} c_{d\bar{\beta}}^\dagger c_{d\beta} c_{k'\bar{\beta}} c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger \frac{1}{\omega^- - H_1} \\
&= - \sum_{q\beta k k'} J_t^2 \hat{n}_{q\beta} \hat{n}_{d\bar{\beta}} c_{d\beta} c_{k'\bar{\beta}} c_{d\beta}^\dagger c_{k\bar{\beta}}^\dagger \frac{1}{\omega^- - H_1} \\
&= \sum_{q\beta k k'} J_t^2 \hat{n}_{q\beta} \hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta}) c_{k'\bar{\beta}} c_{k\bar{\beta}}^\dagger \frac{1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \\
&= -J_t^2 \sum_{q\beta k k'} c_{k\bar{\beta}}^\dagger c_{k'\beta} \frac{\hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}})}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} + J_t^2 \sum_{qk\beta} \frac{\hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta})}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}
\end{aligned} \tag{0.90}$$

Scaling equations for hole sector

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

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

0.4 Particle-Hole symmetry

The Anderson model Hamiltonian, eq. 0.7, has an impurity particle-hole symmetry for a certain condition of the couplings. To see this, we apply the particle-hole transformation

$c_k \rightarrow c_k^\dagger, c_d \rightarrow -c_d^\dagger$ 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

$$\epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} \rightarrow 2\epsilon_d - \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} \quad (0.91)$$

$$U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \rightarrow U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} - U \sum_{\sigma} \hat{n}_{d\sigma} + U \quad (0.92)$$

$$\sum_{k\sigma} V(k) c_{k\sigma}^\dagger c_{d\sigma} + hc \rightarrow \sum_{k\sigma} -V(k) c_{k\sigma} c_{d\sigma}^\dagger + hc = \sum_{k\sigma} V^*(k) c_{k\sigma}^\dagger c_{d\sigma} + hc \quad (0.93)$$

$$S^z \sum_{kq} s_{kq}^z \rightarrow (-S^z) \sum_{kq} (-s_{kq}^z) = S^z \sum_{kq} s_{kq}^z \quad (0.94)$$

$$S^\pm \sum_{kq} s_{kq}^\mp \rightarrow (-S^\pm) \sum_{kq} (-s_{kq}^\mp) = S^\pm \sum_{kq} s_{kq}^\mp \quad (0.95)$$

The transformation of the spin terms, eqs. 0.94 and 0.95, 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: $\hat{S} = \hat{n} - \frac{1}{2} \rightarrow \frac{1}{2} - \hat{n} = -\hat{S}$. 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. 0.93,

$$V(k) \left(c_{k\sigma}^\dagger c_{d\sigma} + c_{d\sigma}^\dagger c_{k\sigma} \right) \rightarrow V(k) \left(c_{d\sigma}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger c_{d\sigma} \right) \quad (0.96)$$

The impurity diagonal terms, ϵ_d and U , require a specific condition. Combining eqs. 0.91 and 0.92,

$$\epsilon_d \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \rightarrow (-\epsilon_d - U) \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \quad (0.97)$$

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

$$\epsilon_d = -\epsilon_d - U \implies \epsilon_d + \frac{1}{2}U = 0 \quad (0.98)$$

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. 0.98.

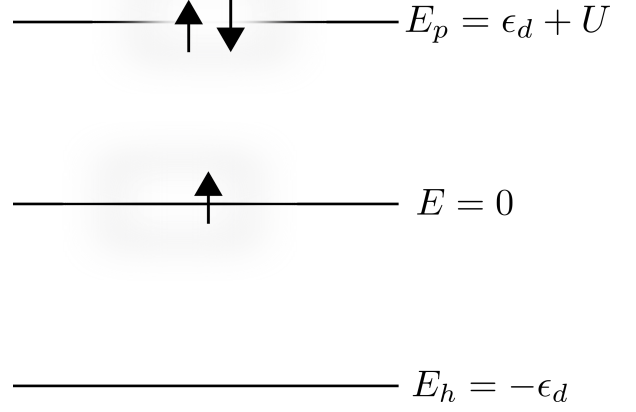


Figure 1: Particle and hole excitations of the impurity

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

$$\Delta \left(\epsilon_d + \frac{1}{2}U \right) = 0 \quad (0.99)$$

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

$$\begin{aligned} \Delta^+ \gamma &\equiv \Delta^+ \left(\epsilon_d + \frac{1}{2}U \right) = \sum_q |V(q)|^2 \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \\ \Delta^- \gamma &\equiv \Delta^- \left(\epsilon_d + \frac{1}{2}U \right) = - \sum_q |V(q)|^2 \frac{1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \end{aligned} \quad (0.100)$$

At this point, we must note that ω^+ and ω^- , 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 $\eta(\omega^-) = (\eta^\dagger(\omega^+))^\dagger$. This condition constrains the relation between ω^\pm . To see what the relation is, we can demand $\Delta\gamma \equiv \Delta^+\gamma + \Delta^-\gamma = 0$. That gives

$$\omega^+ - \frac{1}{2}\epsilon_q = \omega^- + \frac{1}{2}\epsilon_q \quad (0.101)$$

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

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

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

$$\delta\epsilon_d = - \sum_q \frac{|V_q|^2}{\omega^+ - \epsilon_q} \quad (0.102)$$

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

$$\sum_q = \sum_{\epsilon_q \in [D - |\delta D|, D]} = \rho(D) |\delta D| \quad (0.103)$$

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

$$\delta\epsilon_d = - \frac{\Delta |\delta D|}{\omega^+ - D} \quad (0.104)$$

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

$$\frac{d\epsilon_d}{dD} = - \frac{\Delta}{D} \quad (0.105)$$

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

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

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

$$2\Delta J_z = 2\Delta J_t = \Delta J = -J^2 \sum_q \frac{1}{\omega^+ - \epsilon_q - \epsilon_d + \frac{1}{4}J} \quad (0.106)$$

In order to reach the Kondo RG equations, we need to make the appropriate physical change; the difference between the Anderson model and the Kondo model is that the impurity charge fluctuations are frozen at single occupation in the latter. This means that the ground state

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

$$2\Delta J_z = 2\Delta J_t = \Delta J = -J^2 \sum_q \frac{1}{\tilde{\omega}^+ - \epsilon_q + \frac{1}{4}J} \quad (0.107)$$

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

$$\Delta J = -J^2 \sum_q \frac{1}{-\epsilon_q} \quad (0.108)$$

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

$$\sum_q = \rho(D)\Delta D \quad (0.109)$$

The flow equation of J becomes

$$\Delta J = J^2 \rho(D) \frac{|\Delta D|}{D} \quad (0.110)$$

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,

$$\frac{dJ}{d \ln D} = -J^2 \rho(D) \quad (0.111)$$

0.7 Connection with Kondo URG result

Recall eq. 0.107.

$$\Delta J = -J^2 \sum_q \frac{1}{\tilde{\omega}^+ - \epsilon_q + \frac{1}{4}J} \quad (0.112)$$

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

$$\Delta J = 2J^2 \sum_q \frac{1}{D - \frac{1}{2}J} \quad (0.113)$$

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

0.8 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:

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

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.

$$\Delta U = \frac{|V|^2 U n(D)}{(\omega^- - D) (\omega^- - D - \frac{1}{2}U)} \quad (0.114)$$

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

$$\Delta U = \frac{|V|^2 U n(D)}{D (D - \frac{1}{2}U)} \quad (0.115)$$

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.

$$U^* = 2D^* \quad (0.116)$$

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

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

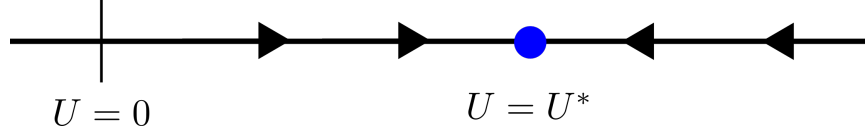


Figure 2: Flows towards local moment for $J = 0$

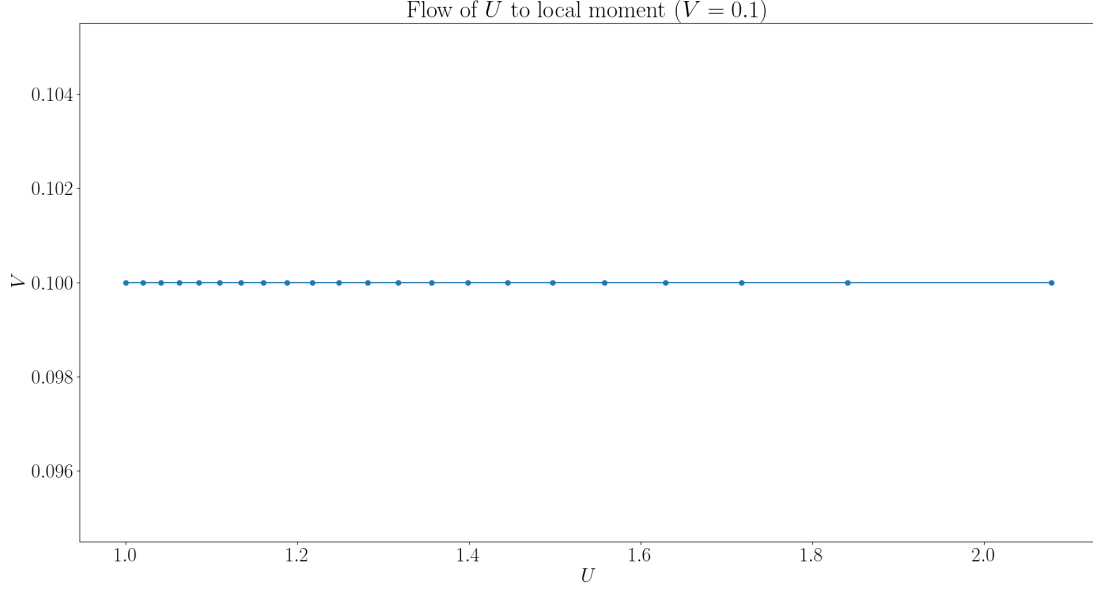


Figure 3: Plot of a particular flow from free orbital (leftmost) to local moment (rightmost) for $J = 0$

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

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

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

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

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

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

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

$$\begin{aligned}\Delta U &= \frac{1}{2} \frac{|V|^2 J n(D)}{(D - \frac{1}{4}J) (D - \frac{1}{2}J)} > 0 \\ \Delta V &= \frac{3}{4} J n(D) V \frac{1}{D - \frac{1}{4}J} > 0 \\ \Delta J &= \frac{1}{2} J^2 n(D) \frac{1}{D - \frac{1}{4}J} > 0\end{aligned}$$

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.

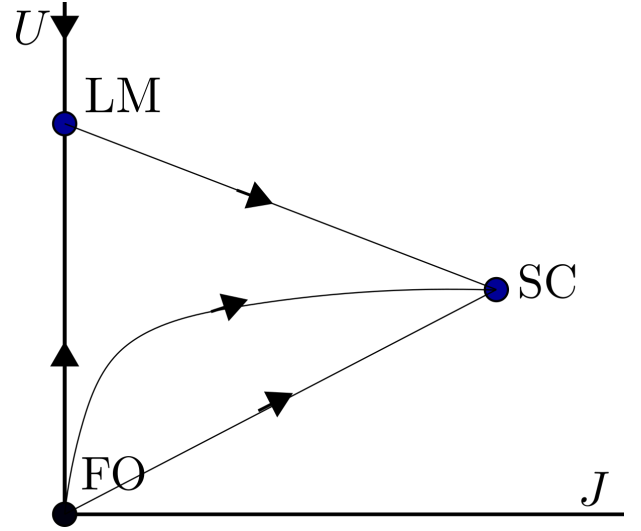


Figure 4: Schematic flows from local moment and free orbital to strong-coupling

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

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

$$\left(\hat{\mathcal{H}}_0 + \hat{V}\right) |\Psi\rangle = E |\Psi\rangle \quad (1.1)$$

$\hat{\mathcal{H}}_0$ is the diagonal part of the Hamiltonian. Starting from the definition of \hat{T} -matrix,

$$\hat{T} |\Psi_0\rangle = \hat{V} |\Psi\rangle \quad (1.2)$$

where $|\Psi_0\rangle$ is an eigenstate of $\hat{\mathcal{H}}_0$, we can write an equation for the \hat{T} -matrix (see eq. ??):

$$\hat{T} = \hat{V} + \hat{V} \left(E - \hat{\mathcal{H}}_0\right)^{-1} \hat{T} \quad (1.3)$$

Define the non-interacting Green's function

$$G_0 = \left(E - \hat{\mathcal{H}}_0\right)^{-1} \quad (1.4)$$

Substituting the expression of \hat{T} back into the right hand side gives an infinite sum. PMS typically requires up to $O(V^2)$:

$$\begin{aligned} \hat{T} &= \hat{V} + \hat{V} G_0 \left[\hat{V} + \hat{V} G_0 \left(\hat{V} + \hat{V} G_0 \right) \dots \right] \\ &= \hat{V} + \hat{V} G_0 \hat{V} + \hat{V} G_0 \hat{V} G_0 \hat{V} + \dots \\ &= \hat{V} + \hat{V} G \hat{V} \end{aligned} \quad (1.5)$$

where G is the total interacting Green's function:

$$G = G_0 + G_0 \hat{V} G_0 + \dots = \frac{1}{E - \hat{\mathcal{H}}} \quad (1.6)$$

The current bandwidth is D . We want to find a Hamiltonian with bandwidth $D - \delta D$. That is, we intend to integrate out all conduction band states in the range $\epsilon_k \in [D - \delta D, D]$. The crudest approximation would be to directly project out all such states. We call this the zeroth approximation:

$$\hat{\mathcal{H}}^{(0)}(D - \delta D) = P \hat{\mathcal{H}}(D) P = P \hat{\mathcal{H}}_0 P + P \hat{V} P \quad (1.7)$$

where

$$P(D - \delta D) = \sum_{k_1, k_2 < D - \delta D} |n_{k_1}\rangle \langle n_{k_2}| \quad (1.8)$$

projects out states above $D - \delta D$. This zeroth approximation retains no information about the eliminated subspace. A better approximation would be to retain the effects of the high

energy subspace through virtual transitions to those states and then back to the low energy subspace. The way we do this is by calculating the T -matrix to arbitrary order, by taking into account those transitions that connect the high and low energy subspaces. Note that since the total scattering has to be inside the low energy subspace, we need atleast two scatterings, one that takes me into the high energy subspace and one that brings me back. Consequently, there is no first order V contribution:

$$\Delta T = \hat{V} G \hat{V} \quad (1.9)$$

As mentioned already, \hat{V} refers to all those processes that connect the two subspaces. If we now write the T -matrix for the low energy subspace up to second order by replacing \hat{T} with \hat{V} in eq. 1.3, the change $\Delta \hat{T}$ can be interpreted as a renormalization in \hat{V} itself.

$$\hat{T} \rightarrow \hat{V} \implies \Delta \hat{T} = \Delta \hat{V} \quad (1.10)$$

This gives us an exact equation for the renormalization of \hat{V} :

$$\Delta \hat{V} = \hat{V} \frac{1}{E - \hat{\mathcal{H}}_0 - \hat{V}} \hat{V} \quad (1.11)$$

with the understanding that the \hat{V} 's in the numerators must connect the two subspaces in order to renormalize \hat{V} . For PMS, we typically expand the denominator and keep only the lowest order.

$$\Delta \hat{V}_P = \hat{V} \frac{1}{E - \hat{\mathcal{H}}_0} \hat{V} \quad (1.12)$$

To make the connection with URG, note that instead of eq. 1.1, the problem URG is trying to solve is:

$$\hat{\mathcal{H}} |\Psi\rangle = \hat{\mathcal{H}}' |\Psi\rangle \quad (1.13)$$

That is, while PMS intends to solve the entire problem, URG tries to decouple just one degree of freedom at each step. The difference is that PMS deals with a scalar energy E , while URG deals with an operator $\hat{\mathcal{H}}'$. Hence, we can make a similar transformation in eq. 1.11:

$$\Delta \hat{V}_U = \hat{V} \frac{1}{\hat{\mathcal{H}}' - \hat{\mathcal{H}}_0 - \hat{V}} \hat{V} \quad (1.14)$$

We can separate the term \hat{V} into two parts; one part V^D consists of diagonal terms that may arise from the scattering term like an $S^z s_z$ term that arises from a Heisenberg-like term, and the other part is the purly scattering part which we call \hat{V}_i .

$$\Delta \hat{V}_U = \hat{V} \frac{1}{\hat{\mathcal{H}}' - \hat{V}_i - \hat{\mathcal{H}}_0 - V^D} \hat{V} \quad (1.15)$$

We now define a new quantity $\hat{\omega} = \hat{\mathcal{H}}' - \hat{V}_i$:

$$\Delta \hat{V}_U = \hat{V} \frac{1}{\hat{\omega} - \hat{\mathcal{H}}_0 - V^D} \hat{V} \quad (1.16)$$

Comparing the two equations 1.12 and 1.16, we can note the following points:

- The scalar E in PMS refers to the energy eigenvalue of the many-body eigenstate $|\Psi\rangle$, while the operator $\hat{\omega}$ in URG contains both the renormalized Hamiltonian as well as the purely scattering term V^i . The difference is that while PMS ignores the scattering in the denominator, URG accounts for it, atleast in principle, inside the $\hat{\omega}$.
- URG has an extra term in the denominator, the diagonal term V^D that arises from the scattering term. This term is not there in PMS because the PMS result is the lowest order term in an expansion.

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

$$\Delta V_P = c_{d\uparrow}^\dagger c_{q\uparrow} \frac{1}{E - \hat{\mathcal{H}}_0} c_{q\uparrow}^\dagger c_{d\uparrow} \quad (1.17)$$

The intermediate energy (at the propagator) is

$$E_1 = \epsilon_d \hat{n}_{d\bar{\beta}} + \epsilon_q \quad (1.18)$$

which gives

$$\begin{aligned} \Delta V_P &= c_{d\uparrow}^\dagger c_{q\uparrow} \frac{1}{E - \epsilon_q - \epsilon_d \hat{n}_{d\bar{\beta}}} c_{q\uparrow}^\dagger c_{d\uparrow} \\ &= \frac{1}{E - \epsilon_q - \epsilon_d \hat{n}_{d\bar{\beta}}} c_{d\uparrow}^\dagger c_{q\uparrow} c_{q\uparrow}^\dagger c_{d\uparrow} \\ &= \left(\frac{\hat{n}_{d\bar{\beta}}}{E^a - \epsilon_q - \epsilon_d} + \frac{1 - \hat{n}_{d\bar{\beta}}}{E^b - \epsilon_q} \right) c_{d\uparrow}^\dagger c_{q\uparrow} c_{q\uparrow}^\dagger c_{d\uparrow} \end{aligned} \quad (1.19)$$

There are two terms. The two terms differ in their initial states; one starts from $n_{d\bar{\beta}} = 1$ (corresponding to E^a) and the other starts from $n_{d\bar{\beta}} = 0$ (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:

$$\begin{aligned} E_0 &= \epsilon_d + (\epsilon_d + U) \hat{n}_{d\bar{\beta}} \\ \implies E_0^a &= 2\epsilon_d + U \\ E_0^b &= \epsilon_d \end{aligned} \quad (1.20)$$

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

$$\begin{aligned} \Delta V_P &= \left(\frac{\hat{n}_{d\bar{\beta}}}{\xi + E_0^a - \epsilon_q - \epsilon_d} + \frac{1 - \hat{n}_{d\bar{\beta}}}{\xi + E_0^b - \epsilon_q} \right) c_{d\uparrow}^\dagger c_{q\uparrow} c_{q\uparrow}^\dagger c_{d\uparrow} \\ &= \left(\frac{\hat{n}_{d\bar{\beta}}}{\xi - \epsilon_q + \epsilon_d + U} + \frac{1 - \hat{n}_{d\bar{\beta}}}{\xi - \epsilon_q + \epsilon_d} \right) c_{d\uparrow}^\dagger c_{q\uparrow} c_{q\uparrow}^\dagger c_{d\uparrow} \end{aligned} \quad (1.21)$$

The quantity ξ 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 ϵ_q . This gives the ground state of the total Hamiltonian.

$$\Delta V_P = - \left(\frac{\hat{n}_{d\bar{\beta}}}{\epsilon_q - \epsilon_d - U} + \frac{1 - \hat{n}_{d\bar{\beta}}}{\epsilon_q - \epsilon_d} \right) c_{d\uparrow}^\dagger c_{q\uparrow} c_{q\uparrow}^\dagger c_{d\uparrow} \quad (1.22)$$

The URG calculation proceeds similarly with the ω replacing the E .

$$\Delta V_U = \left(\frac{\hat{n}_{d\bar{\beta}}}{\omega - \epsilon_q + \epsilon_d + U} + \frac{1 - \hat{n}_{d\bar{\beta}}}{\omega - \epsilon_q + \epsilon_d} \right) c_{d\uparrow}^\dagger c_{q\uparrow} c_{q\uparrow}^\dagger c_{d\uparrow} \quad (1.23)$$

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

$$\eta_p = \frac{1}{E - \hat{\mathcal{H}}_0} V, \eta_p^\dagger = \frac{1}{E - \hat{\mathcal{H}}_0} V^\dagger \quad (1.24)$$

Here V destroys a high energy electron and V^\dagger creates one.

References