1 Anderson Model URG

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

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

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

$$\mathcal{H}_I = \underbrace{\sum_{k,k',\sigma,\sigma'} u_1 \hat{n}_{d\sigma'} c^\dagger_{k\sigma} c_{k'\sigma}}_{\text{spin-preserving scattering}} + \overbrace{\sum_{k,k',\sigma} u_2 c^\dagger_{d\overline{\sigma}} c_{d\sigma} c^\dagger_{k\sigma} c_{k'\overline{\sigma}}}^{\text{spin-flip scattering}} \tag{0.2}$$

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

$$\mathcal{H}_{I,N} = \sum_{k,k',\sigma,\sigma'} u_P \hat{n}_{d\sigma'} c^\dagger_{k\sigma} c_{k'\sigma} + \sum_{k,k',\sigma} u_A c^\dagger_{d\overline{\sigma}} c_{d\sigma} c^\dagger_{k\sigma} c_{k'\overline{\sigma}} \tag{0.3}$$

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

$$u_{\uparrow\uparrow} \hat{n}_{d\uparrow} c^\dagger_{k\uparrow} c_{k'\uparrow} + u_{\downarrow\downarrow} \hat{n}_{d\downarrow} c^\dagger_{k\downarrow} c_{k'\uparrow} + u_{\uparrow\downarrow} \hat{n}_{d\uparrow} c^\dagger_{k\downarrow} c_{k'\downarrow} + u_{\downarrow\uparrow} \hat{n}_{d\downarrow} c^\dagger_{k\uparrow} c_{k'\uparrow} \tag{0.4}$$

We define J_c, J_z and J_t such that the interaction can be written as

$$\begin{aligned}\mathcal{H}_I &= \frac{1}{2} J_c \hat{n}_d \sum_{kk'} \left(c^\dagger_{k\uparrow} c_{k'\uparrow} + c^\dagger_{k\downarrow} c_{k'\downarrow} \right) + J_z \frac{\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow}}{2} \sum_{kk'} \left(c^\dagger_{k\uparrow} c_{k'\uparrow} - c^\dagger_{k\downarrow} c_{k'\downarrow} \right) + J_t \sum_{kk'} \Big[c^\dagger_{d\uparrow} c_{d\downarrow} c^\dagger_{k\downarrow} c_{k'\uparrow} + c^\dagger_{d\downarrow} c_{d\uparrow} c^\dagger_{k} \\ &= \frac{1}{2} J_c \hat{n}_d \sum_{kk'} \left(c^\dagger_{k\uparrow} c_{k'\uparrow} + c^\dagger_{k\downarrow} c_{k'\downarrow} \right) + 2 J_z S^z_d s^z + J_t \left(S^+_d s^- + S^-_d s^+ \right)\end{aligned} \tag{0.5}$$

The spin-like operators are defined as

$$\begin{aligned} S^z_d &\equiv \frac{1}{2} \left(\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow} \right) & S^+_d &\equiv c^\dagger_{d\uparrow} c_{d\downarrow} & S^-_d &\equiv c^\dagger_{d\downarrow} c_{d\uparrow} \\ s^z_{kk'} &\equiv \frac{1}{2} \left(c^\dagger_{k\uparrow} c_{k'\uparrow} - c^\dagger_{k\downarrow} c_{k'\downarrow} \right) & s^+_{kk'} &\equiv c^\dagger_{k\uparrow} c_{k'\downarrow} & s^-_{kk'} &\equiv c^\dagger_{k\downarrow} c_{k'\uparrow} \\ & & s^a &\equiv \sum_{kk'} s^a_{kk'} \end{aligned} \tag{0.6}$$

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

$$\begin{aligned}\mathcal{H}_N = H_{N-1} + H_{\text{imp}} + \left(\epsilon_q + \frac{1}{2}J_c\hat{n}_d + \beta J_z S_d^z\right)\hat{n}_{q\beta} + V_q c^\dagger_{q\beta}c_{d\beta} + \text{h.c.} + \\ + \sum_{k<\Lambda_N}\left[\left(\frac{1}{2}J_c\hat{n}_d + J_z S_d^z\beta\right)\left(c^\dagger_{k\beta}c_{q\beta} + c^\dagger_{q\beta}c_{k\beta}\right) + J_t\left(c^\dagger_{d\beta}c_{d\overline{\beta}}c^\dagger_{k\overline{\beta}}c_{q\beta} + c^\dagger_{d\overline{\beta}}c_{d\beta}c^\dagger_{q\beta}c_{k\overline{\beta}}\right)\right]\end{aligned} \tag{0.7}$$

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

$$H_{N-1} = \sum_{k<\Lambda_N,\sigma}\left[\left(\epsilon_k + \frac{1}{2}J_c\hat{n}_d + \sigma J_z S_d^z\right)\hat{n}_{k\sigma} + V_k c^\dagger_{k\sigma}c_{d\sigma} + \text{h.c.}\right] + H_{I,N-1} \tag{0.8}$$

1.1 Particle sector

The renormalization in the Hamiltonian in the particle sector is

$$\begin{aligned}\Delta^+\mathcal{H}_N = \sum_{q\beta}\left[V_q^* c^\dagger_{d\beta}c_{q\beta} + \left(\frac{1}{2}J_c\hat{n}_d + J_z\beta S_d^z\right)\sum_k c^\dagger_{k\beta}c_{q\beta} + J_t\sum_k c^\dagger_{d\beta}c_{d\overline{\beta}}c^\dagger_{k\overline{\beta}}c_{q\beta}\right] \times \frac{1}{\hat{\omega}^+ - \mathcal{H}_D^+} \\ \times\left[V_q c^\dagger_{q\beta}c_{d\beta} + \left(\frac{1}{2}J_c\hat{n}_d + J_z\beta S_d^z\right)\sum_k c^\dagger_{q\beta}c_{k\beta} + J_t\sum_k c^\dagger_{d\overline{\beta}}c_{d\beta}c^\dagger_{q\beta}c_{k\overline{\beta}}\right]\end{aligned} \tag{0.9}$$

The $\mathcal{H}_D$ is the diagonal part of the Hamiltonian, and the superscript $\pm$ signifies that its the particle(hole) sector part, with respect to the electron presently being disentangled ($q\beta$).

$$\mathcal{H}_D^+ \equiv \text{Tr}_{q\beta}\left[\mathcal{H}\hat{n}_{q\beta}\right] = \sum_{k<\Lambda_N,\sigma}\left(\epsilon_k + \frac{1}{2}J_c\hat{n}_d + \sigma J_z S_d^z\right)\hat{n}_{k\sigma} + \left(\epsilon_q + \frac{1}{2}J_c\hat{n}_d + \beta J_z S_d^z\right) + H_{imp} \tag{0.10}$$

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.

1.

$$\Delta_1^+\mathcal{H}_N = \sum_{q\beta}|V_q|^2 c^\dagger_{d\beta}c_{q\beta}\frac{1}{\hat{\omega}^+ - \mathcal{H}_D^+}c^\dagger_{q\beta}c_{d\beta} \tag{0.11}$$

The final expression in the propagator will involve the energy difference between the initial state and the intermediate state at the propagator. As such, we will only consider the operators to the right of the propagator while calculating the energy values; those on the left will get canceled in the difference. Also, we will worry only about the energy of the on-shell conduction electrons in the denominator.

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

$$\begin{aligned} H_1 \equiv \mathcal{H}_D^+ &= \left[\epsilon_q + \frac{1}{2}J_c\hat{n}_d + \beta J_z S_d^z\right] + \epsilon_d \hat{n}_{d\overline{\beta}} \\ &= \left[\epsilon_q + \frac{1}{2}J_c\hat{n}_{d\overline{\beta}} - \frac{1}{2}\beta\beta J_t \hat{n}_{d\overline{\beta}}\right] + \epsilon_d \hat{n}_{d\overline{\beta}} \\ &= \left[\epsilon_q + \frac{1}{2}J_c\hat{n}_{d\overline{\beta}} - \frac{1}{2}J_t \hat{n}_{d\overline{\beta}}\right] + \epsilon_d \hat{n}_{d\overline{\beta}} \end{aligned} \tag{0.12}$$

H_1 is the intermediate state Hamiltonian. As a simplification, we replace $\hat{\omega}^+$ with its eigenvalue ω^+. Since the propagator, in this form, does not depend on $q\beta$ or $d\beta$ (they have been resolved inside H_1), we can move the propagator to the front:

$$\begin{aligned} \Delta_1^+\mathcal{H}_N &= \sum_{q\beta} |V_q|^2 c^\dagger_{d\beta} c_{q\beta} c^\dagger_{q\beta} c_{d\beta} \frac{1}{\omega^+ - H_1} \\ &= \sum_{q\beta} |V_q|^2 \hat{n}_{d\beta}\left(1 - \hat{n}_{q\beta}\right) \frac{1}{\omega^+ - H_1} \end{aligned} \tag{0.13}$$

We will now write the denominator in terms of the initial energy, H_0. The initial state is characterized by $\hat{n}_{q\beta} = 0, \hat{n}_{d\beta} = 1$:

$$\begin{aligned} H_0 &= \epsilon_d + (\epsilon_d + U)\hat{n}_{d\overline{\beta}} \\ &= H_1 + \epsilon_d + U\hat{n}_{d\overline{\beta}} - \epsilon_q - \frac{1}{2}J_c\hat{n}_{d\overline{\beta}} + \frac{J_z}{2}\hat{n}_{d\overline{\beta}} \end{aligned} \tag{0.14}$$

If we measure the quantum fluctuation ω^+ from the initial (diagonal) state energy which does not have any quantum fluctuations, we can set $H_0 = 0$ in the denominator. Also, since $q\beta$ is on the upper band edge, we can assume it is unoccupied in the initial state. Then,

$$\begin{aligned} \Delta_1^+\mathcal{H}_N &= \sum_{q\beta} |V_q|^2 \hat{n}_{d\beta} \frac{1}{\omega^+ - \epsilon_q + \epsilon_d + \left(U - \frac{1}{2}J_c + \frac{1}{2}J_z\right)\hat{n}_{d\overline{\beta}}} \\ &= \sum_{q\beta} \hat{n}_{d\beta}\left[\frac{|V_q^1|^2 \hat{n}_{d\overline{\beta}}}{\omega^+ - \epsilon_q + \epsilon_d + \left(U - \frac{1}{2}J_c + \frac{1}{2}J_z\right)} + \frac{|V_q^0|^2\left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega^+ - \epsilon_q + \epsilon_d}\right] \\ &= \sum_{q\beta} \hat{n}_{d\beta}\left[\frac{|V_q^0|^2}{\omega^+ - \epsilon_q + \epsilon_d} + \hat{n}_{d\overline{\beta}}\left(\frac{|V_q^1|^2}{\omega^+ - \epsilon_q + \epsilon_d + \left(U - \frac{1}{2}J_c + \frac{1}{2}J_z\right)} - \frac{|V_q^0|^2}{\omega^+ - \epsilon_q + \epsilon_d}\right)\right] \end{aligned} \tag{0.15}$$

2.

$$\Delta_2^+\mathcal{H}_N = \sum_{q\beta k} V_q^* c^\dagger_{d\beta} c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+}\left(\frac{1}{2}J_c\hat{n}_d + J_z\beta S_d^z\right) c^\dagger_{q\beta} c_{k\beta} \tag{0.16}$$

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 $c^\dagger_{d\beta}$, and therefore

$$c^\dagger_{d\beta}\left(\frac{1}{2}J_c\hat{n}_d + J_z\beta S_d^z\right) = c^\dagger_{d\beta}\frac{1}{2}\left(J_c - J_z\right)\hat{n}_{d\overline{\beta}} \tag{0.17}$$

The expression simplifies to

$$\Delta_2^+\mathcal{H}_N = \frac{1}{2}\left(J_c - J_z\right)\sum_{q\beta k} V_q^* c^\dagger_{d\beta}c_{q\beta}\hat{n}_{d\overline{\beta}}\frac{1}{\omega^+ - \mathcal{H}_D^+}c^\dagger_{q\beta}c_{k\beta} \tag{0.18}$$

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

$$H_1 = \epsilon_q + \left(\frac{1}{2}J_c\hat{n}_d + J_z\beta S_d^z\right) + \epsilon_d = \epsilon_q + \frac{1}{2}\left(J_c - J_z\right) + \epsilon_d \tag{0.19}$$

The first term $\epsilon_q + \left(\frac{1}{2}J_c\hat{n}_d + J_z\beta S_d^z\right)$ 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.

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

$$H_0 = \epsilon_d = H_1 - \epsilon_q - \frac{1}{2}\left(J_c - J_z\right) \tag{0.20}$$

$$\begin{aligned}\Delta_2^+\mathcal{H}_N &= \frac{1}{2}\left(J_c - J_z\right)\sum_{q\beta k} V_q^* c^\dagger_{d\beta}c_{q\beta}\hat{n}_{d\overline{\beta}}c^\dagger_{q\beta}c_{k\beta}\frac{1}{\omega^+ - H_1 - \epsilon_q - \frac{1}{2}\left(J_c - J_z\right)} \\ &= \frac{1}{2}\left(J_c - J_z\right)\sum_{q\beta k} c^\dagger_{d\beta}c_{k\beta}\frac{\hat{n}_{d\overline{\beta}}V_q^{1^*}}{\omega^+ - \epsilon_q - \frac{1}{2}\left(J_c - J_z\right)}\end{aligned} \tag{0.21}$$

3.

$$\Delta_3^+\mathcal{H}_N = \sum_{q\beta k} V_q^* c^\dagger_{d\beta}c_{q\beta}\frac{1}{\omega^+ - \mathcal{H}_D^+}J_t c^\dagger_{d\overline{\beta}}c_{d\beta}c^\dagger_{q\beta}c_{k\overline{\beta}} \tag{0.22}$$

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

$$H_1 = \epsilon_q + \frac{1}{2}\left(J_c - J_z\right) + \epsilon_d \tag{0.23}$$

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

$$H_0 = \epsilon_d = H_1 - \epsilon_q - \frac{1}{2}\left(J_c - J_z\right) \tag{0.24}$$

$$
\begin{aligned}
\Delta_3^+\mathcal{H}_N &= \sum_{q\beta k} J_t V_q^* c^\dagger_{d\beta} c_{q\beta} c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k\overline{\beta}} \frac{1}{\omega^+ - H_1 - \epsilon_q - \frac{1}{2}(J_c - J_z)} \\
&= \sum_{q\beta k} -J_t V_q^* \hat{n}_{d\beta}\left(1 - \hat{n}_{q\beta}\right) c^\dagger_{d\overline{\beta}} c_{k\overline{\beta}} \frac{1}{\omega^+ - H_1 - \epsilon_q - \frac{1}{2}(J_c - J_z)} \\
&= -J_t \sum_{q\beta k} c^\dagger_{d\beta} c_{k\beta} \frac{V_q^{1^*} \hat{n}_{d\overline{\beta}}}{\omega^+ - \epsilon_q - \frac{1}{2}(J_c - J_z)}
\end{aligned} \tag{0.25}
$$

4.

$$
\Delta_4^+\mathcal{H}_N = \sum_{q\beta k\sigma} \left(\frac{1}{2} J_c \hat{n}_d + J_z \beta S_d^z\right) c^\dagger_{k\beta} c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} V_q c^\dagger_{q\beta} c_{d\beta} \tag{0.26}
$$

The first step is a simplification:

$$
\left(\frac{1}{2} J_c \hat{n}_d + J_z \beta S_d^z\right) c_{d\beta} = \frac{1}{2}(J_c - J_z)\, \hat{n}_{d\overline{\beta}} c_{d\beta} \tag{0.27}
$$

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

$$
H_1 = \epsilon_q + \frac{1}{2}(J_c - J_z) + \epsilon_d \tag{0.28}
$$

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

$$
H_0 = 2\epsilon_d + U = H_1 + \epsilon_d + U - \epsilon_q - \frac{1}{2}(J_c - J_z) \tag{0.29}
$$

$$
\begin{aligned}
\Delta_4^+\mathcal{H}_N &= \sum_{q\beta k} \frac{1}{2}(J_c - J_z) V_q \hat{n}_{d\overline{\beta}} c^\dagger_{k\beta} c_{q\beta} c^\dagger_{q\beta} c_{d\beta} \frac{1}{\omega^+ - H_0 + \epsilon_d + U - \epsilon_q - \frac{1}{2}(J_c - J_z)} \\
&= \sum_{q\beta k} \frac{1}{2}(J_c - J_z) V_q \hat{n}_{d\overline{\beta}}\left(1 - \hat{n}_{q\beta}\right) c^\dagger_{k\beta} c_{d\beta} \frac{1}{\omega^+ + \epsilon_d + U - \epsilon_q - \frac{1}{2}(J_c - J_z)} \\
&= \frac{1}{2}(J_c - J_z) \sum_{q\beta k} c^\dagger_{k\beta} c_{d\beta} \frac{V_q^1 \hat{n}_{d\overline{\beta}}}{\omega^+ - \epsilon_q + \epsilon_d + U - \frac{1}{2}(J_c - J_z)}
\end{aligned} \tag{0.30}
$$

5.

$$
\Delta_5^+\mathcal{H}_N = \sum_{q\beta k\sigma} J_t c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} V_q c^\dagger_{q\beta} c_{d\beta} \tag{0.31}
$$

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

$$
H_1 = \epsilon_q + \frac{1}{2}(J_c - J_z) + \epsilon_d + \mathcal{E}_0 \tag{0.32}
$$

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

$$H_0 = 2\epsilon_d + U + \mathcal{E}_0 = H_1 + \epsilon_d + U - \epsilon_q - \frac{1}{2}(J_c - J_z) \tag{0.33}$$

$$\begin{aligned}\Delta_5^+\mathcal{H}_N &= \sum_{q\beta k} J_t V_q c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{q\beta} c^\dagger_{q\beta} c_{d\beta} \frac{1}{\omega^+ - H_0 + \epsilon_d + U - \epsilon_q - \frac{1}{2}(J_c - J_z)} \\ &= -\sum_{q\beta k} J_t V_q \left(1 - \hat{n}_{q\beta}\right) \hat{n}_{d\beta} c^\dagger_{k\overline{\beta}} c_{d\overline{\beta}} \frac{1}{\omega^+ + \epsilon_d + U - \epsilon_q - \frac{1}{2}(J_c - J_z)} \\ &= -J_t \sum_{q\beta k} c^\dagger_{k\beta} c_{d\beta} \frac{V_q^1 \hat{n}_{d\overline{\beta}}}{\omega^+ - \epsilon_q + \epsilon_d + U - \frac{1}{2}(J_c - J_z)}\end{aligned} \tag{0.34}$$

6.

$$\Delta_6^+\mathcal{H}_N = \sum_{k'q\beta k} \left(\frac{1}{2} J_c \hat{n}_d + J_z S_d^z \beta\right) c^\dagger_{k\beta} c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} \left(\frac{1}{2} J_c \hat{n}_d + J_z S_d^z \beta\right) c^\dagger_{q\beta} c_{k'\beta} \tag{0.35}$$

Since the impurity parts are diagonal, we keep them as is for the time-being:

$$\hat{d}^2 = \left(\frac{1}{2} J_c \hat{n}_d + J_z S_d^z \beta\right)^2 \tag{0.36}$$

$$\Delta_6^+\mathcal{H}_N = \sum_{k'q\beta k} \hat{d}^2 c^\dagger_{k\beta} c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} c^\dagger_{q\beta} c_{k'\beta} \tag{0.37}$$

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

$$H_1 = \epsilon_q + \frac{1}{2} J_c \hat{n}_d + \beta J_z S_d^z + H_{imp} \tag{0.38}$$

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

$$H_0 = H_{imp} = H_1 - \epsilon_q - \beta J_z S_d^z - \frac{1}{2} J_c \hat{n}_d = H_1 - \epsilon_q - \hat{d} \tag{0.39}$$

$$\begin{aligned}\Delta_6^+\mathcal{H}_N &= \sum_{k'q\beta k} \hat{d}^2 c^\dagger_{k\beta} c_{q\beta} c^\dagger_{q\beta} c_{k'\beta} \frac{1}{\omega^+ - H_1} \\ &= \sum_{k'q\beta k} \hat{d}^2 \left(1 - \hat{n}_{q\beta}\right) c^\dagger_{k\beta} c_{k'\beta} \frac{1}{\omega^+ - H_0 - \epsilon_q - \hat{d}} \\ &= \sum_{k'q\beta k} \hat{d}^2 c^\dagger_{k\beta} c_{k'\beta} \frac{1}{\omega^+ - \epsilon_q - \hat{d}}\end{aligned} \tag{0.40}$$

The operator $\hat{d}$ takes the values

$$\hat{d} = \begin{cases} 0 & \hat{n}_{d\beta} = \hat{n}_{d\overline{\beta}} = 0 \\ \frac{1}{2}(J_c + J_z) & \hat{n}_{d\beta} = 1 - \hat{n}_{d\overline{\beta}} = 0 \\ \frac{1}{2}(J_c - J_z) & 1 - \hat{n}_{d\beta} = \hat{n}_{d\overline{\beta}} = 0 \\ J_c & \hat{n}_{d\beta} = \hat{n}_{d\overline{\beta}} = 1 \end{cases} \tag{0.41}$$

Expanding in this basis gives

$$\Delta_6^+ \mathcal{H}_N = \sum_{k'q\beta k} c^\dagger_{k\beta} c_{k'\beta} \left[\frac{\frac{1}{4}(J_c + J_z)^2 \hat{n}_{d\beta}\left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega^+ - \epsilon_q - \frac{1}{2}(J_c + J_z)} + \frac{\frac{1}{4}(J_c - J_z)^2 \hat{n}_{d\overline{\beta}}\left(1 - \hat{n}_{d\beta}\right)}{\omega^+ - \epsilon_q - \frac{1}{2}(J_c - J_z)} + \frac{J_c^2 \hat{n}_{d\beta}\hat{n}_{d\overline{\beta}}}{\omega^+ - \epsilon_q - J_c} \right] \tag{0.42}$$

7.

$$\Delta_7^+ \mathcal{H}_N = \sum_{q\beta kk'} \left(\frac{1}{2} J_c \hat{n}_d + J_z S_d^z \beta \right) c^\dagger_{k\beta} c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_t c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k'\overline{\beta}} \tag{0.43}$$

The first step is a simplification:

$$\left(\frac{1}{2} J_c \hat{n}_d + J_z S_d^z \beta \right) c^\dagger_{d\overline{\beta}} c_{d\beta} = \frac{1}{2}(J_c - J_z) c^\dagger_{d\overline{\beta}} c_{d\beta} \tag{0.44}$$

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

$$H_1 = \epsilon_q + \frac{1}{2} J_c + \beta J_z S_d^z + \epsilon_d = \epsilon_q + \frac{1}{2}(J_c - J_z) + \epsilon_d \tag{0.45}$$

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

$$H_0 = \epsilon_d = H_1 - \epsilon_q - \frac{1}{2}(J_c - J_z) \tag{0.46}$$

$$\begin{aligned} \Delta_7^+ \mathcal{H}_N &= \sum_{q\beta kk'} \frac{1}{2}(J_c - J_z) J_t c^\dagger_{k\beta} c_{q\beta} c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k'\overline{\beta}} \frac{1}{\omega^+ - H_1} \\ &= \frac{1}{2}(J_c - J_z) J_t \sum_{q\beta kk'} \left(1 - \hat{n}_{q\beta}\right) c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{k\beta} c_{k'\overline{\beta}} \frac{1}{\omega^+ - \epsilon_q - \frac{1}{2}(J_c - J_z)} \\ &= \frac{1}{2}(J_c - J_z) J_t \sum_{q\beta kk'} c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{k\beta} c_{k'\overline{\beta}} \frac{1}{\omega^+ - \epsilon_q - \frac{1}{2}(J_c - J_z)} \end{aligned} \tag{0.47}$$

8.

$$\Delta_8^+\mathcal{H}_N = \sum_{q\beta kk'} J_t c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+}\left(\frac{1}{2}J_c\hat{n}_d + J_z S_d^z \beta\right) c^\dagger_{q\beta} c_{k'\beta} \tag{0.48}$$

The first step is a simplification:

$$c^\dagger_{d\beta} c_{d\overline{\beta}}\left(\frac{1}{2}J_c\hat{n}_d + J_z S_d^z \beta\right) = \frac{1}{2}\left(J_c - J_z\right) c^\dagger_{d\beta} c_{d\overline{\beta}} \tag{0.49}$$

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

$$H_1 = \epsilon_q + \left(\frac{1}{2}J_c + \beta J_z S_d^z\right) + \epsilon_d = \epsilon_q + \frac{1}{2}\left(J_c - J_z\right) + \epsilon_d \tag{0.50}$$

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

$$H_0 = \epsilon_d = H_1 - \epsilon_q - \frac{1}{2}\left(J_c - J_z\right) \tag{0.51}$$

$$\begin{aligned}
\Delta_8^+\mathcal{H}_N &= \frac{1}{2}\left(J_c - J_z\right) J_t \sum_{q\beta kk'} c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{q\beta} c^\dagger_{q\beta} c_{k'\beta} \frac{1}{\omega^+ - \epsilon_q - \frac{1}{2}\left(J_c - J_z\right)} \\
&= \frac{1}{2}\left(J_c - J_z\right) J_t \sum_{q\beta kk'} \left(1 - \hat{n}_{q\beta}\right) c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{k'\beta} \frac{1}{\omega^+ - \epsilon_q - \frac{1}{2}\left(J_c - J_z\right)} \\
&= \frac{1}{2}\left(J_c - J_z\right) J_t \sum_{q\beta kk'} c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{k'\beta} \frac{1}{\omega^+ - \epsilon_q - \frac{1}{2}\left(J_c - J_z\right)}
\end{aligned} \tag{0.52}$$

9.

$$\Delta_9^+\mathcal{H}_N = \sum_{q\beta kk'} J_t c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_t c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k'\overline{\beta}} \tag{0.53}$$

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

$$H_1 = \epsilon_q + \frac{1}{2}\left(J_c - J_z\right) + \epsilon_d \tag{0.54}$$

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

$$H_0 = \epsilon_d = H_1 - \epsilon_q - \frac{1}{2}\left(J_c - J_z\right) \tag{0.55}$$

$$\begin{aligned}
\Delta_9^+\mathcal{H}_N &= \sum_{q\beta kk'} J_t^2 c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{q\beta} c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k'\overline{\beta}} \frac{1}{\omega^+ - \epsilon_q - \frac{1}{2}\left(J_c - J_z\right)} \\
&= \sum_{q\beta kk'} \left(1 - \hat{n}_{q\beta}\right) \hat{n}_{d\beta} \left(1 - \hat{n}_{d\overline{\beta}}\right) c^\dagger_{k\overline{\beta}} c_{k'\overline{\beta}} \frac{J_t^2}{\omega^+ - \epsilon_q - \frac{1}{2}\left(J_c - J_z\right)} \\
&= \sum_{q\beta kk'} c^\dagger_{k\beta} c_{k'\beta} \frac{J_t^2 \hat{n}_{d\overline{\beta}}\left(1 - \hat{n}_{d\beta}\right)}{\omega^+ - \epsilon_q - \frac{1}{2}\left(J_c - J_z\right)}
\end{aligned} \tag{0.56}$$

1.2 Hole sector

The renormalization in the Hamiltonian in the hole sector is

$$\Delta^{-}\mathcal{H}_N = \sum_{q\beta}\left[V_q c^\dagger_{q\beta}c_{d\beta} + \left(\frac{1}{2}J_c\hat{n}_d + J_z\beta S_d^z\right)\sum_{k\sigma}c_{k\beta}c^\dagger_{q\beta} + J_t\sum_{k\sigma}c^\dagger_{d\overline{\beta}}c^\dagger_{q\beta}c_{d\beta}c_{k\overline{\beta}}\right]\times\frac{-1}{\hat{\omega}^- - \mathcal{H}_D^-}$$
$$\times\left[V_q^* c^\dagger_{d\beta}c_{q\beta} + \left(\frac{1}{2}J_c\hat{n}_d + J_z\beta S_d^z\right)\sum_{k\sigma}c_{q\beta}c^\dagger_{k\beta} + J_t\sum_{k\sigma}c^\dagger_{d\beta}c^\dagger_{k\overline{\beta}}c_{d\overline{\beta}}c_{q\beta}\right] \tag{0.57}$$

The propagator can be written as

$$\frac{-1}{\hat{\omega}^- - \mathcal{H}_D^-} = \frac{1}{\omega^- + \mathcal{H}_D^-} \tag{0.58}$$

where we substitute $\hat{\omega}^- = 2\omega^-\tau^- = -\omega^-$. $\mathcal{H}_D^-$ is the energy of the hole state. The kinetic energy and spin of this hole will be the negative of those of the particle, due to conservation.

$$\mathcal{H}_D^- = -\epsilon_q - \frac{1}{2}J_c\hat{n}_d - \beta J_z S_d^z + H_{\text{imp}} \tag{0.59}$$

1.

$$\Delta_1^-\mathcal{H}_N = \sum_{q\beta}|V_q|^2 c^\dagger_{q\beta}c_{d\beta}\frac{1}{\omega^- + \mathcal{H}_D^-}c^\dagger_{d\beta}c_{q\beta} \tag{0.60}$$

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

$$\begin{aligned} H_1 &= \epsilon_d + (\epsilon_d + U)\hat{n}_{d\overline{\beta}} - \epsilon_q - (J_c\hat{n}_d + \beta J_z S_d^z) \\ &= -\epsilon_q - \frac{1}{2}\left[J_c\left(1 + \hat{n}_{d\overline{\beta}}\right) + J_z\left(1 - \hat{n}_{d\overline{\beta}}\right)\right] + \epsilon_d + (\epsilon_d + U)\hat{n}_{d\overline{\beta}} \end{aligned} \tag{0.61}$$

Therefore,

$$\Delta_1^-\mathcal{H}_N = \sum_{q\beta}|V_q|^2\hat{n}_{q\beta}\left(1 - \hat{n}_{d\beta}\right)\frac{1}{\omega^- + H_1} \tag{0.62}$$

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

$$\begin{aligned} H_0 &= \epsilon_d\hat{n}_{d\overline{\beta}} \\ &= H_1 + \epsilon_q - \epsilon_d - U\hat{n}_{d\overline{\beta}} + \frac{1}{2}\left[J_c\left(1 + \hat{n}_{d\overline{\beta}}\right) + J_z\left(1 - \hat{n}_{d\overline{\beta}}\right)\right] \end{aligned} \tag{0.63}$$

As before, we set $H_0 = 0$ and keep $H_1 - H_0$ in the denominator.

$$\begin{aligned}
&\Delta_1^- \mathcal{H}_N \\
&= \sum_{q\beta} |V_q|^2 \hat{n}_{q\beta} \left(1 - \hat{n}_{d\beta}\right) \frac{1}{\omega^- - \epsilon_q + \epsilon_d + U\hat{n}_{d\overline{\beta}} - \frac{1}{2}\left[J_c\left(1 + \hat{n}_{d\overline{\beta}}\right) + J_z\left(1 - \hat{n}_{d\overline{\beta}}\right)\right]} \\
&= \sum_{q\beta} \left(1 - \hat{n}_{d\beta}\right) \left[\frac{|V_q^1|^2 \hat{n}_{d\overline{\beta}}}{\omega^- - \epsilon_q + \epsilon_d + U - J_c} + \frac{|V_q^0|^2 \left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega - \epsilon_q + \epsilon_d - \frac{1}{2}\left(J_c + J_z\right)}\right] \\
&= \sum_{q\beta} \left[\hat{n}_{d\overline{\beta}} \left(\frac{|V_q^1|^2}{\omega - \epsilon_q + \epsilon_d + U - J_c} - \frac{2|V_q^0|^2}{\omega - \epsilon_q + \epsilon_d - \frac{1}{2}\left(J_c + J_z\right)}\right)\right. \\
&\qquad \left. + \hat{n}_{d\uparrow}\hat{n}_{d\downarrow} \left(\frac{|V_q^0|^2}{\omega - \epsilon_q + \epsilon_d - \frac{1}{2}\left(J_c + J_z\right)} - \frac{|V_q^1|^2}{\omega - \epsilon_q + \epsilon_d + U - J_c}\right)\right]
\end{aligned} \tag{0.64}$$

2.

$$\Delta_2^- \mathcal{H}_N = \sum_{q\beta k} V_q c_{q\beta}^\dagger c_{d\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} \left(\frac{1}{2} J_c \hat{n}_d + J_z \beta S_d^z\right) c_{k\beta}^\dagger c_{q\beta} \tag{0.65}$$

The first step is a simplification:

$$\begin{aligned}
c_{d\beta} \left(\frac{1}{2} J_c \hat{n}_d + J_z \beta S_d^z\right) &= c_{d\beta} \frac{1}{2} \left[\left(J_c + J_z\right) + \left(J_c - J_z\right) \hat{n}_{d\overline{\beta}}\right] \\
&= c_{d\beta} \frac{1}{2} \left[2J_c \hat{n}_{d\overline{\beta}} + \left(J_c + J_z\right)\left(1 - \hat{n}_{d\overline{\beta}}\right)\right]
\end{aligned} \tag{0.66}$$

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

$$H_1 = -\epsilon_q + \epsilon_d + \left(\epsilon_d + U\right) \hat{n}_{d\overline{\beta}} - \frac{1}{2} \left[2J_c \hat{n}_{d\overline{\beta}} + \left(J_c + J_z\right)\left(1 - \hat{n}_{d\overline{\beta}}\right)\right] \tag{0.67}$$

The initial state ($\hat{n}_{q\beta} = \hat{n}_{d\beta} = 1$) energy is

$$\begin{aligned}
H_0 &= \epsilon_d + \left(\epsilon_d + U\right) \hat{n}_{d\overline{\beta}} \\
&= H_1 + \epsilon_q + \frac{1}{2} \left[2J_c \hat{n}_{d\overline{\beta}} + \left(J_c + J_z\right)\left(1 - \hat{n}_{d\overline{\beta}}\right)\right]
\end{aligned} \tag{0.68}$$

$$\begin{aligned}
\Delta_2^- \mathcal{H}_N &= \sum_{q\beta k} \frac{1}{2} \left[2J_c \hat{n}_{d\overline{\beta}} + \left(J_c + J_z\right)\left(1 - \hat{n}_{d\overline{\beta}}\right)\right] V_q c_{q\beta}^\dagger c_{d\beta} \left(1 - \hat{n}_{d\overline{\beta}}\right) c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega^- + H_1} \\
&= -\sum_{q\beta k} \hat{n}_{q\beta} c_{k\beta}^\dagger c_{d\beta} \frac{V_q \frac{1}{2} \left[2J_c \hat{n}_{d\overline{\beta}} + \left(J_c + J_z\right)\left(1 - \hat{n}_{d\overline{\beta}}\right)\right]}{\omega^- - \epsilon_q - \frac{1}{2} \left[2J_c \hat{n}_{d\overline{\beta}} + \left(J_c + J_z\right)\left(1 - \hat{n}_{d\overline{\beta}}\right)\right]} \\
&= -\sum_{q\beta k} \hat{n}_{q\beta} c_{k\beta}^\dagger c_{d\beta} \left[\frac{J_c V_q^1 \hat{n}_{d\overline{\beta}}}{\omega^- - \epsilon_q - J_c} + \frac{\frac{1}{2}\left(J_c + J_z\right) V_q^0 \left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega^- - \epsilon_q - \frac{1}{2}\left(J_c + J_z\right)}\right]
\end{aligned} \tag{0.69}$$

3.

$$\Delta_3^- \mathcal{H}_N = \sum_{q\beta k} V_q c^\dagger_{q\beta} c_{d\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_t c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{q\beta} \tag{0.70}$$

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

$$H_1 = \epsilon_d - \epsilon_q - \left(\frac{1}{2} J_c \hat{n}_d + J_z \beta S_d^z\right) = \epsilon_d - \epsilon_q - \frac{1}{2}\left(J_c + J_z\right) \tag{0.71}$$

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

$$H_0 = \epsilon_q + \epsilon_d = H_1 + \epsilon_q + \frac{1}{2}\left(J_c + J_z\right) \tag{0.72}$$

$$\begin{aligned}
\Delta_3^- \mathcal{H}_N &= \sum_{q\beta k} J_t V_q c^\dagger_{q\beta} c_{d\beta} c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{q\beta} \frac{1}{\omega^- + H_1} \\
&= \sum_{q\beta k} J_t V_q \hat{n}_{q\beta} \left(1 - \hat{n}_{d\beta}\right) c^\dagger_{k\overline{\beta}} c_{d\overline{\beta}} \frac{-1}{\omega^- - \epsilon_q - \frac{1}{2}\left(J_c + J_z\right)} \\
&= -J_t \sum_{q\beta k} c^\dagger_{k\beta} c_{d\beta} \frac{V_q^0 \left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega^- - \epsilon_q^- - \frac{1}{2}\left(J_c + J_z\right)}
\end{aligned} \tag{0.73}$$

4.

$$\Delta_4^- \mathcal{H}_N = \sum_{q\beta k} \left(\frac{1}{2} J_c \hat{n}_d + J_z \beta S_d^z\right) c^\dagger_{q\beta} c_{k\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} V_q^* c^\dagger_{d\beta} c_{q\beta} \tag{0.74}$$

There is a simplification:

$$\left(\frac{1}{2} J_c \hat{n}_d + J_z \beta S_d^z\right) c^\dagger_{d\beta} = \frac{1}{2}\left[2 J_c \hat{n}_{d\overline{\beta}} + \left(J_c + J_z\right)\left(1 - \hat{n}_{d\overline{\beta}}\right)\right] c^\dagger_{d\beta} \tag{0.75}$$

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

$$H_1 = -\epsilon_q + \epsilon_d + \left(\epsilon_d + U\right) \hat{n}_{d\overline{\beta}} - \frac{1}{2}\left[2 J_c \hat{n}_{d\overline{\beta}} + \left(J_c + J_z\right)\left(1 - \hat{n}_{d\overline{\beta}}\right)\right] \tag{0.76}$$

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

$$\begin{aligned}
H_0 &= \epsilon_d \hat{n}_{d\overline{\beta}} \\
&= H_1 + \epsilon_q + \frac{1}{2}\left[2 J_c \hat{n}_{d\overline{\beta}} + \left(J_c + J_z\right)\left(1 - \hat{n}_{d\overline{\beta}}\right)\right] - \epsilon_d - U \hat{n}_{d\overline{\beta}} \\
&= H_1 + \epsilon_q + \frac{1}{2}\left(J_c + J_z\right)\left(1 - \hat{n}_{d\overline{\beta}}\right) - \epsilon_d + \left(J_c - U\right) \hat{n}_{d\overline{\beta}}
\end{aligned} \tag{0.77}$$

$$
\begin{aligned}
\Delta_4^- \mathcal{H}_N &= \sum_{q\beta k} V_q^* c_{q\beta}^\dagger c_{k\beta} c_{d\beta}^\dagger c_{q\beta} \frac{\frac{1}{2}\left[2J_c \hat{n}_{d\overline{\beta}} + (J_c + J_z)\left(1 - \hat{n}_{d\overline{\beta}}\right)\right]}{\omega^- - H_0 - \epsilon_q - \frac{1}{2}(J_c + J_z)\left(1 - \hat{n}_{d\overline{\beta}}\right) + \epsilon_d - (J_c - U)\hat{n}_{d\overline{\beta}}} \\
&= \sum_{q\beta k} \hat{n}_{q\beta} V_q^* c_{k\beta} c_{d\beta}^\dagger \frac{\frac{1}{2}\left[2J_c \hat{n}_{d\overline{\beta}} + (J_c + J_z)\left(1 - \hat{n}_{d\overline{\beta}}\right)\right]}{\omega^- - \epsilon_q - \frac{1}{2}(J_c + J_z)\left(1 - \hat{n}_{d\overline{\beta}}\right) + \epsilon_d - (J_c - U)\hat{n}_{d\overline{\beta}}} \\
&= -\sum_{q\beta k} c_{k\beta} c_{d\beta}^\dagger \left[\frac{V_q^{1*} J_c \hat{n}_{d\overline{\beta}}}{\omega^- - \epsilon_q + \epsilon_d + (U - J_c)} + \frac{V_q^{0*} \frac{1}{2}(J_c + J_z)\left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega^- - \epsilon_q - \frac{1}{2}(J_c + J_z) + \epsilon_d}\right]
\end{aligned} \tag{0.78}
$$

5.

$$
\Delta_5^- \mathcal{H}_N = \sum_{q\beta k} J_t c_{d\overline{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\overline{\beta}} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} V_q^* c_{d\beta}^\dagger c_{q\beta} \tag{0.79}
$$

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

$$
H_1 = -\epsilon_q + \epsilon_d - \frac{1}{2}(J_c + J_z) \tag{0.80}
$$

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

$$
H_0 = 0 \tag{0.81}
$$

$$
\begin{aligned}
\Delta_5^- \mathcal{H}_N &= \sum_{q\beta k} J_t V_q^* c_{d\overline{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\overline{\beta}} c_{d\beta}^\dagger c_{q\beta} \frac{1}{\hat{\omega}^- - \epsilon_q + \epsilon_d - \frac{1}{2}(J_c + J_z)} \\
&= -J_t \sum_{q\beta k} V_q^* \hat{n}_{q\beta}\left(1 - \hat{n}_{d\beta}\right) c_{d\overline{\beta}}^\dagger c_{k\overline{\beta}} \frac{1}{\omega^- - \epsilon_q + \epsilon_d - \frac{1}{2}(J_c + J_z)} \\
&= -J_t \sum_{q\beta k} c_{d\beta}^\dagger c_{k\beta} \frac{V_q^{0*}\left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega^- - \epsilon_q + \epsilon_d - \frac{1}{2}(J_c + J_z)}
\end{aligned} \tag{0.82}
$$

6.

$$
\Delta_6^- \mathcal{H}_N = \sum_{q\beta k k'} \left(\frac{1}{2} J_c \hat{n}_d + J_z \beta S_d^z\right) c_{q\beta}^\dagger c_{k'\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} \left(\frac{1}{2} J_c \hat{n}_d + J_z \beta S_d^z\right) c_{k\beta}^\dagger c_{q\beta} \tag{0.83}
$$

We again label

$$
\left(\frac{1}{2} J_c \hat{n}_d + J_z \beta S_d^z\right)^2 = \hat{d}^2 \tag{0.84}
$$

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

$$
H_1 = H_{\text{imp}} - \epsilon_q - \hat{d} \tag{0.85}
$$

The initial state ($\hat{n}_{q\beta} = 1$) energy is

$$H_0 = H_{\text{imp}} = H_1 + \epsilon_q + \hat{d} \tag{0.86}$$

$$\begin{aligned}
\Delta_6^- \mathcal{H}_N &= \sum_{q\beta kk'} \hat{d}^2 c^\dagger_{q\beta} c_{k'\beta} c^\dagger_{k\beta} c_{q\beta} \frac{1}{\omega^- + H_1} \\
&= \sum_{q\beta kk'} \hat{n}_{q\beta} \hat{d}^2 c_{k'\beta} c^\dagger_{k\beta} \frac{1}{\omega^- - \epsilon_q - \hat{d}} \\
&= -\sum_{k'q\beta k} c^\dagger_{k\beta} c_{k'\beta} \left[\frac{\frac{1}{4}(J_c + J_z)^2 \hat{n}_{d\beta}\left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega^- - \epsilon_q - \frac{1}{2}(J_c + J_z)} + \frac{\frac{1}{4}(J_c - J_z)^2 \hat{n}_{d\overline{\beta}}\left(1 - \hat{n}_{d\beta}\right)}{\omega^- - \epsilon_q - \frac{1}{2}(J_c - J_z)} + \frac{J_c^2 \hat{n}_{d\beta} \hat{n}_{d\overline{\beta}}}{\omega^- - \epsilon_q - J_c} \right] \\
&\quad + \sum_{q\beta k} \left[\frac{\frac{1}{4}(J_c + J_z)^2 \hat{n}_{d\beta}\left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega^- - \epsilon_q - \frac{1}{2}(J_c + J_z)} + \frac{\frac{1}{4}(J_c - J_z)^2 \hat{n}_{d\overline{\beta}}\left(1 - \hat{n}_{d\beta}\right)}{\omega^- - \epsilon_q - \frac{1}{2}(J_c - J_z)} + \frac{J_c^2 \hat{n}_{d\beta} \hat{n}_{d\overline{\beta}}}{\omega^- - \epsilon_q - J_c} \right]
\end{aligned} \tag{0.87}$$

7.

$$\Delta_7^- \mathcal{H}_N = \sum_{q\beta kk'} \left(\frac{1}{2} J_c \hat{n}_d + J_z \beta S_d^z \right) c^\dagger_{q\beta} c_{k'\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_t c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{q\beta} \tag{0.88}$$

Simplification:

$$\left(\frac{1}{2} J_c \hat{n}_d + J_z \beta S_d^z \right) c^\dagger_{d\beta} c_{d\overline{\beta}} = \frac{1}{2}(J_c + J_z) c^\dagger_{d\beta} c_{d\overline{\beta}} \tag{0.89}$$

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

$$H_1 = \epsilon_d - \epsilon_q - \frac{1}{2}(J_c + J_z) \tag{0.90}$$

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

$$H_0 = \epsilon_d = H_1 + \epsilon_q + \frac{1}{2} J_z \tag{0.91}$$

$$\begin{aligned}
\Delta_7^- \mathcal{H}_N &= \frac{1}{2}(J_c + J_z) J_t \sum_{q\beta kk'} c^\dagger_{q\beta} c_{k'\beta} c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{q\beta} \frac{1}{\omega^- - H_1} \\
&= -\frac{1}{2}(J_c + J_z) J_t \sum_{q\beta kk'} \hat{n}_{q\beta} c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{k'\beta} \frac{1}{\omega^- - \epsilon_q - \frac{1}{2}(J_c + J_z)} \\
&= -\frac{1}{2}(J_c + J_z) J_t \sum_{q\beta kk'} c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{k'\beta} \frac{1}{\omega^- - \epsilon_q - \frac{1}{2}(J_c + J_z)} \\
&= -\frac{1}{2}(J_c + J_z) J_t \sum_{q\beta kk'} c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{k\beta} c_{k'\overline{\beta}} \frac{1}{\omega^- - \epsilon_q - \frac{1}{2}(J_c + J_z)}
\end{aligned} \tag{0.92}$$

8.

$$\Delta_8^- \mathcal{H}_N = \sum_{q\beta kk'} J_t c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k'\overline{\beta}} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} \left(\frac{1}{2} J_c \hat{n}_d + J_z \beta S_d^z\right) c^\dagger_{k\beta} c_{q\beta} \tag{0.93}$$

Simplification:

$$c^\dagger_{d\overline{\beta}} c_{d\beta} \left(\frac{1}{2} J_c \hat{n}_d + J_z \beta S_d^z\right) = \frac{1}{2}\left(J_c + J_z\right) c^\dagger_{d\overline{\beta}} c_{d\beta} \tag{0.94}$$

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

$$H_1 = -\epsilon_q - \frac{1}{2}\left(J_c + J_z\right) + \epsilon_d \tag{0.95}$$

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

$$H_0 = \epsilon_d = H_1 + \epsilon_q + \frac{1}{2}\left(J_c + J_z\right) \tag{0.96}$$

$$\begin{aligned}
\Delta_8^- \mathcal{H}_N &= \frac{1}{2}\left(J_c + J_z\right) J_t \sum_{q\beta kk'} c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k'\overline{\beta}} c^\dagger_{k\beta} c_{q\beta} \frac{1}{\omega^- - H_1} \\
&= \frac{1}{2}\left(J_c + J_z\right) J_t \sum_{q\beta kk'} \hat{n}_{q\beta} c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{k\beta} c_{k'\overline{\beta}} \frac{-1}{\omega^- - \epsilon_q - \frac{1}{2}\left(J_c + J_z\right)} \\
&= -\frac{1}{2}\left(J_c + J_z\right) J_t \sum_{q\beta kk'} c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{k\beta} c_{k'\overline{\beta}} \frac{1}{\omega^- - \epsilon_q - \frac{1}{2}\left(J_c + J_z\right)}
\end{aligned} \tag{0.97}$$

9.

$$\Delta_9^- \mathcal{H}_N = \sum_{q\beta kk'} J_t c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k'\overline{\beta}} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_t c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{q\beta} \tag{0.98}$$

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

$$H_1 = -\epsilon_q - \frac{1}{2}\left(J_c + J_z\right) + \epsilon_d \tag{0.99}$$

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

$$H_0 = \epsilon_d = H_1 + \epsilon_q + \frac{1}{2}\left(J_c + J_z\right) \tag{0.100}$$

$$
\begin{aligned}
\Delta_9^- \mathcal{H}_N &= \sum_{q\beta kk'} J_t^2 c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k'\overline{\beta}} c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{q\beta} \frac{1}{\omega^- - H_1} \\
&= \sum_{q\beta kk'} J_t^2 \hat{n}_{q\beta} c^\dagger_{d\overline{\beta}} c_{d\beta} c_{k'\overline{\beta}} c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} \frac{1}{\omega^- - H_1} \\
&= -\sum_{q\beta kk'} J_t^2 \hat{n}_{q\beta} \hat{n}_{d\overline{\beta}} c_{d\beta} c_{k'\overline{\beta}} c^\dagger_{d\beta} c^\dagger_{k\overline{\beta}} \frac{1}{\omega^- - H_1} \\
&= \sum_{q\beta kk'} J_t^2 \hat{n}_{q\beta} \hat{n}_{d\overline{\beta}} \left(1 - \hat{n}_{d\beta}\right) c_{k'\overline{\beta}} c^\dagger_{k\overline{\beta}} \frac{1}{\omega^- - \epsilon_q^- - \frac{1}{2}\left(J_c + J_z\right)} \\
&= -J_t^2 \sum_{q\beta kk'} c^\dagger_{k\beta} c_{k'\beta} \frac{\hat{n}_{d\beta}\left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega^- - \epsilon_q^- - \frac{1}{2}\left(J_c + J_z\right)} + J_t^2 \sum_{qk\beta} \frac{\hat{n}_{d\overline{\beta}}\left(1 - \hat{n}_{d\beta}\right)}{\omega^- - \epsilon_q^- - \frac{1}{2}\left(J_c + J_z\right)}
\end{aligned}
\tag{0.101}
$$

1.3 Scaling equations

$$\Delta\epsilon_d = \sum_q \Bigg[\frac{|V_q^0|^2}{\omega^+ - \epsilon_q + \epsilon_d} + \frac{|V_q^1|^2}{\omega^- - \epsilon_q + \epsilon_d + U - J_c} - \frac{2|V_q^0|^2}{\omega^- - \epsilon_q + \epsilon_d - \frac{1}{2}(J_c + J_z)}$$
$$+ \sum_k \left(\frac{J_t^2 + \frac{1}{4}(J_c + J_z)^2}{\omega^- - \epsilon_q - \frac{1}{2}(J_c + J_z)} + \frac{\frac{1}{4}(J_c - J_z)^2}{\omega - \epsilon_q - \frac{1}{2}(J_c - J_z)} \right) \Bigg]$$

$$\Delta U = \sum_q 2 \Bigg[\frac{|V_q^1|^2}{\omega^+ - \epsilon_q + \epsilon_d + U - \frac{1}{2}(J_c - J_z)} - \frac{|V_q^0|^2}{\omega^+ - \epsilon_q + \epsilon_d} + \frac{|V_q^0|^2}{\omega^- - \epsilon_q + \epsilon_d - \frac{1}{2}(J_c + J_z)}$$
$$- \frac{|V_q^1|^2}{\omega^- - \epsilon_q + \epsilon_d + U - J_c} + \sum_k \left(\frac{J_c^2}{\omega^- - \epsilon_q - J_c} - \frac{J_t^2 + \frac{1}{4}(J_c + J_z)^2}{\omega^- - \epsilon_q - \frac{1}{2}(J_c + J_z)} - \frac{\frac{1}{4}(J_c - J_z)^2}{\omega - \epsilon_q - \frac{1}{2}(J_c - J_z)} \right) \Bigg]$$

$$\Delta V_1 = \sum_q V_1(q) \left(\frac{\frac{1}{2}(J_c - J_z) - J_t}{\omega^+ - \epsilon_q + \epsilon_d + U - \frac{1}{2}(J_c - J_z)} - \frac{J_c}{\omega^- - \epsilon_q - J_c} \right)$$

$$\Delta V_1^* = \sum_q V_1^*(q) \left(\frac{\frac{1}{2}(J_c - J_z) - J_t}{\omega^+ - \epsilon_q - \frac{1}{2}(J_c - J_z)} - \frac{J_c}{\omega^- - \epsilon_q + \epsilon_d + U - J_c} \right)$$

$$\Delta V_0 = -\sum_q V_0(q) \frac{\frac{1}{2}(J_c + J_z) + J_t}{\omega^- - \epsilon_q - \frac{1}{2}(J_c + J_z)}$$

$$\Delta V_0^* = -\sum_q V_0(q)^* \frac{\frac{1}{2}(J_c + J_z) + J_t}{\omega^- - \epsilon_q + \epsilon_d - \frac{1}{2}(J_c + J_z)}$$

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

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

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

1.4 SU(2) invariance and Kondo 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:

$$2\Delta J_z = 2\Delta J_t = \Delta J = -\frac{1}{2}J^2 \sum_q \left(\frac{1}{\omega^+ - \epsilon_q + \frac{1}{4}J} + \frac{1}{\omega^- - \epsilon_q - \frac{1}{4}J} \right) \tag{0.102}$$

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

$$\Delta J = -\frac{1}{2}J^2 \sum_q \frac{2}{-\epsilon_q} \tag{0.103}$$

For an isotropic dispersion, we can use $\epsilon_q = D$, where D is the current(running) bandwidth. The sum can then be evaluated as

$$\sum_q = \rho(D)\Delta D \tag{0.104}$$

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. The flow equation of J becomes

$$\Delta J = J^2 \rho(D)\frac{|\Delta D|}{D} \tag{0.105}$$

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,

$$\frac{\mathrm{d}J}{\mathrm{d}\ln D} = -J^2\rho(D) \tag{0.106}$$

1.5 Particle-hole symmetry of impurity levels and Anderson model one-loop form

The terms of order J^2 in $\Delta\epsilon_d$ and ΔU already satisfy $\Delta\epsilon_d + \frac{1}{2}\Delta U = 0$. They are not relevant to the one-loop form either, because the lowest order is J. So we can ignore those terms in this discussion. The RG equation for the asymmetry factor $(\epsilon_d + \frac{1}{2}U)$ becomes (after making some obvious cancellations)

$$\Delta\epsilon_d + \frac{1}{2}\Delta U = \sum_q \left[-\frac{|V_q^0|^2}{\omega^- - \epsilon_q + \epsilon_d - \frac{1}{2}J_z} + \frac{|V_q^1|^2}{\omega^+ - \epsilon_q + \epsilon_d + U + \frac{1}{2}J_z} \right] \tag{0.107}$$

For a particle-hole symmetric model, we have $\omega^+ = \omega^- = \omega$ and $|V_q^0|^2 = |V_q^1|^2 = |V_q|^2$. Also, in the URG formalism, the hole contribution comes with an additional minus sign on the excited energy, so we need to invert that sign to compare the particle and hole terms. This involves, for the first term, taking $\epsilon_d \to -\epsilon_d$ and $J_z \to -J_z$. These give

$$\Delta\epsilon_d + \frac{1}{2}\Delta U = \sum_q |V_q|^2 \left[-\frac{1}{\omega - \epsilon_q - \epsilon_d + \frac{1}{2}J_z} + \frac{1}{\omega - \epsilon_q + \epsilon_d + U + \frac{1}{2}J_z} \right] \tag{0.108}$$

We can now use the particle-hole symmetry condition $\epsilon_d + U = -\epsilon_d$ to see that the two terms cancel and we get $\Delta\epsilon_d + \frac{1}{2}\Delta U = 0$.

In the limit of $\epsilon_d, J \gg D \gg U$, the equation for ϵ_d becomes

$$\Delta\epsilon_d = -\sum_q \frac{|V_q|^2}{\omega - \epsilon_q} \tag{0.109}$$

Under the same assumptions as previously, we get

$$\begin{aligned} \Delta\epsilon_d &= \frac{|V|^2}{D}\rho(D)|\Delta D| \\ \frac{\mathrm{d}\epsilon_d}{\mathrm{d}\ln D} &+ \frac{\Delta}{\pi} = 0 \end{aligned}$$