

1 Anderson Model URG

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

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

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_c, J_z and J_t such that the interaction can be written as

$$\begin{aligned} \mathcal{H}_I &= \frac{1}{2} J_c \hat{n}_d \sum_{k\sigma} \hat{n}_{k\sigma} + J_z \frac{\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow}}{2} \sum_{kk'} (c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow}) + J_t \sum_{kk'} [c_{d\uparrow}^\dagger c_{d\downarrow} c_{k\downarrow}^\dagger c_{k'\uparrow} + c_{d\downarrow}^\dagger c_{d\uparrow} c_{k\uparrow}^\dagger c_{k'\downarrow}] \\ &= \frac{1}{2} J_c \hat{n}_d \sum_{k\sigma} \hat{n}_{k\sigma} + 2J_z S_d^z s^z + J_t (S_d^+ s^- + S_d^- s^+) \end{aligned} \quad (0.5)$$

The spin-like operators are defined as

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

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

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

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

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

1.1 Particle sector

The renormalization in the Hamiltonian in the particle sector is

$$\begin{aligned} \Delta^+ \mathcal{H}_N = & \sum_{q\beta} \left[V_q^* c_{d\beta}^\dagger c_{q\beta} + J_z \beta S_d^z \sum_k c_{k\beta}^\dagger c_{q\beta} + J_t \sum_k c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \right] \times \frac{1}{\hat{\omega}^+ - \mathcal{H}_D^+} \\ & \times \left[V_q c_{q\beta}^\dagger c_{d\beta} + J_z \beta S_d^z \sum_k c_{q\beta}^\dagger c_{k\beta} + J_t \sum_k c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\bar{\beta}} \right] \end{aligned} \quad (0.9)$$

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 ($q\beta$).

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

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.

$$\Delta_1^+ \mathcal{H}_N = \sum_{q\beta} |V_q|^2 c_{d\beta}^\dagger c_{q\beta} \frac{1}{\hat{\omega}^+ - \mathcal{H}_D^+} c_{q\beta}^\dagger c_{d\beta} \quad (0.11)$$

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

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

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:

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

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

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

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,

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

2.

$$\Delta_2^+ \mathcal{H}_N = \sum_{q\beta k} V_q^* c_{d\beta}^+ c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_z \beta S_d^z c_{q\beta}^+ c_{k\beta} \quad (0.16)$$

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 $c_{d\beta}^\dagger$, and therefore

$$c_{d\beta}^\dagger J_z \beta S_d^z = c_{d\beta}^\dagger \frac{1}{2} (-J_z) \hat{n}_{d\bar{\beta}} \quad (0.17)$$

The expression simplifies to

$$\Delta_2^+ \mathcal{H}_N = \frac{1}{2} (J_c - J_z) \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{q\beta} \hat{n}_{d\bar{\beta}} \frac{1}{\omega^+ - \mathcal{H}_D^+} c_{q\beta}^\dagger c_{k\beta} \quad (0.18)$$

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

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

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

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

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

3.

$$\Delta_3^+ \mathcal{H}_N = \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_t c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\bar{\beta}} \quad (0.22)$$

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

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

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

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

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

4.

$$\Delta_4^+ \mathcal{H}_N = \sum_{q\beta k\sigma} J_z \beta S_d^z c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} V_q c_{q\beta}^\dagger c_{d\beta} \tag{0.26}$$

The first step is a simplification:

$$J_z \beta S_d^z c_{d\beta} = \frac{1}{2} (-J_z) \hat{n}_{d\bar{\beta}} c_{d\beta} \tag{0.27}$$

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

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

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

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

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

5.

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

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

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

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

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

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

6.

$$\Delta_6^+ \mathcal{H}_N = \sum_{k'q\beta k} J_z S_d^z \beta c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_z S_d^z \beta c_{q\beta}^\dagger c_{k'\beta} \quad (0.35)$$

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

$$\hat{d}^2 = (J_z S_d^z \beta)^2 = J_c^2 (S_d^z)^2 \quad (0.36)$$

$$\Delta_6^+ \mathcal{H}_N = \sum_{k'q\beta k} \hat{d}^2 c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} c_{q\beta}^\dagger c_{k'\beta} \quad (0.37)$$

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

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

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

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

$$\begin{aligned} \Delta_6^+ \mathcal{H}_N &= \sum_{k'q\beta k} \hat{d}^2 c_{k\beta}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{k'\beta} \frac{1}{\omega^+ - H_1} \\ &= \sum_{k'q\beta k} \hat{d}^2 (1 - \hat{n}_{q\beta}) c_{k\beta}^\dagger c_{k'\beta} \frac{1}{\omega^+ - H_0 - \epsilon_q - \beta J_z S_d^z - \frac{1}{2}J_c \hat{n}_d} \\ &= \sum_{k'q\beta k} \hat{d}^2 c_{k\beta}^\dagger c_{k'\beta} \frac{1}{\omega^+ - \epsilon_q - \beta J_z S_d^z - \frac{1}{2}J_c \hat{n}_d} \end{aligned} \quad (0.40)$$

The operator in the denominator takes the values

$$\hat{d} = \begin{cases} 0 & \hat{n}_{d\beta} = \hat{n}_{d\bar{\beta}} = 0 \\ \frac{1}{2}J_z & \hat{n}_{d\beta} = 1 - \hat{n}_{d\bar{\beta}} = 0 \\ -\frac{1}{2}J_z & 1 - \hat{n}_{d\beta} = \hat{n}_{d\bar{\beta}} = 0 \\ 0 & \hat{n}_{d\beta} = \hat{n}_{d\bar{\beta}} = 1 \end{cases} \quad (0.41)$$

Expanding in this basis gives

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

7.

$$\Delta_7^+ \mathcal{H}_N = \sum_{q\beta k k'} J_z S_d^z \beta c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_t c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\bar{\beta}} \quad (0.43)$$

The first step is a simplification:

$$J_z S_d^z \beta c_{d\bar{\beta}}^\dagger c_{d\beta} = -\frac{1}{2} J_z c_{d\bar{\beta}}^\dagger c_{d\beta} \quad (0.44)$$

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

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

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

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

$$\begin{aligned} \Delta_7^+ \mathcal{H}_N &= \sum_{q\beta k k'} -\frac{1}{2} J_z J_t c_{k\beta}^\dagger c_{q\beta} c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\bar{\beta}} \frac{1}{\omega^+ - H_1} \\ &= -\frac{1}{2} J_z J_t \sum_{q\beta k k'} (1 - \hat{n}_{q\beta}) c_{d\bar{\beta}}^\dagger c_{d\beta} c_{k\beta}^\dagger c_{k'\bar{\beta}} \frac{1}{\omega^+ - \epsilon_q - \frac{1}{2}(J_c - J_z)} \\ &= -\frac{1}{2} J_z J_t \sum_{q\beta k k'} c_{d\bar{\beta}}^\dagger c_{d\beta} c_{k\beta}^\dagger c_{k'\bar{\beta}} \frac{1}{\omega^+ - \epsilon_q - \frac{1}{2}(J_c - J_z)} \end{aligned} \quad (0.47)$$

8.

$$\Delta_8^+ \mathcal{H}_N = \sum_{q\beta k k'} J_t c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_z S_d^z \beta c_{q\beta}^\dagger c_{k'\beta} \quad (0.48)$$

The first step is a simplification:

$$c_{d\beta}^\dagger c_{d\bar{\beta}} \frac{1}{2} J_z S_d^z \beta = -\frac{1}{2} J_z c_{d\beta}^\dagger c_{d\bar{\beta}} \quad (0.49)$$

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

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

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

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

$$\begin{aligned} \Delta_8^+ \mathcal{H}_N &= -\frac{1}{2} J_z J_t \sum_{q\beta k k'} c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{k'\beta} \frac{1}{\omega^+ - \epsilon_q - \frac{1}{2} (J_c - J_z)} \\ &= -\frac{1}{2} J_z J_t \sum_{q\beta k k'} (1 - \hat{n}_{q\beta}) c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{k'\beta} \frac{1}{\omega^+ - \epsilon_q - \frac{1}{2} (J_c - J_z)} \\ &= -\frac{1}{2} J_z J_t \sum_{q\beta k k'} c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{k'\beta} \frac{1}{\omega^+ - \epsilon_q - \frac{1}{2} (J_c - J_z)} \end{aligned} \quad (0.52)$$

9.

$$\Delta_9^+ \mathcal{H}_N = \sum_{q\beta k k'} J_t c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D} J_t c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\bar{\beta}} \quad (0.53)$$

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

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

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

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

$$\begin{aligned} \Delta_9^+ \mathcal{H}_N &= \sum_{q\beta k k'} J_t^2 c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\bar{\beta}} \frac{1}{\omega^+ - \epsilon_q - \frac{1}{2} (J_c - J_z)} \\ &= \sum_{q\beta k k'} (1 - \hat{n}_{q\beta}) \hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}}) c_{k\bar{\beta}}^\dagger c_{k'\bar{\beta}} \frac{J_t^2}{\omega^+ - \epsilon_q - \frac{1}{2} (J_c - J_z)} \\ &= \sum_{q\beta k k'} c_{k\bar{\beta}}^\dagger c_{k'\bar{\beta}} \frac{J_t^2 \hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta})}{\omega^+ - \epsilon_q - \frac{1}{2} (J_c - J_z)} \end{aligned} \quad (0.56)$$

1.2 Hole sector

The renormalization in the Hamiltonian in the hole sector is

$$\begin{aligned} \Delta^- \mathcal{H}_N = \sum_{q\beta} \left[V_q c_{q\beta}^\dagger c_{d\beta} + J_z \beta S_d^z \sum_{k\sigma} c_{k\beta} c_{q\beta}^\dagger + J_t \sum_{k\sigma} c_{d\bar{\beta}}^\dagger c_{q\beta}^\dagger c_{d\beta} c_{k\bar{\beta}} \right] \times \frac{-1}{\hat{\omega}^- - \mathcal{H}_D^-} \\ \times \left[V_q^* c_{d\beta}^\dagger c_{q\beta} + J_z \beta S_d^z \sum_{k\sigma} c_{q\beta} c_{k\beta}^\dagger + J_t \sum_{k\sigma} c_{d\beta}^\dagger c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} c_{q\beta} \right] \end{aligned} \quad (0.57)$$

The propagator can be written as

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

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.

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

1.

$$\Delta_1^- \mathcal{H}_N = \sum_{q\beta} |V_q|^2 c_{q\beta}^\dagger c_{d\beta} \frac{1}{\omega^- + \mathcal{H}_D^-} c_{d\beta}^\dagger c_{q\beta} \quad (0.60)$$

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

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

Therefore,

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

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

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

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

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

2.

$$\Delta_2^- \mathcal{H}_N = \sum_{q\beta k} V_q c_{q\beta}^\dagger c_{d\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_z \beta S_d^z c_{k\beta}^\dagger c_{q\beta} \tag{0.65}$$

The first step is a simplification:

$$c_{d\beta} J_z \beta S_d^z = c_{d\beta} \frac{1}{2} J_z (1 - \hat{n}_{d\bar{\beta}}) \tag{0.66}$$

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

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

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

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

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

3.

$$\Delta_3^- \mathcal{H}_N = \sum_{q\beta k} V_q c_{q\beta}^\dagger c_{d\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_t c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \quad (0.70)$$

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

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

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

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

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

4.

$$\Delta_4^- \mathcal{H}_N = \sum_{q\beta k} \frac{1}{2} J_z \beta S_d^z c_{q\beta}^\dagger c_{k\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} V_q^* c_{d\beta}^\dagger c_{q\beta} \quad (0.74)$$

There is a simplification:

$$\frac{1}{2} J_z \beta S_d^z c_{d\beta}^\dagger = \frac{1}{2} J_z (1 - \hat{n}_{d\bar{\beta}}) c_{d\beta}^\dagger \quad (0.75)$$

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

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

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

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

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

5.

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

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

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

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

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

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

6.

$$\Delta_6^- \mathcal{H}_N = \sum_{q\beta k k'} J_z \beta S_d^z c_{q\beta}^\dagger c_{k'\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_z \beta S_d^z c_{k\beta}^\dagger c_{q\beta} \tag{0.83}$$

We again label

$$(J_z \beta S_d^z)^2 = \hat{d}^2 \tag{0.84}$$

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

$$H_1 = H_{\text{imp}} - \epsilon_q - \frac{1}{2} J_c \hat{n}_d - J_z \beta S_d^z \tag{0.85}$$

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

$$H_0 = H_{\text{imp}} = H_1 + \epsilon_q + \frac{1}{2}J_c\hat{n}_d + J_z\beta S_d^z \quad (0.86)$$

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

7.

$$\Delta_7^- \mathcal{H}_N = \sum_{q\beta k k'} J_z\beta S_d^z c_{q\beta}^\dagger c_{k'\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D} J_t c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \quad (0.88)$$

Simplification:

$$J_z\beta S_d^z c_{d\beta}^\dagger c_{d\bar{\beta}} = \frac{1}{2}J_z c_{d\beta}^\dagger c_{d\bar{\beta}} \quad (0.89)$$

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

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

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

$$H_0 = \epsilon_d = H_1 + \epsilon_q + \frac{1}{2}J_z \quad (0.91)$$

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

8.

$$\Delta_8^- \mathcal{H}_N = \sum_{q\beta kk'} J_t c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\bar{\beta}} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_z \beta S_d^z c_{k\beta}^\dagger c_{q\beta} \quad (0.93)$$

Simplification:

$$c_{d\bar{\beta}}^\dagger c_{d\beta} J_z \beta S_d^z = \frac{1}{2} J_z c_{d\bar{\beta}}^\dagger c_{d\beta} \quad (0.94)$$

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

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

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

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

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

9.

$$\Delta_9^- \mathcal{H}_N = \sum_{q\beta kk'} J_t c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\bar{\beta}} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_t c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\beta}^\dagger c_{q\beta} \quad (0.98)$$

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

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

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

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

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

1.3 Scaling equations

$$\begin{aligned}
\Delta \epsilon_d &= \sum_q \left[\frac{|V_q^0|^2}{\omega^+ - \epsilon_q + \epsilon_d} + \frac{|V_q^1|^2}{\omega^- - \epsilon_q + \epsilon_d + U - J_c} - \frac{2|V_q^0|^2}{\omega^- - \epsilon_q + \epsilon_d - \frac{1}{2}(J_c + J_z)} \right. \\
&\quad \left. + \sum_k \left(\frac{J_t^2 + \frac{1}{4}J_z^2}{\omega^- - \epsilon_q - \frac{1}{2}(J_c + J_z)} + \frac{\frac{1}{4}J_z^2}{\omega^- - \epsilon_q - \frac{1}{2}(J_c - J_z)} \right) \right] \\
\Delta U &= \sum_q 2 \left[\frac{|V_q^1|^2}{\omega^+ - \epsilon_q + \epsilon_d + U - \frac{1}{2}(J_c - J_z)} - \frac{|V_q^0|^2}{\omega^+ - \epsilon_q + \epsilon_d} + \frac{|V_q^0|^2}{\omega^- - \epsilon_q + \epsilon_d - \frac{1}{2}(J_c + J_z)} \right. \\
&\quad \left. - \frac{|V_q^1|^2}{\omega^- - \epsilon_q + \epsilon_d + U - J_c} - \sum_k \left(\frac{J_t^2 + \frac{1}{4}J_z^2}{\omega^- - \epsilon_q - \frac{1}{2}(J_c + J_z)} + \frac{\frac{1}{4}J_z^2}{\omega^- - \epsilon_q - \frac{1}{2}(J_c - J_z)} \right) \right] \\
\Delta V_1 &= - \sum_q V_1(q) \left(\frac{\frac{1}{2}J_z + J_t}{\omega^+ - \epsilon_q + \epsilon_d + U - \frac{1}{2}(J_c - J_z)} \right) \\
\Delta V_1^* &= - \sum_q V_1^*(q) \left(\frac{\frac{1}{2}J_z + J_t}{\omega^+ - \epsilon_q - \frac{1}{2}(J_c - J_z)} \right) \\
\Delta V_0 &= - \sum_q V_0(q) \frac{\frac{1}{2}J_z + J_t}{\omega^- - \epsilon_q - \frac{1}{2}(J_c + J_z)} \\
\Delta V_0^* &= - \sum_q V_0(q)^* \frac{\frac{1}{2}J_z + J_t}{\omega^- - \epsilon_q + \epsilon_d - \frac{1}{2}(J_c + J_z)} \\
\Delta J_c &= -J_t^2 \sum_q \left(\frac{1}{\omega^+ - \epsilon_q - \frac{1}{2}(J_c - J_z)} - \frac{1}{\omega^- - \epsilon_q - \frac{1}{2}(J_c + J_z)} \right) \\
\Delta J_z &= -J_t^2 \sum_q \left(\frac{1}{\omega^+ - \epsilon_q - \frac{1}{2}(J_c - J_z)} + \frac{1}{\omega^- - \epsilon_q - \frac{1}{2}(J_c + J_z)} \right) \\
\Delta J_t &= -J_z J_t \sum_q \left(\frac{1}{\omega^+ - \epsilon_q - \frac{1}{2}(J_c - J_z)} + \frac{1}{\omega^- - \epsilon_q - \frac{1}{2}(J_c + J_z)} \right)
\end{aligned}$$