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

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

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

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

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

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

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

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

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:

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

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

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

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.

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

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

$$c_{d\beta}^\dagger J_z \beta S_d^z = c_{d\beta}^\dagger \frac{1}{2} \left(-J_z\right) \hat{n}_{d\overline{\beta}} \tag{0.17}$$

The expression simplifies to

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

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

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

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

3.

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

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

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

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

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:

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

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

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

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

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

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

5.

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

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

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

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

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

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

6.

$$\Delta_6^+\mathcal{H}_N = \sum_{k'q\beta k} J_z S_d^z \beta c^\dagger_{k\beta} c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_z S_d^z \beta c^\dagger_{q\beta} c_{k'\beta} \tag{0.35}$$

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

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

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

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

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

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

The operator in the denominator takes the values

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

Expanding in this basis gives

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

7.

$$\Delta_7^+\mathcal{H}_N = \sum_{q\beta kk'} J_zS_d^z\beta c^\dagger_{k\beta}c_{q\beta}\frac{1}{\omega^+-\mathcal{H}_D^+}J_tc^\dagger_{d\overline{\beta}}c_{d\beta}c^\dagger_{q\beta}c_{k'\overline{\beta}} \tag{0.43}$$

The first step is a simplification:

$$J_zS_d^z\beta c^\dagger_{d\overline{\beta}}c_{d\beta} = -\frac{1}{2}J_zc^\dagger_{d\overline{\beta}}c_{d\beta} \tag{0.44}$$

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

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

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

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

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

8.

$$\Delta_8^+\mathcal{H}_N = \sum_{q\beta kk'} J_tc^\dagger_{d\beta}c_{d\overline{\beta}}c^\dagger_{k\overline{\beta}}c_{q\beta}\frac{1}{\omega^+-\mathcal{H}_D^+}J_zS_d^z\beta c^\dagger_{q\beta}c_{k'\beta} \tag{0.48}$$

The first step is a simplification:

$$c^\dagger_{d\beta}c_{d\overline{\beta}}\frac{1}{2}J_zS_d^z\beta = -\frac{1}{2}J_zc^\dagger_{d\beta}c_{d\overline{\beta}} \tag{0.49}$$

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

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

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

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

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

9.

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

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

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

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

1.2 Hole sector

The renormalization in the Hamiltonian in the hole sector is

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

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.

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

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.

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

2.

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

The first step is a simplification:

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

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

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

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

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

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

3.

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

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

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

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

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

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

4.

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

There is a simplification:

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

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

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

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

5.

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

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

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

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

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

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

6.

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

We again label

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

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

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

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

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

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

7.

$$\Delta_7^- \mathcal{H}_N = \sum_{q\beta kk'} J_z \beta S_d^z c^\dagger_{q\beta} c_{k'\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_t c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{q\beta} \tag{0.88}$$

Simplification:

$$J_z \beta S_d^z c^\dagger_{d\beta} c_{d\overline{\beta}} = \frac{1}{2} J_z c^\dagger_{d\beta} c_{d\overline{\beta}} \tag{0.89}$$

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

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

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

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

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

8.

$$\Delta_8^- \mathcal{H}_N = \sum_{q\beta kk'} J_t c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k'\overline{\beta}} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_z \beta S_d^z c^\dagger_{k\beta} c_{q\beta} \tag{0.93}$$

Simplification:

$$c^\dagger_{d\overline{\beta}} c_{d\beta} J_z \beta S_d^z = \frac{1}{2} J_z c^\dagger_{d\overline{\beta}} c_{d\beta} \tag{0.94}$$

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

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

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

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

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

To make the conduction bath particle-hole symmetric, we can write the following term in a particle-hole symmetric fashion:

$$\frac{1}{2}J_c \sum_{k\sigma\beta} \hat{n}_{d\beta}\hat{n}_{k\sigma'} = \frac{1}{2}J_c \sum_{k\sigma\beta} \left(\hat{n}_{d\beta} - \frac{1}{2} \right) \left(\hat{n}_{k\sigma'} - \frac{1}{2} \right) + \frac{1}{4}J_c \sum_{k\sigma\beta} \hat{n}_{d\beta} + \frac{1}{4}J_c \sum_{k\sigma\beta} \hat{n}_{k\sigma} \tag{0.102}$$

The last term can be combined with a chemical potential term:

$$\frac{1}{4}J_c \sum_{k\sigma\beta} \hat{n}_{k\sigma} - \mu \sum_{k\sigma} \hat{n}_{k\sigma} = -\left(\mu - \frac{1}{2}J_c \right) \sum_{k\sigma} \hat{n}_{k\sigma} \tag{0.103}$$

to define an effective chemical potential $\mu_{\text{eff}} = \mu - \frac{1}{2}J_c$. If we set the chemical potential $\mu = \frac{1}{2}J_c$, this term disappears from the Hamiltonian. Shifting the chemical potential to $\mu = \frac{1}{2}J_c$ is equivalent to replacing $\epsilon_q \to \epsilon_q - \frac{1}{2}J_c$.

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

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

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

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

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

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

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

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

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

1.4 Marginality of J_c

The second fraction in ΔJ_c is in the hole sector, so we need to change $J_z \to -J_z$:

$$\Delta J_c = -J_t^2 \sum_q \left(\frac{1}{\omega^+ - \epsilon_q + \frac{1}{2}J_z} - \frac{1}{\omega^- - \epsilon_q + \frac{1}{2}J_z} \right) = 0 \tag{0.104}$$

This ensures that if there is no off-diagonal term of the form $\hat{n}_d \sum_{kk'\sigma} c^\dagger_{k\sigma} c_{k'\sigma}$ in the bare Hamiltonian, it will not be generated along the flow.

1.5 Particle-hole symmetry

The particle-hole asymmetry parameter RG equation is

$$\Delta\left(\epsilon_d+\frac{1}{2}U\right)=\sum_q\left[\frac{|V_q^1|^2}{\omega^+-\epsilon_q+\epsilon_d+U+\frac{1}{2}J_z}-\frac{|V_q^0|^2}{\omega^--\epsilon_q+\epsilon_d-\frac{1}{2}J_z}\right] \tag{0.105}$$

Again making the change $\epsilon_d, J_z \to -\epsilon_d, -J_z$ for the hole term and setting $|V^1|^2=|V^0|^2$ for a particle-hole symmetric Hamiltonian, we get

$$\Delta\left(\epsilon_d+\frac{1}{2}U\right)=\sum_q|V_q|^2\left[\frac{1}{\omega^+-\epsilon_q+\epsilon_d+U+\frac{1}{2}J_z}-\frac{1}{\omega^--\epsilon_q-\epsilon_d+\frac{1}{2}J_z}\right] \tag{0.106}$$

This becomes zero when $\epsilon_d=-\epsilon_d-U$.

1.6 Hermiticity

The equations in consideration are those of ΔV_1 and ΔV_1^*. The superscript 1 signifies that $d\overline{\beta}$ is filled. For the moment, we label the ω^+ in ΔV_1^* as ω^{+^*} - the quantum fluctuation energy for the process $\hat{n}_{d\overline{\beta}}c^\dagger_{d\beta}c_k$ - to distinguish it from the ω^+ that characterizes the process $\hat{n}_{d\overline{\beta}}c^\dagger_k c_{d\beta}$. In other words, ω^+ is the fluctuation energy scale for the singly-occupied state, while ω^{+^*} is the fluctuation energy scale for the doubly-occupied state. The difference between the two scales is ϵ_d+U, so we can write $\omega^{+^*}=\omega^++\epsilon_d+U$. Assuming $V_1=V_1^*$ in the bare model, the two RG equations now becomes

$$\Delta V_1=-\sum_q V_1(q)\left(\frac{\frac{1}{2}J_z+J_t}{\omega^+-\epsilon_q+\epsilon_d+U+\frac{1}{2}J_z}\right)=\Delta V_1^* \tag{0.107}$$

Similarly, if we take the RG equations for ΔV_0 and ΔV_0^*, the two quantum fluctuation scales ω^- and ω^{-^*} correspond to those of the singly-occupied and empty states respectively. Since the difference between these states is ϵ_d, we can write $\omega^- - \omega^{-^*}=\epsilon_d$.

$$\Delta V_0=-\sum_q V_0(q)\frac{\frac{1}{2}J_z+J_t}{\omega^- * -\epsilon_q+\epsilon_d-\frac{1}{2}J_z}=\Delta V_0^* \tag{0.108}$$

1.7 Scaling equations that satisfy all checks (with appropriate shifts and sign changes)

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

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

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

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

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

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