# 1 Without higher order scattering

$$\mathcal{H}_N = H_{N-1} + \epsilon_q \hat{n}_{q\beta} + V_q c^\dagger_{q\beta} c_{d\beta} + \text{h.c.} + \epsilon_d \sum_\sigma \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \tag{0.1}$$

where $H_{N-1} \equiv \sum_{k<\Lambda_N,\sigma} \left(\epsilon_k \hat{n}_{k\sigma} + V_k c^\dagger_{k\sigma} c_{d\sigma} + \text{h.c.}\right)$ features the electrons below the shell. *In the absence of higher order scattering, the only renormalization is in $\epsilon_d$ and $U$, so we do not need to split the $V_q$ into $V_q^1 \hat{n}_{d\overline{\beta}} + V_q^0 \left(1 - \hat{n}_{d\overline{\beta}}\right)$. These will appear at third order in $V_q$.*

## 1.1 Particle sector

The excited states consist of particles on the higher band edge ($+D$).

$$\Delta^+ \mathcal{H}_N = \sum_{q\beta} \eta_{q\beta} c^\dagger_{q\beta} \text{Tr}\left[\mathcal{H}_N c_{q\beta}\right] \tag{0.2}$$

where[1] $c^\dagger_{q\beta} \text{Tr}\left[\mathcal{H}_N c_{q\beta}\right]$ is the part of $\mathcal{H}_N$ that scatters from $|\hat{n}_{q\beta} = 0\rangle$ to $|\hat{n}_{q\beta} = 1\rangle$:

$$c^\dagger_{q\beta} \text{Tr}\left[\mathcal{H}_N c_{q\beta}\right] = V_q c^\dagger_{q\beta} c_{d\beta} \tag{0.3}$$

and

$$\eta_{q\beta} = \text{Tr}\left[c^\dagger_{q\beta} \mathcal{H}_N\right] \frac{1}{\hat{\omega} - \mathcal{H}_N^{D,1}} = V_q^* c^\dagger_{d\beta} c_{q\beta} \frac{1}{\hat{\omega} - \left[H^C_{N-1} + \epsilon_q^+ + H_{imp}\right] \hat{n}_{q\beta}} \tag{0.4}$$

$\epsilon_q^+$ is the energy of a particle excitation in the momentum $q$. $\mathcal{H}_N^{D,1} \equiv \text{Tr}\left(\mathcal{H}_N \hat{n}_{q\beta}\right) \hat{n}_{q\beta}$ is the diagonal part of $\mathcal{H}_N$ in the particle sector, $H^C_{N-1}$ is the remaining conduction band part of the Hamiltonian and $H_{imp}$ is the impurity-diagonal part ($\equiv \epsilon_d \sum_\sigma \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow}$). Putting it all together,

$$\Delta^+ \mathcal{H}_N = \sum_{q\beta} V_q^* c^\dagger_{d\beta} c_{q\beta} \frac{1}{\hat{\omega} - \left[H^C_{N-1} + \epsilon_q^+ + H_{imp}\right] \hat{n}_{q\beta}} V_q c^\dagger_{q\beta} c_{d\beta} \tag{0.5}$$

Since the internal propagator is preceded by a $c^\dagger_{q\beta} c_{d\beta}$, we can set $\hat{n}_{q\beta} = 1$ and $\hat{n}_{d\beta} = 0$ inside the propagator. $H_{imp}$ then becomes $\epsilon_d \hat{n}_{d\overline{\beta}}$.

$$\Delta^+ \mathcal{H}_N = \sum_{q\beta} V_q^* c^\dagger_{d\beta} c_{q\beta} \frac{1}{\hat{\omega} - \left[H^C_{N-1} + \epsilon_q^+ + \epsilon_d \hat{n}_{d\overline{\beta}}\right]} V_q c^\dagger_{q\beta} c_{d\beta} \tag{0.6}$$

Since the propagator is devoid of any operator in $q\beta$ or $d\beta$ now, it can be pushed to the end:

$$\begin{aligned} \Delta^+ \mathcal{H}_N &= \sum_{q\beta} |V_q|^2 c^\dagger_{d\beta} c_{q\beta} c^\dagger_{q\beta} c_{d\beta} \frac{1}{\hat{\omega} - \left[H^C_{N-1} + \epsilon_q^+ + \epsilon_d \hat{n}_{d\overline{\beta}}\right]} \\ &= \sum_{q\beta} |V_q|^2 \hat{n}_{d\beta} \left(1 - \hat{n}_{q\beta}\right) \frac{1}{\hat{\omega} - \left[H^C_{N-1} + \epsilon_d \hat{n}_{d\overline{\beta}}\right] - \epsilon_q^+} \end{aligned} \tag{0.7}$$

[1] all traces in this subsection are partial in $q\beta$

The $1-\hat{n}_{q\beta}$ ensures that the state we act on has no excited state $q\beta$, so it is a ground state. Similarly, the $\hat{n}_{d\beta}$ ensures we need to have $\hat{n}_{d\beta}=1$ in that state. We now add and subtract a $\epsilon_d\hat{n}_{d\beta}+U\hat{n}_{d\beta}\hat{n}_{d\overline{\beta}}=\epsilon_d+U\hat{n}_{d\overline{\beta}}$ in the propagator:

$$\Delta^+\mathcal{H}_N=\sum_{q\beta}|V_q|^2\hat{n}_{d\beta}\left(1-\hat{n}_{q\beta}\right)\frac{1}{\hat{\omega}-\left[H^C_{N-1}+\epsilon_d\hat{n}_{d\overline{\beta}}+\epsilon_d\hat{n}_{d\beta}+U\hat{n}_{d\beta}\hat{n}_{d\overline{\beta}}\right]-\epsilon^+_q+\epsilon_d+U\hat{n}_{d\overline{\beta}}} \tag{0.8}$$

Note that

$$H^G\equiv H^C_{N-1}+\epsilon_d\hat{n}_{d\overline{\beta}}+\epsilon_d\hat{n}_{d\beta}+U\hat{n}_{d\beta}\hat{n}_{d\overline{\beta}}=H^C_{N-1}+H_{imp} \tag{0.9}$$

is the Hamiltonian consisting of the remaining conduction band electrons and the impurity, so it gives the energy of the ground state upon which we create the excitations to the band edges.

$$\Delta^+\mathcal{H}_N=\sum_{q\beta}|V_q|^2\hat{n}_{d\beta}\left(1-\hat{n}_{q\beta}\right)\frac{1}{\hat{\omega}-H^G-\epsilon^+_q+\epsilon_d+U\hat{n}_{d\overline{\beta}}} \tag{0.10}$$

*If we measure the quantum fluctuation energy scale relative to the ground state energy $H^G$, we can set $H^G$ to* 0. A further simplification is made when we replace $\hat{\omega}$ by its eigenvalue $\omega$:

$$\Delta^+\mathcal{H}_N=\sum_{q\beta}|V_q|^2\hat{n}_{d\beta}\left(1-\hat{n}_{q\beta}\right)\frac{1}{\omega-\epsilon^+_q+\epsilon_d+U\hat{n}_{d\overline{\beta}}} \tag{0.11}$$

*Assuming there are no excited states on the band edges to begin with,* we can set $\hat{n}_{q\beta}=0$.

$$\Delta^+\mathcal{H}_N=\sum_{q\beta}\hat{n}_{d\beta}|V_q|^2\frac{1}{\omega-\epsilon^+_q+\epsilon_d+U\hat{n}_{d\overline{\beta}}} \tag{0.12}$$

To lift the $\hat{n}_{d\overline{\beta}}$ from the denominator into the numerator, we can expand the propagator in the basis of $\hat{n}_{d\overline{\beta}}$:

$$\begin{aligned}\frac{1}{\omega-\epsilon^+_q+\epsilon_d+U\hat{n}_{d\overline{\beta}}}&=\frac{\hat{n}_{d\overline{\beta}}}{\omega-\epsilon^+_q+\epsilon_d+U}+\frac{1-\hat{n}_{d\overline{\beta}}}{\omega-\epsilon^+_q+\epsilon_d}\\&=\hat{n}_{d\overline{\beta}}\left(\frac{1}{\omega-\epsilon^+_q+\epsilon_d+U}-\frac{1}{\omega-\epsilon^+_q+\epsilon_d}\right)+\frac{1}{\omega-\epsilon^+_q+\epsilon_d}\end{aligned} \tag{0.13}$$

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

$$\begin{aligned}\Delta^+\mathcal{H}_N&=\sum_{q\beta}|V_q|^2\hat{n}_{d\beta}\left[\frac{1}{\omega-\epsilon^+_q+\epsilon_d}+\hat{n}_{d\overline{\beta}}\left(\frac{1}{\omega-\epsilon^+_q+\epsilon_d+U}-\frac{1}{\omega-\epsilon^+_q+\epsilon_d}\right)\right]\\&=\sum_\beta\hat{n}_{d\beta}\sum_q|V_q|^2\frac{1}{\omega-\epsilon^+_q+\epsilon_d}+\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\sum_q 2|V_q|^2\left(\frac{1}{\omega-\epsilon^+_q+\epsilon_d+U}-\frac{1}{\omega-\epsilon^+_q+\epsilon_d}\right)\end{aligned} \tag{0.14}$$

There I used $\sum_\beta \hat{n}_{d\beta}\hat{n}_{d\overline{\beta}} = 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}$. Comparing with the bare impurity Hamiltonian we get the following scaling equations for the particle sector:

$$\begin{aligned}\Delta^+\epsilon_d &= \sum_q |V_q|^2 \frac{1}{\omega - \epsilon_q^+ + \epsilon_d} \\ \Delta^+ U &= \sum_q 2|V_q|^2 \left(\frac{1}{\omega - \epsilon_q^+ + \epsilon_d + U} - \frac{1}{\omega - \epsilon_q^+ + \epsilon_d}\right)\end{aligned} \tag{0.15}$$

## 1.2 Hole sector

The excited states consist of holes on the lower band edge ($-D$).

$$\Delta^- \mathcal{H}_N = \sum_{q\beta} c^\dagger_{q\beta} \text{Tr}\left[\mathcal{H}_N c_{q\beta}\right] \eta_{q\beta} \tag{0.16}$$

where[2] and

$$\eta_{q\beta} = \frac{1}{\hat{\omega} - \mathcal{H}_N^{D,0}} \text{Tr}\left[c^\dagger_{q\beta}\mathcal{H}_N\right] = V_q^* c^\dagger_{d\beta} c_{q\beta} \frac{1}{\hat{\omega} - \left[H^C_{N-1} + H_{imp}\right]\left(1 - \hat{n}_{q\beta}\right)} \tag{0.17}$$

$\mathcal{H}_N^{D,0} \equiv \text{Tr}\left(\mathcal{H}_N\left(1 - \hat{n}_{q\beta}\right)\right)\left(1 - \hat{n}_{q\beta}\right)$ is the diagonal part of $\mathcal{H}_N$ in the hole sector, $H^C_{N-1}$ is the remaining conduction band part of the Hamiltonian and $H_{imp}$ is the impurity-diagonal part ($\equiv \epsilon_d \sum_\sigma \hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}$). Putting it all together,

$$\Delta^- \mathcal{H}_N = \sum_{q\beta} V_q c^\dagger_{q\beta} c_{d\beta} \frac{1}{\hat{\omega} - \left[H^C_{N-1} + H_{imp}\right]\left(1 - \hat{n}_{q\beta}\right)} V_q^* c^\dagger_{d\beta} c_{q\beta} \tag{0.18}$$

Since the internal propagator is preceded by a $c^\dagger_{d\beta}c_{q\beta}$, we can set $\hat{n}_{q\beta} = 0$ and $\hat{n}_{d\beta} = 1$ inside the propagator. $H_{imp}$ then becomes $\epsilon_d + (\epsilon_d + U)\,\hat{n}_{d\overline{\beta}}$.

$$\Delta^- \mathcal{H}_N = \sum_{q\beta} V_q c^\dagger_{q\beta} c_{d\beta} \frac{1}{\hat{\omega} - \left[H^C_{N-1} + \epsilon_d + (\epsilon_d + U)\,\hat{n}_{d\overline{\beta}}\right]} V_q^* c^\dagger_{d\beta} c_{q\beta} \tag{0.19}$$

Since the propagator is devoid of any operator in $q\beta$ or $d\beta$ now, it can be pushed to the end:

$$\begin{aligned}\Delta^- \mathcal{H}_N &= \sum_{q\beta} V_q c^\dagger_{q\beta} c_{d\beta} V_q^* c^\dagger_{d\beta} c_{q\beta} \frac{1}{\hat{\omega} - \left[H^C_{N-1} + \epsilon_d + (\epsilon_d + U)\,\hat{n}_{d\overline{\beta}}\right]} \\ &= \sum_{q\beta} |V_q|^2 \hat{n}_{q\beta}\left(1 - \hat{n}_{d\beta}\right) \frac{1}{\hat{\omega} - \left[H^C_{N-1} + \epsilon_d \hat{n}_{d\overline{\beta}}\right] - \epsilon_d - U\hat{n}_{d\overline{\beta}}}\end{aligned} \tag{0.20}$$

[2] all traces in this subsection are partial in $q\beta$

The $\hat{n}_{q\beta}$ ensures that the state we act on must have a state on the lower band edge at $-D$. Similarly, the $1-\hat{n}_{d\beta}$ ensures we need to have $\hat{n}_{d\beta}=0$ in that state. We can hence subtract a $\epsilon_d\hat{n}_{d\beta}+U\hat{n}_{d\beta}\hat{n}_{d\overline{\beta}}=0$ in the propagator:

$$\Delta^{-}\mathcal{H}_N=\sum_{q\beta}|V_q|^2\hat{n}_{q\beta}\left(1-\hat{n}_{d\beta}\right)\frac{1}{\hat{\omega}-\left[H^C_{N-1}+\epsilon_d\hat{n}_{d\overline{\beta}}+\epsilon_d\hat{n}_{d\beta}+U\hat{n}_{d\beta}\hat{n}_{d\overline{\beta}}\right]-\epsilon_d-U\hat{n}_{d\overline{\beta}}} \tag{0.21}$$

In order to convert the term in [ ] into the ground state energy $H^G$, we need to also add the energy of the state $-D$ which is of course a part of the ground state (it is far inside the Fermi surface and hence most likely to be filled) but is not a part of $H^C_{N-1}$ (because we are reducing the bandwidth and the state at $-D$ has just gone out of the bandwidth). Adding and subtracting $\epsilon_q\hat{n}_{q\beta}=\epsilon_q^-$ gives

$$\begin{aligned}\Delta^{-}\mathcal{H}_N&=\sum_{q\beta}|V_q|^2\hat{n}_{q\beta}\left(1-\hat{n}_{d\beta}\right)\frac{1}{\hat{\omega}-\left[H^C_{N-1}+\epsilon_q^-\hat{n}_{q\beta}+H_{imp}\right]+\epsilon_q^--\epsilon_d-U\hat{n}_{d\overline{\beta}}}\\&=\sum_{q\beta}|V_q|^2\hat{n}_{q\beta}\left(1-\hat{n}_{d\beta}\right)\frac{1}{\hat{\omega}-H^G+\epsilon_q^--\epsilon_d-U\hat{n}_{d\overline{\beta}}}\end{aligned} \tag{0.22}$$

Doing similar simplifications as in the previous section ($\hat{\omega}-H^G=\omega,\hat{n}_{q\beta}=1$) gives

$$\begin{aligned}\Delta^{-}\mathcal{H}_N&=\sum_{q\beta}|V_q|^2\left(1-\hat{n}_{d\beta}\right)\frac{1}{\omega+\epsilon_q^--\epsilon_d-U\hat{n}_{d\overline{\beta}}}\\&=\sum_{q\beta}|V_q|^2\left(1-\hat{n}_{d\beta}\right)\left[\hat{n}_{d\overline{\beta}}\left(\frac{1}{\omega+\epsilon_q^--\epsilon_d-U}-\frac{1}{\omega+\epsilon_q^--\epsilon_d}\right)+\frac{1}{\omega+\epsilon_q^--\epsilon_d}\right]\\&=\sum_{\beta}\hat{n}_{d\beta}\sum_q|V_q|^2\left(\frac{1}{\omega+\epsilon_q^--\epsilon_d-U}-\frac{2}{\omega+\epsilon_q^--\epsilon_d}\right)\\&\quad+\sum_{\beta}\hat{n}_{d\beta}\hat{n}_{d\overline{\beta}}\sum_q2|V_q|^2\left(\frac{1}{\omega+\epsilon_q^--\epsilon_d}-\frac{1}{\omega+\epsilon_q^--\epsilon_d-U}\right)\end{aligned} \tag{0.23}$$

We get the following scaling equations for the hole sector:

$$\begin{aligned}\Delta^{-}\epsilon_d&=\sum_q|V_q|^2\left(\frac{1}{\omega+\epsilon_q^--\epsilon_d-U}-\frac{2}{\omega+\epsilon_q^--\epsilon_d}\right)\\\Delta^{-}U&=\sum_q2|V_q|^2\left(\frac{1}{\omega+\epsilon_q^--\epsilon_d}-\frac{1}{\omega+\epsilon_q^--\epsilon_d-U}\right)\end{aligned} \tag{0.24}$$

### 1.3 Scaling equations

Combining the two sectors, the scaling equations become

$$\begin{aligned}\Delta\epsilon_d &= \sum_q |V_q|^2\left(\frac{1}{\omega-\epsilon_q^+ +\epsilon_d}+\frac{1}{\omega+\epsilon_q^- -\epsilon_d-U}-\frac{2}{\omega+\epsilon_q^- -\epsilon_d}\right)\\ \Delta U &= \sum_q 2|V_q|^2\left(\frac{1}{\omega-\epsilon_q^+ +\epsilon_d+U}-\frac{1}{\omega-\epsilon_q^+ +\epsilon_d}+\frac{1}{\omega+\epsilon_q^- -\epsilon_d}-\frac{1}{\omega+\epsilon_q^- -\epsilon_d-U}\right)\end{aligned} \tag{0.25}$$

### 1.4 Particle-hole symmetric case

For $U=-2\epsilon_d$ (and setting $\epsilon_q^+=-\epsilon_q^-$), the equations become

$$\begin{aligned}\Delta\epsilon_d &= \sum_q |V_q|^2\left(\frac{1}{\omega-\epsilon_q^+ +\epsilon_d}+\frac{1}{\omega-\epsilon_q^+ +\epsilon_d}-\frac{2}{\omega-\epsilon_q^+ -\epsilon_d}\right)\\ &= \sum_q |V_q|^2\left(\frac{2}{\omega-\epsilon_q^+ +\epsilon_d}-\frac{2}{\omega-\epsilon_q^+ -\epsilon_d}\right)\\ \frac{1}{2}\Delta U &= \sum_q |V_q|^2\left(\frac{1}{\omega-\epsilon_q^+ -\epsilon_d}-\frac{1}{\omega-\epsilon_q^+ +\epsilon_d}+\frac{1}{\omega-\epsilon_q^+ -\epsilon_d}-\frac{1}{\omega-\epsilon_q^+ +\epsilon_d}\right)\\ &= \sum_q |V_q|^2\left(\frac{2}{\omega-\epsilon_q^+ -\epsilon_d}-\frac{2}{\omega-\epsilon_q^+ +\epsilon_d}\right)\end{aligned}$$

$$\implies \Delta\epsilon_d+\frac{1}{2}\Delta U = 0$$

*The particle-hole symmetry is maintained for all $\omega$.*

### 1.5 Matching poor man's scaling

*Assuming a spherical shell ($\epsilon_q^+=D, \epsilon_q^-=-D$) and momentum-independent scattering ($\sum_q |V_q|^2=|V|^2\rho|\delta D|=|\delta D|\frac{\Delta}{\pi}$) and setting $\omega=0$,*

$$\begin{aligned}\delta\epsilon_d &= |\delta D|\frac{\Delta}{\pi}\left(\frac{1}{-D+\epsilon_d}+\frac{1}{-D-\epsilon_d-U}-\frac{2}{-D-\epsilon_d}\right)\\ &= |\delta D|\frac{\Delta}{\pi}\left(\frac{2}{D+\epsilon_d}-\frac{1}{D-\epsilon_d}-\frac{1}{D+\epsilon_d+U}\right)\\ \delta U &= |\delta D|\frac{2\Delta}{\pi}\left(\frac{1}{-D+\epsilon_d+U}-\frac{1}{-D+\epsilon_d}+\frac{1}{-D-\epsilon_d}-\frac{1}{-D-\epsilon_d-U}\right)\\ &= |\delta D|\frac{2\Delta}{\pi}\left(\frac{1}{D-\epsilon_d}-\frac{1}{D-\epsilon_d-U}-\frac{1}{D+\epsilon_d}+\frac{1}{D+\epsilon_d+U}\right)\end{aligned} \tag{0.26}$$

These are identical to equation set 3.61 in Hewson.

## 2 With higher order scattering

$$\mathcal{H} = \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{k\sigma} \left( V_k c^\dagger_{k\sigma} c_{d\sigma} + h.c. \right) + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \sum_{\substack{kk' \\ \sigma\sigma'}} V_2 c^\dagger_{d\sigma'} c^\dagger_{k\sigma} c_{d\sigma} c_{k'\sigma'} \tag{0.27}$$

Such an interaction allows both spin-flip ($d\sigma \to d\overline{\sigma}$) as well as spin-preserving ($d\sigma \to d\sigma$) scattering.

$$\begin{aligned} \mathcal{H}_N = H_{N-1} + H_{\text{imp}} + \left( \epsilon_q + V_2 \hat{n}_{d\beta} \right) \hat{n}_{q\beta} + V_q c^\dagger_{q\beta} c_{d\beta} + \text{h.c.} \\ + \sum_{k\sigma} V_2 \left( c^\dagger_{q\beta} c^\dagger_{d\sigma} c_{k\sigma} c_{d\beta} + c^\dagger_{d\beta} c^\dagger_{k\sigma} c_{d\sigma} c_{q\beta} \right) \end{aligned} \tag{0.28}$$

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

$$\mathcal{H}_I = \sum_{k,q,\sigma_i} u c^\dagger_{k\sigma_1} c^\dagger_{d\sigma_2} c_{q\sigma_3} c_{d\sigma_4} \delta_{(\sigma_1+\sigma_2=\sigma_3+\sigma_4)} \tag{0.29}$$

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

$$\mathcal{H}_I = \underbrace{\sum_{k,q,\sigma,\sigma'} u_1 c^\dagger_{k\sigma} c^\dagger_{d\sigma'} c_{q\sigma} c_{d\sigma'}}_{\text{spin-preserving scattering}} + \overbrace{\sum_{k,q,\sigma} u_2 c^\dagger_{k\sigma} c^\dagger_{d\overline{\sigma}} u_2 c_{q\overline{\sigma}} c_{d\sigma}}^{\text{spin-flip scattering}} \tag{0.30}$$

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

$$\mathcal{H}_{I,N} = \sum_{k,q,\sigma,\sigma'} u_P c^\dagger_{k\sigma} c^\dagger_{d\sigma'} c_{q\sigma} c_{d\sigma'} + \sum_{k,q,\sigma} u_A c^\dagger_{k\sigma} c^\dagger_{d\overline{\sigma}} c_{q\overline{\sigma}} c_{d\sigma} \tag{0.31}$$

where the $N$ in the denominator means the sum is over all momenta up to $|k| = \Lambda_N$.

The total Hamiltonian can be written as

$$\begin{aligned} \mathcal{H} = \sum_{k} \left( \epsilon_k \hat{n}_{k\sigma} + V_k c^\dagger_{k\sigma} c_{d\sigma} + \text{h.c.} \right) + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \sum_{k,k',\sigma} u_A c^\dagger_{k\sigma} c^\dagger_{d\overline{\sigma}} c_{k'\overline{\sigma}} c_{d\sigma} \\ + \sum_{k,k',\sigma,\sigma'} u_P c^\dagger_{k\sigma} c^\dagger_{d\sigma'} c_{k'\sigma} c_{d\sigma'} \end{aligned} \tag{0.32}$$

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

$$\begin{aligned}\mathcal{H}_N = H_{N-1} + H_{imp} + \left(\epsilon_q - u_P\hat{n}_d\right)\hat{n}_{q\beta} + V_q c^\dagger_{q\beta}c_{d\beta} + \text{h.c.} + \sum_{k<\Lambda_N} u_A\left(c^\dagger_{q\beta}c^\dagger_{d\overline{\beta}}c_{k\overline{\beta}}c_{d\beta} + c^\dagger_{k\overline{\beta}}c^\dagger_{d\beta}c_{q\beta}c_{d\overline{\beta}}\right)\\ + \sum_{k<\Lambda_N\sigma}\frac{u_P}{2}\left(c^\dagger_{q\beta}c^\dagger_{d\sigma}c_{k\beta}c_{d\sigma} + c^\dagger_{k\beta}c^\dagger_{d\sigma}c_{q\beta}c_{d\sigma}\right)\end{aligned} \tag{0.33}$$

where $\hat{n}_d = \sum_\sigma \hat{n}_{d\sigma}$ is the total number operator for the impurity site, $H_{imp}$ is the impurity-diagonal part of the Hamiltonian ($\epsilon_d\hat{n}_d + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}$) and

$$H_{N-1} = \sum_{k<\Lambda_N,\sigma}\left[\left(\epsilon_k - u_P\hat{n}_d\right)\hat{n}_{k\sigma} + V_k c^\dagger_{k\sigma}c_{d\sigma} + \text{h.c.}\right] + H_{I,N-1} \tag{0.34}$$

## 2.1 Particle sector

The renormalization in the Hamiltonian in the particle sector is

$$\begin{aligned}\Delta^+\mathcal{H}_N = \sum_{q\beta}\left[V_q^* c^\dagger_{d\beta}c_{q\beta} + u_P\sum_{k\sigma}\hat{n}_{d\sigma}c_{q\beta}c^\dagger_{k\beta} + u_A\sum_{k\sigma}c^\dagger_{d\beta}c^\dagger_{k\overline{\beta}}c_{d\overline{\beta}}c_{q\beta}\right]\times\frac{1}{\hat{\omega} - \mathcal{H}^+_D}\\ \times\left[V_q c^\dagger_{q\beta}c_{d\beta} + u_P\sum_{k\sigma}\hat{n}_{d\sigma}c_{k\beta}c^\dagger_{q\beta} + u_A\sum_{k\sigma}c^\dagger_{d\overline{\beta}}c^\dagger_{q\beta}c_{d\beta}c_{k\overline{\beta}}\right]\end{aligned} \tag{0.35}$$

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 ($q\beta$).

$$\begin{aligned}\mathcal{H}^+_D &= \sum_{k<\Lambda_N,\sigma}\left(\epsilon_k - u_P\hat{n}_d\right)\hat{n}_{k\sigma} + \left(\epsilon_q - u_P\hat{n}_d\right)\hat{n}_{q\beta} + H_{imp}\\ \mathcal{H}^-_D &= \sum_{k<\Lambda_N,\sigma}\left(\epsilon_k - u_P\hat{n}_d\right)\hat{n}_{k\sigma} + H_{imp}\end{aligned} \tag{0.36}$$

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

**1.**

$$\Delta_1^+ \mathcal{H}_N = \sum_{q\beta} |V_q|^2 c^\dagger_{d\beta} c_{q\beta} \frac{1}{\hat{\omega} - \mathcal{H}_D^+} c^\dagger_{q\beta} c_{d\beta} \tag{0.37}$$

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

$$H_1 \equiv \mathcal{H}_D^+ = \sum_{k<\Lambda_N,\sigma} \left(\epsilon_k - u_P \hat{n}_{d\overline{\beta}}\right) \hat{n}_{k\sigma} + \left(\epsilon_q^+ - u_P \hat{n}_{d\overline{\beta}}\right) + \epsilon_d \hat{n}_{d\overline{\beta}} \tag{0.38}$$

$H_1$ is the intermediate state Hamiltonian. As a simplification, we replace $\hat{\omega}$ with its eigenvalue $\omega$. 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:

$$\begin{aligned} \Delta_1^+ \mathcal{H}_N &= \sum_{q\beta} |V_q|^2 c^\dagger_{d\beta} c_{q\beta} c^\dagger_{q\beta} c_{d\beta} \frac{1}{\omega - H_1} \\ &= \sum_{q\beta} |V_q|^2 \hat{n}_{d\beta} \left(1 - \hat{n}_{q\beta}\right) \frac{1}{\omega - H_1} \end{aligned} \tag{0.39}$$

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

$$\begin{aligned} H_0 &= \sum_{k<\Lambda_N,\sigma} \left(\epsilon_k - u_P \left(\hat{n}_{d\overline{\beta}} + 1\right)\right) \hat{n}_{k\sigma} + \epsilon_d + (\epsilon_d + U)\, \hat{n}_{d\overline{\beta}} \\ &= H_1 + \epsilon_d + U \hat{n}_{d\overline{\beta}} - u_P \sum_{k<\Lambda_N \sigma} \hat{n}_{k,\sigma} - \left(\epsilon_q^+ - u_P \hat{n}_{d\overline{\beta}}\right) \end{aligned} \tag{0.40}$$

We now approximate the denominator by dropping the correlations with the lower electrons;

$$\Delta_1^+ \mathcal{H}_N = \sum_{q\beta} |V_q|^2 \hat{n}_{d\beta} \left(1 - \hat{n}_{q\beta}\right) \frac{1}{\omega - H_0 + \epsilon_d + U \hat{n}_{d\overline{\beta}} - \left(\epsilon_q^+ - u_P \hat{n}_{d\overline{\beta}}\right)} \tag{0.41}$$

From this point on, we will not bother to keep track of the energies of the lower shell electrons, unless they appear in the scattering process itself (and hence their number operator can be resolved into an eigenvalue). If we measure the quantum fluctuation $\omega$ from the initial (diagonal) state energy which does not have any quantum fluctuations, we can set $H_0 = 0$. Also, since $q\beta$ is on the upper band edge, we can assume it is unoccupied in the initial state. Then,

$$
\begin{aligned}
\Delta_1^+\mathcal{H}_N &= \sum_{q\beta} |V_q|^2 \hat{n}_{d\beta} \frac{1}{\omega - \epsilon_q^+ + \epsilon_d + (U + u_P)\,\hat{n}_{d\overline{\beta}}} \\
&= \sum_{q\beta} \hat{n}_{d\beta} \left[ \frac{|V_q^1|^2 \hat{n}_{d\overline{\beta}}}{\omega - \epsilon_q^+ + \epsilon_d + (U + u_P)} + \frac{|V_q^0|^2 \left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega - \epsilon_q^+ + \epsilon_d} \right] \\
&= \sum_{q\beta} \hat{n}_{d\beta} \left[ \frac{|V_q^0|^2}{\omega - \epsilon_q^+ + \epsilon_d} + \hat{n}_{d\overline{\beta}} \left( \frac{|V_q^1|^2}{\omega - \epsilon_q^+ + \epsilon_d + (U + u_P)} - \frac{|V_q^0|^2}{\omega - \epsilon_q^+ + \epsilon_d} \right) \right]
\end{aligned}
\tag{0.42}
$$

**2.**

$$
\Delta_2^+\mathcal{H}_N = \sum_{q\beta k\sigma} u_P V_q^* c_{d\beta}^\dagger c_{q\beta} \frac{1}{\omega - \mathcal{H}_D^+} \hat{n}_{d\sigma} c_{k\beta} c_{q\beta}^\dagger
\tag{0.43}
$$

This can be simplified by noting that since the propagator is diagonal, the only operator that changes $\hat{n}_d$ is the $c_{d\beta}^\dagger$, and therefore

$$
c_{d\beta}^\dagger \sum_\sigma \hat{n}_{d\sigma} = c_{d\beta}^\dagger \hat{n}_{d\overline{\beta}}
\tag{0.44}
$$

The expression simplifies to

$$
\Delta_2^+\mathcal{H}_N = \sum_{q\beta k\sigma} u_P V_q^* c_{d\beta}^\dagger c_{q\beta} \hat{n}_{d\overline{\beta}} \frac{1}{\omega - \mathcal{H}_D^+} c_{k\beta} c_{q\beta}^\dagger
\tag{0.45}
$$

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

$$
H_1 = \epsilon_q^+ - u_P + \epsilon_d
\tag{0.46}
$$

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

$$
H_0 = \epsilon_k - u_P + \epsilon_d = H_1 + \epsilon_k - \epsilon_q^+
\tag{0.47}
$$

$$
\begin{aligned}
\Delta_2^+\mathcal{H}_N &= \sum_{q\beta k\sigma} u_P V_q^* c_{d\beta}^\dagger c_{q\beta} \hat{n}_{d\overline{\beta}} c_{k\beta} c_{q\beta}^\dagger \frac{1}{\omega - H_1 + \epsilon_k - \epsilon_q^+} \\
&= \sum_{q\beta k\sigma} c_{d\beta}^\dagger c_{k\beta} \frac{-\hat{n}_{d\overline{\beta}} u_P V_q^{1*}}{\omega - \epsilon_q^+ + \epsilon_k}
\end{aligned}
\tag{0.48}
$$

**3.**

$$\Delta_3^+\mathcal{H}_N = \sum_{q\beta k} u_A V_q^* c^\dagger_{d\beta} c_{q\beta} \frac{1}{\omega - \mathcal{H}_D^+} c^\dagger_{d\overline{\beta}} c^\dagger_{q\beta} c_{d\beta} c_{k\overline{\beta}} \tag{0.49}$$

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

$$H_1 = \epsilon_q^+ - u_P + \epsilon_d \tag{0.50}$$

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

$$H_0 = \epsilon_k - u_P + \epsilon_d = H_1 + \epsilon_k - \epsilon_q^+ \tag{0.51}$$

$$\begin{aligned}
\Delta_2^+\mathcal{H}_N &= \sum_{q\beta k} u_A V_q^* c^\dagger_{d\beta} c_{q\beta} c^\dagger_{d\overline{\beta}} c^\dagger_{q\beta} c_{d\beta} c_{k\overline{\beta}} \frac{1}{\omega - H_1 + \epsilon_k - \epsilon_q^+} \\
&= \sum_{q\beta k} u_A V_q^* \hat{n}_{d\beta} \left(1 - \hat{n}_{q\beta}\right) c^\dagger_{d\overline{\beta}} c_{k\overline{\beta}} \frac{1}{\omega - H_1 + \epsilon_k - \epsilon_q^+} \\
&= \sum_{q\beta k} c^\dagger_{d\beta} c_{k\beta} \frac{u_A V_q^{1^*} \hat{n}_{d\overline{\beta}}}{\omega + \epsilon_k - \epsilon_q^+}
\end{aligned} \tag{0.52}$$

**4.**

$$\Delta_4^+\mathcal{H}_N = \sum_{q\beta k\sigma} u_P V_q \hat{n}_{d\sigma} c_{q\beta} c^\dagger_{k\beta} \frac{1}{\omega - \mathcal{H}_D^+} c^\dagger_{q\beta} c_{d\beta} \tag{0.53}$$

The first step is a simplification:

$$\sum_\sigma \hat{n}_{d\sigma} c_{d\beta} = \hat{n}_{d\overline{\beta}} c_{d\beta} \tag{0.54}$$

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

$$H_1 = \epsilon_q^+ - u_P + \epsilon_d \tag{0.55}$$

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

$$H_0 = 2\epsilon_d + U = H_1 + \epsilon_d + U - \epsilon_q^+ + u_P \tag{0.56}$$

$$
\begin{aligned}
\Delta_4^+\mathcal{H}_N &= \sum_{q\beta k} u_P V_q \hat{n}_{d\overline{\beta}} c_{q\beta} c^\dagger_{k\beta} c^\dagger_{q\beta} c_{d\beta} \frac{1}{\omega - H_0 + \epsilon_d + U - \epsilon_q^+ + u_P} \\
&= \sum_{q\beta k} u_P V_q \hat{n}_{d\overline{\beta}} \left(1 - \hat{n}_{q\beta}\right) c^\dagger_{k\beta} c_{d\beta} \frac{-1}{\omega + \epsilon_d + U - \epsilon_q^+ + u_P} \\
&= \sum_{q\beta k} c^\dagger_{k\beta} c_{d\beta} \frac{-u_P V_q^1 \hat{n}_{d\overline{\beta}}}{\omega - \epsilon_q^+ + \epsilon_d + U + u_P}
\end{aligned} \tag{0.57}
$$

**5.**

$$
\Delta_5^+\mathcal{H}_N = \sum_{q\beta k\sigma} u_A V_q c^\dagger_{d\beta} c^\dagger_{k\overline{\beta}} c_{d\overline{\beta}} c_{q\beta} \frac{1}{\omega - \mathcal{H}_D^+} c^\dagger_{q\beta} c_{d\beta} \tag{0.58}
$$

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

$$
H_1 = \epsilon_q^+ - u_P + \epsilon_d \tag{0.59}
$$

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

$$
H_0 = 2\epsilon_d + U = H_1 + \epsilon_d + U - \epsilon_q^+ + u_P \tag{0.60}
$$

$$
\begin{aligned}
\Delta_5^+\mathcal{H}_N &= \sum_{q\beta k} u_A V_q c^\dagger_{d\beta} c^\dagger_{k\overline{\beta}} c_{d\overline{\beta}} c_{q\beta} c^\dagger_{q\beta} c_{d\beta} \frac{1}{\omega - H_0 + \epsilon_d + U - \epsilon_q^+ + u_P} \\
&= \sum_{q\beta k} u_A V_q \left(1 - \hat{n}_{q\beta}\right) \hat{n}_{d\beta} c^\dagger_{k\overline{\beta}} c_{d\overline{\beta}} \frac{1}{\omega + \epsilon_d + U - \epsilon_q^+ + u_P} \\
&= \sum_{q\beta k} c^\dagger_{k\overline{\beta}} c_{d\overline{\beta}} \frac{u_A V_q^1 \hat{n}_{d\beta}}{\omega - \epsilon_q^+ + \epsilon_d + U + u_P}
\end{aligned} \tag{0.61}
$$

**6.**

$$\Delta_4^+\mathcal{H}_N = \sum_{q\beta k\sigma\sigma'} u_P^2 \hat{n}_{d\sigma} c_{q\beta} c_{k\beta}^\dagger \frac{1}{\omega - \mathcal{H}_D^+} \hat{n}_{d\sigma'} c_{k'\beta} c_{q\beta}^\dagger \tag{0.62}$$

The first step is a simplification:

$$\begin{aligned}\sum_{\sigma\sigma'} \hat{n}_{d\sigma}\hat{n}_{d\sigma'} = \sum_{\sigma} \hat{n}_{d\sigma}\left(\hat{n}_{d\sigma} + \hat{n}_{d\overline{\sigma}}\right) &= \sum_{\sigma} \hat{n}_{d\sigma}\left(1 + \hat{n}_{d\overline{\sigma}}\right) \\ &= \hat{n}_d + 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\end{aligned} \tag{0.63}$$

$$\Delta_4^+\mathcal{H}_N = \sum_{q\beta k} u_P^2 \left(\hat{n}_d + 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right) c_{q\beta} c_{k\beta}^\dagger \frac{1}{\omega - \mathcal{H}_D^+} c_{k'\beta} c_{q\beta}^\dagger$$

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

$$H_1 = \epsilon_q^+ - u_P\hat{n}_d + \epsilon_d\hat{n}_d + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} \tag{0.64}$$

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

$$H_0 = \epsilon_{k'} - u_P\hat{n}_d + \epsilon_d\hat{n}_d + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} = H_1 - \epsilon_q^+ + \epsilon_{k'} \tag{0.65}$$

$$\begin{aligned}\Delta_6^+\mathcal{H}_N &= \sum_{q\beta k} u_P^2 \left(\hat{n}_d + 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right) c_{q\beta} c_{k\beta}^\dagger c_{k'\beta} c_{q\beta}^\dagger \frac{1}{\omega - H_1} \\ &= \sum_{q\beta k} u_P^2 \left(\hat{n}_d + 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right)\left(1 - \hat{n}_{q\beta}\right) c_{k\beta}^\dagger c_{k'\beta} \frac{1}{\omega - H_0 - \epsilon_q^+ + \epsilon_{k'}}\end{aligned} \tag{0.66}$$

The first term gives

$$\sum_{q\beta k\sigma} u_P^2 \hat{n}_{d\sigma} c_{k\beta}^\dagger c_{k'\beta} \frac{1}{\omega - \epsilon_q^+ + \epsilon_{k'}} = \sum_{q\beta k\sigma} c_{k\beta}^\dagger c_{d\sigma}^\dagger c_{k'\beta} c_{d\sigma} \frac{-u_P^2}{\omega - \epsilon_q^+ + \epsilon_{k'}} \tag{0.67}$$

The second term gives

$$\sum_{q\beta k} \hat{n}_{d\uparrow}\hat{n}_{d\downarrow} c_{k\beta}^\dagger c_{k'\beta} \frac{2u_P^2}{\omega - \epsilon_q^+ + \epsilon_{k'}} \tag{0.68}$$

In total,

$$\Delta_6^+\mathcal{H}_N = \sum_{q\beta k\sigma} c_{k\beta}^\dagger c_{d\sigma}^\dagger c_{k'\beta} c_{d\sigma} \frac{-u_P^2}{\omega - \epsilon_q^+ + \epsilon_{k'}} + \sum_{q\beta k} \hat{n}_{d\uparrow}\hat{n}_{d\downarrow} c_{k\beta}^\dagger c_{k'\beta} \frac{2u_P^2}{\omega - \epsilon_q^+ + \epsilon_{k'}} \tag{0.69}$$

**7.**

$$\Delta_7^+\mathcal{H}_N = \sum_{q\beta kk'\sigma} u_P u_A \hat{n}_{d\sigma} c_{q\beta} c^\dagger_{k'\beta} \frac{1}{\omega - \mathcal{H}_D^+} c^\dagger_{d\overline{\beta}} c^\dagger_{q\beta} c_{d\beta} c_{k\overline{\beta}} \tag{0.70}$$

The first step is a simplification:

$$\sum_\sigma \hat{n}_{d\sigma} c^\dagger_{d\overline{\beta}} c_{d\beta} = c^\dagger_{d\overline{\beta}} c_{d\beta} \tag{0.71}$$

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

$$H_1 = \epsilon_q^+ - u_P + \epsilon_d \tag{0.72}$$

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

$$H_0 = \epsilon_k - u_P + \epsilon_d = H_1 - \epsilon_{q^+} + \epsilon_k \tag{0.73}$$

$$\begin{aligned}
\Delta_7^+\mathcal{H}_N &= \sum_{q\beta kk'} u_P u_A c_{q\beta} c^\dagger_{k'\beta} c^\dagger_{d\overline{\beta}} c^\dagger_{q\beta} c_{d\beta} c_{k\overline{\beta}} \frac{1}{\omega - H_1} \\
&= \sum_{q\beta kk'} \left(1 - \hat{n}_{q\beta}\right) c^\dagger_{k'\beta} c^\dagger_{d\overline{\beta}} c_{k\overline{\beta}} c_{d\beta} \frac{-u_P u_A}{\omega - \epsilon_{q^+} + \epsilon_k} \\
&= \sum_{q\beta kk'} c^\dagger_{k\beta} c^\dagger_{d\overline{\beta}} c_{k'\overline{\beta}} c_{d\beta} \frac{-u_P u_A}{\omega - \epsilon_{q^+} + \epsilon_{k'}}
\end{aligned} \tag{0.74}$$

**8.**

$$\Delta_8^+\mathcal{H}_N = \sum_{q\beta kk'\sigma} u_A u_P c^\dagger_{d\beta} c^\dagger_{k'\overline{\beta}} c_{d\overline{\beta}} c_{q\beta} \frac{1}{\omega - \mathcal{H}_D^+} \hat{n}_{d\sigma} c_{k\beta} c^\dagger_{q\beta} \tag{0.75}$$

The first step is a simplification:

$$c^\dagger_{d\beta} c_{d\overline{\beta}} \sum_\sigma \hat{n}_{d\sigma} = c^\dagger_{d\beta} c_{d\overline{\beta}} \tag{0.76}$$

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

$$H_1 = \epsilon_q^+ - u_P + \epsilon_d \tag{0.77}$$

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

$$H_0 = \epsilon_k - u_P + \epsilon_d = H_1 - \epsilon_q^+ + \epsilon_k \tag{0.78}$$

$$
\begin{aligned}
\Delta_8^+\mathcal{H}_N &= \sum_{q\beta kk'} u_A u_P c^\dagger_{d\beta} c^\dagger_{k'\overline{\beta}} c_{d\overline{\beta}} c_{q\beta} c_{k\beta} c^\dagger_{q\beta} \frac{1}{\omega - H_0 - \epsilon_q^+ + \epsilon_k} \\
&= \sum_{q\beta kk'} \left(1 - \hat{n}_{q\beta}\right) c^\dagger_{k'\overline{\beta}} c^\dagger_{d\beta} c_{k\beta} c_{d\overline{\beta}} \frac{-u_A u_P}{\omega - H_0 - \epsilon_q^+ + \epsilon_k} \\
&= \sum_{q\beta kk'} c^\dagger_{k\beta} c^\dagger_{d\overline{\beta}} c_{k'\overline{\beta}} c_{d\beta} \frac{-u_A u_P}{\omega - \epsilon_q^+ + \epsilon_{k'}}
\end{aligned}
\tag{0.79}
$$

**9.**

$$
\Delta_9^+\mathcal{H}_N = \sum_{q\beta kk'} u_A^2 c^\dagger_{d\beta} c^\dagger_{k\overline{\beta}} c_{d\overline{\beta}} c_{q\beta} \frac{1}{\omega - \mathcal{H}_D^+} c^\dagger_{d\overline{\beta}} c^\dagger_{q\beta} c_{d\beta} c_{k'\overline{\beta}}
\tag{0.80}
$$

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

$$
H_1 = \epsilon_q^+ - u_P + \epsilon_d
\tag{0.81}
$$

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

$$
H_0 = \epsilon_{k'} - u_P + \epsilon_d = H_1 - \epsilon_q^+ + \epsilon_{k'}
\tag{0.82}
$$

$$
\begin{aligned}
\Delta_9^+\mathcal{H}_N &= \sum_{q\beta kk'} u_A^2 c^\dagger_{d\beta} c^\dagger_{k\overline{\beta}} c_{d\overline{\beta}} c_{q\beta} c^\dagger_{d\overline{\beta}} c^\dagger_{q\beta} c_{d\beta} c_{k'\overline{\beta}} \frac{1}{\omega - H_0 - \epsilon_q^+ + \epsilon_{k'}} \\
&= \sum_{q\beta kk'} \left(1 - \hat{n}_{q\beta}\right)\left(1 - \hat{n}_{d\overline{\beta}}\right) c^\dagger_{k\overline{\beta}} c^\dagger_{d\beta} c_{k'\overline{\beta}} c_{d\beta} \frac{u_A^2}{\omega - H_0 - \epsilon_q^+ + \epsilon_{k'}} \\
&= \sum_{q\beta kk'} \left(1 - \hat{n}_{d\beta}\right) c^\dagger_{k\beta} c^\dagger_{d\overline{\beta}} c_{k'\beta} c_{d\overline{\beta}} \frac{u_A^2}{\omega - H_0 - \epsilon_q^+ + \epsilon_{k'}}
\end{aligned}
\tag{0.83}
$$

## 2.2 Hole sector

The renormalization in the Hamiltonian in the hole sector is

$$
\begin{aligned}
\Delta^+\mathcal{H}_N = \sum_{q\beta} &\left[ V_q c^\dagger_{q\beta} c_{d\beta} + u_P \sum_{k\sigma} \hat{n}_{d\sigma} c_{k\beta} c^\dagger_{q\beta} + u_A \sum_{k\sigma} c^\dagger_{d\overline{\beta}} c^\dagger_{q\beta} c_{d\beta} c_{k\overline{\beta}} \right] \times \frac{1}{\hat{\omega} - \mathcal{H}_D^-} \\
&\times \left[ V_q^* c^\dagger_{d\beta} c_{q\beta} + u_P \sum_{k\sigma} \hat{n}_{d\sigma} c_{q\beta} c^\dagger_{k\beta} + u_A \sum_{k\sigma} c^\dagger_{d\beta} c^\dagger_{k\overline{\beta}} c_{d\overline{\beta}} c_{q\beta} \right]
\end{aligned}
\tag{0.84}
$$

**1.**

$$\Delta_1^- \mathcal{H}_N = \sum_{q\beta} |V_q|^2 c^\dagger_{q\beta} c_{d\beta} \frac{1}{\hat{\omega} - \mathcal{H}_D^-} c^\dagger_{d\beta} c_{q\beta} \tag{0.85}$$

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

$$H_1 = \epsilon_d + (\epsilon_d + U)\,\hat{n}_{d\overline{\beta}} \tag{0.86}$$

$$\Delta_1^- \mathcal{H}_N = \sum_{q\beta} |V_q|^2 \hat{n}_{q\beta} \left(1 - \hat{n}_{d\beta}\right) \frac{1}{\omega - H_1} \tag{0.87}$$

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

$$\begin{aligned} H_0 &= \epsilon_q^- - u_P \hat{n}_{d\overline{\beta}} + \epsilon_d \hat{n}_{d\overline{\beta}} \\ &= H_1 + \epsilon_q^- - \epsilon_d - (U + u_P)\,\hat{n}_{d\overline{\beta}} \end{aligned} \tag{0.88}$$

$$\begin{aligned} \Delta_1^- \mathcal{H}_N &= \sum_{q\beta} |V_q|^2 \hat{n}_{q\beta} \left(1 - \hat{n}_{d\beta}\right) \frac{1}{\omega - H_0 + \epsilon_q^- - \epsilon_d - (U + u_P)\,\hat{n}_{d\overline{\beta}}} \\ &= \sum_{q\beta} |V_q|^2 \left(1 - \hat{n}_{d\beta}\right) \frac{1}{\omega + \epsilon_q^- - \epsilon_d - (U + u_P)\,\hat{n}_{d\overline{\beta}}} \\ &= \sum_{q\beta} \left(1 - \hat{n}_{d\beta}\right) \left[ \frac{|V_q^1|^2 \hat{n}_{d\overline{\beta}}}{\omega + \epsilon_q^- - \epsilon_d - (U + u_P)} + \frac{|V_q^0|^2 \left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega + \epsilon_q^- - \epsilon_d} \right] \\ &= \sum_{q\beta} \left[ \hat{n}_{d\overline{\beta}} \left( \frac{|V_q^1|^2}{\omega + \epsilon_q^- - \epsilon_d - (U + u_P)} - \frac{2|V_q^0|^2}{\omega + \epsilon_q^- - \epsilon_d} \right) \right. \\ &\qquad \left. + \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \left( \frac{|V_q^0|^2}{\omega + \epsilon_q^- - \epsilon_d} - \frac{|V_q^1|^2}{\omega + \epsilon_q^- - \epsilon_d - (U + u_P)} \right) \right] \end{aligned} \tag{0.89}$$

**2.**

$$\Delta_2^- \mathcal{H}_N = \sum_{q\beta\sigma k} u_P V_q c_{q\beta}^\dagger c_{d\beta} \frac{1}{\hat{\omega} - \mathcal{H}_D^-} \hat{n}_{d\sigma} c_{q\beta} c_{k\beta}^\dagger \tag{0.90}$$

The first step is a simplification:

$$c_{d\beta} \sum_\sigma \hat{n}_{d\sigma} = c_{d\beta}\left(1 + \hat{n}_{d\overline{\beta}}\right) \tag{0.91}$$

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

$$H_1 = \epsilon_k - u_P\left(1 + \hat{n}_{d\overline{\beta}}\right) + \epsilon_d + (\epsilon_d + U)\,\hat{n}_{d\overline{\beta}} \tag{0.92}$$

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

$$\begin{aligned} H_0 &= \epsilon_q^- - u_P\left(1 + \hat{n}_{d\overline{\beta}}\right) + \epsilon_d + (\epsilon_d + U)\,\hat{n}_{d\overline{\beta}} \\ &= H_1 + \epsilon_q^- - \epsilon_k \end{aligned} \tag{0.93}$$

$$\begin{aligned} \Delta_2^- \mathcal{H}_N &= \sum_{q\beta k} u_P V_q c_{q\beta}^\dagger c_{d\beta}\left(1 + \hat{n}_{d\overline{\beta}}\right) c_{q\beta} c_{k\beta}^\dagger \frac{1}{\omega - H_1} \\ &= \sum_{q\beta k} \hat{n}_{q\beta}\left(1 + \hat{n}_{d\overline{\beta}}\right) c_{k\beta}^\dagger c_{d\beta} \frac{u_P V_q}{\omega + \epsilon_q^- - \epsilon_k} \\ &= \sum_{q\beta k} c_{k\beta}^\dagger c_{d\beta}\left[\frac{2u_P V_q^1 \hat{n}_{d\overline{\beta}}}{\omega + \epsilon_q^- - \epsilon_k} + \frac{u_P V_q^0\left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega + \epsilon_q^- - \epsilon_k}\right] \end{aligned} \tag{0.94}$$

**3.**

$$\Delta_3^- \mathcal{H}_N = \sum_{q\beta k} u_A V_q c_{q\beta}^\dagger c_{d\beta} \frac{1}{\hat{\omega} - \mathcal{H}_D^-} c_{d\beta}^\dagger c_{k\overline{\beta}}^\dagger c_{d\overline{\beta}} c_{q\beta} \tag{0.95}$$

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

$$H_1 = \epsilon_k - u_P + \epsilon_d \tag{0.96}$$

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

$$H_0 = \epsilon_q^- - u_P + \epsilon_d = H_1 + \epsilon_q^- - \epsilon_k \tag{0.97}$$

$$
\begin{aligned}
\Delta_3^- \mathcal{H}_N &= \sum_{q\beta k} u_A V_q c^\dagger_{q\beta} c_{d\beta} c^\dagger_{d\beta} c^\dagger_{k\overline{\beta}} c_{d\overline{\beta}} c_{q\beta} \frac{1}{\omega - H_1} \\
&= \sum_{q\beta k} u_A V_q \hat{n}_{q\beta} \left(1 - \hat{n}_{d\beta}\right) c^\dagger_{k\overline{\beta}} c_{d\overline{\beta}} \frac{1}{\omega + \epsilon_q^- - \epsilon_k} \\
&= \sum_{q\beta k} c^\dagger_{k\beta} c_{d\beta} \frac{u_A V_q^0 \left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega + \epsilon_q^- - \epsilon_k}
\end{aligned} \tag{0.98}
$$

**4.**

$$
\Delta_4^- \mathcal{H}_N = \sum_{q\beta k\sigma} u_P V_q^* \hat{n}_{d\sigma} c_{k\beta} c^\dagger_{q\beta} \frac{1}{\hat{\omega} - \mathcal{H}_D^-} c^\dagger_{d\beta} c_{q\beta} \tag{0.99}
$$

There is a simplification:

$$
\sum_\sigma \hat{n}_{d\sigma} c^\dagger_{d\beta} = \left(1 + \hat{n}_{d\overline{\beta}}\right) c^\dagger_{d\beta} \tag{0.100}
$$

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

$$
H_1 = \epsilon_k - u_P \left(1 + \hat{n}_{d\overline{\beta}}\right) + \epsilon_d + \left(\epsilon_d + U\right) \hat{n}_{d\overline{\beta}} \tag{0.101}
$$

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

$$
H_0 = \epsilon_k - u_P \hat{n}_{d\overline{\beta}} + \epsilon_q^- - u_P \hat{n}_{d\overline{\beta}} + \epsilon_d \hat{n}_{d\overline{\beta}} = H_1 + \epsilon_q^- + u_P \left(1 - \hat{n}_{d\overline{\beta}}\right) - \epsilon_d - U \hat{n}_{d\overline{\beta}} \tag{0.102}
$$

$$
\begin{aligned}
\Delta_4^- \mathcal{H}_N &= \sum_{q\beta k} u_P V_q^* \left(1 + \hat{n}_{d\overline{\beta}}\right) c_{k\beta} c^\dagger_{q\beta} c^\dagger_{d\beta} c_{q\beta} \frac{1}{\omega - H_0 + \epsilon_q^- + u_P \left(1 - \hat{n}_{d\overline{\beta}}\right) - \epsilon_d - U \hat{n}_{d\overline{\beta}}} \\
&= \sum_{q\beta k} u_P V_q^* \left(1 + \hat{n}_{d\overline{\beta}}\right) \hat{n}_{q\beta} c^\dagger_{d\beta} c_{k\beta} \left( \frac{\hat{n}_{d\overline{\beta}}}{\omega - H_0 + \epsilon_q^- - \epsilon_d - U} + \frac{1 - \hat{n}_{d\overline{\beta}}}{\omega - H_0 + \epsilon_q^- + u_P - \epsilon_d} \right) \\
&= \sum_{q\beta k} c^\dagger_{d\beta} c_{k\beta} \left[ \frac{2 u_P V_q^{1^*} \hat{n}_{d\overline{\beta}}}{\omega - H_0 + \epsilon_q^- - \epsilon_d - U} + \frac{u_P V_q^{0^*} \left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega - H_0 + \epsilon_q^- + u_P - \epsilon_d} \right]
\end{aligned} \tag{0.103}
$$

**5.**

$$\Delta_5^- \mathcal{H}_N = \sum_{q\beta k} u_A V_q^* c_{d\overline{\beta}}^\dagger c_{q\beta}^\dagger c_{d\beta} c_{k\overline{\beta}} \frac{1}{\hat{\omega} - \mathcal{H}_D^-} c_{d\beta}^\dagger c_{q\beta} \tag{0.104}$$

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

$$H_1 = \epsilon_k - u_P + \epsilon_d \tag{0.105}$$

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

$$H_0 = \epsilon_q^- + \epsilon_k = H_1 + \epsilon_q^- + u_P - \epsilon_d \tag{0.106}$$

$$\begin{aligned}
\Delta_5^- \mathcal{H}_N &= \sum_{q\beta k} u_A V_q^* c_{d\overline{\beta}}^\dagger c_{q\beta}^\dagger c_{d\beta} c_{k\overline{\beta}} c_{d\beta}^\dagger c_{q\beta} \frac{1}{\hat{\omega} - H_0 + \epsilon_q^- + u_P - \epsilon_d} \\
&= \sum_{q\beta k} u_A V_q^* \hat{n}_{q\beta} \left(1 - \hat{n}_{d\beta}\right) c_{d\overline{\beta}}^\dagger c_{k\overline{\beta}} \frac{1}{\omega + \epsilon_q^- + u_P - \epsilon_d} \\
&= \sum_{q\beta k} c_{d\overline{\beta}}^\dagger c_{k\overline{\beta}} \frac{u_A V_q^{0*} \left(1 - \hat{n}_{d\beta}\right)}{\omega + \epsilon_q^- + u_P - \epsilon_d}
\end{aligned} \tag{0.107}$$

**6.**

$$\Delta_6^- \mathcal{H}_N = \sum_{q\beta k k' \sigma\sigma'} u_P^2 \hat{n}_{d\sigma} c_{k\beta} c_{q\beta}^\dagger \frac{1}{\hat{\omega} - \mathcal{H}_D^-} \hat{n}_{d\sigma'} c_{q\beta} c_{k'\beta}^\dagger \tag{0.108}$$

From eq. 0.63,

$$\sum_{\sigma\sigma'} \hat{n}_{d\sigma} \hat{n}_{d\sigma'} = \hat{n}_d + 2\hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \tag{0.109}$$

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

$$H_1 = \epsilon_{k'} - u_P \hat{n}_d + \epsilon_d \hat{n}_d + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \tag{0.110}$$

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

$$H_0 = \epsilon_q^- - u_P \hat{n}_d + \epsilon_d \hat{n}_d + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} = H_1 + \epsilon_q^- - \epsilon_{k'} \tag{0.111}$$

$$\begin{aligned}
\Delta_6^-\mathcal{H}_N &= \sum_{q\beta kk'} u_P^2 \left(\hat{n}_d + 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right) c_{k\beta} c^\dagger_{q\beta} c_{q\beta} c^\dagger_{k'\beta} \frac{1}{\omega - H_1} \\
&= \sum_{q\beta kk'} u_P^2 \hat{n}_{q\beta} \left(\hat{n}_d + 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right) c_{k\beta} c^\dagger_{k'\beta} \frac{1}{\omega - H_0 + \epsilon_q^- - \epsilon_{k'}} \\
&= \sum_{q\beta kk'\sigma} \hat{n}_{d\sigma} c^\dagger_{k'\beta} c_{k\beta} \frac{-u_P^2}{\omega + \epsilon_q^- - \epsilon_{k'}} + \sum_{q\beta kk'} 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} c^\dagger_{k'\beta} c_{k\beta} \frac{-u_P^2}{\omega + \epsilon_q^- - \epsilon_{k'}} \\
&+ \sum_{q\beta k\sigma} \hat{n}_{d\sigma} \frac{u_P^2}{\omega + \epsilon_q^- - \epsilon_k} + \sum_{q\beta k} 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} \frac{u_P^2}{\omega + \epsilon_q^- - \epsilon_k}
\end{aligned} \tag{0.112}$$

**7.**

$$\Delta_7^-\mathcal{H}_N = \sum_{q\beta kk'\sigma} u_A u_P \hat{n}_{d\sigma} c_{k\beta} c^\dagger_{q\beta} \frac{1}{\hat{\omega} - \mathcal{H}_D^-} c^\dagger_{d\beta} c^\dagger_{k'\overline{\beta}} c_{d\overline{\beta}} c_{q\beta} \tag{0.113}$$

Simplification:

$$\sum_\sigma \hat{n}_{d\sigma} c^\dagger_{d\beta} c_{d\overline{\beta}} = c^\dagger_{d\beta} c_{d\overline{\beta}} \tag{0.114}$$

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

$$H_1 = \epsilon_{k'} - u_P + \epsilon_d \tag{0.115}$$

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

$$H_0 = \epsilon_q^- - u_P + \epsilon_d = H_1 + \epsilon_q^- - \epsilon_{k'} \tag{0.116}$$

$$\begin{aligned}
\Delta_7^-\mathcal{H}_N &= \sum_{q\beta kk'} u_A u_P c_{k\beta} c^\dagger_{q\beta} c^\dagger_{d\beta} c^\dagger_{k'\overline{\beta}} c_{d\overline{\beta}} c_{q\beta} \frac{1}{\omega - H_1} \\
&= \sum_{q\beta kk'} u_A u_P \hat{n}_{q\beta} c^\dagger_{d\beta} c^\dagger_{k'\overline{\beta}} c_{d\overline{\beta}} c_{k\beta} \frac{1}{\hat{\omega} - H_0 + \epsilon_q^- - \epsilon_{k'}} \\
&= \sum_{q\beta kk'} c^\dagger_{k\overline{\beta}} c^\dagger_{d\beta} c_{k'\beta} c_{d\overline{\beta}} \frac{u_A u_P}{\omega + \epsilon_q^- - \epsilon_k}
\end{aligned} \tag{0.117}$$

**8.**

$$\Delta_8^- \mathcal{H}_N = \sum_{q\beta kk'\sigma} u_A u_P c^\dagger_{d\overline{\beta}} c^\dagger_{q\beta} c_{d\beta} c_{k\overline{\beta}} \frac{1}{\hat{\omega} - \mathcal{H}_D^-} \hat{n}_{d\sigma} c_{q\beta} c^\dagger_{k'\beta} \tag{0.118}$$

Simplification:

$$c^\dagger_{d\overline{\beta}} c_{d\beta} \sum_\sigma \hat{n}_{d\sigma} = c^\dagger_{d\overline{\beta}} c_{d\beta} \tag{0.119}$$

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

$$H_1 = \epsilon_{k'} - u_P + \epsilon_d \tag{0.120}$$

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

$$H_0 = \epsilon_q^- - u_P + \epsilon_d = H_1 + \epsilon_q^- - \epsilon_k \tag{0.121}$$

$$\begin{aligned}
\Delta_8^- \mathcal{H}_N &= \sum_{q\beta kk'\sigma} u_A u_P c^\dagger_{d\overline{\beta}} c^\dagger_{q\beta} c_{d\beta} c_{k\overline{\beta}} c_{q\beta} c^\dagger_{k'\beta} \frac{1}{\omega - H_1} \\
&= \sum_{q\beta kk'} u_A u_P \hat{n}_{q\beta} c^\dagger_{k'\beta} c^\dagger_{d\overline{\beta}} c_{k\overline{\beta}} c_{d\beta} \frac{1}{\omega - H_0 + \epsilon_q^- - \epsilon_k} \\
&= \sum_{q\beta kk'} c^\dagger_{k\beta} c^\dagger_{d\overline{\beta}} c_{k'\overline{\beta}} c_{d\beta} \frac{u_A u_P}{\omega + \epsilon_q^- - \epsilon_k}
\end{aligned} \tag{0.122}$$

**9.**

$$\Delta_9^- \mathcal{H}_N = \sum_{q\beta kk'} u_A^2 c^\dagger_{d\overline{\beta}} c^\dagger_{q\beta} c_{d\beta} c_{k'\overline{\beta}} \frac{1}{\hat{\omega} - \mathcal{H}_D^-} c^\dagger_{d\beta} c^\dagger_{k\overline{\beta}} c_{d\overline{\beta}} c_{q\beta} \tag{0.123}$$

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

$$H_1 = \epsilon_k - u_P + \epsilon_d \tag{0.124}$$

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

$$H_0 = \epsilon_q^- - u_P + \epsilon_d = H_1 + \epsilon_q^- - \epsilon_k \tag{0.125}$$

$$
\begin{aligned}
\Delta_9^- \mathcal{H}_N &= \sum_{q\beta kk'} u_A^2 c^\dagger_{d\overline{\beta}} c^\dagger_{q\beta} c_{d\beta} c_{k'\overline{\beta}} c^\dagger_{d\beta} c^\dagger_{k\overline{\beta}} c_{d\overline{\beta}} c_{q\beta} \frac{1}{\omega - H_1} \\
&= \sum_{q\beta kk'} \hat{n}_{q\beta} \left(1 - \hat{n}_{d\beta}\right) c^\dagger_{d\overline{\beta}} c_{k'\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{d\overline{\beta}} \frac{u_A u_P}{\omega + \epsilon_q^- - \epsilon_k} \\
&= \sum_{q\beta kk'} \left(1 - \hat{n}_{d\beta}\right) c^\dagger_{k\overline{\beta}} c^\dagger_{d\overline{\beta}} c_{k'\overline{\beta}} c_{d\overline{\beta}} \frac{u_A u_P}{\omega + \epsilon_q^- - \epsilon_k} + \sum_{q\beta k} \left(1 - \hat{n}_{d\beta}\right) \hat{n}_{d\overline{\beta}} \frac{u_A u_P}{\omega + \epsilon_q^- - \epsilon_k}
\end{aligned}
\tag{0.126}
$$

## 2.3 Scaling equations

$$
\begin{aligned}
\Delta \epsilon_d &= \sum_q \left( \frac{|V_q^0|^2}{\omega - \epsilon_q^+ + \epsilon_d} + \frac{|V_q^1|^2}{\omega + \epsilon_q^- - \epsilon_d - U - u_P} - \frac{2|V_q^0|^2}{\omega + \epsilon_q^- - \epsilon_d} \right) \\
\Delta U &= \sum_q 2 \left( \frac{|V_q^1|^2}{\omega - \epsilon_q^+ + \epsilon_d + U + u_P} - \frac{|V_q^0|^2}{\omega - \epsilon_q^+ + \epsilon_d} - \frac{|V_q^1|^2}{\omega + \epsilon_q^- - \epsilon_d - U - u_P} + \frac{|V_q^0|^2}{\omega + \epsilon_q^- - \epsilon_d} \right) \\
\Delta V_k^1 &= \sum_q V_q^1 \left[ \frac{2u_P}{\omega + \epsilon_q^- - \epsilon_k^+} + \frac{u_A - u_P}{\omega - \epsilon_q^+ + \epsilon_d + U + u_P} \right] \\
\Delta V_k^{1*} &= \sum_q V_q^{1*} \left[ \frac{u_A - u_P}{\omega + \epsilon_k^- - \epsilon_q^+} + \frac{2u_P}{\omega + \epsilon_q^- - \epsilon_d - U - u_P} \right] \\
\Delta V_k^0 &= \sum_q V_q^0 \frac{u_P + u_A}{\omega + \epsilon_q^- - \epsilon_k^+} \\
\Delta V_k^{0*} &= \sum_q V_q^{0*} \frac{u_P + u_A}{\omega + \epsilon_q^- - \epsilon_d - u_P} \\
\Delta u_P &= u_P^2 \left( \frac{1}{\omega - \epsilon_q^+ + \epsilon_{k'}^-} - \frac{1}{\omega - \epsilon_q^+ + \epsilon_k^-} \right) \\
\Delta u_A &= 2u_P u_A \left( \frac{1}{\omega - \epsilon_q^+ + \epsilon_{k'}^-} - \frac{1}{\omega - \epsilon_q^+ + \epsilon_k^-} \right)
\end{aligned}
\tag{0.127}
$$

**Note:** The reason for the lack of a $u_P$ or $u_A$ in the denominators of the last two equations is the following: The dispersion of the conduction electrons in the presence of the 4-Fermi scattering term is $\epsilon_k - u_P n_d$, $n_d$ being the number of impurity electrons. The scattering processes that give rise to the last two RG equations involve a $c_k^\dagger c_q$ or its h.c. in front of the propagator. Such a process creates a conduction electron by destroying another. The net change in energy in this process is $(\epsilon_q - u_P n_d) - (\epsilon_k - u_P n_d)$. It is clear that $u_P$ will vanish from such a difference.