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 ϵ_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

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

ϵ_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 ω:

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

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 ($-D$).

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

where[2] and

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

$\mathcal{H}_N^{D,0} \equiv \mathrm{Tr}\left(\mathcal{H}_N \left(1 - \hat{n}_{q\beta}\right)\right)\left(1 - \hat{n}_{q\beta}\right)$ 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

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

We get the following scaling equations for the hole sector:

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

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 ω.

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 (only spin-spin, dropping all lower shell electrons)

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

$$\mathcal{H}_I = \sum_{k,k',\sigma_i} u c^\dagger_{d\sigma_2} c_{d\sigma_4} c_{k'\sigma_3} c^\dagger_{k\sigma_1} \delta_{(\sigma_1+\sigma_2=\sigma_3+\sigma_4)} \tag{0.27}$$

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

$$\mathcal{H}_I = \underbrace{\sum_{k,k',\sigma,\sigma'} u_1 \hat{n}_{d\sigma'} c^\dagger_{k\sigma} c_{k'\sigma}}_{\text{spin-preserving scattering}} + \overbrace{\sum_{k,k',\sigma} u_2 c^\dagger_{d\overline{\sigma}} c_{d\sigma} c^\dagger_{k\sigma} c_{k'\overline{\sigma}}}^{\text{spin-flip scattering}} \tag{0.28}$$

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.

$$\mathcal{H}_{I,N} = \sum_{k,k',\sigma,\sigma'} u_P \hat{n}_{d\sigma'} c^\dagger_{k\sigma} c_{k'\sigma} + \sum_{k,k',\sigma} u_A c^\dagger_{d\overline{\sigma}} c_{d\sigma} c^\dagger_{k\sigma} c_{k'\overline{\sigma}} \tag{0.29}$$

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

$$u_{\uparrow\uparrow} \hat{n}_{d\uparrow} c^\dagger_{k\uparrow} c_{k'\uparrow} + u_{\downarrow\downarrow} \hat{n}_{d\downarrow} c^\dagger_{k\downarrow} c_{k'\uparrow} + u_{\uparrow\downarrow} \hat{n}_{d\uparrow} c^\dagger_{k\downarrow} c_{k'\downarrow} + u_{\downarrow\uparrow} \hat{n}_{d\downarrow} c^\dagger_{k\uparrow} c_{k'\uparrow} \tag{0.30}$$

We define $u_{\sigma,\sigma'} = u_C + \sigma\sigma' u_S$ such that the parallel term can be written as

$$u_C \hat{n}_d \sum_{kk'\sigma} c^\dagger_{k\sigma} c_{k'\sigma} + u_S \hat{m}_d \sum_{kk'\sigma} \sigma c^\dagger_{k\sigma} c_{k'\sigma} = u_C \hat{n}_d \sum_{kk'\sigma} c^\dagger_{k\sigma} c_{k'\sigma} + u_S \hat{S}^z_d \sum_{kk'\sigma} \sigma c^\dagger_{k\sigma} c_{k'\sigma} \tag{0.31}$$

$\hat{n}_d = \sum_\sigma \hat{n}_{d\sigma}$ is the total impurity charge and $\hat{S}^z_d = \hat{n}_{d\uparrow} - \hat{n}_{d\downarrow}$ is the impurity spin magnetization.

$$\mathcal{H}_{I,N} = \sum_{kk'\sigma} \left[\left(u_C \hat{n}_d + u_S \sigma \hat{m}_d \right) c^\dagger_{k\sigma} c_{k'\sigma} + u_A c^\dagger_{d\overline{\sigma}} c_{d\sigma} c^\dagger_{k\sigma} c_{k'\overline{\sigma}} \right] \tag{0.32}$$

For the time being, we will keep just the spin interaction part. The interaction can be written down in the expanded form:

$$\mathcal{H}_{I,N} = u_S \hat{S}^z_d \sum_{kk'} \left(c^\dagger_{k\uparrow} c_{k'\uparrow} - c^\dagger_{k\downarrow} c_{k'\downarrow} \right) + u_A \sum_{kk'} \left(S^+_d c^\dagger_{k\downarrow} c_{k'\uparrow} + S^-_d c^\dagger_{k\uparrow} c_{k'\downarrow} \right) \tag{0.33}$$

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

$$\begin{aligned}\mathcal{H}_N &= H_{N-1} + H_{imp} + \left(\epsilon_q + \beta u_s \hat{m}_d\right)\hat{n}_{q\beta} + V_q c^\dagger_{q\beta}c_{d\beta} + \text{h.c.}\\ &\quad + \sum_{k<\Lambda_N}\left[u_S\beta\hat{m}_d\left(c^\dagger_{k\beta}c_{q\beta} + c^\dagger_{q\beta}c_{k\beta}\right) + u_A\left(c^\dagger_{d\beta}c_{d\overline{\beta}}c^\dagger_{k\overline{\beta}}c_{q\beta} + c^\dagger_{d\overline{\beta}}c_{d\beta}c^\dagger_{q\beta}c_{k\overline{\beta}}\right)\right]\end{aligned} \tag{0.34}$$

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

$$H_{N-1} = \sum_{k<\Lambda_N,\sigma}\left[\left(\epsilon_k + \sigma u_S \hat{S}^z_d\right)\hat{n}_{k\sigma} + V_k c^\dagger_{k\sigma}c_{d\sigma} + \text{h.c.}\right] + H_{I,N-1} \tag{0.35}$$

Some useful expressions

- $\hat{m}_d = \beta\left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right)$
- $\tilde{\epsilon}_{k\beta} = \epsilon_k + \beta u_S\hat{m}_d = \epsilon_k + u_S\left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right)$

2.1 Particle sector

The renormalization in the Hamiltonian in the particle sector is

$$\begin{aligned}\Delta^+\mathcal{H}_N &= \sum_{q\beta}\left[V^*_q c^\dagger_{d\beta}c_{q\beta} + \beta u_S\hat{m}_d\sum_k c^\dagger_{k\beta}c_{q\beta} + u_A\sum_k c^\dagger_{d\beta}c_{d\overline{\beta}}c^\dagger_{k\overline{\beta}}c_{q\beta}\right]\times\frac{1}{\hat{\omega} - \mathcal{H}^+_D}\\ &\qquad\times\left[V_q c^\dagger_{q\beta}c_{d\beta} + \beta u_S\hat{m}_d\sum_k c^\dagger_{q\beta}c_{k\beta} + u_A\sum_k c^\dagger_{d\overline{\beta}}c_{d\beta}c^\dagger_{q\beta}c_{k\overline{\beta}}\right]\\ &= \sum_{q\beta}\left[V^*_q c^\dagger_{d\beta}c_{q\beta} + u_S\left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right)\sum_k c^\dagger_{k\beta}c_{q\beta} + u_A\sum_k c^\dagger_{d\beta}c_{d\overline{\beta}}c^\dagger_{k\overline{\beta}}c_{q\beta}\right]\times\frac{1}{\hat{\omega} - \mathcal{H}^+_D}\\ &\qquad\times\left[V_q c^\dagger_{q\beta}c_{d\beta} + u_S\left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right)\sum_k c^\dagger_{q\beta}c_{k\beta} + u_A\sum_k c^\dagger_{d\overline{\beta}}c_{d\beta}c^\dagger_{q\beta}c_{k\overline{\beta}}\right]\end{aligned} \tag{0.36}$$

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 $(q\beta)$.

$$\begin{aligned}\mathcal{H}^+_D &= \sum_{k<\Lambda_N,\sigma}\left(\epsilon_k + \sigma u_S\hat{m}_d\right)\hat{n}_{k\sigma} + \left(\epsilon_q + \beta u_S\hat{m}_d\right)\hat{n}_{q\beta} + H_{imp}\\ \mathcal{H}^-_D &= \sum_{k<\Lambda_N,\sigma}\left(\epsilon_k + \sigma u_S\hat{m}_d\right)\hat{n}_{k\sigma} + H_{imp}\end{aligned} \tag{0.37}$$

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.

$$\Delta_1^+ \mathcal{H}_N = \sum_{q\beta} |V_q|^2 c^\dagger_{d\beta} c_{q\beta} \frac{1}{\hat{\omega} - \mathcal{H}_D^+} c^\dagger_{q\beta} c_{d\beta} \tag{0.38}$$

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

$$\begin{aligned} H_1 \equiv \mathcal{H}_D^+ &= \sum_{k<\Lambda_N,\sigma} \left(\epsilon_k + \sigma u_s(k) \hat{m}_d\right) \hat{n}_{k\sigma} + \left(\epsilon_q^+ + \beta u_s(q^+) \hat{m}_d\right) + \epsilon_d \hat{n}_{d\overline{\beta}} \\ &= \sum_{k<\Lambda_N,\sigma} \left(\epsilon_k - \sigma\beta u_s(k) \hat{n}_{d\overline{\beta}}\right) \hat{n}_{k\sigma} + \left(\epsilon_q^+ - \beta\beta u_s(q^+) \hat{n}_{d\overline{\beta}}\right) + \epsilon_d \hat{n}_{d\overline{\beta}} \\ &= \sum_{k<\Lambda_N,\sigma} \left(\epsilon_k - \sigma\beta u_s(k) \hat{n}_{d\overline{\beta}}\right) \hat{n}_{k\sigma} + \left[\epsilon_q^+ - u_S(q^+) \hat{n}_{d\overline{\beta}}\right] + \epsilon_d \hat{n}_{d\overline{\beta}} \end{aligned} \tag{0.39}$$

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

$$\begin{aligned} \Delta_1^+ \mathcal{H}_N &= \sum_{q\beta} |V_q|^2 c^\dagger_{d\beta} c_{q\beta} c^\dagger_{q\beta} c_{d\beta} \frac{1}{\omega - H_1} \\ &= \sum_{q\beta} |V_q|^2 \hat{n}_{d\beta} \left(1 - \hat{n}_{q\beta}\right) \frac{1}{\omega - H_1} \end{aligned} \tag{0.40}$$

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

$$\begin{aligned} H_0 &= \sum_{k<\Lambda_N,\sigma} \left[\epsilon_k + \sigma\beta u_s(k) \left(1 - \hat{n}_{d\overline{\beta}}\right)\right] \hat{n}_{k\sigma} + \epsilon_d + (\epsilon_d + U) \hat{n}_{d\overline{\beta}} \\ &= H_1 + \epsilon_d + U \hat{n}_{d\overline{\beta}} + \sum_{k<\Lambda_N \sigma} \sigma\beta u_S(k) \hat{n}_{k,\sigma} - \left(\epsilon_q^+ - u_S(q^+) \hat{n}_{d\overline{\beta}}\right) \end{aligned} \tag{0.41}$$

The third term has a sum over all the shells below the one we are decoupling right now. It can be written as

$$\mathcal{E}_0 = \sum_{k<\Lambda_N} u_S(k) \left(\beta^2 \hat{n}_{k,\beta} + \beta(-\beta) \hat{n}_{k,\overline{\beta}}\right) = \sum_{k<\Lambda_N} u_S(k) \left(\hat{n}_{k\uparrow} - \hat{n}_{k\downarrow}\right) \tag{0.42}$$

For a time-reversal symmetric Hamiltonian, we can expect that the number of electrons with spin $\uparrow$ is equal to that with $\downarrow$, so $\mathcal{E}_0$ will vanish.

$$\Delta_1^+ \mathcal{H}_N = \sum_{q\beta} |V_q|^2 \hat{n}_{d\beta} \left(1 - \hat{n}_{q\beta}\right) \frac{1}{\omega - H_0 + \epsilon_d + U \hat{n}_{d\overline{\beta}} - \left(\epsilon_q^+ - u_S \hat{n}_{d\overline{\beta}}\right)} \tag{0.43}$$

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

$$\begin{aligned}
\Delta_1^+\mathcal{H}_N &= \sum_{q\beta} |V_q|^2 \hat{n}_{d\beta} \frac{1}{\omega - \epsilon_q^+ + \epsilon_d + (U + u_S(q^+))\,\hat{n}_{d\bar{\beta}}} \\
&= \sum_{q\beta} \hat{n}_{d\beta} \left[\frac{|V_q^1|^2 \hat{n}_{d\bar{\beta}}}{\omega - \epsilon_q^+ + \epsilon_d + (U + u_S(q^+))} + \frac{|V_q^0|^2 \left(1 - \hat{n}_{d\bar{\beta}}\right)}{\omega - \epsilon_q^+ + \epsilon_d} \right] \\
&= \sum_{q\beta} \hat{n}_{d\beta} \left[\frac{|V_q^0|^2}{\omega - \epsilon_q^+ + \epsilon_d} + \hat{n}_{d\bar{\beta}} \left(\frac{|V_q^1|^2}{\omega - \epsilon_q^+ + \epsilon_d + (U + u_S(q^+))} - \frac{|V_q^0|^2}{\omega - \epsilon_q^+ + \epsilon_d} \right) \right]
\end{aligned} \tag{0.44}$$

2.

$$\Delta_2^+\mathcal{H}_N = \sum_{q\beta k\sigma} u_S V_q^* c_{d\beta}^\dagger c_{q\beta} \frac{1}{\omega - \mathcal{H}_D^+} \left(\hat{n}_{d\beta} - \hat{n}_{d\bar{\beta}} \right) c_{q\beta}^\dagger c_{k\beta} \tag{0.45}$$

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

$$c_{d\beta}^\dagger \left(\hat{n}_{d\beta} - \hat{n}_{d\bar{\beta}} \right) = -c_{d\beta}^\dagger \hat{n}_{d\bar{\beta}} \tag{0.46}$$

The expression simplifies to

$$\Delta_2^+\mathcal{H}_N = -\sum_{q\beta k} u_S V_q^* c_{d\beta}^\dagger c_{q\beta} \hat{n}_{d\bar{\beta}} \frac{1}{\omega - \mathcal{H}_D^+} c_{q\beta}^\dagger c_{k\beta} \tag{0.47}$$

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

$$H_1 = \epsilon_q^+ + u_S \beta m_d + \epsilon_d + \mathcal{E}_0 = \epsilon_q^+ - u_S + \epsilon_d \tag{0.48}$$

The first term $\epsilon_q^+ - u_S$ 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 background energy $\mathcal{E}_0$ is of course zero as shown in the previous section.

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

$$H_0 = \mathcal{E}_0 + \epsilon_d = H_1 - \epsilon_q^+ + u_S \tag{0.49}$$

$$\begin{aligned}
\Delta_2^+\mathcal{H}_N &= -\sum_{q\beta k} u_S V_q^* c_{d\beta}^\dagger c_{q\beta} \hat{n}_{d\bar{\beta}} c_{q\beta}^\dagger c_{k\beta} \frac{1}{\omega - H_1 - \epsilon_q^+ + u_S} \\
&= \sum_{q\beta k} c_{d\beta}^\dagger c_{k\beta} \frac{-\hat{n}_{d\bar{\beta}} u_S V_q^{1*}}{\omega - \epsilon_q^+ + u_S}
\end{aligned} \tag{0.50}$$

3.

$$\Delta_3^+\mathcal{H}_N = \sum_{q\beta k} u_A V_q^* c^\dagger_{d\beta} c_{q\beta} \frac{1}{\omega - \mathcal{H}_D^+} c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k\overline{\beta}} \tag{0.51}$$

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

$$H_1 = \epsilon_q^+ - u_S + \epsilon_d + \mathcal{E}_0 \tag{0.52}$$

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

$$H_0 = \epsilon_k + \mathcal{E}_0 + \epsilon_d = H_1 - \epsilon_q^+ + u_S \tag{0.53}$$

$$\begin{aligned}
\Delta_2^+\mathcal{H}_N &= \sum_{q\beta k} u_A V_q^* c^\dagger_{d\beta} c_{q\beta} c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k\overline{\beta}} \frac{1}{\omega - H_1 - \epsilon_q^+ + u_S} \\
&= \sum_{q\beta k} -u_A V_q^* \hat{n}_{d\beta} \left(1 - \hat{n}_{q\beta}\right) c^\dagger_{d\overline{\beta}} c_{k\overline{\beta}} \frac{1}{\omega - H_1 - \epsilon_q^+ + u_S} \\
&= \sum_{q\beta k} c^\dagger_{d\beta} c_{k\beta} \frac{-u_A {V_q^1}^* \hat{n}_{d\overline{\beta}}}{\omega - \epsilon_q^+ + u_S}
\end{aligned} \tag{0.54}$$

4.

$$\Delta_4^+\mathcal{H}_N = \sum_{q\beta k\sigma} u_S V_q \left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right) c^\dagger_{k\beta} c_{q\beta} \frac{1}{\omega - \mathcal{H}_D^+} c^\dagger_{q\beta} c_{d\beta} \tag{0.55}$$

The first step is a simplification:

$$\left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right) = -\hat{n}_{d\overline{\beta}} c_{d\beta} \tag{0.56}$$

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

$$H_1 = \epsilon_q^+ - u_S + \epsilon_d + \mathcal{E}_0 \tag{0.57}$$

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

$$H_0 = 2\epsilon_d + U + \mathcal{E}_0 = H_1 + \epsilon_d + U - \epsilon_q^+ + u_S \tag{0.58}$$

$$\begin{aligned}
\Delta_4^+\mathcal{H}_N &= -\sum_{q\beta k} u_S V_q \hat{n}_{d\overline{\beta}} c^\dagger_{k\beta} c_{q\beta} c^\dagger_{q\beta} c_{d\beta} \frac{1}{\omega - H_0 + \epsilon_d + U - \epsilon_q^+ + u_S} \\
&= \sum_{q\beta k} u_S V_q \hat{n}_{d\overline{\beta}} \left(1 - \hat{n}_{q\beta}\right) c^\dagger_{k\beta} c_{d\beta} \frac{-1}{\omega + \epsilon_d + U - \epsilon_q^+ + u_S} \\
&= \sum_{q\beta k} c^\dagger_{k\beta} c_{d\beta} \frac{-u_S V_q^1 \hat{n}_{d\overline{\beta}}}{\omega - \epsilon_q^+ + \epsilon_d + U + u_S}
\end{aligned} \tag{0.59}$$

5.

$$\Delta_5^+\mathcal{H}_N = \sum_{q\beta k\sigma} u_A V_q c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{q\beta} \frac{1}{\omega - \mathcal{H}_D^+} c^\dagger_{q\beta} c_{d\beta} \tag{0.60}$$

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

$$H_1 = \epsilon_q^+ - u_S + \epsilon_d + \mathcal{E}_0 \tag{0.61}$$

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

$$H_0 = 2\epsilon_d + U + \mathcal{E}_0 = H_1 + \epsilon_d + U - \epsilon_q^+ + u_S \tag{0.62}$$

$$\begin{aligned}\Delta_5^+\mathcal{H}_N &= \sum_{q\beta k} u_A V_q c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{q\beta} c^\dagger_{q\beta} c_{d\beta} \frac{1}{\omega - H_0 + \epsilon_d + U - \epsilon_q^+ + u_S} \\ &= -\sum_{q\beta k} u_A V_q \left(1 - \hat{n}_{q\beta}\right) \hat{n}_{d\beta} c^\dagger_{k\overline{\beta}} c_{d\overline{\beta}} \frac{1}{\omega + \epsilon_d + U - \epsilon_q^+ + u_S} \\ &= \sum_{q\beta k} c^\dagger_{k\beta} c_{d\beta} \frac{-u_A V_q^1 \hat{n}_{d\overline{\beta}}}{\omega - \epsilon_q^+ + \epsilon_d + U + u_S}\end{aligned} \tag{0.63}$$

6.

$$\Delta_6^+\mathcal{H}_N = \sum_{k'q\beta k} u_S(k,q) u_S(q,k') \left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right) c^\dagger_{k\beta} c_{q\beta} \frac{1}{\omega - \mathcal{H}_D^+} \left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right) c^\dagger_{q\beta} c_{k'\beta} \tag{0.64}$$

The first step is a simplification:

$$\left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right)^2 = \hat{n}_{d\beta} + \hat{n}_{d\overline{\beta}} - 2\hat{n}_{d\beta}\hat{n}_{d\overline{\beta}} = \hat{n}_d - 2\hat{n}_{d\beta}\hat{n}_{d\overline{\beta}} \tag{0.65}$$

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

$$H_1 = \epsilon_q^+ + u_S(q^+)\left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right) + \epsilon_d \hat{n}_d + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + \mathcal{E}_0 \tag{0.66}$$

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

$$H_0 = \mathcal{E}_0 + \epsilon_d \hat{n}_d + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} = H_1 - \epsilon_q^+ - u_S(q^+)\left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right) \tag{0.67}$$

$$
\begin{aligned}
\Delta_6^+\mathcal{H}_N &= \sum_{k'q\beta k} \left(\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right) c^\dagger_{k\beta} c_{q\beta} c^\dagger_{q\beta} c_{k'\beta} \frac{u_S(k,q)u_S(q,k')}{\omega - H_1} \\
&= \sum_{k'q\beta k} \left(\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right)\left(1 - \hat{n}_{q\beta}\right) c^\dagger_{k\beta} c_{k'\beta} \frac{u_S(k,q)u_S(q,k')}{\omega - H_0 - \epsilon_q^+ - u_S(q^+)\left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right)} \\
&= \sum_{k'q\beta k} c^\dagger_{k\beta} c_{k'\beta} \frac{u_S(k,q)u_S(q,k')\left(\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right)}{\omega - \epsilon_q^+ - u_S(q^+)\left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right)} \\
&= \sum_{k'q\beta k} c^\dagger_{k\beta} c_{k'\beta} \left[\frac{u_S(k,q)u_S(q,k')\hat{n}_{d\beta}\left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega - \epsilon_q^+ - u_S(q^+)} + \frac{u_S(k,q)u_S(q,k')\hat{n}_{d\overline{\beta}}\left(1 - \hat{n}_{d\beta}\right)}{\omega - \epsilon_q^+ + u_S(q^+)}\right]
\end{aligned}
\tag{0.68}
$$

In the last step, we used the fact that $\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}$ is not zero only in the singly occupied subspace, hence we can expand it into $\hat{n}_\uparrow(1-\hat{n}_\downarrow) + \mathrm{p} \leftrightarrow \mathrm{h}$.

7.

$$
\Delta_7^+\mathcal{H}_N = \sum_{q\beta kk'} u_S(k,q)u_A(q,k')\left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right) c^\dagger_{k\beta} c_{q\beta} \frac{1}{\omega - \mathcal{H}_D^+} c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k'\overline{\beta}} \tag{0.69}
$$

The first step is a simplification:

$$
\left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right) c^\dagger_{d\overline{\beta}} c_{d\beta} = -c^\dagger_{d\overline{\beta}} c_{d\beta} \tag{0.70}
$$

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

$$
H_1 = \epsilon_q^+ - u_S(q^+) + \epsilon_d + \mathcal{E}_0 \tag{0.71}
$$

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

$$
H_0 = \mathcal{E}_0 + \epsilon_d = H_1 - \epsilon_q^+ + u_S(q^+) \tag{0.72}
$$

$$
\begin{aligned}
\Delta_7^+\mathcal{H}_N &= \sum_{q\beta kk'} u_S(k,q)u_A(q,k') c^\dagger_{k\beta} c_{q\beta} c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k'\overline{\beta}} \frac{-1}{\omega - H_1} \\
&= \sum_{q\beta kk'} \left(1 - \hat{n}_{q\beta}\right) c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{k\beta} c_{k'\overline{\beta}} \frac{-u_S(k,q)u_A(q,k')}{\omega - \epsilon_q^+ + u_S(q^+)} \\
&= \sum_{q\beta kk'} c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{k\beta} c_{k'\overline{\beta}} \frac{-u_S(k,q)u_A(q,k')}{\omega - \epsilon_q^+ + u_S(q^+)}
\end{aligned}
\tag{0.73}
$$

8.

$$
\Delta_8^+\mathcal{H}_N = \sum_{q\beta kk'} u_A(k,q)u_S(q,k') c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{q\beta} \frac{1}{\omega - \mathcal{H}_D^+} \left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right) c^\dagger_{q\beta} c_{k'\beta} \tag{0.74}
$$

The first step is a simplification:

$$c^\dagger_{d\beta}c_{d\overline{\beta}}\left(\hat{n}_{d\beta}-\hat{n}_{d\overline{\beta}}\right)=-c^\dagger_{d\beta}c_{d\overline{\beta}} \tag{0.75}$$

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

$$H_1=\epsilon_q^+-u_S(q^+)+\epsilon_d+\mathcal{E}_0 \tag{0.76}$$

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

$$H_0=\mathcal{E}_0+\epsilon_d=H_1-\epsilon_q^++u_S(q^+) \tag{0.77}$$

$$\begin{aligned}\Delta_8^+\mathcal{H}_N&=-\sum_{q\beta kk'}u_A(k,q)u_S(q,k')c^\dagger_{d\beta}c_{d\overline{\beta}}c^\dagger_{k\overline{\beta}}c_{q\beta}c^\dagger_{q\beta}c_{k'\beta}\frac{1}{\omega-H_0-\epsilon_q^++u_S(q^+)}\\&=\sum_{q\beta kk'}\left(1-\hat{n}_{q\beta}\right)c^\dagger_{d\beta}c_{d\overline{\beta}}c^\dagger_{k\overline{\beta}}c_{k'\beta}\frac{-u_A(k,q)u_S(q,k')}{\omega-H_0-\epsilon_q^++u_S(q^+)}\\&=\sum_{q\beta kk'}c^\dagger_{d\beta}c_{d\overline{\beta}}c^\dagger_{k\overline{\beta}}c_{k'\beta}\frac{-u_A(k,q)u_S(q,k')}{\omega-\epsilon_q^++u_S(q^+)}\end{aligned} \tag{0.78}$$

9.

$$\Delta_9^+\mathcal{H}_N=\sum_{q\beta kk'}u_A(k,q)u_A(q,k')c^\dagger_{d\beta}c_{d\overline{\beta}}c^\dagger_{k\overline{\beta}}c_{q\beta}\frac{1}{\omega-\mathcal{H}_D^+}c^\dagger_{d\overline{\beta}}c_{d\beta}c^\dagger_{q\beta}c_{k'\overline{\beta}} \tag{0.79}$$

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

$$H_1=\epsilon_q^+-u_S(q^+)+\epsilon_d+\mathcal{E}_0 \tag{0.80}$$

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

$$H_0=\mathcal{E}_0+\epsilon_d=H_1-\epsilon_q^++u_S(q^+) \tag{0.81}$$

$$\begin{aligned}\Delta_9^+\mathcal{H}_N&=\sum_{q\beta kk'}u_A(k,q)u_A(q,k')c^\dagger_{d\beta}c_{d\overline{\beta}}c^\dagger_{k\overline{\beta}}c_{q\beta}c^\dagger_{d\overline{\beta}}c_{d\beta}c^\dagger_{q\beta}c_{k'\overline{\beta}}\frac{1}{\omega-H_0-\epsilon_q^++u_S(q^+)}\\&=\sum_{q\beta kk'}\left(1-\hat{n}_{q\beta}\right)\hat{n}_{d\beta}\left(1-\hat{n}_{d\overline{\beta}}\right)c^\dagger_{k\overline{\beta}}c_{k'\overline{\beta}}\frac{u_A(k,q)u_A(q,k')}{\omega-H_0-\epsilon_q^++u_S(q^+)}\\&=\sum_{q\beta kk'}c^\dagger_{k\beta}c_{k'\beta}\frac{u_A(k,q)u_A(q,k')\hat{n}_{d\overline{\beta}}\left(1-\hat{n}_{d\beta}\right)}{\omega-\epsilon_q^++u_S(q^+)}\end{aligned} \tag{0.82}$$

2.2 Hole sector

The renormalization in the Hamiltonian in the hole sector is

$$\begin{aligned}\Delta^{+}\mathcal{H}_N = \sum_{q\beta}\left[V_q c^\dagger_{q\beta}c_{d\beta} + u_P\sum_{k\sigma}\hat{n}_{d\sigma}c_{k\beta}c^\dagger_{q\beta} + u_A\sum_{k\sigma}c^\dagger_{d\overline{\beta}}c^\dagger_{q\beta}c_{d\beta}c_{k\overline{\beta}}\right]\times\frac{1}{\hat{\omega}-\mathcal{H}^{-}_D}\\ \times\left[V^*_q c^\dagger_{d\beta}c_{q\beta} + u_P\sum_{k\sigma}\hat{n}_{d\sigma}c_{q\beta}c^\dagger_{k\beta} + u_A\sum_{k\sigma}c^\dagger_{d\beta}c^\dagger_{k\overline{\beta}}c_{d\overline{\beta}}c_{q\beta}\right]\end{aligned} \tag{0.83}$$

1.

$$\Delta^{-}_1\mathcal{H}_N = \sum_{q\beta}|V_q|^2 c^\dagger_{q\beta}c_{d\beta}\frac{1}{\hat{\omega}-\mathcal{H}^{-}_D}c^\dagger_{d\beta}c_{q\beta} \tag{0.84}$$

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

$$H_1 = \epsilon_d + (\epsilon_d + U)\,\hat{n}_{d\overline{\beta}} + \mathcal{E}_0 - u_S \tag{0.85}$$

$$\Delta^{-}_1\mathcal{H}_N = \sum_{q\beta}|V_q|^2\hat{n}_{q\beta}\left(1-\hat{n}_{d\beta}\right)\frac{1}{\omega - H_1} \tag{0.86}$$

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

$$\begin{aligned}H_0 &= \epsilon^{-}_q + \epsilon_d\hat{n}_{d\overline{\beta}} + \mathcal{E}_0\\ &= H_1 + \epsilon^{-}_q - \epsilon_d - (U-u_S)\,\hat{n}_{d\overline{\beta}}\end{aligned} \tag{0.87}$$

$$\begin{aligned}\Delta^{-}_1\mathcal{H}_N &= \sum_{q\beta}|V_q|^2\hat{n}_{q\beta}\left(1-\hat{n}_{d\beta}\right)\frac{1}{\omega - H_0 + \epsilon^{-}_q - \epsilon_d - (U-u_S)\,\hat{n}_{d\overline{\beta}}}\\ &= \sum_{q\beta}|V_q|^2\left(1-\hat{n}_{d\beta}\right)\frac{1}{\omega + \epsilon^{-}_q - \epsilon_d - (U-u_S)\,\hat{n}_{d\overline{\beta}}}\\ &= \sum_{q\beta}\left(1-\hat{n}_{d\beta}\right)\left[\frac{|V^1_q|^2\hat{n}_{d\overline{\beta}}}{\omega+\epsilon^{-}_q-\epsilon_d-(U-u_S)} + \frac{|V^0_q|^2\left(1-\hat{n}_{d\overline{\beta}}\right)}{\omega+\epsilon^{-}_q-\epsilon_d}\right]\\ &= \sum_{q\beta}\left[\hat{n}_{d\overline{\beta}}\left(\frac{|V^1_q|^2}{\omega+\epsilon^{-}_q-\epsilon_d-U+u_S} - \frac{2|V^0_q|^2}{\omega+\epsilon^{-}_q-\epsilon_d}\right)\right.\\ &\qquad\left. + \hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\left(\frac{|V^0_q|^2}{\omega+\epsilon^{-}_q-\epsilon_d} - \frac{|V^1_q|^2}{\omega+\epsilon^{-}_q-\epsilon_d-U+u_S}\right)\right]\end{aligned} \tag{0.88}$$

2.

$$\Delta_2^- \mathcal{H}_N = \sum_{q\beta k} u_S V_q c_{q\beta}^\dagger c_{d\beta} \frac{1}{\hat{\omega} - \mathcal{H}_D^-} \left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right) c_{k\beta}^\dagger c_{q\beta} \tag{0.89}$$

The first step is a simplification:

$$c_{d\beta}\left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right) = c_{d\beta}\left(1 - \hat{n}_{d\overline{\beta}}\right) \tag{0.90}$$

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

$$H_1 = \epsilon_d + (\epsilon_d + U)\hat{n}_{d\overline{\beta}} + \mathcal{E}_0 - u_S\left(1 - \hat{n}_{d\overline{\beta}}\right) \tag{0.91}$$

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

$$\begin{aligned} H_0 &= \epsilon_q^- + \mathcal{E}_0 + \epsilon_d + (\epsilon_d + U)\hat{n}_{d\overline{\beta}} \\ &= H_1 + \epsilon_q^- + u_S\left(1 - \hat{n}_{d\overline{\beta}}\right) \end{aligned} \tag{0.92}$$

$$\begin{aligned} \Delta_2^- \mathcal{H}_N &= \sum_{q\beta k} u_S V_q c_{q\beta}^\dagger c_{d\beta}\left(1 - \hat{n}_{d\overline{\beta}}\right) c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega - H_1} \\ &= \sum_{q\beta k} \hat{n}_{q\beta}\left(1 - \hat{n}_{d\overline{\beta}}\right) c_{k\beta}^\dagger c_{d\beta} \frac{-u_S V_q}{\omega + \epsilon_q^- + u_S} \\ &= \sum_{q\beta k} c_{k\beta}^\dagger c_{d\beta} \frac{-u_S V_q^0\left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega + \epsilon_q^- + u_S} \end{aligned} \tag{0.93}$$

3.

$$\Delta_3^- \mathcal{H}_N = \sum_{q\beta k} u_A V_q c_{q\beta}^\dagger c_{d\beta} \frac{1}{\hat{\omega} - \mathcal{H}_D^-} c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{q\beta} \tag{0.94}$$

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

$$H_1 = \epsilon_d + \mathcal{E}_0 - u_S \tag{0.95}$$

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

$$H_0 = \epsilon_q^- + \mathcal{E}_0 + \epsilon_d = H_1 + \epsilon_q^- + u_S \tag{0.96}$$

$$\begin{aligned} \Delta_3^- \mathcal{H}_N &= \sum_{q\beta k} u_A V_q c_{q\beta}^\dagger c_{d\beta} c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{q\beta} \frac{1}{\omega - H_1} \\ &= \sum_{q\beta k} u_A V_q \hat{n}_{q\beta}\left(1 - \hat{n}_{d\beta}\right) c_{k\overline{\beta}}^\dagger c_{d\overline{\beta}} \frac{-1}{\omega + \epsilon_q^- + u_S} \\ &= \sum_{q\beta k} c_{k\beta}^\dagger c_{d\beta} \frac{-u_A V_q^0\left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega + \epsilon_q^- + u_S} \end{aligned} \tag{0.97}$$

4.

$$\Delta_4^- \mathcal{H}_N = \sum_{q\beta k} u_S V_q^* \left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right) c_{q\beta}^\dagger c_{k\beta} \frac{1}{\hat{\omega} - \mathcal{H}_D^-} c_{d\beta}^\dagger c_{q\beta} \tag{0.98}$$

There is a simplification:

$$\left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right) c_{d\beta}^\dagger = \left(1 - \hat{n}_{d\overline{\beta}}\right) c_{d\beta}^\dagger \tag{0.99}$$

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

$$H_1 = \epsilon_d + (\epsilon_d + U)\, \hat{n}_{d\overline{\beta}} + \mathcal{E}_0 - u_S \tag{0.100}$$

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

$$H_0 = \mathcal{E}_0 + \epsilon_q^- + \epsilon_d \hat{n}_{d\overline{\beta}} = H_1 + \epsilon_q^- + u_S - \epsilon_d - U \hat{n}_{d\overline{\beta}} \tag{0.101}$$

$$\begin{aligned}
\Delta_4^- \mathcal{H}_N &= \sum_{q\beta k} u_S V_q^* \left(1 - \hat{n}_{d\overline{\beta}}\right) c_{q\beta}^\dagger c_{k\beta} c_{d\beta}^\dagger c_{q\beta} \frac{1}{\omega - H_0 + \epsilon_q^- + u_S - \epsilon_d - U \hat{n}_{d\overline{\beta}}} \\
&= \sum_{q\beta k} \hat{n}_{q\beta} u_S V_q^* \left(1 - \hat{n}_{d\overline{\beta}}\right) c_{k\beta} c_{d\beta}^\dagger \frac{1}{\omega + \epsilon_q^- + u_S - \epsilon_d - U \hat{n}_{d\overline{\beta}}} \\
&= \sum_{q\beta k} c_{d\beta}^\dagger c_{k\beta} \frac{-u_S V_q^{0*} \left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega + \epsilon_q^- - \epsilon_d + u_S}
\end{aligned} \tag{0.102}$$

5.

$$\Delta_5^- \mathcal{H}_N = \sum_{q\beta k} u_A V_q^* c_{d\overline{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\overline{\beta}} \frac{1}{\hat{\omega} - \mathcal{H}_D^-} c_{d\beta}^\dagger c_{q\beta} \tag{0.103}$$

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

$$H_1 = \mathcal{E}_0 - u_S + \epsilon_d \tag{0.104}$$

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

$$H_0 = \mathcal{E}_0 + \epsilon_q^- = H_1 + \epsilon_q^- + u_S - \epsilon_d \tag{0.105}$$

$$\begin{aligned}
\Delta_5^- \mathcal{H}_N &= \sum_{q\beta k} u_A V_q^* c_{d\overline{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\overline{\beta}} c_{d\beta}^\dagger c_{q\beta} \frac{1}{\hat{\omega} - H_0 + \epsilon_q^- + u_S - \epsilon_d} \\
&= \sum_{q\beta k} u_A V_q^* \hat{n}_{q\beta} \left(1 - \hat{n}_{d\beta}\right) c_{d\overline{\beta}}^\dagger c_{k\overline{\beta}} \frac{-1}{\omega + \epsilon_q^- + u_S - \epsilon_d} \\
&= \sum_{q\beta k} c_{d\overline{\beta}}^\dagger c_{k\overline{\beta}} \frac{-u_A V_q^{0*} \left(1 - \hat{n}_{d\beta}\right)}{\omega + \epsilon_q^- - \epsilon_d + u_S}
\end{aligned} \tag{0.106}$$

6.

$$\Delta_6^- \mathcal{H}_N = \sum_{q\beta kk'} u_S(q,k')u_S(k,q)\left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right)c^\dagger_{q\beta}c_{k'\beta}\frac{1}{\hat{\omega} - \mathcal{H}_D^-}\left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right)c^\dagger_{k\beta}c_{q\beta} \tag{0.107}$$

From eq. 0.65,

$$\left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right)^2 = \hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} \tag{0.108}$$

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

$$H_1 = \epsilon_d \hat{n}_d + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + \mathcal{E}_0 - u_S(q^-)\left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right) \tag{0.109}$$

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

$$H_0 = \epsilon_q^- + \mathcal{E}_0 + \epsilon_d\hat{n}_d + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} = H_1 + \epsilon_q^- + u_S(q^-)\left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right) \tag{0.110}$$

$$\begin{aligned}
\Delta_6^- \mathcal{H}_N &= \sum_{q\beta kk'} u_S(q,k')u_S(k,q)\left(\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right)c^\dagger_{q\beta}c_{k'\beta}c^\dagger_{k\beta}c_{q\beta}\frac{1}{\omega - H_1} \\
&= \sum_{q\beta kk'} \hat{n}_{q\beta}\left(\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right)c_{k'\beta}c^\dagger_{k\beta}\frac{u_S(q,k')u_S(k,q)}{\omega - H_0 + \epsilon_q^- + u_S(q^-)\left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right)} \\
&= -\sum_{q\beta kk'} c^\dagger_{k\beta}c_{k'\beta}\left[\frac{u_S(q,k')u_S(k,q)\hat{n}_{d\beta}\left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega + \epsilon_q^- + u_S(q^-)} + \frac{u_S(q,k')u_S(k,q)\hat{n}_{d\overline{\beta}}\left(1 - \hat{n}_{d\beta}\right)}{\omega + \epsilon_q^- - u_S(q^-)}\right] \\
&\quad + \sum_{q\beta k} u_S(q,k')u_S(k,q)\left[\frac{\hat{n}_{d\beta}\left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega + \epsilon_q^- + u_S(q^-)} + \frac{\hat{n}_{d\overline{\beta}}\left(1 - \hat{n}_{d\beta}\right)}{\omega + \epsilon_q^- - u_S(q^-)}\right]
\end{aligned} \tag{0.111}$$

7.

$$\Delta_7^- \mathcal{H}_N = \sum_{q\beta kk'} u_S(q,k')u_A(k,q)\left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right)c^\dagger_{q\beta}c_{k'\beta}\frac{1}{\hat{\omega} - \mathcal{H}_D^-}c^\dagger_{d\beta}c_{d\overline{\beta}}c^\dagger_{k\overline{\beta}}c_{q\beta} \tag{0.112}$$

Simplification:

$$\left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right)c^\dagger_{d\beta}c_{d\overline{\beta}} = c^\dagger_{d\beta}c_{d\overline{\beta}} \tag{0.113}$$

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

$$H_1 = \epsilon_d + \mathcal{E}_0 - u_S(q^-) \tag{0.114}$$

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

$$H_0 = \epsilon_q^- + \mathcal{E}_0 + \epsilon_d = H_1 + \epsilon_q^- + u_S(q^-) \tag{0.115}$$

$$
\begin{aligned}
\Delta_7^- \mathcal{H}_N &= \sum_{q\beta kk'} u_S(q,k')u_A(k,q)c^\dagger_{q\beta}c_{k'\beta}c^\dagger_{d\beta}c_{d\overline{\beta}}c^\dagger_{k\overline{\beta}}c_{q\beta}\frac{1}{\omega - H_1} \\
&= \sum_{q\beta kk'} u_S(q,k')u_A(k,q)\hat{n}_{q\beta}c^\dagger_{d\beta}c_{d\overline{\beta}}c^\dagger_{k\overline{\beta}}c_{k'\beta}\frac{-1}{\omega - H_0 + \epsilon_q^- + u_S(q^-)} \\
&= \sum_{q\beta kk'} c^\dagger_{d\beta}c_{d\overline{\beta}}c^\dagger_{k\overline{\beta}}c_{k'\beta}\frac{-u_S(q,k')u_A(k,q)}{\omega + \epsilon_q^- + u_S(q^-)} \\
&= \sum_{q\beta kk'} c^\dagger_{d\overline{\beta}}c_{d\beta}c^\dagger_{k\beta}c_{k'\overline{\beta}}\frac{-u_S(q,k')u_A(k,q)}{\omega + \epsilon_q^- + u_S(q^-)}
\end{aligned}
\tag{0.116}
$$

8.

$$
\Delta_8^- \mathcal{H}_N = \sum_{q\beta kk'} u_A(q,k')u_S(k,q)c^\dagger_{d\overline{\beta}}c_{d\beta}c^\dagger_{q\beta}c_{k'\overline{\beta}}\frac{1}{\hat{\omega} - \mathcal{H}_D^-}\left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right)c^\dagger_{k\beta}c_{q\beta} \tag{0.117}
$$

Simplification:

$$
c^\dagger_{d\overline{\beta}}c_{d\beta}\left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right) = c^\dagger_{d\overline{\beta}}c_{d\beta} \tag{0.118}
$$

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

$$
H_1 = \mathcal{E}_0 - u_S(q^-) + \epsilon_d \tag{0.119}
$$

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

$$
H_0 = \epsilon_q^- + \mathcal{E}_0 + \epsilon_d = H_1 + \epsilon_q^- + u_S(q^-) \tag{0.120}
$$

$$
\begin{aligned}
\Delta_8^- \mathcal{H}_N &= \sum_{q\beta kk'} u_A(q,k')u_S(k,q)c^\dagger_{d\overline{\beta}}c_{d\beta}c^\dagger_{q\beta}c_{k'\overline{\beta}}c^\dagger_{k\beta}c_{q\beta}\frac{1}{\omega - H_1} \\
&= \sum_{q\beta kk'} u_A(q,k')u_S(k,q)\hat{n}_{q\beta}c^\dagger_{d\overline{\beta}}c_{d\beta}c^\dagger_{k\beta}c_{k'\overline{\beta}}\frac{-1}{\omega - H_0 + \epsilon_q^- + u_S(q^-)} \\
&= \sum_{q\beta kk'} c^\dagger_{d\overline{\beta}}c_{d\beta}c^\dagger_{k\beta}c_{k'\overline{\beta}}\frac{-u_A(q,k')u_S(k,q)}{\omega + \epsilon_q^- + u_S(q^-)}
\end{aligned}
\tag{0.121}
$$

9.

$$
\Delta_9^- \mathcal{H}_N = \sum_{q\beta kk'} u_A(q,k')u_A(k,q)c^\dagger_{d\overline{\beta}}c_{d\beta}c^\dagger_{q\beta}c_{k'\overline{\beta}}\frac{1}{\hat{\omega} - \mathcal{H}_D^-}c^\dagger_{d\beta}c_{d\overline{\beta}}c^\dagger_{k\overline{\beta}}c_{q\beta} \tag{0.122}
$$

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

$$
H_1 = \mathcal{E}_0 - u_S(q^-) + \epsilon_d \tag{0.123}
$$

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

$$H_0 = \epsilon_q^- + \epsilon_d = H_1 + \epsilon_q^- + u_S(q^-) \tag{0.124}$$

$$\begin{aligned}
\Delta_9^- \mathcal{H}_N &= \sum_{q\beta kk'} u_A^2 c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k'\overline{\beta}} c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{q\beta} \frac{1}{\omega - H_1} \\
&= \sum_{q\beta kk'} u_A^2 \hat{n}_{q\beta} c^\dagger_{d\overline{\beta}} c_{d\beta} c_{k'\overline{\beta}} c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} \frac{1}{\omega - H_1} \\
&= -\sum_{q\beta kk'} u_A^2 \hat{n}_{q\beta} \hat{n}_{d\overline{\beta}} c_{d\beta} c_{k'\overline{\beta}} c^\dagger_{d\beta} c^\dagger_{k\overline{\beta}} \frac{1}{\omega - H_1} \\
&= \sum_{q\beta kk'} u_A^2 \hat{n}_{q\beta} \hat{n}_{d\overline{\beta}} \left(1 - \hat{n}_{d\beta}\right) c_{k'\overline{\beta}} c^\dagger_{k\overline{\beta}} \frac{1}{\omega + \epsilon_q^- + u_S(q^-)} \\
&= \sum_{q\beta kk'} c^\dagger_{k\beta} c_{k'\beta} \frac{-u_A^2 \hat{n}_{d\beta} \left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega + \epsilon_q^- + u_S(q^-)} + \sum_{qk} \frac{u_A^2 \left(\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right)}{\omega + \epsilon_q^- + u_S(q^-)}
\end{aligned} \tag{0.125}$$

2.3 Scaling equations

$$\Delta\epsilon_d = \sum_q \left(\frac{|V_q^0|^2}{\omega - \epsilon_q^+ + \epsilon_d} + \frac{|V_q^1|^2}{\omega + \epsilon_q^- - \epsilon_d - U + u_S} - \frac{2|V_q^0|^2}{\omega + \epsilon_q^- - \epsilon_d} + \sum_k \frac{u_S^2 + u_A^2}{\omega + \epsilon_q^- - \epsilon_k} \right)$$

$$\Delta U = \sum_q 2 \left(\frac{|V_q^1|^2}{\omega - \epsilon_q^+ + \epsilon_d + U + u_S} - \frac{|V_q^0|^2}{\omega - \epsilon_q^+ + \epsilon_d} - \frac{|V_q^1|^2}{\omega + \epsilon_q^- - \epsilon_d - U + u_S} + \frac{|V_q^0|^2}{\omega + \epsilon_q^- - \epsilon_d} - \sum_k \frac{4u_S^2 + 2u_A^2}{\omega + \epsilon_q^- - \epsilon_k} \right)$$

$$\Delta V_k^{1*} = -\sum_q V_q^1 \left(\frac{u_A}{\omega - \epsilon_q^+ + \epsilon_d + U + 2u_S} + \frac{u_S}{\omega - \epsilon_q^+ + \epsilon_d + U} \right)$$

$$\Delta V_k^1 = -\sum_q V_q^{1*} \frac{u_A + u_S}{\omega + \epsilon_k - \epsilon_q^+ + u_S}$$

$$\Delta V_k^0 = -\sum_q V_q^0 \left(\frac{u_S}{\omega + \epsilon_q^- - \epsilon_k} + \frac{u_A}{\omega + \epsilon_q^- - \epsilon_k + 2u_S} \right)$$

$$\Delta V_k^{0*} = -\sum_q V_q^{0*} \frac{u_S + u_A}{\omega + \epsilon_q^- - \epsilon_d + u_S}$$

$$\Delta u_S = -\sum_q \frac{u_A^2}{2} \left(\frac{1}{\omega - \epsilon_q^+ + \epsilon_{k'} + 2u_S} + \frac{1}{\omega + \epsilon_q^- - \epsilon_k + 2u_S} \right)$$

$$\Delta u_A = -\sum_q u_S u_A \left(\frac{1}{\omega + \epsilon_q^- - \epsilon_k} + \frac{1}{\omega - \epsilon_q^+ + \epsilon_{k'}} + \frac{1}{\omega + \epsilon_q^- - \epsilon_k + 2u_S} + \frac{1}{\omega - \epsilon_q^+ + \epsilon_{k'} + 2u_S} \right)$$