

Contents

1	Anderson Model URG
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2

1 Anderson Model URG

$$\mathcal{H} = \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{k\sigma} \left(V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right) + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \quad (1.1)$$

Without higher order scattering

$$\mathcal{H}_N = H_{N-1} + \epsilon_q \hat{n}_{q\beta} + V_q c_{q\beta}^\dagger c_{d\beta} + h.c. + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \quad (1.2)$$

where $H_{N-1} \equiv \sum_{k < \Lambda_{N,\sigma}} \left(\epsilon_k \hat{n}_{k\sigma} + V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right)$ 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 $V_q^1 \hat{n}_{d\bar{\beta}} + V_q^0 (1 - \hat{n}_{d\bar{\beta}})$. These will appear at third order in V_q .*

Particle sector

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

$$\Delta^+ \mathcal{H}_N = \sum_{q\beta} \eta_{q\beta} c_{q\beta}^\dagger \text{Tr} [\mathcal{H}_N c_{q\beta}] \quad (1.3)$$

where¹ $c_{q\beta}^\dagger \text{Tr} [\mathcal{H}_N c_{q\beta}]$ is the part of \mathcal{H}_N that scatters from $|\hat{n}_{q\beta} = 0\rangle$ to $|\hat{n}_{q\beta} = 1\rangle$:

$$c_{q\beta}^\dagger \text{Tr} [\mathcal{H}_N c_{q\beta}] = V_q c_{q\beta}^\dagger c_{d\beta} \quad (1.4)$$

and

$$\eta_{q\beta} = \text{Tr} [c_{q\beta}^\dagger \mathcal{H}_N] \frac{1}{\hat{\omega} - \mathcal{H}_N^{D,1}} = V_q^* c_{d\beta}^\dagger c_{q\beta} \frac{1}{\hat{\omega} - [H_{N-1}^C + \epsilon_q^+ + H_{imp}] \hat{n}_{q\beta}} \quad (1.5)$$

ϵ_q^+ is the energy of a particle excitation in the momentum q . $\mathcal{H}_N^{D,1} \equiv \text{Tr} (\mathcal{H}_N \hat{n}_{q\beta}) \hat{n}_{q\beta}$ is the diagonal part of \mathcal{H}_N in the particle sector, H_{N-1}^C 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,

$$\Delta^+ \mathcal{H}_N = \sum_{q\beta} V_q^* c_{d\beta}^\dagger c_{q\beta} \frac{1}{\hat{\omega} - [H_{N-1}^C + \epsilon_q^+ + H_{imp}] \hat{n}_{q\beta}} V_q c_{q\beta}^\dagger c_{d\beta} \quad (1.6)$$

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

$$\Delta^+ \mathcal{H}_N = \sum_{q\beta} V_q^* c_{d\beta}^\dagger c_{q\beta} \frac{1}{\hat{\omega} - [H_{N-1}^C + \epsilon_q^+ + \epsilon_d \hat{n}_{d\bar{\beta}}]} V_q c_{q\beta}^\dagger c_{d\beta} \quad (1.7)$$

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

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

$$\begin{aligned}\Delta^+\mathcal{H}_N &= \sum_{q\beta} |V_q|^2 c_{d\beta}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{d\beta} \frac{1}{\hat{\omega} - [H_{N-1}^C + \epsilon_q^+ + \epsilon_d \hat{n}_{d\bar{\beta}}]} \\ &= \sum_{q\beta} |V_q|^2 \hat{n}_{d\beta} (1 - \hat{n}_{q\beta}) \frac{1}{\hat{\omega} - [H_{N-1}^C + \epsilon_d \hat{n}_{d\bar{\beta}}] - \epsilon_q^+}\end{aligned}\quad (1.8)$$

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 $\epsilon_d \hat{n}_{d\beta} + U \hat{n}_{d\beta} \hat{n}_{d\bar{\beta}} = \epsilon_d + U \hat{n}_{d\bar{\beta}}$ in the propagator:

$$\Delta^+\mathcal{H}_N = \sum_{q\beta} |V_q|^2 \hat{n}_{d\beta} (1 - \hat{n}_{q\beta}) \frac{1}{\hat{\omega} - [H_{N-1}^C + \epsilon_d \hat{n}_{d\bar{\beta}} + \epsilon_d \hat{n}_{d\beta} + U \hat{n}_{d\beta} \hat{n}_{d\bar{\beta}}] - \epsilon_q^+ + \epsilon_d + U \hat{n}_{d\bar{\beta}}}\quad (1.9)$$

Note that

$$H^G \equiv H_{N-1}^C + \epsilon_d \hat{n}_{d\bar{\beta}} + \epsilon_d \hat{n}_{d\beta} + U \hat{n}_{d\beta} \hat{n}_{d\bar{\beta}} = H_{N-1}^C + H_{imp}\quad (1.10)$$

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.

$$\Delta^+\mathcal{H}_N = \sum_{q\beta} |V_q|^2 \hat{n}_{d\beta} (1 - \hat{n}_{q\beta}) \frac{1}{\hat{\omega} - H^G - \epsilon_q^+ + \epsilon_d + U \hat{n}_{d\bar{\beta}}}\quad (1.11)$$

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 :

$$\Delta^+\mathcal{H}_N = \sum_{q\beta} |V_q|^2 \hat{n}_{d\beta} (1 - \hat{n}_{q\beta}) \frac{1}{\omega - \epsilon_q^+ + \epsilon_d + U \hat{n}_{d\bar{\beta}}}\quad (1.12)$$

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

$$\Delta^+\mathcal{H}_N = \sum_{q\beta} \hat{n}_{d\beta} |V_q|^2 \frac{1}{\omega - \epsilon_q^+ + \epsilon_d + U \hat{n}_{d\bar{\beta}}}\quad (1.13)$$

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

$$\begin{aligned}\frac{1}{\omega - \epsilon_q^+ + \epsilon_d + U \hat{n}_{d\bar{\beta}}} &= \frac{\hat{n}_{d\bar{\beta}}}{\omega - \epsilon_q^+ + \epsilon_d + U} + \frac{1 - \hat{n}_{d\bar{\beta}}}{\omega - \epsilon_q^+ + \epsilon_d} \\ &= \hat{n}_{d\bar{\beta}} \left(\frac{1}{\omega - \epsilon_q^+ + \epsilon_d + U} - \frac{1}{\omega - \epsilon_q^+ + \epsilon_d} \right) + \frac{1}{\omega - \epsilon_q^+ + \epsilon_d}\end{aligned}\quad (1.14)$$

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

$$\begin{aligned}\Delta^+ \mathcal{H}_N &= \sum_{q\beta} |V_q|^2 \hat{n}_{d\beta} \left[\frac{1}{\omega - \epsilon_q^+ + \epsilon_d} + \hat{n}_{d\bar{\beta}} \left(\frac{1}{\omega - \epsilon_q^+ + \epsilon_d + U} - \frac{1}{\omega - \epsilon_q^+ + \epsilon_d} \right) \right] \\ &= \sum_{\beta} \hat{n}_{d\beta} \sum_q |V_q|^2 \frac{1}{\omega - \epsilon_q^+ + \epsilon_d} + \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \sum_q 2|V_q|^2 \left(\frac{1}{\omega - \epsilon_q^+ + \epsilon_d + U} - \frac{1}{\omega - \epsilon_q^+ + \epsilon_d} \right)\end{aligned}\quad (1.15)$$

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

$$\begin{aligned}\Delta^+ \epsilon_d &= \sum_q |V_q|^2 \frac{1}{\omega - \epsilon_q^+ + \epsilon_d} \\ \Delta^+ U &= \sum_q 2|V_q|^2 \left(\frac{1}{\omega - \epsilon_q^+ + \epsilon_d + U} - \frac{1}{\omega - \epsilon_q^+ + \epsilon_d} \right)\end{aligned}\quad (1.16)$$

Hole sector

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

$$\Delta^- \mathcal{H}_N = \sum_{q\beta} c_{q\beta}^\dagger \text{Tr} [\mathcal{H}_N c_{q\beta}] \eta_{q\beta} \quad (1.17)$$

where² and

$$\eta_{q\beta} = \frac{1}{\hat{\omega} - \mathcal{H}_N^{D,0}} \text{Tr} [c_{q\beta}^\dagger \mathcal{H}_N] = V_q^* c_{d\beta}^\dagger c_{q\beta} \frac{1}{\hat{\omega} - [H_{N-1}^C + H_{imp}] (1 - \hat{n}_{q\beta})} \quad (1.18)$$

$\mathcal{H}_N^{D,0} \equiv \text{Tr} (\mathcal{H}_N (1 - \hat{n}_{q\beta})) (1 - \hat{n}_{q\beta})$ is the diagonal part of \mathcal{H}_N in the hole sector, H_{N-1}^C 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,

$$\Delta^- \mathcal{H}_N = \sum_{q\beta} V_q c_{q\beta}^\dagger c_{d\beta} \frac{1}{\hat{\omega} - [H_{N-1}^C + H_{imp}] (1 - \hat{n}_{q\beta})} V_q^* c_{d\beta}^\dagger c_{q\beta} \quad (1.19)$$

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

$$\Delta^- \mathcal{H}_N = \sum_{q\beta} V_q c_{q\beta}^\dagger c_{d\beta} \frac{1}{\hat{\omega} - [H_{N-1}^C + \epsilon_d + (\epsilon_d + U) \hat{n}_{d\bar{\beta}}]} V_q^* c_{d\beta}^\dagger c_{q\beta} \quad (1.20)$$

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

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

$$\begin{aligned}\Delta^- \mathcal{H}_N &= \sum_{q\beta} V_q c_{q\beta}^\dagger c_{d\beta} V_q^* c_{d\beta}^\dagger c_{q\beta} \frac{1}{\hat{\omega} - [H_{N-1}^C + \epsilon_d + (\epsilon_d + U) \hat{n}_{d\bar{\beta}}]} \\ &= \sum_{q\beta} |V_q|^2 \hat{n}_{q\beta} (1 - \hat{n}_{d\beta}) \frac{1}{\hat{\omega} - [H_{N-1}^C + \epsilon_d \hat{n}_{d\bar{\beta}}] - \epsilon_d - U \hat{n}_{d\bar{\beta}}}\end{aligned}\quad (1.21)$$

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 $\epsilon_d \hat{n}_{d\beta} + U \hat{n}_{d\beta} \hat{n}_{d\bar{\beta}} = 0$ in the propagator:

$$\Delta^- \mathcal{H}_N = \sum_{q\beta} |V_q|^2 \hat{n}_{q\beta} (1 - \hat{n}_{d\beta}) \frac{1}{\hat{\omega} - [H_{N-1}^C + \epsilon_d \hat{n}_{d\bar{\beta}} + \epsilon_d \hat{n}_{d\beta} + U \hat{n}_{d\beta} \hat{n}_{d\bar{\beta}}] - \epsilon_d - U \hat{n}_{d\bar{\beta}}}\quad (1.22)$$

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_{N-1}^C (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

$$\begin{aligned}\Delta^- \mathcal{H}_N &= \sum_{q\beta} |V_q|^2 \hat{n}_{q\beta} (1 - \hat{n}_{d\beta}) \frac{1}{\hat{\omega} - [H_{N-1}^C + \epsilon_q^- \hat{n}_{q\beta} + H_{imp}] + \epsilon_q^- - \epsilon_d - U \hat{n}_{d\bar{\beta}}} \\ &= \sum_{q\beta} |V_q|^2 \hat{n}_{q\beta} (1 - \hat{n}_{d\beta}) \frac{1}{\hat{\omega} - H^G + \epsilon_q^- - \epsilon_d - U \hat{n}_{d\bar{\beta}}}\end{aligned}\quad (1.23)$$

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

$$\begin{aligned}\Delta^- \mathcal{H}_N &= \sum_{q\beta} |V_q|^2 (1 - \hat{n}_{d\beta}) \frac{1}{\omega + \epsilon_q^- - \epsilon_d - U \hat{n}_{d\bar{\beta}}} \\ &= \sum_{q\beta} |V_q|^2 (1 - \hat{n}_{d\beta}) \left[\hat{n}_{d\bar{\beta}} \left(\frac{1}{\omega + \epsilon_q^- - \epsilon_d - U} - \frac{1}{\omega + \epsilon_q^- - \epsilon_d} \right) + \frac{1}{\omega + \epsilon_q^- - \epsilon_d} \right] \\ &= \sum_{\beta} \hat{n}_{d\beta} \sum_q |V_q|^2 \left(\frac{1}{\omega + \epsilon_q^- - \epsilon_d - U} - \frac{2}{\omega + \epsilon_q^- - \epsilon_d} \right) \\ &\quad + \sum_{\beta} \hat{n}_{d\beta} \hat{n}_{d\bar{\beta}} \sum_q 2 |V_q|^2 \left(\frac{1}{\omega + \epsilon_q^- - \epsilon_d} - \frac{1}{\omega + \epsilon_q^- - \epsilon_d - U} \right)\end{aligned}\quad (1.24)$$

We get the following scaling equations for the hole sector:

$$\begin{aligned}\Delta^- \epsilon_d &= \sum_q |V_q|^2 \left(\frac{1}{\omega + \epsilon_q^- - \epsilon_d - U} - \frac{2}{\omega + \epsilon_q^- - \epsilon_d} \right) \\ \Delta^- U &= \sum_q 2|V_q|^2 \left(\frac{1}{\omega + \epsilon_q^- - \epsilon_d} - \frac{1}{\omega + \epsilon_q^- - \epsilon_d - U} \right)\end{aligned}\tag{1.25}$$

Scaling equations

Combining the two sectors, the scaling equations become

$$\begin{aligned}\Delta \epsilon_d &= \sum_q |V_q|^2 \left(\frac{1}{\omega - \epsilon_q^+ + \epsilon_d} + \frac{1}{\omega + \epsilon_q^- - \epsilon_d - U} - \frac{2}{\omega + \epsilon_q^- - \epsilon_d} \right) \\ \Delta U &= \sum_q 2|V_q|^2 \left(\frac{1}{\omega - \epsilon_q^+ + \epsilon_d + U} - \frac{1}{\omega - \epsilon_q^+ + \epsilon_d} + \frac{1}{\omega + \epsilon_q^- - \epsilon_d} - \frac{1}{\omega + \epsilon_q^- - \epsilon_d - U} \right)\end{aligned}\tag{1.26}$$

Particle-hole symmetric case

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

$$\begin{aligned}\Delta \epsilon_d &= \sum_q |V_q|^2 \left(\frac{1}{\omega - \epsilon_q^+ + \epsilon_d} + \frac{1}{\omega - \epsilon_q^+ + \epsilon_d} - \frac{2}{\omega - \epsilon_q^+ - \epsilon_d} \right) \\ &= \sum_q |V_q|^2 \left(\frac{2}{\omega - \epsilon_q^+ + \epsilon_d} - \frac{2}{\omega - \epsilon_q^+ - \epsilon_d} \right) \\ \frac{1}{2} \Delta U &= \sum_q |V_q|^2 \left(\frac{1}{\omega - \epsilon_q^+ - \epsilon_d} - \frac{1}{\omega - \epsilon_q^+ + \epsilon_d} + \frac{1}{\omega - \epsilon_q^+ - \epsilon_d} - \frac{1}{\omega - \epsilon_q^+ + \epsilon_d} \right) \\ &= \sum_q |V_q|^2 \left(\frac{2}{\omega - \epsilon_q^+ - \epsilon_d} - \frac{2}{\omega - \epsilon_q^+ + \epsilon_d} \right) \\ \implies \Delta \epsilon_d + \frac{1}{2} \Delta U &= 0\end{aligned}$$

The particle-hole symmetry is maintained for all ω .

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 $\omega = 0$,

$$\begin{aligned}\delta\epsilon_d &= |\delta D| \frac{\Delta}{\pi} \left(\frac{1}{-D + \epsilon_d} + \frac{1}{-D - \epsilon_d - U} - \frac{2}{-D - \epsilon_d} \right) \\ &= |\delta D| \frac{\Delta}{\pi} \left(\frac{2}{D + \epsilon_d} - \frac{1}{D - \epsilon_d} - \frac{1}{D + \epsilon_d + U} \right) \\ \delta U &= |\delta D| \frac{2\Delta}{\pi} \left(\frac{1}{-D + \epsilon_d + U} - \frac{1}{-D + \epsilon_d} + \frac{1}{-D - \epsilon_d} - \frac{1}{-D - \epsilon_d - U} \right) \\ &= |\delta D| \frac{2\Delta}{\pi} \left(\frac{1}{D - \epsilon_d} - \frac{1}{D - \epsilon_d - U} - \frac{1}{D + \epsilon_d} + \frac{1}{D + \epsilon_d + U} \right)\end{aligned}\tag{1.27}$$

These are identical to equation set 3.61 in Hewson.

With higher order scattering

$$\mathcal{H} = \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{k\sigma} \left(V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right) + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \sum_{\substack{kk' \\ \sigma\sigma'}} V_2 c_{d\sigma'}^\dagger c_{k\sigma}^\dagger c_{d\sigma} c_{k'\sigma'}\tag{1.28}$$

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

$$\begin{aligned}\mathcal{H}_N &= H_{N-1} + H_{\text{imp}} + (\epsilon_q + V_2 \hat{n}_{d\beta}) \hat{n}_{q\beta} + V_q c_{q\beta}^\dagger c_{d\beta} + h.c. \\ &\quad + \sum_{k\sigma} V_2 \left(c_{q\beta}^\dagger c_{d\sigma}^\dagger c_{k\sigma} c_{d\beta} + c_{d\beta}^\dagger c_{k\sigma}^\dagger c_{d\sigma} c_{q\beta} \right)\end{aligned}\tag{1.29}$$

Particle sector: The intermediate state consists of particle states, obtained by exciting electrons to the upper bandwidth edge ($+D$).

$$\begin{aligned}\Delta^+ \mathcal{H}_N &= \sum_{q\beta} c_{d\beta}^\dagger \left[V_q^* + \sum_{k'\sigma'} V_2 c_{k'\sigma'}^\dagger c_{d\sigma'} \right] c_{q\beta} \frac{1}{\hat{\omega} - (H_{N-1}^C + H_{\text{imp}} + V_2 \hat{n}_{d\beta} + \epsilon_q) \hat{n}_{q\beta}} \\ &\quad c_{q\beta}^\dagger \left[V_q + \sum_{k\sigma} V_2 c_{d\sigma}^\dagger c_{k\sigma} \right] c_{d\beta}\end{aligned}\tag{1.30}$$

Since the Greens function is preceded by $c_{q\beta}^\dagger$, we can substitute $\hat{n}_{q\beta} = 1$ in the denominator.

$$\frac{1}{\hat{\omega} - (H_{\text{imp}} + V_2 \hat{n}_{d\beta} + \epsilon_q) \hat{n}_{q\beta}} c_{q\beta}^\dagger = \frac{1}{\hat{\omega} - (H_{N-1}^C + H_{\text{imp}} + V_2 \hat{n}_{d\beta} + \epsilon_q^+)} c_{q\beta}^\dagger\tag{1.31}$$

$$\Delta^+ \mathcal{H}_N = \sum_{q\beta} c_{q\beta} c_{d\beta}^\dagger \left[V_q^* + \sum_{k'\sigma'} V_2 c_{k'\sigma'}^\dagger c_{d\sigma'} \right] \frac{1}{\omega - H_{N-1}^C - H_{\text{imp}} - V_2 \hat{n}_{d\beta} - \epsilon_q^+} \times \left[V_q + \sum_{k\sigma} V_2 c_{d\sigma}^\dagger c_{k\sigma} \right] c_{d\beta} c_{q\beta}^\dagger \quad (1.32)$$

There are four scattering processes. The changes will be labeled as $\Delta_i^+ \mathcal{H}_N$.

1. This was calculated in the previous section. The only addition is the splitting of the hybridisation coupling:

$$\begin{aligned} |V_q|^2 &= [V_q^1 \hat{n}_{d\bar{\beta}} + V_q^0 (1 - \hat{n}_{d\bar{\beta}})] \times [(V_q^1)^* \hat{n}_{d\bar{\beta}} + (V_q^0)^* (1 - \hat{n}_{d\bar{\beta}})] \\ &= |V_q^1|^2 \hat{n}_{d\bar{\beta}} + |V_q^0|^2 (1 - \hat{n}_{d\bar{\beta}}) \\ &= (|V_q^1|^2 - |V_q^0|^2) \hat{n}_{d\bar{\beta}} + |V_q^0|^2 \end{aligned} \quad (1.33)$$

From eq. 1.14,

$$\begin{aligned} \Delta_1^+ \mathcal{H} &= \sum_{q\beta} \hat{n}_{d\beta} |V_q|^2 \left[\frac{\hat{n}_{d\bar{\beta}}}{\omega - \epsilon_q^+ + \epsilon_d + U} + \frac{1 - \hat{n}_{d\bar{\beta}}}{\omega - \epsilon_q^+ + \epsilon_d} \right] \\ &= \sum_{q\beta} \hat{n}_{d\beta} \left[\frac{|V_q^1|^2 \hat{n}_{d\bar{\beta}}}{\omega - \epsilon_q^+ + \epsilon_d + U} + \frac{|V_q^0|^2 (1 - \hat{n}_{d\bar{\beta}})}{\omega - \epsilon_q^+ + \epsilon_d} \right] \\ &= \sum_{q\beta} \hat{n}_{d\beta} \frac{|V_q^0|^2}{\omega - \epsilon_q^+ + \epsilon_d} + 2 \sum_q \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \left[\frac{|V_q^1|^2}{\omega - \epsilon_q^+ + \epsilon_d + U} - \frac{|V_q^0|^2}{\omega - \epsilon_q^+ + \epsilon_d} \right] \end{aligned} \quad (1.34)$$

2.

$$\begin{aligned} \Delta_2^+ \mathcal{H}_N &= \sum_{q\beta k\sigma} c_{q\beta} c_{d\beta}^\dagger \frac{V_q^* V_2}{\hat{\omega} - H_{N-1}^C - H_{\text{imp}} - V_2 \hat{n}_{d\beta} - \epsilon_q^+} c_{d\sigma}^\dagger c_{k\sigma} c_{d\beta} c_{q\beta}^\dagger \\ &= \sum_{q\beta k} c_{q\beta} c_{d\beta}^\dagger \frac{V_q^* V_2}{\hat{\omega} - H_{N-1}^C - H_{\text{imp}} - V_2 \hat{n}_{d\beta} - \epsilon_q^+} c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}} c_{d\beta} c_{q\beta}^\dagger \quad [c_\beta^\dagger c_\sigma^\dagger = \delta_{\beta\sigma} c_\beta^\dagger] \\ &= \sum_{q\beta k} c_{q\beta} c_{d\beta}^\dagger \frac{V_q^* V_2}{\hat{\omega} - H_{N-1}^C - \epsilon_d \hat{n}_{d\bar{\beta}} - \epsilon_q^+} c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}} c_{d\beta} c_{q\beta}^\dagger \quad [\hat{n}_{d\beta} = 0 \text{ in propagator}] \end{aligned} \quad (1.35)$$

We cannot directly push the propagator to the end, because it still has an $\hat{n}_{d\bar{\beta}}$. We can use an identity. If A and B are two entities that commute with $c_{d\bar{\beta}}^\dagger$, then

$$\begin{aligned} (A - B \hat{n}_{d\bar{\beta}}) c_{d\bar{\beta}}^\dagger &= A c_{d\bar{\beta}}^\dagger - B c_{d\bar{\beta}}^\dagger (1 - \hat{n}_{d\bar{\beta}}) = c_{d\bar{\beta}}^\dagger (A - B + B \hat{n}_{d\bar{\beta}}) \\ \implies \frac{1}{A - B \hat{n}_{d\bar{\beta}}} c_{d\bar{\beta}}^\dagger &= c_{d\bar{\beta}}^\dagger \frac{1}{A - B + B \hat{n}_{d\bar{\beta}}} \end{aligned}$$

This gives

$$\frac{1}{\hat{\omega} - H_{N-1}^C - \epsilon_d \hat{n}_{d\bar{\beta}} - \epsilon_q^+} c_{d\bar{\beta}}^\dagger = c_{d\bar{\beta}}^\dagger \frac{1}{\hat{\omega} - H_{N-1}^C - \epsilon_d + \epsilon_d \hat{n}_{d\bar{\beta}} - \epsilon_q^+} \quad (1.36)$$

A similar process gives

$$\begin{aligned} \frac{1}{\hat{\omega} - H_{N-1}^{C,(k\bar{\beta})} - \epsilon_k \hat{n}_{k\bar{\beta}} - \epsilon_d + \epsilon_d \hat{n}_{d\bar{\beta}} - \epsilon_q^+} c_{k\bar{\beta}} &= c_{k\bar{\beta}} \frac{1}{\hat{\omega} - H_{N-1}^{C,(k\bar{\beta})} - \epsilon_d + \epsilon_d \hat{n}_{d\bar{\beta}} - \epsilon_q^+} \\ &= c_{k\bar{\beta}} \frac{1}{\hat{\omega} - H_{N-1}^C + \epsilon_k \hat{n}_{k\bar{\beta}} - \epsilon_d + \epsilon_d \hat{n}_{d\bar{\beta}} - \epsilon_q^+} \\ &= c_{k\bar{\beta}} \frac{1}{\hat{\omega} - H_{N-1}^C + \epsilon_k^- - \epsilon_d + \epsilon_d \hat{n}_{d\bar{\beta}} - \epsilon_q^+} \end{aligned} \quad (1.37)$$

$(H_{N-1}^{C,(k\sigma)} = H_{N-1}^C - \epsilon_k \hat{n}_{k\sigma})$. The change in \mathcal{H} becomes

$$\sum_{q\beta k} V_q^* V_2 (1 - \hat{n}_{q\beta}) \hat{n}_{d\beta} c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}} \frac{1}{\hat{\omega} - H_{N-1}^C + \epsilon_k^- - \epsilon_d + \epsilon_d \hat{n}_{d\bar{\beta}} - \epsilon_q^+} \quad (1.38)$$

Since this term must act on a state with $\hat{n}_{d\beta} = 1 - \hat{n}_{d\bar{\beta}} = 1$, we can write

$$\begin{aligned} \hat{\omega} - H_{N-1}^C - \epsilon_d + \epsilon_d \hat{n}_{d\bar{\beta}} - \epsilon_q^+ &= \hat{\omega} - H_{N-1}^C - \epsilon_d \hat{n}_{d\beta} - \epsilon_d \hat{n}_{d\bar{\beta}} - U \hat{n}_{d\beta} \hat{n}_{d\bar{\beta}} - \epsilon_q^+ \\ &= \hat{\omega} - H^G - \epsilon_q^+ \\ &= \omega - \epsilon_q^+ \end{aligned} \quad (1.39)$$

Therefore,

$$\begin{aligned} \Delta_2^+ \mathcal{H}_N &= \sum_{q\beta k} V_q^* V_2 (1 - \hat{n}_{q\beta}) \hat{n}_{d\beta} c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}} \frac{1}{\omega + \epsilon_k^- - \epsilon_q^+} \\ &= \sum_{q\beta k} V_q^* V_2 \hat{n}_{d\beta} c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}} \frac{1}{\omega + \epsilon_k^- - \epsilon_q^+} \\ &= \sum_{q\beta k} (V_q^1)^* V_2 \hat{n}_{d\beta} c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}} \frac{1}{\omega + \epsilon_k^- - \epsilon_q^+} \quad [V_q = V_q^1 \hat{n}_{d\bar{\beta}} + V_q^0 (1 - \hat{n}_{d\bar{\beta}})] \\ &= \sum_{q\beta k} (V_q^1)^* V_2 \hat{n}_{d\bar{\beta}} c_{d\beta}^\dagger c_{k\beta} \frac{1}{\omega + \epsilon_k^- - \epsilon_q^+} \end{aligned} \quad (1.40)$$

This renormalizes the $(V_q^1)^*$ coupling.

3.

$$\begin{aligned}
\Delta_3^+ \mathcal{H}_N &= \sum_{q\beta k\sigma} c_{q\beta} c_{d\beta}^\dagger c_{k\sigma}^\dagger c_{d\sigma} \frac{V_q V_2}{\hat{\omega} - H_{N-1}^C - H_{\text{imp}} - V_2 \hat{n}_{d\beta} - \epsilon_q^+} c_{d\beta} c_{q\beta}^\dagger \\
&= \sum_{q\beta k\sigma} c_{q\beta} c_{d\beta}^\dagger c_{k\sigma}^\dagger c_{d\sigma} \frac{V_q V_2}{\hat{\omega} - H_{N-1}^C - H_{\text{imp}} - \epsilon_q^+} c_{d\beta} c_{q\beta}^\dagger \\
&= \sum_{q\beta k\sigma} c_{q\beta} c_{d\beta}^\dagger c_{k\sigma}^\dagger c_{d\sigma} c_{d\beta} c_{q\beta}^\dagger \frac{V_q V_2}{\omega - \epsilon_q^+ + \epsilon_d + U \hat{n}_{d\bar{\beta}}} \quad [\text{from prev. section}] \\
&= \sum_{q\beta k} (1 - \hat{n}_{q\beta}) \hat{n}_{d\beta} c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} \frac{V_q V_2}{\omega - \epsilon_q^+ + \epsilon_d + U \hat{n}_{d\bar{\beta}}} \\
&= \sum_{q\beta k} (1 - \hat{n}_{q\beta}) \hat{n}_{d\beta} c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} \frac{V_q V_2}{\omega - \epsilon_q^+ + \epsilon_d} \\
&= \sum_{q\beta k} \hat{n}_{d\beta} c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} \frac{V_q^1 V_2}{\omega - \epsilon_q^+ + \epsilon_d}
\end{aligned} \tag{1.41}$$

This renormalizes the V_q^1 coupling.

4. $O(V_2^2)$, ignore for now.

Hole sector The intermediate state consists of hole states, obtained by exciting electrons from the lower bandwidth edge ($-D$).

$$\Delta^- \mathcal{H}_N = \sum_{q\beta} c_{q\beta}^\dagger \left[V_q + \sum_{k\sigma} V_2 c_{d\sigma}^\dagger c_{k\sigma} \right] c_{d\beta} \frac{1}{\hat{\omega} - H_{N-1}^C - H_{\text{imp}}} c_{d\beta}^\dagger \left[V_q^* + \sum_{k'\sigma'} V_2 c_{k'\sigma'}^\dagger c_{d\sigma'} \right] c_{q\beta} \tag{1.42}$$

The Green's function simplifies as

$$\begin{aligned}
c_{d\beta} \frac{1}{\hat{\omega} - H_{N-1}^C - H_{\text{imp}}} c_{d\beta}^\dagger &= c_{d\beta} \frac{1}{\hat{\omega} - H_{N-1}^C - \epsilon_d - (\epsilon_d + U) \hat{n}_{d\bar{\beta}}} c_{d\beta}^\dagger \\
&= (1 - \hat{n}_{d\beta}) \frac{1}{\hat{\omega} - H_{N-1}^C - \epsilon_d - (\epsilon_d + U) \hat{n}_{d\bar{\beta}}}
\end{aligned} \tag{1.43}$$

1.

$$\begin{aligned}
\Delta_1^- \mathcal{H}_N &= \sum_{q\beta} |V_q|^2 \hat{n}_{q\beta} (1 - \hat{n}_{d\beta}) \frac{1}{\hat{\omega} - H_{N-1}^C - \epsilon_d - (\epsilon_d + U) \hat{n}_{d\bar{\beta}}} \\
&= \sum_{q\beta} |V_q|^2 \hat{n}_{q\beta} (1 - \hat{n}_{d\beta}) \frac{1}{\hat{\omega} - H_{N-1}^C - \epsilon_d \hat{n}_{d\beta} - \epsilon_d \hat{n}_{d\bar{\beta}} - U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} - \epsilon_d - U \hat{n}_{d\bar{\beta}}} \\
&= \sum_{q\beta} |V_q|^2 (1 - \hat{n}_{d\beta}) \frac{1}{\omega + \epsilon_q^- - \epsilon_d - U \hat{n}_{d\bar{\beta}}} \\
&= \sum_{q\beta} (1 - \hat{n}_{d\beta}) \left[\hat{n}_{d\bar{\beta}} \left(\frac{|V_q^1|^2}{\omega + \epsilon_q^- - \epsilon_d - U} - \frac{|V_q^0|^2}{\omega + \epsilon_q^- - \epsilon_d} \right) + \frac{|V_q^0|^2}{\omega + \epsilon_q^- - \epsilon_d} \right] \\
&= \sum_{q\beta} \hat{n}_{d\beta} \left(\frac{|V_q^1|^2}{\omega + \epsilon_q^- - \epsilon_d - U} - \frac{2|V_q^0|^2}{\omega + \epsilon_q^- - \epsilon_d} \right) \\
&\quad + \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \sum_{q\beta} 2 \left(\frac{|V_q^0|^2}{\omega + \epsilon_q^- - \epsilon_d} - \frac{|V_q^1|^2}{\omega + \epsilon_q^- - \epsilon_d - U} \right) \\
&\quad + \sum_{q\beta} \frac{|V_q^0|^2}{\omega + \epsilon_q^- - \epsilon_d}
\end{aligned} \tag{1.44}$$

2.

$$\begin{aligned}
\Delta_2^- \mathcal{H}_N &= \frac{1}{2} \sum_{k\sigma q\beta} V_2 V_q \hat{n}_{q\beta} (1 - \hat{n}_{d\beta}) \frac{1}{\hat{\omega} - H_{N-1}^C - \epsilon_d - (\epsilon_d + U) \hat{n}_{d\bar{\beta}}} c_{k\sigma}^\dagger c_{d\sigma} \\
&= \sum_{kq\beta} V_2 V_q \hat{n}_{q\beta} (1 - \hat{n}_{d\beta}) \frac{1}{\hat{\omega} - H_{N-1}^C - \epsilon_d - (\epsilon_d + U) \hat{n}_{d\bar{\beta}}} \left(c_{k\beta}^\dagger c_{d\beta} + c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} \right) \\
&= \sum_{kq\beta} V_2 V_q \hat{n}_{q\beta} c_{k\beta}^\dagger c_{d\beta} \frac{1}{\hat{\omega} - \epsilon_k^+ - H_{N-1}^C - \epsilon_d - (\epsilon_d + U) \hat{n}_{d\bar{\beta}}} \\
&\quad + \sum_{kq\beta} V_2 V_q \hat{n}_{q\beta} (1 - \hat{n}_{d\beta}) c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} \frac{1}{\hat{\omega} - \epsilon_k^+ - H_{N-1}^C - \epsilon_d} \\
&= \sum_{kq\beta} V_2 V_q c_{k\beta}^\dagger c_{d\beta} \frac{1}{\omega - \epsilon_k^+ + \epsilon_q^-} + \sum_{kq\beta} V_2 V_q (1 - \hat{n}_{d\bar{\beta}}) c_{k\beta}^\dagger c_{d\beta} \frac{1}{\omega - \epsilon_k^+ + \epsilon_q^-} \\
&= \sum_{kq\beta} V_2 \hat{n}_{d\bar{\beta}} c_{k\beta}^\dagger c_{d\beta} \frac{V_q^1}{\omega - \epsilon_k^+ + \epsilon_q^-} + \sum_{kq\beta} V_2 (1 - \hat{n}_{d\bar{\beta}}) c_{k\beta}^\dagger c_{d\beta} \frac{2V_q^0}{\omega - \epsilon_k^+ + \epsilon_q^-}
\end{aligned} \tag{1.45}$$

3.

$$\begin{aligned}
& \Delta_3^- \mathcal{H}_N \\
&= \sum_{k\sigma q\beta} V_q^* V_2 \hat{n}_{q\beta} c_{d\sigma}^\dagger c_{k\sigma} (1 - \hat{n}_{d\beta}) \frac{1}{\hat{\omega} - H_{N-1}^C - \epsilon_d - (\epsilon_d + U) \hat{n}_{d\bar{\beta}}} \\
&= \sum_{kq\beta} V_q^* V_2 \hat{n}_{q\beta} \left(c_{d\beta}^\dagger c_{k\beta} + c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}} \right) (1 - \hat{n}_{d\beta}) \frac{1}{\hat{\omega} - H_{N-1}^C - \epsilon_d - (\epsilon_d + U) \hat{n}_{d\bar{\beta}}} \\
&= \sum_{kq\beta} V_q^* V_2 \hat{n}_{q\beta} c_{d\beta}^\dagger c_{k\beta} \frac{1}{\hat{\omega} - H_{N-1}^C - \epsilon_d - (\epsilon_d + U) \hat{n}_{d\bar{\beta}}} \\
&+ \sum_{kq\beta} V_q^* V_2 \hat{n}_{q\beta} (1 - \hat{n}_{d\beta}) c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}} \frac{1}{\hat{\omega} - H_{N-1}^C - \epsilon_d - (\epsilon_d + U) \hat{n}_{d\bar{\beta}}} \\
&= \sum_{kq\beta} \hat{n}_{q\beta} c_{d\beta}^\dagger c_{k\beta} \frac{V_q^* V_2}{\omega + \epsilon_q^- - (\epsilon_d + U \hat{n}_{d\bar{\beta}})} + \sum_{kq\beta} \hat{n}_{q\beta} (1 - \hat{n}_{d\beta}) c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}} \frac{V_q^* V_2}{\omega + \epsilon_q^- - \epsilon_d - U} \\
&= \sum_{kq\beta} V_2 c_{d\beta}^\dagger c_{k\beta} \left(\frac{(V_q^1)^* \hat{n}_{d\bar{\beta}}}{\omega + \epsilon_q^- - \epsilon_d - U} + \frac{(V_q^0)^* (1 - \hat{n}_{d\bar{\beta}})}{\omega + \epsilon_q^- - \epsilon_d} \right) + \sum_{kq\beta} c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}} \frac{V_2 (V_q^0)^* (1 - \hat{n}_{d\bar{\beta}})}{\omega + \epsilon_q^- - \epsilon_d - U} \\
&= \sum_{kq\beta} c_{d\beta}^\dagger c_{k\beta} \frac{V_2 (V_q^1)^* \hat{n}_{d\bar{\beta}}}{\omega + \epsilon_q^- - \epsilon_d - U} + \sum_{kq\beta} c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}} \left\{ \frac{V_2 (V_q^0)^* (1 - \hat{n}_{d\bar{\beta}})}{\omega + \epsilon_q^- - \epsilon_d} + \frac{V_2 (V_q^0)^* (1 - \hat{n}_{d\bar{\beta}})}{\omega + \epsilon_q^- - \epsilon_d - U} \right\}
\end{aligned} \tag{1.46}$$

Scaling equations

$$\begin{aligned}
\Delta \epsilon_d &= \sum_q \left(\frac{|V_q^0|^2}{\omega - \epsilon_q^+ + \epsilon_d} + \frac{|V_q^1|^2}{\omega + \epsilon_q^- - \epsilon_d - U} - \frac{2|V_q^0|^2}{\omega + \epsilon_q^- - \epsilon_d} \right) \\
\Delta U &= \sum_q 2 \left(\frac{|V_q^1|^2}{\omega - \epsilon_q^+ + \epsilon_d + U} - \frac{|V_q^1|^2}{\omega + \epsilon_q^- - \epsilon_d - U} + \frac{|V_q^0|^2}{\omega + \epsilon_q^- - \epsilon_d} - \frac{|V_q^0|^2}{\omega - \epsilon_q^+ + \epsilon_d} \right) \\
\Delta V_q^1 &= \frac{V_2 V_q^1}{\omega - \epsilon_q^+ + \epsilon_d} + \frac{V_2 V_q^1}{\omega + \epsilon_q^- - \epsilon_k^+} \\
\Delta V_q^{1*} &= \frac{V_2 V_q^{1*}}{\omega + \epsilon_k^- - \epsilon_q^+} + \frac{V_2 V_q^{1*}}{\omega + \epsilon_q^- - \epsilon_d - U} \\
\Delta V_q^0 &= \frac{2V_2 V_q^0}{\omega + \epsilon_q^- - \epsilon_k^+} \\
\Delta V_q^{0*} &= \frac{V_2 V_q^{0*}}{\omega + \epsilon_q^- - \epsilon_d} + \frac{V_2 V_q^{0*}}{\omega + \epsilon_q^- - \epsilon_d - U}
\end{aligned} \tag{1.47}$$