1 Anderson Model URG

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

Without higher order scattering

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

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.*

Particle sector

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

$$\Delta^+ \mathcal{H}_N = \sum_{q\beta} \eta_{q\beta} c^\dagger_{q\beta} \text{Tr} \left[\mathcal{H}_N c_{q\beta} \right] \tag{1.3}$$

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 $|\hat{n}_{q\beta} = 1\rangle$:

$$c^\dagger_{q\beta} \text{Tr} \left[\mathcal{H}_N c_{q\beta} \right] = V_q c^\dagger_{q\beta} c_{d\beta} \tag{1.4}$$

and

$$\eta_{q\beta} = \text{Tr} \left[c^\dagger_{q\beta} \mathcal{H}_N \right] \frac{1}{\hat{\omega} - \mathcal{H}_N^{D,1}} = V_q^* c^\dagger_{d\beta} c_{q\beta} \frac{1}{\hat{\omega} - \left[H^C_{N-1} + \epsilon_q^+ + H_{imp} \right] \hat{n}_{q\beta}} \tag{1.5}$$

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,

$$\Delta^+ \mathcal{H}_N = \sum_{q\beta} V_q^* c^\dagger_{d\beta} c_{q\beta} \frac{1}{\hat{\omega} - \left[H^C_{N-1} + \epsilon_q^+ + H_{imp} \right] \hat{n}_{q\beta}} V_q c^\dagger_{q\beta} c_{d\beta} \tag{1.6}$$

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 $\epsilon_d \hat{n}_{d\overline{\beta}}$.

$$\Delta^+ \mathcal{H}_N = \sum_{q\beta} V_q^* c^\dagger_{d\beta} c_{q\beta} \frac{1}{\hat{\omega} - \left[H^C_{N-1} + \epsilon_q^+ + \epsilon_d \hat{n}_{d\overline{\beta}} \right]} V_q c^\dagger_{q\beta} c_{d\beta} \tag{1.7}$$

[1] all 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:

$$\begin{aligned}\Delta^+\mathcal{H}_N &= \sum_{q\beta} |V_q|^2 c^\dagger_{d\beta} c_{q\beta} c^\dagger_{q\beta} c_{d\beta} \frac{1}{\hat{\omega} - \left[H^C_{N-1} + \epsilon^+_q + \epsilon_d \hat{n}_{d\overline{\beta}}\right]} \\ &= \sum_{q\beta} |V_q|^2 \hat{n}_{d\beta} \left(1 - \hat{n}_{q\beta}\right) \frac{1}{\hat{\omega} - \left[H^C_{N-1} + \epsilon_d \hat{n}_{d\overline{\beta}}\right] - \epsilon^+_q}\end{aligned} \tag{1.8}$$

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

$$\Delta^+\mathcal{H}_N = \sum_{q\beta} |V_q|^2 \hat{n}_{d\beta} \left(1 - \hat{n}_{q\beta}\right) \frac{1}{\hat{\omega} - \left[H^C_{N-1} + \epsilon_d \hat{n}_{d\overline{\beta}} + \epsilon_d \hat{n}_{d\beta} + U \hat{n}_{d\beta} \hat{n}_{d\overline{\beta}}\right] - \epsilon^+_q + \epsilon_d + U \hat{n}_{d\overline{\beta}}} \tag{1.9}$$

Note that

$$H^G \equiv H^C_{N-1} + \epsilon_d \hat{n}_{d\overline{\beta}} + \epsilon_d \hat{n}_{d\beta} + U \hat{n}_{d\beta} \hat{n}_{d\overline{\beta}} = H^C_{N-1} + H_{imp} \tag{1.10}$$

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.

$$\Delta^+\mathcal{H}_N = \sum_{q\beta} |V_q|^2 \hat{n}_{d\beta} \left(1 - \hat{n}_{q\beta}\right) \frac{1}{\hat{\omega} - H^G - \epsilon^+_q + \epsilon_d + U \hat{n}_{d\overline{\beta}}} \tag{1.11}$$

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:

$$\Delta^+\mathcal{H}_N = \sum_{q\beta} |V_q|^2 \hat{n}_{d\beta} \left(1 - \hat{n}_{q\beta}\right) \frac{1}{\omega - \epsilon^+_q + \epsilon_d + U \hat{n}_{d\overline{\beta}}} \tag{1.12}$$

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

$$\Delta^+\mathcal{H}_N = \sum_{q\beta} \hat{n}_{d\beta} |V_q|^2 \frac{1}{\omega - \epsilon^+_q + \epsilon_d + U \hat{n}_{d\overline{\beta}}} \tag{1.13}$$

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

$$\begin{aligned}\frac{1}{\omega - \epsilon^+_q + \epsilon_d + U \hat{n}_{d\overline{\beta}}} &= \frac{\hat{n}_{d\overline{\beta}}}{\omega - \epsilon^+_q + \epsilon_d + U} + \frac{1 - \hat{n}_{d\overline{\beta}}}{\omega - \epsilon^+_q + \epsilon_d} \\ &= \hat{n}_{d\overline{\beta}} \left(\frac{1}{\omega - \epsilon^+_q + \epsilon_d + U} - \frac{1}{\omega - \epsilon^+_q + \epsilon_d}\right) + \frac{1}{\omega - \epsilon^+_q + \epsilon_d}\end{aligned} \tag{1.14}$$

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

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

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:

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

Hole sector

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

$$\Delta^-\mathcal{H}_N = \sum_{q\beta} c^\dagger_{q\beta} \mathrm{Tr}\left[\mathcal{H}_N c_{q\beta}\right] \eta_{q\beta} \tag{1.17}$$

where[2] and

$$\eta_{q\beta} = \frac{1}{\hat{\omega} - \mathcal{H}_N^{D,0}} \mathrm{Tr}\left[c^\dagger_{q\beta}\mathcal{H}_N\right] = V_q^* c^\dagger_{d\beta} c_{q\beta} \frac{1}{\hat{\omega} - \left[H^C_{N-1} + H_{imp}\right]\left(1 - \hat{n}_{q\beta}\right)} \tag{1.18}$$

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

$$\Delta^-\mathcal{H}_N = \sum_{q\beta} V_q c^\dagger_{q\beta} c_{d\beta} \frac{1}{\hat{\omega} - \left[H^C_{N-1} + H_{imp}\right]\left(1 - \hat{n}_{q\beta}\right)} V_q^* c^\dagger_{d\beta} c_{q\beta} \tag{1.19}$$

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 $\epsilon_d + (\epsilon_d + U)\,\hat{n}_{d\overline{\beta}}$.

$$\Delta^-\mathcal{H}_N = \sum_{q\beta} V_q c^\dagger_{q\beta} c_{d\beta} \frac{1}{\hat{\omega} - \left[H^C_{N-1} + \epsilon_d + (\epsilon_d + U)\,\hat{n}_{d\overline{\beta}}\right]} V_q^* c^\dagger_{d\beta} c_{q\beta} \tag{1.20}$$

[2]all 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:

$$\begin{aligned}\Delta^{-}\mathcal{H}_N &= \sum_{q\beta} V_q c^\dagger_{q\beta} c_{d\beta} V_q^* c^\dagger_{d\beta} c_{q\beta} \frac{1}{\hat{\omega} - \left[H^C_{N-1} + \epsilon_d + \left(\epsilon_d + U\right) \hat{n}_{d\overline{\beta}}\right]} \\ &= \sum_{q\beta} |V_q|^2 \hat{n}_{q\beta} \left(1 - \hat{n}_{d\beta}\right) \frac{1}{\hat{\omega} - \left[H^C_{N-1} + \epsilon_d \hat{n}_{d\overline{\beta}}\right] - \epsilon_d - U\hat{n}_{d\overline{\beta}}}\end{aligned} \tag{1.21}$$

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

$$\Delta^{-}\mathcal{H}_N = \sum_{q\beta} |V_q|^2 \hat{n}_{q\beta} \left(1 - \hat{n}_{d\beta}\right) \frac{1}{\hat{\omega} - \left[H^C_{N-1} + \epsilon_d \hat{n}_{d\overline{\beta}} + \epsilon_d \hat{n}_{d\beta} + U\hat{n}_{d\beta}\hat{n}_{d\overline{\beta}}\right] - \epsilon_d - U\hat{n}_{d\overline{\beta}}} \tag{1.22}$$

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^C_{N-1}. Adding and subtracting $\epsilon_q \hat{n}_{q\beta} = \epsilon^-_q$ gives

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

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

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

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

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

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

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.