Contents

1 Anderson Model URG

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

One electron on shell

At first order, the rotated Hamiltonian is

$$\mathcal{H}_{j-1} = 2^{-n_j} \mathrm{Tr}_{1,2,\ldots,n_j} \mathcal{H}_j + \sum_{q\beta} \tau_{q\beta} \left\{ c^\dagger_{q\beta} \mathrm{Tr}_{q\beta} \left(\mathcal{H} c_{q\beta} \right), \eta_{q\beta} \right\} \tag{1.2}$$

n_j is the number of states on the shell Λ_j. We take the full Hamiltonian as our $\mathcal{H}_j$. Since this is the first step of the RG, the shell being decoupled is the highest one, which we call Λ_N.

Calculation of first term The first term, the initial trace, is a sequential trace over all the states on the shell being disentangled. At each trace, we consider only electrons on the current degree of freedom and on shells below the current shell:

$$\begin{aligned} \frac{1}{2} \mathrm{Tr}_{q\uparrow} \mathcal{H}_j &= \sum_{k<\Lambda_N, \sigma} \epsilon_k \hat{n}_{k\sigma} + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \frac{1}{2} \mathrm{Tr}_{q\uparrow} \left\{ \epsilon_k \hat{n}_{q\uparrow} \right\} \\ &= \sum_{k<\Lambda_N, \sigma} \epsilon_k \hat{n}_{k\sigma} + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \frac{1}{2} \epsilon_q \\ \frac{1}{2} \mathrm{Tr}_{q\downarrow} \frac{1}{2} \mathrm{Tr}_{q\uparrow} \mathcal{H}_j &= \sum_{k<\Lambda_N, \sigma} \epsilon_k \hat{n}_{k\sigma} + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \epsilon_q \end{aligned} \tag{1.3}$$

$$\implies 2^{-n_j} \mathrm{Tr}_{1,2,\ldots,n_j} \mathcal{H}_j = \sum_{k<\Lambda_N, \sigma} \epsilon_k \hat{n}_{k\sigma} + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \sum_{|q|=\Lambda_N} \epsilon_q \tag{1.4}$$

Calculation of second term The second term involves some other traces:

$$\begin{aligned} \mathrm{Tr}_{q\beta} \left(\mathcal{H} c_{q\beta} \right) &= \sum_{k\sigma} V_k \mathrm{Tr}_{q\beta} \left(c^\dagger_{k\sigma} c_{d\sigma} c_{q\beta} \right) \\ &= \sum_{k\sigma} V_k c_{d\sigma} \delta_{\sigma\beta} \delta_{kq} \\ &= V_q c_{d\beta} \\ \mathrm{Tr}_{q\beta} \left(c^\dagger_{q\beta} \mathcal{H} \right) &= V_q^* c^\dagger_{d\beta} \end{aligned} \tag{1.5}$$

$$
\begin{aligned}
\mathcal{H}^D &= \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \epsilon_d \sum_\sigma \hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} \\
\mathrm{Tr}_{q\beta}\left(\mathcal{H}^D \hat{n}_{q\beta}\right) &= \sum_{k<\Lambda_N,\sigma} \epsilon_k \hat{n}_{k\sigma} + \epsilon_d \sum_\sigma \hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + \epsilon_q \\
\eta_{q\beta} &= \mathrm{Tr}_{q\beta}\left(c^\dagger_{q\beta}\mathcal{H}\right) c_{q\beta} \frac{1}{\hat{\omega} - \mathrm{Tr}_{q\beta}\left(\mathcal{H}^D \hat{n}_{q\beta}\right)\hat{n}_{q\beta}} \\
&= V_q^* c^\dagger_{d\beta} c_{q\beta} \frac{1}{\hat{\omega} - \left(\sum_{k<\Lambda_N,\sigma} \epsilon_k \hat{n}_{k\sigma} + \epsilon_d \sum_\sigma \hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} - \epsilon_q\right)\hat{n}_{q\beta}} \\
&= V_q^* c^\dagger_{d\beta} c_{q\beta} \frac{1}{\omega\tau_{q\beta} - \left(\epsilon_d \sum_\sigma \hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + \epsilon_q\right)\tau_{q\beta}}
\end{aligned} \tag{1.6}
$$

At the last step, **I replaced $\hat{\omega} - \sum_{k<\Lambda_N,\sigma} \epsilon_k \hat{n}_{k\sigma}\hat{n}_{q\beta} - \frac{1}{2}\left(\epsilon_d \sum_\sigma \hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + \epsilon_q\right)$ with $\omega\tau_{q\beta}$**. Note that since this term has a $c^\dagger_{d\beta}$, it will not vanish only when acting on a state with $\hat{n}_{d\beta} = 0$. Hence we can drop the terms $\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}$ and $\epsilon_{d\beta}\hat{n}_{d\beta}$ in the denominator. Also, since it has a $c_{q\beta}$, we can set the $\tau_{q\beta}$ in the denominator to $\frac{1}{2}$. Putting together the individual pieces, we can now write the second term:

$$
\begin{aligned}
\sum_{q\beta} \tau_{q\beta} \left\{ c^\dagger_{q\beta} \mathrm{Tr}_{q\beta}\left(\mathcal{H} c_{q\beta}\right), \eta_{q\beta} \right\} &= \sum_{q\beta} \tau_{q\beta} \left\{ V_q c^\dagger_{q\beta} c_{d\beta}, V_q^* c^\dagger_{d\beta} c_{q\beta} \frac{1}{\frac{1}{2}\left(\omega - \epsilon_q - \epsilon_d \hat{n}_{d\overline{\beta}}\right)} \right\} \\
&= \sum_{q\beta} 2\tau_{q\beta} \left\{ V_q c^\dagger_{q\beta} c_{d\beta}, V_q^* c^\dagger_{d\beta} c_{q\beta} \frac{1}{\omega - \epsilon_q - \epsilon_d \hat{n}_{d\overline{\beta}}} \right\}
\end{aligned} \tag{1.7}
$$

We now note that the factor with ω can be written as follows:

$$
\begin{aligned}
\frac{1}{\omega - \epsilon_q - \epsilon_d \hat{n}_{d\overline{\beta}}} &= \frac{\hat{n}_{d\overline{\beta}}}{\omega - \epsilon_q - \epsilon_d} + \frac{1 - \hat{n}_{d\overline{\beta}}}{\omega - \epsilon_q} \\
&= \hat{n}_{d\overline{\beta}} \frac{\epsilon_d}{\left(\omega - \epsilon_q - \epsilon_d\right)\left(\omega - \epsilon_q\right)} + \frac{1}{\omega - \epsilon_q}
\end{aligned} \tag{1.8}
$$

Since these terms commute with the other terms, they can be taken out of the anticommutator; what's left is

$$
\left\{ V_q c^\dagger_{q\beta} c_{d\beta}, V_q^* c^\dagger_{d\beta} c_{q\beta} \right\} = \left|V_q\right|^2 \left[\hat{n}_{q\beta}\left(1 - \hat{n}_{d\beta}\right) + \hat{n}_{d\beta}\left(1 - \hat{n}_{q\beta}\right)\right] \tag{1.9}
$$

The τ and the $\hat{n}$ can be multiplied:

$$
2\tau_{q\beta}\left(1 - \hat{n}_{q\beta}\right) = \left(\hat{n}_{q\beta} - 1\right) \tag{1.10}
$$

$$
2\tau_{q\beta}\hat{n}_{q\beta} = \hat{n}_{q\beta} \tag{1.11}
$$

The total thing becomes

$$\begin{aligned}\sum_{q\beta}|V_q|^2\left[\hat{n}_{d\beta}\left(\hat{n}_{q\beta}-1\right)+\hat{n}_{q\beta}\left(1-\hat{n}_{d\beta}\right)\right]\left[\hat{n}_{d\overline{\beta}}\frac{\epsilon_d}{\left(\omega-\epsilon_q-\epsilon_d\right)\left(\omega-\epsilon_q\right)}+\frac{1}{\omega-\epsilon_q}\right]\\=\sum_{q\beta}|V_q|^2\left[\hat{n}_{q\beta}-\hat{n}_{d\beta}\right]\left[\hat{n}_{d\overline{\beta}}\frac{\epsilon_d}{\left(\omega-\epsilon_q-\epsilon_d\right)\left(\omega-\epsilon_q\right)}+\frac{1}{\omega-\epsilon_q}\right]\end{aligned}\tag{1.12}$$

Putting $\hat{n}_{q\beta}=1$, and dropping the non-operator terms, we get

$$\sum_\beta \hat{n}_{d\beta}\sum_q|V_q|^2\frac{\epsilon_q-\omega+2\epsilon_d}{\left(\omega-\epsilon_q\right)\left(\omega-\epsilon_q-\epsilon_d\right)}-\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\sum_{q\beta}|V_q|^2\frac{\epsilon_d}{\left(\omega-\epsilon_q\right)\left(\omega-\epsilon_q-\epsilon_d\right)}\tag{1.13}$$

The first term is the renormalization in on-site energy, $\sum_\beta \hat{n}_{d\beta}\Delta\epsilon_{d\beta}$, and the second term is the renormalization in the onsite repulsion, $\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\Delta U$.

Renormalized Hamiltonian Combining eqs. 1.4 and 1.13, we get

$$\mathcal{H}_{N-1}=\sum_{k<\Lambda_N,\sigma}\epsilon_k\hat{n}_{k\sigma}+\sum_{|q|=\Lambda_N}\epsilon_q+\sum_\sigma\left(\epsilon_{d\sigma}+\Delta\epsilon_{d\sigma}\right)\hat{n}_{d\sigma}+\left(U+\Delta U\right)\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\tag{1.14}$$

The second term is the renormalization in the kinetic energy of the disentangled electrons, the third term is the renormalized impurity site energy and the fourth term is the renormalized onsite repulsion.

$$\Delta\epsilon_d^N\equiv\epsilon_d\big|_{N-1}-\epsilon_d\big|_N=\sum_q|V_q|^2\frac{\epsilon_q-\omega+2\epsilon_d}{\left(\omega-\epsilon_q\right)\left(\omega-\epsilon_q-\epsilon_d\right)}\tag{1.15}$$

According to Hewson eq. 3.62 (page 68),

$$\frac{\mathrm{d}\epsilon_d}{\mathrm{d}\ln D}=-\frac{\Delta}{\pi}+O(V^3)=-\rho_0|V|^2+O(V^3)\tag{1.16}$$

in the limit of $U+\epsilon_d\gg D$ and $|\epsilon_d|\ll D$, under the assumptions that V_k is independent of k and the conduction band is flat ($\rho(\epsilon)=\rho_0$ for $\epsilon\in[-D,D]$).

Assuming that we integrate out a ring at energy D and of thickness $-|\delta D|$, such that $\epsilon_q=D$ everywhere on the ring, the number of available states is

$$\delta n=\frac{\mathrm{d}n}{\mathrm{d}E}\times\delta E=\rho(D)\times|\delta D|\tag{1.17}$$

We can then replace the summation in eq. 1.15 by δn:

$$\delta\epsilon_d(D)=|V|^2\rho(D)|\delta D|\frac{D-\omega+2\epsilon_d}{\left(\omega-D\right)\left(\omega-D-\epsilon_d\right)}\tag{1.18}$$

where $\rho(D)$ is the number of single-spin states on the shell D. This can be compared to eq. 1.16. In two dimensions, the energy density of states is independent of energy. **Setting $\omega = 0$**, we get

$$\begin{aligned} \delta\epsilon_d(D) &= |V|^2 \rho(D) |\delta D| \frac{D + 2\epsilon_d}{D\,(D+\epsilon_d)} \\ &= |V|^2 \rho(D) \frac{|\delta D|}{D} \frac{D+2\epsilon_d}{D+\epsilon_d} \end{aligned} \tag{1.19}$$

I used $\delta D = -|\delta D|$. Changing to continuum equation,

$$\frac{\mathrm{d}\epsilon_d}{\mathrm{d}\ln D} = -\frac{\Delta}{\pi} \frac{D+2\epsilon_d}{D+\epsilon_d} \tag{1.20}$$

In the regime where the single-occupied impurity level is comfortably inside the conduction band ($D \gg |\epsilon_d|$), we can approximate both the numerator and denominator as simply D. Then,

$$\frac{\mathrm{d}\epsilon_d}{\mathrm{d}\ln D} = -\frac{\Delta}{\pi} \tag{1.21}$$

$$\implies \epsilon_d + \frac{\Delta}{\pi} \log D = \text{constant} \tag{1.22}$$

Turning to the general equation 1.15, under the assumption of momentum-independent scattering, the continuum equation is

$$\begin{aligned} \frac{\mathrm{d}\epsilon_d}{\mathrm{d}\ln D} &= |V|^2 n(D) \frac{\omega - D - 2\epsilon_d}{(\omega - D)\,(\omega - D - \epsilon_d)} \\ &= |V|^2 n(D) \left(\frac{2}{\omega - D} - \frac{1}{\omega - D - \epsilon_d} \right) \end{aligned} \tag{1.23}$$

$n(D)$ is not the density of states, but the total number of states on the shell at energy D. Similarly, the renormalization in U is

$$\begin{aligned} \delta U &= -\sum_{q\beta} |V_q|^2 \frac{\epsilon_d}{(\omega - \epsilon_q)\,(\omega - \epsilon_q - \epsilon_d)} \\ &= -|V|^2 n(D) \sum_{\beta} \frac{\epsilon_d}{(\omega - D)\,(\omega - D - \epsilon_d)} \\ &= -2|V|^2 n(D) \frac{\epsilon_d}{(\omega - D)\,(\omega - D - \epsilon_d)} \\ \implies \frac{\mathrm{d}U}{\mathrm{d}\ln D} &= 2|V|^2 n(D) \frac{\epsilon_d}{(\omega - D)\,(\omega - D - \epsilon_d)} \\ &= 2|V|^2 n(D) \left(\frac{1}{\omega - D - \epsilon_d} - \frac{1}{\omega - D} \right) \end{aligned} \tag{1.24}$$

In the penultimate step, I used the fact that since the onsite energy for either spin is same, the summation just returns a factor of 2.

Putting $\omega = 0$,

$$\begin{aligned}
\frac{\mathrm{d}\epsilon_d}{\mathrm{d}\ln D} &= |V|^2 n(D)\left(\frac{1}{D+\epsilon_d} - \frac{2}{D}\right) \\
\frac{\mathrm{d}U}{\mathrm{d}\ln D} &= 2|V|^2 n(D)\left(\frac{1}{D} - \frac{1}{D+\epsilon_d}\right)
\end{aligned} \tag{1.25}$$

With higher order scattering

$$\mathcal{H} = \sum_{k\sigma}\epsilon_k \hat{n}_{k\sigma} + \sum_{k\sigma}\left(V_k c^\dagger_{k\sigma}c_{d\sigma} + h.c.\right) + \epsilon_d\sum_\sigma \hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + \sum_{\substack{kk'\\ \sigma}} V_2 c^\dagger_{k\sigma}c^\dagger_{d\overline{\sigma}}c_{d\sigma}c_{k'\overline{\sigma}} \tag{1.26}$$

One electron on shell:

$$\mathcal{H}_N = H_0 + H_{\text{imp}} + \epsilon_q\hat{n}_{q\beta} + V_q c^\dagger_{q\beta}c_{d\beta} + V_q^* c^\dagger_{d\beta}c_{q\beta} + \sum_k V_2 c^\dagger_{q\beta}c^\dagger_{d\overline{\beta}}c_{d\beta}c_{k\overline{\beta}} + \sum_{k'} V_2 c^\dagger_{k'\overline{\beta}}c^\dagger_{d\beta}c_{d\overline{\beta}}c_{q\beta} \tag{1.27}$$

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

$$\begin{aligned}
\Delta\mathcal{H}_N &= \sum_{q\beta}\tau_{q\beta}c^\dagger_{q\beta}\left[V_q + \sum_k V_2 c_{k\overline{\beta}}c^\dagger_{d\overline{\beta}}\right]c_{d\beta}\times c^\dagger_{d\beta}\left[V_q^* + \sum_{k'}V_2 c_{d\overline{\beta}}c^\dagger_{k'\overline{\beta}}\right]c_{q\beta}\frac{1}{\hat{\omega} - \left(H_{\text{imp}}+\epsilon_q\right)\hat{n}_{q\beta}} \\
&= \sum_{q\beta}\tau_{q\beta}\hat{n}_{q\beta}\left(1-\hat{n}_{d\beta}\right)\left[V_q + \sum_k V_2 c_{k\overline{\beta}}c^\dagger_{d\overline{\beta}}\right]\times\left[V_q^* + V_2\sum_{k'}c_{d\overline{\beta}}c^\dagger_{k'\overline{\beta}}\right]\frac{2}{\omega - \left(H_{\text{imp}}+\epsilon_q\right)} \\
&= \sum_{q\beta}\left[|V_q|^2 + \sum_{k'}V_q V_2 c_{d\overline{\beta}}c^\dagger_{k'\overline{\beta}} + \sum_k V_q^* V_2 c_{k\overline{\beta}}c^\dagger_{d\overline{\beta}} + \sum_{kk'}V_2^2\hat{n}_{d\overline{\beta}}c_{k\overline{\beta}}c^\dagger_{k'\overline{\beta}}\right]\frac{\left(1-\hat{n}_{d\beta}\right)\hat{n}_{q\beta}}{\omega - \left(H_{\text{imp}}+\epsilon_q\right)}
\end{aligned} \tag{1.28}$$

The first term in $\Delta\mathcal{H}_N$ is (calculated in the previous section)

$$\sum_{q\beta}|V_q|^2\left(1-\hat{n}_{d\beta}\right)\frac{1}{\omega - \left(H_{\text{imp}}+\epsilon_q\right)} = \sum_{q\beta}|V_q|^2\frac{\hat{n}_{d\beta}\left(\epsilon_q - \omega + 2\epsilon_d\right) - \hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\epsilon_d}{\left(\omega-\epsilon_q\right)\left(\omega-\epsilon_q-\epsilon_d\right)} \tag{1.29}$$

Just as in the previous section, they renormalize the onsite energy ϵ_d and double-occupation penalty U. The second term gives

$$\sum_{k'\beta}c_{d\overline{\beta}}c^\dagger_{k'\overline{\beta}}\sum_q V_q V_2\frac{\left(1-\hat{n}_{d\beta}\right)}{\omega - \left(H_{\text{imp}}+\epsilon_q\right)} = \sum_{k'\beta}c_{d\overline{\beta}}c^\dagger_{k'\overline{\beta}}\sum_q V_q V_2\left(1-\hat{n}_{d\beta}\right)\frac{1}{\omega - \left(\epsilon_d+\epsilon_q\right)} \tag{1.30}$$

The first of the two terms renormalizes the coupling V_k. The third term is the Hermitian conjugate of this term. The fourth term produces a potential scattering term.