4 Anderson Model URG

$$\mathcal{H} = \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{k\sigma} \left(V_k c^\dagger_{k\sigma} c_{d\sigma} + h.c. \right) + \sum_{\sigma} \epsilon_{d\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \tag{4.1}$$

One electron on shell

At first order, the rotated Hamiltonian is

$$\mathcal{H}_{j-1} = 2^{-n_j} \mathrm{Tr}_{1,2,\ldots,n_j} \mathcal{H}_j + \sum_{q\beta} \tau_{q\beta} \left\{ c^\dagger_{q\beta} \mathrm{Tr}_{q\beta} \left(\mathcal{H} c_{q\beta} \right), \eta_{q\beta} \right\} \tag{4.2}$$

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:

$$\begin{aligned}
\frac{1}{2} \mathrm{Tr}_{q\uparrow} \mathcal{H}_j &= \sum_{k<\Lambda_N,\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{\sigma} \epsilon_{d\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \frac{1}{2} \mathrm{Tr}_{q\uparrow} \left\{ \epsilon_k \hat{n}_{q\uparrow} \right\} \\
&= \sum_{k<\Lambda_N,\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{\sigma} \epsilon_{d\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \frac{1}{2} \epsilon_q \\
\frac{1}{2} \mathrm{Tr}_{q\downarrow} \frac{1}{2} \mathrm{Tr}_{q\uparrow} \mathcal{H}_j &= \sum_{k<\Lambda_N,\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{\sigma} \epsilon_{d\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \epsilon_q
\end{aligned} \tag{4.3}$$

$$\implies 2^{-n_j} \mathrm{Tr}_{1,2,\ldots,n_j} \mathcal{H}_j = \sum_{k<\Lambda_N,\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{\sigma} \epsilon_{d\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \sum_{|q|=\Lambda_N} \epsilon_q \tag{4.4}$$

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

$$\begin{aligned}
\mathrm{Tr}_{q\beta} \left(\mathcal{H} c_{q\beta} \right) &= \sum_{k\sigma} V_k \mathrm{Tr}_{q\beta} \left(c^\dagger_{k\sigma} c_{d\sigma} c_{q\beta} \right) \\
&= \sum_{k\sigma} V_k c_{d\sigma} \delta_{\sigma\beta} \delta_{kq} \\
&= V_q c_{d\beta}
\end{aligned} \tag{4.5}$$

$$\mathrm{Tr}_{q\beta} \left(c^\dagger_{q\beta} \mathcal{H} \right) = V^*_q c^\dagger_{d\beta} \tag{4.6}$$

$$
\begin{aligned}
\mathcal{H}^D &= \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{\sigma} \epsilon_{d\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \\
\text{Tr}_{q\beta}\left(\mathcal{H}^D \hat{n}_{q\beta}\right) &= \sum_{k<\Lambda_N,\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{\sigma} \epsilon_{d\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \epsilon_q \\
\eta_{q\beta} &= \text{Tr}_{q\beta}\left(c^\dagger_{q\beta}\mathcal{H}\right) c_{q\beta} \frac{1}{\hat{\omega} - \text{Tr}_{q\beta}\left(\mathcal{H}^D \hat{n}_{q\beta}\right)\hat{n}_{q\beta}} \\
&= V_q^* c^\dagger_{d\beta} c_{q\beta} \frac{1}{\hat{\omega} - \left(\sum_{k<\Lambda_N,\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_\sigma \epsilon_{d\sigma}\hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right)\hat{n}_{q\beta} - \epsilon_q \hat{n}_{q\beta}} \\
&= V_q^* c^\dagger_{d\beta} c_{q\beta} \frac{1}{\omega\tau_{q\beta} - \epsilon_q \tau_{q\beta} - \epsilon_{d\beta}\tau_{d\beta}}
\end{aligned}
\tag{4.7}
$$

At the last step, **I replaced $\hat{\omega} - \sum_{k<\Lambda_N,\sigma} \epsilon_k \hat{n}_{k\sigma}\hat{n}_{q\beta} - \epsilon_{d\overline{\beta}}\hat{n}_{d\overline{\beta}}$ with $\omega\tau_{q\beta} + \frac{\epsilon_{d\beta}}{2} + \frac{\epsilon_q}{2}$**.Also, **I assumed there are no two-particle correlations such that** $\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} = 0$. Putting together the individual pieces, we can now write the second term:

$$
\sum_{q\beta} \tau_{q\beta} \left\{ c^\dagger_{q\beta} \text{Tr}_{q\beta}\left(\mathcal{H} c_{q\beta}\right), \eta_{q\beta} \right\} = \sum_{q\beta} \tau_{q\beta} \left\{ V_q c^\dagger_{q\beta} c_{d\beta}, V_q^* c^\dagger_{d\beta} c_{q\beta} \frac{1}{\omega\tau_{q\beta} - \epsilon_q\tau_{q\beta} - \epsilon_{d\beta}\tau_{d\beta}} \right\}
\tag{4.8}
$$

We now note that the factor with ω can be made a scalar as follows:

$$
\begin{aligned}
\left(1 - \hat{n}_{d\beta}\right)\hat{n}_{q\beta} \frac{1}{\omega\tau_{q\beta} - \epsilon_q\tau_{q\beta} - \epsilon_{d\beta}\tau_{d\beta}} \left|n_{q\beta}, n_{d\beta}\right\rangle &= \begin{cases} \frac{2}{\omega - \epsilon_q + \epsilon_{d\beta}} \left|1, 0\right\rangle & \hat{n}_{q\beta} = 1, \hat{n}_{d\beta} = 0 \\ 0 & \text{otherwise} \end{cases} \\
&= 2\left(1 - \hat{n}_{d\beta}\right)\hat{n}_{q\beta}\left(\omega - \epsilon_q + \epsilon_{d\beta}\right)^{-1} \\
c^\dagger_{d\beta} c_{q\beta} \frac{1}{\omega\tau_{q\beta} - \epsilon_q\tau_{q\beta} - \epsilon_{d\beta}\tau_{d\beta}} c^\dagger_{q\beta} c_{d\beta} \left|n_{q\beta}, n_{d\beta}\right\rangle &= 2\hat{n}_{d\beta}\left(1 - \hat{n}_{q\beta}\right)\left(\omega - \epsilon_q + \epsilon_{d\beta}\right)^{-1}
\end{aligned}
\tag{4.9}
$$

The anticommutator becomes

$$
\sum_{q\beta} \tau_{q\beta} \left\{ c^\dagger_{q\beta} \text{Tr}_{q\beta}\left(\mathcal{H} c_{q\beta}\right), \eta_{q\beta} \right\} = \sum_{q\beta} 2\tau_{q\beta} |V_q|^2 \left[\hat{n}_{d\beta}\left(1 - \hat{n}_{q\beta}\right) + \hat{n}_{q\beta}\left(1 - \hat{n}_{d\beta}\right)\right]\left(\omega - \epsilon_q + \epsilon_{d\beta}\right)^{-1}
\tag{4.10}
$$

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

$$
2\tau_{q\beta}\left(1 - \hat{n}_{q\beta}\right) = \hat{n}_{q\beta} - 1 \tag{4.11}
$$

$$
2\tau_{q\beta}\hat{n}_{q\beta} = \hat{n}_{q\beta} \tag{4.12}
$$

This simplifies the expression of the anticommutator:

$$
\begin{aligned}
\sum_{q\beta} \tau_{q\beta} \left\{ c^\dagger_{q\beta} \text{Tr}_{q\beta}\left(\mathcal{H} c_{q\beta}\right), \eta_{q\beta} \right\} &= \sum_{q\beta} |V_q|^2 \left[\hat{n}_{d\beta}\left(\hat{n}_{q\beta} - 1\right) + \hat{n}_{q\beta}\left(1 - \hat{n}_{d\beta}\right)\right]\left(\omega - \epsilon_q + \epsilon_{d\beta}\right)^{-1} \\
&= \sum_{q\beta} |V_q|^2 \left(\hat{n}_{q\beta} - \hat{n}_{d\beta}\right)\left(\omega - \epsilon_q + \epsilon_{d\beta}\right)^{-1}
\end{aligned}
\tag{4.13}
$$

Renormalized Hamiltonian Combining eqs. 4.4 and 4.13, we get

$$\mathcal{H}_{N-1} = \sum_{k<\Lambda_N,\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{\sigma} \epsilon_{d\sigma}\hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + \sum_{|q|=\Lambda_N} \epsilon_q + \sum_{q\beta} \frac{|V_q|^2}{\omega - \epsilon_q + \epsilon_{d\beta}} \left(\hat{n}_{q\beta} - \hat{n}_{d\beta}\right) \tag{4.14}$$

Dropping the constant (non-operator) term and gathering the terms into conduction electron and impurity electron groups:

$$\mathcal{H}_{N-1} = \sum_{k<\Lambda_N,\sigma} \epsilon_k \hat{n}_{k\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + \sum_{q\beta} \frac{|V_q|^2}{\omega - \epsilon_q + \epsilon_{d\beta}} \hat{n}_{q\beta} + \sum_{\beta} \left(\epsilon_{d\beta} - \sum_{q} \frac{|V_q|^2}{\omega - \epsilon_q + \epsilon_{d\beta}} \right) \hat{n}_{d\beta} \tag{4.15}$$

The third term is the renormalization in the kinetic energy of the disentangled electrons and the fourth term is the renormalization in the impurity site energy:

$$\Delta\epsilon_{d\beta}^{N} \equiv \epsilon_{d\beta}\big|_{N-1} - \epsilon_{d\beta}\big|_{N} = -\sum_{q} \frac{|V_q|^2}{\omega - \epsilon_q + \epsilon_{d\beta}} \tag{4.16}$$

Since the equation is same for $\beta =\uparrow,\downarrow$, we can drop the β index. According to Hewson eq. 3.62 (page 68),

$$\frac{d\epsilon_d}{d\ln D} = -\frac{\Delta}{\pi} + O(V^3) = -\rho_0|V|^2 + O(V^3) \tag{4.17}$$

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

$$\delta n = \frac{dn}{dE} \times \delta E = \rho(D) \times \delta D \tag{4.18}$$

We can then replace the summation by δn:

$$\delta\epsilon_d(D) = |V|^2 \sum_{q} \frac{1}{\omega(D) - D + \epsilon_d} = \delta D \rho(D)|V|^2 \frac{1}{\omega - D + \epsilon_d} \tag{4.19}$$

where $\rho(\epsilon_N)$ is the number of single-spin states on the shell. This can be compared to eq. 4.17. In two dimensions, the energy density of states is independent of energy. **Setting $\omega = 0$**, we get

$$\begin{aligned} \delta\epsilon_d(D) &= -\delta D \rho(D)|V|^2 \frac{1}{D - \epsilon_d} \\ &= -\delta D \frac{\Delta}{\pi} \frac{1}{D - \epsilon_d} \end{aligned} \tag{4.20}$$

Changing to continuum equation,

$$\frac{d\epsilon_d}{dD} = -\frac{\Delta}{\pi}\frac{1}{D-\epsilon_d} \tag{4.21}$$

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

$$\frac{d\epsilon_d}{dD} = -\frac{\Delta}{\pi}\frac{1}{D} \tag{4.22}$$

$$\implies \epsilon_d + \frac{\Delta}{\pi}\log D = \text{constant} \tag{4.23}$$

This is eq. 3.65 in Hewson.

Turning to the general equation 4.16, under the assumption of momentum-independent scattering, the continuum equation is

$$\frac{d\epsilon_d}{dD} = \frac{|V|^2 n(D)}{\omega - D + \epsilon_d} \tag{4.24}$$

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

- $\omega = 2D$ gives a fixed point at $D = \epsilon_d$. According to Haldane, such a fixed point arises for the regime $\epsilon_d^* \gg \Delta$.
- $\omega = 0$ gives a fixed point at $D = -\epsilon_d$. Such a fixed point arises when $\epsilon_d^* \ll -\Delta$.
- Intermediate values of ω might correspond to the mixed valence regime.

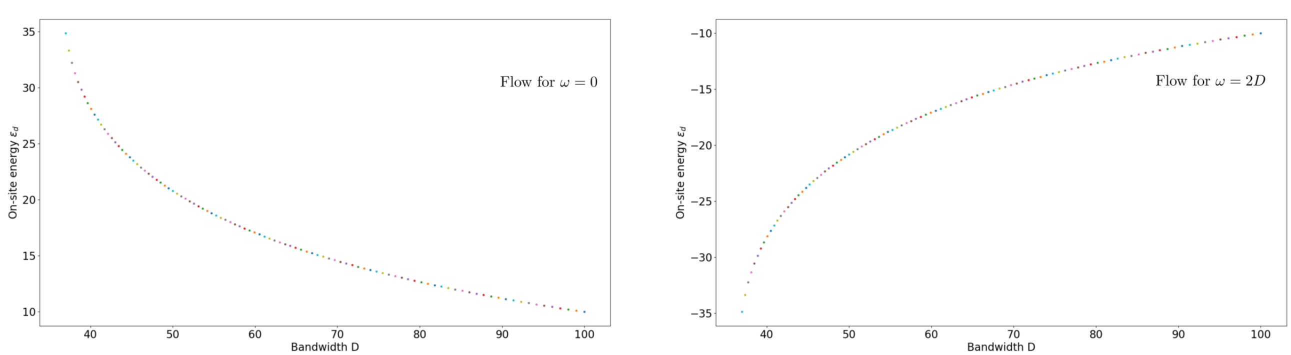

Figure 6: Variation of on-site energy for $\omega = 0, 2D$