Contents

1 Anderson Model URG

 $\mathbf{2}$

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

With four-Fermion interaction

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

$$\tag{1.2}$$

Considering one electron on the shell,

$$\mathcal{H} = \sum_{\substack{k < \Lambda_N \\ \sigma}} \left[\epsilon_k \hat{n}_{k\sigma} + V_k c_{k\sigma}^{\dagger} c_{d\sigma} + \text{h.c.} \right] + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \sum_{\substack{k,k',q \\ \sigma\sigma'}} v_q c_{k+q,\sigma}^{\dagger} c_{k'-q,\sigma'}^{\dagger} c_{k,\sigma} c_{k',\sigma'} + \epsilon_q \hat{n}_{q\beta} + V_q c_{q\beta}^{\dagger} c_{d\beta} + \text{h.c.} + \sum_{\substack{k,p \\ (k,k+p,q-p<\Lambda_N)}} \left[v_p c_{k+p,\sigma}^{\dagger} c_{q-p,\beta}^{\dagger} c_{k\sigma} c_{q\beta} + \text{h.c.} \right] + \sum_{k<\Lambda_N,\sigma} v_{k-q} \hat{n}_{k\sigma} \hat{n}_{q\beta}$$

$$(1.3)$$

Define

$$H_0 \equiv \sum_{\substack{k < \Lambda_N \\ \sigma}} \left[\epsilon_k \hat{n}_{k\sigma} + V_k c_{k\sigma}^{\dagger} c_{d\sigma} + \text{h.c.} \right] + \sum_{\substack{k,k',q \\ \sigma\sigma'}} v_q c_{k+q,\sigma}^{\dagger} c_{k'-q,\sigma'}^{\dagger} c_{k,\sigma} c_{k',\sigma'}$$
(1.4)

$$H_{\rm imp} = \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \tag{1.5}$$

Then,

$$\mathcal{H}_{1} = \frac{1}{2} \operatorname{Tr}_{\text{all}} (\mathcal{H}) + \sum_{q\beta} \tau_{q\beta} \left\{ c_{q\beta}^{\dagger} \operatorname{Tr}_{q\beta} (\mathcal{H} c_{q\beta}), \eta_{q\beta} \right\}$$
(1.6)

The first term is

$$\frac{1}{2} \operatorname{Tr}_{\text{all}} (\mathcal{H}) = H_0 + H_{\text{imp}} + \frac{1}{2} \sum_{q\beta} \left[\epsilon_q + \sum_{k < \Lambda_N, \sigma} v_{k-q} \hat{n}_{k\sigma} \right]$$
 (1.7)

The second term is:

$$c_{q\beta}^{\dagger} \operatorname{Tr}_{q\beta} (\mathcal{H} c_{q\beta}) = V_{q} c_{q\beta}^{\dagger} c_{d\beta} + \sum_{k,p} v_{p}^{*} c_{q\beta}^{\dagger} c_{k\sigma}^{\dagger} c_{k+p,\sigma} c_{q-p,\beta}$$

$$= c_{q\beta}^{\dagger} \left(V_{q} c_{d\beta} + \sum_{k,p} v_{p}^{*} c_{k\sigma}^{\dagger} c_{k+p,\sigma} c_{q-p,\beta} \right)$$

$$(1.8)$$

$$\eta_{q\beta} = \left[V_{q}^{*} c_{d\beta}^{\dagger} c_{q\beta} + \sum_{k,p} v_{p} c_{k+p,\sigma}^{\dagger} c_{q-p,\beta}^{\dagger} c_{k\sigma} c_{q\beta} \right] \frac{1}{\hat{\omega} - \left[H_{0}^{D} + H_{imp} + \epsilon_{q} + \sum_{k<\Lambda_{N},\sigma} v_{k-q} \hat{n}_{k\sigma} \right] \hat{n}_{q\beta}}$$

$$= \left[\left(V_{q}^{*} c_{d\beta}^{\dagger} + \sum_{k,p} v_{p} c_{q-p,\beta}^{\dagger} c_{k+p,\sigma}^{\dagger} c_{k\sigma} \right) c_{q\beta} \right] \frac{2}{\omega - \left[\epsilon_{d} \hat{n}_{d\overline{\beta}} + \epsilon_{q} \right]}$$

$$\sum_{q\beta} \tau_{q\beta} \left\{ c_{q\beta}^{\dagger} \operatorname{Tr}_{q\beta} \left(\mathcal{H} c_{q\beta} \right), \eta_{q\beta} \right\} = \sum_{q\beta} \frac{2\tau_{q\beta}}{\omega - \left[\epsilon_{d} \hat{n}_{d\overline{\beta}} + \epsilon_{q} \right]} \left\{ c_{q\beta}^{\dagger} \left(V_{q} c_{d\beta} + \sum_{k,p} v_{p}^{*} c_{k\sigma}^{\dagger} c_{k+p,\sigma} c_{q-p,\beta} \right) \right\}$$

$$\left(V_{q}^{*} c_{d\beta}^{\dagger} + \sum_{k,p} v_{p} c_{q-p,\beta}^{\dagger} c_{k+p,\sigma}^{\dagger} c_{k\sigma} \right) c_{q\beta} \right\}$$

$$\left(V_{q}^{*} c_{d\beta}^{\dagger} + \sum_{k,p} v_{p} c_{q-p,\beta}^{\dagger} c_{k+p,\sigma}^{\dagger} c_{k\sigma} \right) c_{q\beta} \right\}$$

$$\left(V_{q}^{*} c_{d\beta}^{\dagger} + \sum_{k,p} v_{p} c_{q-p,\beta}^{\dagger} c_{k+p,\sigma}^{\dagger} c_{k\sigma} \right) c_{q\beta} \right\}$$

$$\left(V_{q}^{*} c_{d\beta}^{\dagger} + \sum_{k,p} v_{p} c_{q-p,\beta}^{\dagger} c_{k+p,\sigma}^{\dagger} c_{k\sigma} \right) c_{q\beta} \right\}$$

$$\left(V_{q}^{*} c_{d\beta}^{\dagger} + \sum_{k,p} v_{p} c_{q-p,\beta}^{\dagger} c_{k+p,\sigma}^{\dagger} c_{k\sigma} \right) c_{q\beta}$$

$$\left(V_{q}^{*} c_{d\beta}^{\dagger} + \sum_{k,p} v_{p} c_{q-p,\beta}^{\dagger} c_{k+p,\sigma}^{\dagger} c_{k\sigma} \right) c_{q\beta} \right\}$$

$$\left(V_{q}^{*} c_{d\beta}^{\dagger} + \sum_{k,p} v_{p} c_{q-p,\beta}^{\dagger} c_{k+p,\sigma}^{\dagger} c_{k\sigma} \right) c_{q\beta}$$

Because $2\tau_{q\beta}c_{q\beta} = -c_{q\beta}$ and $2\tau_{q\beta}c_{q\beta}^{\dagger} = c_{q\beta}^{\dagger}$, we get

$$\sum_{q\beta} \frac{1}{\omega - \left[\epsilon_{d}\hat{n}_{d\overline{\beta}} + \epsilon_{q}\right]} \left[c_{q\beta}^{\dagger} \left(V_{q}c_{d\beta} + \sum_{k,p} v_{p}^{*} c_{k\sigma}^{\dagger} c_{k+p,\sigma} c_{q-p,\beta} \right), \left(V_{q}^{*} c_{d\beta}^{\dagger} + \sum_{k,p} v_{p} c_{q-p,\beta}^{\dagger} c_{k+p,\sigma}^{\dagger} c_{k\sigma} \right) c_{q\beta} \right]$$
(1.11)

The first commutator renormalizes the impurity site energy:

$$\[V_q c_{q\beta}^{\dagger} c_{d\beta}, V_q^* c_{d\beta}^{\dagger} c_{q\beta} \] = |V_q|^2 \left(\hat{n}_{q\beta} - \hat{n}_{d\beta} \right) \tag{1.12}$$

The second term gives:

$$\begin{bmatrix}
V_{q}c_{q\beta}^{\dagger}c_{d\beta}, \sum_{k,p,\sigma}v_{p}c_{q-p,\beta}^{\dagger}c_{k+p,\sigma}^{\dagger}c_{k\sigma}c_{q\beta}
\end{bmatrix} = \sum_{k,p,\sigma}V_{q}v_{p}\left[c_{q\beta}^{\dagger}c_{d\beta}, c_{q-p,\beta}^{\dagger}c_{k+p,\sigma}^{\dagger}c_{k,\sigma}c_{q,\beta}\right]$$

$$= -\sum_{k,p,\sigma}V_{q}v_{p}c_{d\beta}c_{k+p,\sigma}^{\dagger}c_{q-p,\beta}^{\dagger}c_{k,\sigma}$$

$$= -\sum_{k,p,\sigma}V_{q}v_{p}c_{d\beta}c_{k+p,\sigma}^{\dagger}\left(\delta_{q=k+p,\sigma}^{q=k+p} - c_{k,\sigma}c_{q-p,\beta}^{\dagger}\right)$$

$$= \sum_{k,p,\sigma}V_{q}v_{p}c_{d\beta}c_{k+p,\sigma}^{\dagger}c_{k,\sigma}c_{q-p,\beta}$$

$$= \sum_{k,p,\sigma}V_{q}v_{p}c_{d\beta}c_{k+p,\sigma}^{\dagger}c_{k,\sigma}c_{q-p,\beta}$$

$$= \sum_{k,p,\sigma}V_{q}v_{p}c_{d\beta}c_{k+p,\sigma}^{\dagger}c_{k,\sigma}c_{q-p,\beta}$$

$$= \sum_{k,p,\sigma}V_{q}v_{p}c_{d\beta}c_{k+p,\sigma}^{\dagger}c_{k,\sigma}c_{q-p,\beta}$$

In the second step, I chose the $\hat{n}_{q\beta} = 1$ sector. In the last step I used the fact that since the only electron on the shell is the one with q, we must have $k + p \neq q$, hence the $\delta_{q=k+p}$

gives zero. The third term is just the Hermitian conjugate:

$$\left[\sum_{k,p,\sigma} v_p^* c_{k\sigma}^{\dagger} c_{q\beta}^{\dagger} c_{k+p,\sigma} c_{q-p,\beta}, V_q^* c_{d\beta}^{\dagger} c_{q\beta}\right] = \sum_{k,p,\sigma} V_q^* v_p^* c_{q-p,\beta} c_{k,\sigma}^{\dagger} c_{k+p,\sigma} c_{d,\beta}^{\dagger}$$
(1.14)

The fourth term gives (using $\hat{n}_{q\beta} = 1$),

$$\left[\sum_{k,p,\sigma} v_{p}^{*} c_{k\sigma}^{\dagger} c_{q\beta}^{\dagger} c_{k+p,\sigma} c_{q-p,\beta}, \sum_{k',p',\sigma'} v_{p}' c_{q-p',\beta}^{\dagger} c_{k'+p',\sigma'}^{\dagger} c_{k'\sigma'} c_{q\beta}\right] \\
= \sum_{k',p'} v_{p'}^{\dagger} c_{k\sigma}^{\dagger} c_{k+p,\sigma} c_{q-p,\beta} c_{q-p',\beta}^{\dagger} c_{k'+p',\sigma'}^{\dagger} c_{k'\sigma'} c_$$

The total renormalization is thus

$$\Delta H = \sum_{q\beta} \frac{1}{\omega - \left[\epsilon_d \hat{n}_{d\overline{\beta}} + \epsilon_q\right]} \left[|V_q|^2 \left(\hat{n}_{q\beta} - \hat{n}_{d\beta} \right) + \sum_{k,p,\sigma} V_q v_p c_{d\beta} c_{k+p,\sigma}^{\dagger} c_{k,\sigma} c_{q-p,\beta}^{\dagger} + \text{h.c.} \right] + \sum_{k,p,\sigma} v_{p'} c_{k\sigma}^{\dagger} c_{k+p,\sigma} c_{q-p,\beta} c_{q-p',\beta}^{\dagger} c_{k'+p',\sigma'}^{\dagger} c_{k'\sigma'} \right]$$

$$(1.16)$$