Introduction

The single-impurity Anderson model (SIAM) is one of the most well-studied models in condensed matter physics and is the prototypical model for magnetism. It shows how strong correlations between electrons give rise to a residual local moment.

1 Anderson Model URG

1.1 Without spin-spin interaction

The model is the usual single-impurity Anderson model Hamiltonian.

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

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.

Particle Sector

The particle sector involves only particle excitations. The state $q\beta$ is occupied in the intermediate (excited) state. This contribution will be given by the first term in the anti-commutator of eq. 1.2.

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:

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

$$\frac{1}{2} \mathrm{Tr}_{q\downarrow} \frac{1}{2} \mathrm{Tr}_{q\uparrow} \mathcal{H}_j = \sum_{k<\Lambda_N,\sigma} \epsilon_k \hat{n}_{k\sigma} + \epsilon_d \sum_\sigma \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + \epsilon_q$$

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

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

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

$$
\begin{aligned}
\mathcal{H}^D &= \sum_{k\sigma}\epsilon_k\hat{n}_{k\sigma} + \epsilon_d\sum_\sigma \hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} \\
\mathrm{Tr}_{q\beta}\left(\mathcal{H}^D\hat{n}_{q\beta}\right) &= \sum_{k<\Lambda_N,\sigma}\epsilon_k\hat{n}_{k\sigma} + \epsilon_d\sum_\sigma \hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + \epsilon_q
\end{aligned}
\tag{1.6}
$$

There is a more straightforward way of getting these expressions. Some thought reveals that $c^\dagger_{q\beta}\mathrm{Tr}_{q\beta}\left(\mathcal{H}c_{q\beta}\right)$ is, by definition, the part of the Hamiltonian that scatters from electrons *not at* $q\beta$ to $q\beta$. In other words, **it is that off-diagonal part of the Hamiltonian that involves a** $c^\dagger_{q\beta}$. That part is, of course, $V_q c^\dagger_{q\beta}c_{d\beta}$. Similarly, $\mathrm{Tr}_{q\beta}\left(c^\dagger_{q\beta}\mathcal{H}\right)c_{q\beta}$ is the off-diagonal part that has a $c_{q\beta}$, $V^*_q c^\dagger_{d\beta}c_{q\beta}$. Finally, the term in the denominator of η is simply the diagonal part of the Hamiltonian, which in our case is the kinetic energies of all the electrons and the impurity diagonal part. The point of this paragraph is that one can write down these terms simply by looking at the Hamiltonian and without carrying out any trace.

$$
\begin{aligned}
\eta_{q\beta} &= \mathrm{Tr}_{q\beta}\left(c^\dagger_{q\beta}\mathcal{H}\right)c_{q\beta}\frac{1}{\hat{\omega} - \mathrm{Tr}_{q\beta}\left(\mathcal{H}^D\hat{n}_{q\beta}\right)\hat{n}_{q\beta}} \\
&= V^*_q c^\dagger_{d\beta}c_{q\beta}\frac{1}{\hat{\omega} - \left(\sum_{k<\Lambda_N,\sigma}\epsilon_k\hat{n}_{k\sigma} + \epsilon_d\sum_\sigma\hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} - \epsilon_q\right)\hat{n}_{q\beta}} \\
&= V^*_q c^\dagger_{d\beta}c_{q\beta}\frac{1}{\omega\tau_{q\beta} - \left(\epsilon_d\sum_\sigma\hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + \epsilon_q\right)\tau_{q\beta}}
\end{aligned}
\tag{1.7}
$$

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:

$$
\begin{aligned}
\sum_{q\beta}\tau_{q\beta}\left\{c^\dagger_{q\beta}\mathrm{Tr}_{q\beta}\left(\mathcal{H}c_{q\beta}\right), \eta_{q\beta}\right\} &= \sum_{q\beta}\tau_{q\beta}\left\{V_q c^\dagger_{q\beta}c_{d\beta}, V^*_q c^\dagger_{d\beta}c_{q\beta}\frac{1}{\frac{1}{2}\left(\omega - \epsilon_q - \epsilon_d\hat{n}_{d\overline{\beta}}\right)}\right\} \\
&= \sum_{q\beta}2\tau_{q\beta}\left\{V_q c^\dagger_{q\beta}c_{d\beta}, V^*_q c^\dagger_{d\beta}c_{q\beta}\frac{1}{\omega - \epsilon_q - \epsilon_d\hat{n}_{d\overline{\beta}}}\right\}
\end{aligned}
\tag{1.8}
$$

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

$$\begin{aligned}\frac{1}{\omega-\epsilon_q-\epsilon_d\hat{n}_{d\overline{\beta}}} &= \frac{\hat{n}_{d\overline{\beta}}}{\omega-\epsilon_q-\epsilon_d}+\frac{1-\hat{n}_{d\overline{\beta}}}{\omega-\epsilon_q} \\ &= \hat{n}_{d\overline{\beta}}\frac{\epsilon_d}{\left(\omega-\epsilon_q-\epsilon_d\right)\left(\omega-\epsilon_q\right)}+\frac{1}{\omega-\epsilon_q}\end{aligned} \tag{1.9}$$

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

$$\left\{V_q c^\dagger_{q\beta}c_{d\beta}, V_q^* c^\dagger_{d\beta}c_{q\beta}\right\} = \left|V_q\right|^2\left[\hat{n}_{q\beta}\left(1-\hat{n}_{d\beta}\right)+\hat{n}_{d\beta}\left(1-\hat{n}_{q\beta}\right)\right] \tag{1.10}$$

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

$$2\tau_{q\beta}\left(1-\hat{n}_{q\beta}\right) = \left(\hat{n}_{q\beta}-1\right) \tag{1.11}$$

$$2\tau_{q\beta}\hat{n}_{q\beta} = \hat{n}_{q\beta} \tag{1.12}$$

The total thing becomes

$$\begin{aligned}&\sum_{q\beta}\left|V_q\right|^2\left[\hat{n}_{d\beta}\left(\hat{n}_{q\beta}-1\right)+\hat{n}_{q\beta}\left(1-\hat{n}_{d\beta}\right)\right]\left[\hat{n}_{d\overline{\beta}}\frac{\epsilon_d}{\left(\omega-\epsilon_q-\epsilon_d\right)\left(\omega-\epsilon_q\right)}+\frac{1}{\omega-\epsilon_q}\right] \\ &\qquad = \sum_{q\beta}\left|V_q\right|^2\left[\hat{n}_{q\beta}-\hat{n}_{d\beta}\right]\left[\hat{n}_{d\overline{\beta}}\frac{\epsilon_d}{\left(\omega-\epsilon_q-\epsilon_d\right)\left(\omega-\epsilon_q\right)}+\frac{1}{\omega-\epsilon_q}\right]\end{aligned} \tag{1.13}$$

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

$$\sum_\beta \hat{n}_{d\beta}\sum_q\left|V_q\right|^2\frac{\epsilon_q-\omega+2\epsilon_d}{\left(\omega-\epsilon_q\right)\left(\omega-\epsilon_q-\epsilon_d\right)} - \hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\sum_{q\beta}\left|V_q\right|^2\frac{\epsilon_d}{\left(\omega-\epsilon_q\right)\left(\omega-\epsilon_q-\epsilon_d\right)} \tag{1.14}$$

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 1.14, we get

$$\mathcal{H}_{N-1} = \sum_{k<\Lambda_N,\sigma}\epsilon_k\hat{n}_{k\sigma} + \sum_{|q|=\Lambda_N}\epsilon_q + \sum_\sigma\left(\epsilon_{d\sigma}+\Delta\epsilon_{d\sigma}\right)\hat{n}_{d\sigma} + \left(U+\Delta U\right)\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} \tag{1.15}$$

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.

$$\Delta\epsilon_d^N \equiv \epsilon_d\big|_{N-1} - \epsilon_d\big|_N = \sum_q\left|V_q\right|^2\frac{\epsilon_q-\omega+2\epsilon_d}{\left(\omega-\epsilon_q\right)\left(\omega-\epsilon_q-\epsilon_d\right)} \tag{1.16}$$

According to Hewson eq. 3.62 (page 68),

$$\frac{\mathrm{d}\epsilon_d}{\mathrm{d}\ln D} = -\frac{\Delta}{\pi} + O(V^3) = -\rho_0|V|^2 + O(V^3) \tag{1.17}$$

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

$$\delta n = \frac{\mathrm{d}n}{\mathrm{d}E} \times \delta E = \rho(D) \times |\delta D| \tag{1.18}$$

We can then replace the summation in eq. 1.16 by δn:

$$\delta\epsilon_d(D) = |V|^2\rho(D)|\delta D|\frac{D - \omega + 2\epsilon_d}{(\omega - D)(\omega - D - \epsilon_d)} \tag{1.19}$$

where $\rho(D)$ is the number of single-spin states on the shell D. This can be compared to eq. 1.17. In two dimensions, the energy density of states is independent of energy. **Setting $\omega = 0$**, we get

$$\begin{aligned} \delta\epsilon_d(D) &= |V|^2\rho(D)|\delta D|\frac{D + 2\epsilon_d}{D(D + \epsilon_d)} \\ &= |V|^2\rho(D)\frac{|\delta D|}{D}\frac{D + 2\epsilon_d}{D + \epsilon_d} \end{aligned} \tag{1.20}$$

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

$$\frac{\mathrm{d}\epsilon_d}{\mathrm{d}\ln D} = -\frac{\Delta}{\pi}\frac{D + 2\epsilon_d}{D + \epsilon_d} \tag{1.21}$$

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,

$$\frac{\mathrm{d}\epsilon_d}{\mathrm{d}\ln D} = -\frac{\Delta}{\pi} \tag{1.22}$$

$$\implies \epsilon_d + \frac{\Delta}{\pi}\log D = \text{constant} \tag{1.23}$$

Turning to the general equation 1.16, under the assumption of momentum-independent scattering, the continuum equation is

$$\begin{aligned} \frac{\mathrm{d}\epsilon_d}{\mathrm{d}\ln D} &= |V|^2 n(D)\frac{\omega - D - 2\epsilon_d}{(\omega - D)(\omega - D - \epsilon_d)} \\ &= |V|^2 n(D)\left(\frac{2}{\omega - D} - \frac{1}{\omega - D - \epsilon_d}\right) \end{aligned} \tag{1.24}$$

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

$$
\begin{aligned}
\delta U &= -\sum_{q\beta} |V_q|^2 \frac{\epsilon_d}{(\omega - \epsilon_q)(\omega - \epsilon_q - \epsilon_d)} \\
&= -|V|^2 n(D) \sum_{\beta} \frac{\epsilon_d}{(\omega - D)(\omega - D - \epsilon_d)} \\
&= -2|V|^2 n(D) \frac{\epsilon_d}{(\omega - D)(\omega - D - \epsilon_d)} \\
\implies \frac{\mathrm{d}U}{\mathrm{d}\ln D} &= 2|V|^2 n(D) \frac{\epsilon_d}{(\omega - D)(\omega - D - \epsilon_d)} \\
&= 2|V|^2 n(D) \left(\frac{1}{\omega - D - \epsilon_d} - \frac{1}{\omega - D} \right)
\end{aligned}
\tag{1.25}
$$

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 $\omega = 0$,

$$
\begin{aligned}
\frac{\mathrm{d}\epsilon_d}{\mathrm{d}\ln D} &= |V|^2 n(D) \left(\frac{1}{D + \epsilon_d} - \frac{2}{D} \right) \\
\frac{\mathrm{d}U}{\mathrm{d}\ln D} &= 2|V|^2 n(D) \left(\frac{1}{D} - \frac{1}{D + \epsilon_d} \right)
\end{aligned}
\tag{1.26}
$$

1.2 With Kondo-like interaction

The four-Fermi interaction we are considering is of the form

$$
\mathcal{H}_I = \sum_{k,k',\sigma_i} u c^\dagger_{d\sigma_2} c_{d\sigma_4} c_{k'\sigma_3} c^\dagger_{k\sigma_1} \delta_{(\sigma_1 + \sigma_2 = \sigma_3 + \sigma_4)} \tag{1.27}
$$

The u in general depends on the spin and the momenta. Expanding the summation by using the delta gives

$$
\mathcal{H}_I = \underbrace{\sum_{k,k',\sigma,\sigma'} u_1 \hat{n}_{d\sigma'} c^\dagger_{k\sigma} c_{k'\sigma}}_{\text{spin-preserving scattering}} + \overbrace{\sum_{k,k',\sigma} u_2 c^\dagger_{d\overline{\sigma}} c_{d\sigma} c^\dagger_{k\sigma} c_{k'\overline{\sigma}}}^{\text{spin-flip scattering}} \tag{1.28}
$$

At this point, we drop the dependence of u on the momenta and assume it depends only on the spin transfer. The first term (attached with u_1) involves no spin-flip between the scattering momenta or the scattering impurity electrons ($k\sigma \to k'\sigma, d\sigma' \to d\sigma'$). We label this coupling as u_P. The other coupling involves a spin-flip scattering, so we label that as

u_A.

$$\mathcal{H}_{I,N} = \sum_{k,k',\sigma,\sigma'} u_P \hat{n}_{d\sigma'} c^\dagger_{k\sigma} c_{k'\sigma} + \sum_{k,k',\sigma} u_A c^\dagger_{d\overline{\sigma}} c_{d\sigma} c^\dagger_{k\sigma} c_{k'\overline{\sigma}} \tag{1.29}$$

where the N in the denominator means the sum is over all momenta up to $|k| = \Lambda_N$. The parallel scattering has two components, when expanded, is of the form

$$u_{\uparrow\uparrow} \hat{n}_{d\uparrow} c^\dagger_{k\uparrow} c_{k'\uparrow} + u_{\downarrow\downarrow} \hat{n}_{d\downarrow} c^\dagger_{k\downarrow} c_{k'\uparrow} + u_{\uparrow\downarrow} \hat{n}_{d\uparrow} c^\dagger_{k\downarrow} c_{k'\downarrow} + u_{\downarrow\uparrow} \hat{n}_{d\downarrow} c^\dagger_{k\uparrow} c_{k'\uparrow} \tag{1.30}$$

We define J_z and J_t such that this term can be written as

$$\begin{aligned} \mathcal{H}_I &= J_z \frac{\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow}}{2} \sum_{kk'} \left(c^\dagger_{k\uparrow} c_{k'\uparrow} - c^\dagger_{k\downarrow} c_{k'\downarrow} \right) + J_t \sum_{kk'} \left[c^\dagger_{d\uparrow} c_{d\downarrow} c^\dagger_{k\downarrow} c_{k'\uparrow} + c^\dagger_{d\downarrow} c_{d\uparrow} c^\dagger_{k\uparrow} c_{k'\downarrow} \right] \\ &= 2 J_z S^z_d s^z + J_t \left(S^+_d s^- + S^-_d s^+ \right) \end{aligned} \tag{1.31}$$

The spin-like operators are defined as

$$\begin{aligned} S^z_d &\equiv \frac{1}{2} \left(\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow} \right) & S^+_d &\equiv c^\dagger_{d\uparrow} c_{d\downarrow} & S^-_d &\equiv c^\dagger_{d\downarrow} c_{d\uparrow} \\ s^z_{kk'} &\equiv \frac{1}{2} \left(c^\dagger_{k\uparrow} c_{k'\uparrow} - c^\dagger_{k\downarrow} c_{k'\downarrow} \right) & s^+_{kk'} &\equiv c^\dagger_{k\uparrow} c_{k'\downarrow} & s^-_{kk'} &\equiv c^\dagger_{k\downarrow} c_{k'\uparrow} \\ & & s^a &\equiv \sum_{kk'} s^a_{kk'} \end{aligned} \tag{1.32}$$

This is the same interaction that constitutes the Kondo model and gives rise to the quenching of the local moment at low energies. The total Hamiltonian for this *Anderson-Kondo model* is thus

$$\mathcal{H} = \sum_{k\sigma} \left(\epsilon_k \hat{n}_{k\sigma} + V_k c^\dagger_{k\sigma} c_{d\sigma} + h.c. \right) + \epsilon_d \sum_\sigma \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + 2 J_z S^z_d s^z + J_t \left(S^+_d s^- + S^-_d s^+ \right) \tag{1.33}$$

For the special case of $2J_z = 2J_t = J$, we get the SU(2) symmetric Heisenberg-like interaction

$$\mathcal{H}_I = J \left[S^z_d s^z + \frac{1}{2} \left(S^+_d s^- + S^-_d s^+ \right) \right] = J \mathbf{S_d} \cdot \mathbf{s} \tag{1.34}$$

The Hamiltonian for a single electron $q\beta$ on the N^{th} shell is

$$\begin{aligned} \mathcal{H}_N = H_{N-1} + H_{\text{imp}} + \left(\epsilon_q + \beta J_z S^z_d \right) \hat{n}_{q\beta} + V_q c^\dagger_{q\beta} c_{d\beta} + \text{h.c.} + \sum_{k<\Lambda_N} \Big[J_z S^z_d \beta \left(c^\dagger_{k\beta} c_{q\beta} + c^\dagger_{q\beta} c_{k\beta} \right) \\ + J_t \left(c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{q\beta} + c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k\overline{\beta}} \right) \Big] \end{aligned} \tag{1.35}$$

where H_{imp} is the impurity-diagonal part of the Hamiltonian $(\epsilon_d \hat{n}_d + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow})$ and

$$H_{N-1} = \sum_{k<\Lambda_N,\sigma} \left[\left(\epsilon_k + \sigma J_z S^z_d \right) \hat{n}_{k\sigma} + V_k c^\dagger_{k\sigma} c_{d\sigma} + \text{h.c.} \right] + H_{I,N-1} \tag{1.36}$$

1.3 Particle sector

The renormalization in the Hamiltonian in the particle sector is

$$\begin{aligned}\Delta^+\mathcal{H}_N = \sum_{q\beta}\left[V_q^* c^\dagger_{d\beta}c_{q\beta} + J_z\beta S_d^z\sum_k c^\dagger_{k\beta}c_{q\beta} + J_t\sum_k c^\dagger_{d\beta}c_{d\overline{\beta}}c^\dagger_{k\overline{\beta}}c_{q\beta}\right]\times\frac{1}{\hat{\omega}^+ - \mathcal{H}_D^+}\\ \times\left[V_q c^\dagger_{q\beta}c_{d\beta} + J_z\beta S_d^z\sum_k c^\dagger_{q\beta}c_{k\beta} + J_t\sum_k c^\dagger_{d\overline{\beta}}c_{d\beta}c^\dagger_{q\beta}c_{k\overline{\beta}}\right]\end{aligned} \tag{1.37}$$

The $\mathcal{H}_D$ is the diagonal part of the Hamiltonian, and the superscript $\pm$ signifies that its the particle(hole) sector part, with respect to the electron presently being disentangled $(q\beta)$.

$$\mathcal{H}_D^+ \equiv \mathrm{Tr}_{q\beta}\left[\mathcal{H}\hat{n}_{q\beta}\right] = \sum_{k<\Lambda_N,\sigma}\left(\epsilon_k + \sigma J_z S_d^z\right)\hat{n}_{k\sigma} + \left(\epsilon_q + \beta J_z S_d^z\right) + H_{imp} \tag{1.38}$$

As a simplification, we will ignore the terms that pertain to the lower electrons $(k < q)$ in $\mathcal{H}_D^+$. The entire renormalization expression has nine terms- one of order $|V_q|^2$, four of order $V_q u_P$ and four of order u_P^2.

1.

$$\Delta_1^+\mathcal{H}_N = \sum_{q\beta}|V_q|^2 c^\dagger_{d\beta}c_{q\beta}\frac{1}{\hat{\omega}^+ - \mathcal{H}_D^+}c^\dagger_{q\beta}c_{d\beta} \tag{1.39}$$

The intermediate state is characterized by $\hat{n}_{d\beta} = 0, \hat{n}_{q\beta} = 1$. Therefore, at the propagator, we have

$$\begin{aligned}H_1 = \mathcal{H}_D^+ &= \left[\epsilon_q + \beta J_z S_d^z\right] + \epsilon_d\hat{n}_{d\overline{\beta}}\\ &= \left[\epsilon_q - \frac{1}{2}\beta\beta J_z\hat{n}_{d\overline{\beta}}\right] + \epsilon_d\hat{n}_{d\overline{\beta}}\\ &= \left[\epsilon_q - \frac{1}{2}J_z\hat{n}_{d\overline{\beta}}\right] + \epsilon_d\hat{n}_{d\overline{\beta}}\end{aligned} \tag{1.40}$$

H_1 is the intermediate state Hamiltonian. As a simplification, we replace $\hat{\omega}^+$ with its eigenvalue $2\omega^+\tau^+ = \omega^+$.

$$\begin{aligned}\Delta_1^+\mathcal{H}_N &= \sum_{q\beta}|V_q|^2 c^\dagger_{d\beta}c_{q\beta}\frac{1}{\hat{\omega}^+ - H_1}c^\dagger_{q\beta}c_{d\beta}\\ &= \sum_{q\beta}|V_q|^2 c^\dagger_{d\beta}c_{q\beta}c^\dagger_{q\beta}c_{d\beta}\frac{1}{\omega^+ - \epsilon_q - \epsilon_d\hat{n}_{d\overline{\beta}} + \frac{1}{2}J_z\hat{n}_{d\overline{\beta}}}\end{aligned} \tag{1.41}$$

Since $q\beta$ is on the upper band edge, we can assume it is unoccupied in the initial state, and set $c_{q\beta}c^\dagger_{q\beta} = 1$. Then,

$$\begin{aligned}
\Delta_1^+\mathcal{H}_N &= \sum_{q\beta} |V_q|^2 \hat{n}_{d\beta} \frac{1}{\omega^+ - \epsilon_q + \left(\frac{J_z}{2} - \epsilon_d\right)\hat{n}_{d\overline{\beta}}} \\
&= \sum_{q\beta} |V(q)|^2 \hat{n}_{d\beta} \left[\frac{\hat{n}_{d\overline{\beta}}}{\omega^+ - \epsilon_q - \epsilon_d + \frac{1}{2}J_z} + \frac{\left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega^+ - \epsilon_q}\right] \\
&= \sum_{q\beta} |V(q)|^2 \hat{n}_{d\beta} \left[\frac{1}{\omega^+ - \epsilon_q} + \hat{n}_{d\overline{\beta}}\left(\frac{1}{\omega^+ - \epsilon_q - \epsilon_d + \frac{1}{2}J_z} - \frac{1}{\omega^+ - \epsilon_q}\right)\right]
\end{aligned} \tag{1.42}$$

2.

$$\Delta_2^+\mathcal{H}_N = \sum_{q\beta k} V_q^* c^\dagger_{d\beta} c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_z \beta S_d^z c^\dagger_{q\beta} c_{k\beta} \tag{1.43}$$

This can be simplified by noting that since the propagator is diagonal, the only operator that changes $\hat{n}_d$ and S_d^z is the $c^\dagger_{d\beta}$, and therefore

$$c^\dagger_{d\beta} J_z \beta S_d^z = c^\dagger_{d\beta} \frac{1}{2}\left(-J_z\right)\hat{n}_{d\overline{\beta}} \tag{1.44}$$

The expression simplifies to

$$\Delta_2^+\mathcal{H}_N = \frac{1}{2}\left(-J_z\right) \sum_{q\beta k} V_q^* c^\dagger_{d\beta} c_{q\beta} \hat{n}_{d\overline{\beta}} \frac{1}{\omega^+ - \mathcal{H}_D^+} c^\dagger_{q\beta} c_{k\beta} \tag{1.45}$$

Intermediate ($\hat{n}_{q\beta} = 1, \hat{n}_{d\overline{\beta}} = 1, \hat{n}_{d\beta} = 0$) energy is

$$H_1 = \mathcal{H}_D^+ = \epsilon_q + J_z \beta S_d^z + \epsilon_d = \epsilon_q - \frac{1}{2}J_z + \epsilon_d \tag{1.46}$$

The first term $\epsilon_q + J_z\beta S_d^z$ is the total dispersion of the electron $q\beta$. The ϵ_d is the impurity energy and the third term is the total background energy.

$$\begin{aligned}
\Delta_2^+\mathcal{H}_N &= -\frac{1}{2}J_z \sum_{q\beta k} V_q^* c^\dagger_{d\beta} c_{q\beta} \hat{n}_{d\overline{\beta}} c^\dagger_{q\beta} c_{k\beta} \frac{1}{\omega^+ - H_1} \\
&= -\frac{1}{2}J_z \sum_{q\beta k} V_q^* c^\dagger_{d\beta} c_{k\beta} \frac{\hat{n}_{d\overline{\beta}}}{\omega^+ - \epsilon_q - \epsilon_d + \frac{1}{2}J_z}
\end{aligned} \tag{1.47}$$

3.

$$\Delta_3^+\mathcal{H}_N = \sum_{q\beta k} V_q^* c^\dagger_{d\beta} c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_t c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k\overline{\beta}} \tag{1.48}$$

Intermediate $(\hat{n}_{d\beta}=0, \hat{n}_{q\beta}=\hat{n}_{d\overline{\beta}}=1)$ energy is

$$H_1=\epsilon_q-\frac{1}{2}J_z+\epsilon_d \tag{1.49}$$

$$\begin{aligned}\Delta_3^+\mathcal{H}_N&=\sum_{q\beta k}J_tV_q^*c_{d\beta}^\dagger c_{q\beta}c_{d\overline{\beta}}^\dagger c_{d\beta}c_{q\beta}^\dagger c_{k\overline{\beta}}\frac{1}{\omega^+-H_1}\\&=-J_t\sum_{q\beta k}V_q^*\hat{n}_{d\beta}\left(1-\hat{n}_{q\beta}\right)c_{d\overline{\beta}}^\dagger c_{k\overline{\beta}}\frac{1}{\omega^+-H_1}\\&=-J_t\sum_{q\beta k}V_q^*c_{d\beta}^\dagger c_{k\beta}\frac{\hat{n}_{d\overline{\beta}}}{\omega^+-\epsilon_q-\epsilon_d+\frac{1}{2}J_z}\end{aligned} \tag{1.50}$$

4.

$$\Delta_4^+\mathcal{H}_N=\sum_{q\beta k\sigma}J_z\beta S_d^zc_{k\beta}^\dagger c_{q\beta}\frac{1}{\omega^+-\mathcal{H}_D^+}V_qc_{q\beta}^\dagger c_{d\beta} \tag{1.51}$$

The first step is a simplification:

$$J_z\beta S_d^zc_{d\beta}=\frac{1}{2}\left(-J_z\right)\hat{n}_{d\overline{\beta}}c_{d\beta} \tag{1.52}$$

Intermediate $(\hat{n}_{d\beta}=0, \hat{n}_{q\beta}=\hat{n}_{d\overline{\beta}}=1)$ energy is

$$H_1=\epsilon_q-\frac{1}{2}J_z+\epsilon_d \tag{1.53}$$

$$\begin{aligned}\Delta_4^+\mathcal{H}_N&=-\frac{1}{2}J_z\sum_{q\beta k}V_q\hat{n}_{d\overline{\beta}}c_{k\beta}^\dagger c_{q\beta}c_{q\beta}^\dagger c_{d\beta}\frac{1}{\omega^+-H_1}\\&=\sum_{q\beta k}-\frac{1}{2}J_zV_q\hat{n}_{d\overline{\beta}}\left(1-\hat{n}_{q\beta}\right)c_{k\beta}^\dagger c_{d\beta}\frac{1}{\omega^+-\epsilon_q-\epsilon_d+\frac{1}{2}J_z}\\&=-\frac{1}{2}J_z\sum_{q\beta k}V_qc_{k\beta}^\dagger c_{d\beta}\frac{\hat{n}_{d\overline{\beta}}}{\omega^+-\epsilon_q-\epsilon_d+\frac{1}{2}J_z}\end{aligned} \tag{1.54}$$

5.

$$\Delta_5^+\mathcal{H}_N=\sum_{q\beta k\sigma}J_tc_{d\beta}^\dagger c_{d\overline{\beta}}c_{k\overline{\beta}}^\dagger c_{q\beta}\frac{1}{\omega^+-\mathcal{H}_D^+}V_qc_{q\beta}^\dagger c_{d\beta} \tag{1.55}$$

Intermediate $(\hat{n}_{d\beta}=0, \hat{n}_{q\beta}=\hat{n}_{d\overline{\beta}}=1)$ energy is

$$H_1=\epsilon_q-\frac{1}{2}J_z+\epsilon_d \tag{1.56}$$

$$\begin{aligned}\Delta_5^+\mathcal{H}_N &= \sum_{q\beta k} J_t V_q c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{q\beta} c^\dagger_{q\beta} c_{d\beta} \frac{1}{\omega^+ - H_1} \\ &= -\sum_{q\beta k} J_t V_q \left(1-\hat{n}_{q\beta}\right)\hat{n}_{d\beta} c^\dagger_{k\overline{\beta}} c_{d\overline{\beta}} \frac{1}{\omega^+ - \epsilon_q - \epsilon_d + \frac{1}{2}J_z} \\ &= -J_t \sum_{q\beta k} V_q c^\dagger_{k\beta} c_{d\beta} \frac{\hat{n}_{d\overline{\beta}}}{\omega^+ - \epsilon_q - \epsilon_d + \frac{1}{2}J_z}\end{aligned} \tag{1.57}$$

6.

$$\Delta_6^+\mathcal{H}_N = \sum_{k'q\beta k} J_z S_d^z \beta c^\dagger_{k\beta} c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_z S_d^z \beta c^\dagger_{q\beta} c_{k'\beta} \tag{1.58}$$

The first step is a simplification:

$$\left(\beta S_d^z\right)^2 = \frac{1}{4}\left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right)^2 = \frac{1}{4}\left(\hat{n}_{d\beta} + \hat{n}_{d\beta} - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right) = \frac{1}{4}\left(\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right) \tag{1.59}$$

Note that this term projects onto the singly-occupied subspace; both the doubly- and zero-occupied states will give zero for this term. Intermediate ($\hat{n}_{q\beta} = 1$) energy is

$$H_1 = \epsilon_q + \beta J_z S_d^z + H_{imp} \tag{1.60}$$

Since the $\left(S^z\right)^2$ term filters out only the single-occupied subspace, we can write $H_{imp} = \epsilon_d$.

$$\begin{aligned}\Delta_6^+\mathcal{H}_N &= \frac{1}{4}J_z^2 \sum_{k'q\beta k} \left(\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right) c^\dagger_{k\beta} c_{q\beta} c^\dagger_{q\beta} c_{k'\beta} \frac{1}{\omega^+ - H_1} \\ &= \frac{1}{4}J_z^2 \sum_{k'q\beta k} \left(\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right)\left(1-\hat{n}_{q\beta}\right) c^\dagger_{k\beta} c_{k'\beta} \frac{1}{\omega^+ - \epsilon_q - H_{imp} - \beta J_z S_d^z} \\ &= \frac{1}{4}J_z^2 \sum_{k'q\beta k} c^\dagger_{k\beta} c_{k'\beta} \frac{\left(\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right)}{\omega^+ - \epsilon_q - \epsilon_d - \beta J_z S_d^z} \\ &= \frac{1}{4}J_z^2 \sum_{k'q\beta k} c^\dagger_{k\beta} c_{k'\beta} \left[\frac{\hat{n}_{d\beta}\left(1-\hat{n}_{d\overline{\beta}}\right)}{\omega^+ - \epsilon_q - \epsilon_d - \frac{1}{2}J_z} + \frac{\hat{n}_{d\overline{\beta}}\left(1-\hat{n}_{d\beta}\right)}{\omega^+ - \epsilon_q - \epsilon_d + \frac{1}{2}J_z}\right]\end{aligned} \tag{1.61}$$

In the last step, we used the fact that $\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}$ is not zero only in the singly occupied subspace, hence we can expand it into $\hat{n}_\uparrow\left(1-\hat{n}_\downarrow\right) + \hat{n}_\downarrow\left(1-\hat{n}_\uparrow\right)$.

7.

$$\Delta_7^+\mathcal{H}_N = \sum_{q\beta kk'} \beta J_z S_d^z c^\dagger_{k\beta} c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_t c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k'\overline{\beta}} \tag{1.62}$$

The first step is a simplification:

$$\beta S_d^z c^\dagger_{d\overline{\beta}} c_{d\beta} = \beta S_d^z S^+_{d\overline{\beta}} = \beta\frac{1}{2}\overline{\beta} S^+_{d\overline{\beta}} = -\frac{1}{2} c^\dagger_{d\overline{\beta}} c_{d\beta} \tag{1.63}$$

Intermediate $(\hat{n}_{d\beta} = 0, \hat{n}_{q\beta} = \hat{n}_{d\overline{\beta}} = 1)$ energy is

$$H_1 = \epsilon_q + \beta J_z S_d^z + \epsilon_d = \epsilon_q - \frac{1}{2} J_z + \epsilon_d \tag{1.64}$$

$$\begin{aligned}
\Delta_7^+ \mathcal{H}_N &= \sum_{q\beta kk'} \frac{1}{2} J_z J_t c^\dagger_{k\beta} c_{q\beta} c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k'\overline{\beta}} \frac{-1}{\omega^+ - H_1} \\
&= -\frac{1}{2} J_z J_t \sum_{q\beta kk'} \left(1 - \hat{n}_{q\beta}\right) c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{k\beta} c_{k'\overline{\beta}} \frac{1}{\omega^+ - \epsilon_q - \epsilon_d + \frac{1}{2} J_z} \\
&= -\frac{1}{2} J_z J_t \sum_{q\beta kk'} c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{k\beta} c_{k'\overline{\beta}} \frac{1}{\omega^+ - \epsilon_q - \epsilon_d + \frac{1}{2} J_z}
\end{aligned} \tag{1.65}$$

8.

$$\Delta_8^+ \mathcal{H}_N = \sum_{q\beta kk'} J_t c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_z \beta S_d^z c^\dagger_{q\beta} c_{k'\beta} \tag{1.66}$$

The first step is a simplification:

$$c^\dagger_{d\beta} c_{d\overline{\beta}} \beta S_d^z = S^+_{d\beta} \beta S_d^z = \beta \frac{1}{2} \overline{\beta} S^+_{d\overline{\beta}} = -\frac{1}{2} c^\dagger_{d\beta} c_{d\overline{\beta}} \tag{1.67}$$

Intermediate $(\hat{n}_{d\beta} = 0, \hat{n}_{q\beta} = \hat{n}_{d\overline{\beta}} = 1)$ energy is

$$H_1 = \epsilon_q + \beta J_z S_d^z + \epsilon_d = \epsilon_q - \frac{1}{2} J_z + \epsilon_d \tag{1.68}$$

$$\begin{aligned}
\Delta_8^+ \mathcal{H}_N &= -\sum_{q\beta kk'} \frac{1}{2} J_z J_t c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{q\beta} c^\dagger_{q\beta} c_{k'\beta} \frac{1}{\omega^+ - H_1} \\
&= -\frac{1}{2} J_z J_t \sum_{q\beta kk'} \left(1 - \hat{n}_{q\beta}\right) c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{k'\beta} \frac{1}{\omega^+ - \epsilon_q - \epsilon_d + \frac{1}{2} J_z} \\
&= -\frac{1}{2} J_z J_t \sum_{q\beta kk'} c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{k'\beta} \frac{1}{\omega^+ - \epsilon_q - \epsilon_d + \frac{1}{2} J_z}
\end{aligned} \tag{1.69}$$

9.

$$\Delta_9^+ \mathcal{H}_N = \sum_{q\beta kk'} J_t c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_t c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k'\overline{\beta}} \tag{1.70}$$

Intermediate $(\hat{n}_{d\beta} = 0, \hat{n}_{q\beta} = \hat{n}_{d\overline{\beta}} = 1)$ energy is

$$H_1 = \epsilon_q - \frac{1}{2} J_z + \epsilon_d \tag{1.71}$$

$$
\begin{aligned}
\Delta_9^+\mathcal{H}_N &= \sum_{q\beta kk\prime} J_t^2 c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{q\beta} c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k'\overline{\beta}} \frac{1}{\omega^+ - H_1} \\
&= J_t^2 \sum_{q\beta kk\prime} \left(1-\hat{n}_{q\beta}\right) \hat{n}_{d\beta} \left(1-\hat{n}_{d\overline{\beta}}\right) c^\dagger_{k\overline{\beta}} c_{k'\overline{\beta}} \frac{1}{\omega^+ - \epsilon_q - \epsilon_d + \frac{1}{2}J_z} \\
&= J_t^2 \sum_{q\beta kk\prime} c^\dagger_{k\beta} c_{k'\beta} \frac{\hat{n}_{d\overline{\beta}}\left(1-\hat{n}_{d\beta}\right)}{\omega^+ - \epsilon_q - \epsilon_d + \frac{1}{2}J_z}
\end{aligned}
\tag{1.72}
$$

Scaling equations for particle sector

The scaling equations are obtained as follows. The first term gives the renormalization in ϵ_d and U. The renormalization in U will come with a factor of 2 because $\sum_\beta \hat{n}_{d\beta}\hat{n}_{d\overline{\beta}} = 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}$. Terms 2 and 3 renormalize V^*. Terms 4 and 5 renormalize V. Since these renormalizations are same, we write just one them. Also, in the terms 2 through 5, the renormalization is actually that of $V\hat{n}_{d\overline{\beta}}$, not strictly of V. In other words, if we split V as $V = V\left[\hat{n}_{d\overline{\beta}} + \left(1-\hat{n}_{d\overline{\beta}}\right)\right] = V^1\hat{n}_{d\overline{\beta}} + V^0\left(1-\hat{n}_{d\overline{\beta}}\right)$, then these terms will renormalize V^1. However, we do not make this distinction here because in the particle sector, we will get the renormalization in V^0, and they will turn out to be the same, so we can just talk about the renormalization in V instead of splitting it. Terms 7 and * renormalize J_t and 9 renormalizes the anti-parallel part of J_z, that is, the part in which the conduction electron has spin $\overline{\beta}$. The other term, with spin β will renormalize in the hole sector. Term 6 can be ignored for now because it will get canceled by an opposite term in the hole sector, see 1.5 just under eq. 1.120. Otherwise it will renormalize J_z.

$$
\begin{aligned}
\Delta^+\epsilon_d &= \sum_q |V(q)|^2 \frac{1}{\omega^+ - \epsilon_q} \\
\Delta^+U &= \sum_q 2|V(q)|^2 \left(\frac{1}{\omega^+ - \epsilon_q - \epsilon_d + \frac{1}{2}J_z} - \frac{1}{\omega^+ - \epsilon_q}\right) \\
\Delta^+V &= -\left(\frac{1}{2}J_z + J_t\right) \sum_q V_q^* \frac{1}{\omega^+ - \epsilon_q - \epsilon_d + \frac{1}{2}J_z} \\
\Delta^+J_t &= -J_zJ_t \sum_q \frac{1}{\omega^+ - \epsilon_q - \epsilon_d + \frac{1}{2}J_z} \\
\Delta^+J_z &= -J_t^2 \sum_q \frac{1}{\omega^+ - \epsilon_q - \epsilon_d + \frac{1}{2}J_z}
\end{aligned}
\tag{1.73}
$$

1.4 Hole sector

The renormalization in the Hamiltonian in the hole sector is

$$\Delta^{-}\mathcal{H}_N = \sum_{q\beta}\left[V_q c^\dagger_{q\beta}c_{d\beta} + J_z\beta S^z_d\sum_{k\sigma}\hat{n}_{d\sigma}c_{k\beta}c^\dagger_{q\beta} + J_t\sum_{k\sigma}c^\dagger_{d\overline{\beta}}c^\dagger_{q\beta}c_{d\beta}c_{k\overline{\beta}}\right]\times\frac{-1}{\hat{\omega}^- - \mathcal{H}^-_D}$$
$$\times\left[V^*_q c^\dagger_{d\beta}c_{q\beta} + J_z\beta S^z_d\sum_{k\sigma}\hat{n}_{d\sigma}c_{q\beta}c^\dagger_{k\beta} + J_t\sum_{k\sigma}c^\dagger_{d\beta}c^\dagger_{k\overline{\beta}}c_{d\overline{\beta}}c_{q\beta}\right] \tag{1.74}$$

The propagator can be written as

$$\frac{-1}{\hat{\omega}^- - \mathcal{H}^-_D} = \frac{1}{\omega^- + \mathcal{H}^-_D} \tag{1.75}$$

where we substitute $\hat{\omega}^- = 2\omega^-\tau^- = -\omega^-$. $\mathcal{H}^-_D$ is the energy of the hole state. The kinetic energy and spin of this hole will be the negative of those of the particle, due to conservation.

$$\mathcal{H}^-_D = -\epsilon_q - \beta J_z S^z_d + H_{\text{imp}} \tag{1.76}$$

1.

$$\Delta^-_1\mathcal{H}_N = \sum_{q\beta}|V_q|^2 c^\dagger_{q\beta}c_{d\beta}\frac{1}{\hat{\omega}^- - \mathcal{H}^-_D}c^\dagger_{d\beta}c_{q\beta} \tag{1.77}$$

The intermediate ($\hat{n}_{q\beta} = 0, \hat{n}_{d\beta} = 1$) energy is

$$H_1 = \epsilon_d + (\epsilon_d + U)\,\hat{n}_{d\overline{\beta}} - \epsilon_q - \beta J_z S^z_d = -\epsilon_q - \frac{J_z}{2}\left(1 - \hat{n}_{d\overline{\beta}}\right) + \epsilon_d + (\epsilon_d + U)\,\hat{n}_{d\overline{\beta}} \tag{1.78}$$

$$\Delta^-_1\mathcal{H}_N = \sum_{q\beta}|V_q|^2\hat{n}_{q\beta}\left(1 - \hat{n}_{d\beta}\right)\frac{1}{\omega^- - H_1} \tag{1.79}$$

For hole excitations, the initial state must be filled, so we can set $\hat{n}_{q\beta} = 1$.

$$\begin{aligned}\Delta^-_1\mathcal{H}_N &= \sum_{q\beta}|V_q|^2\hat{n}_{q\beta}\left(1 - \hat{n}_{d\beta}\right)\frac{1}{\omega^- - \epsilon_q - \frac{J_z}{2}\left(1 - \hat{n}_{d\overline{\beta}}\right) + \epsilon_d + (\epsilon_d + U)\,\hat{n}_{d\overline{\beta}}}\\
&= \sum_{q\beta}\left(1 - \hat{n}_{d\beta}\right)\left[\frac{|V^1_q|^2\hat{n}_{d\overline{\beta}}}{\omega^- - \epsilon_q + 2\epsilon_d + U} + \frac{|V^0_q|^2\left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega - \epsilon_q + \epsilon_d - \frac{1}{2}J_z}\right]\\
&= \sum_{q\beta}|V(q)|^2\left[\hat{n}_{d\overline{\beta}}\left(\frac{1}{\omega - \epsilon_q + 2\epsilon_d + U} - \frac{2}{\omega - \epsilon_q + \epsilon_d - \frac{1}{2}J_z}\right)\right.\\
&\qquad\left. + \hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\left(\frac{1}{\omega - \epsilon_q + \epsilon_d - \frac{1}{2}J_z} - \frac{1}{\omega - \epsilon_q + 2\epsilon_d + U}\right)\right]\end{aligned} \tag{1.80}$$

2.

$$\Delta_2^- \mathcal{H}_N = \sum_{q\beta k} V_q c_{q\beta}^\dagger c_{d\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_z \beta S_d^z c_{k\beta}^\dagger c_{q\beta} \tag{1.81}$$

The first step is a simplification:

$$c_{d\beta} J_z \beta S_d^z = c_{d\beta} \frac{1}{2} J_z \left(1 - \hat{n}_{d\overline{\beta}}\right) \tag{1.82}$$

The intermediate $(\hat{n}_{q\beta} = 0, \hat{n}_{d\beta} = 1)$ energy is

$$H_1 = -\epsilon_q + \epsilon_d + (\epsilon_d + U)\, \hat{n}_{d\overline{\beta}} - \frac{1}{2} J_z \left(1 - \hat{n}_{d\overline{\beta}}\right) \tag{1.83}$$

$$\begin{aligned}
\Delta_2^- \mathcal{H}_N &= \sum_{q\beta k} \frac{1}{2} J_z \left(1 - \hat{n}_{d\overline{\beta}}\right) V_q c_{q\beta}^\dagger c_{d\beta} \left(1 - \hat{n}_{d\overline{\beta}}\right) c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega^- + H_1} \\
&= - \sum_{q\beta k} \hat{n}_{q\beta} c_{k\beta}^\dagger c_{d\beta} \frac{V_q \frac{1}{2} J_z \left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega^- - \epsilon_q + \epsilon_d + (\epsilon_d + U)\, \hat{n}_{d\overline{\beta}} - \frac{1}{2} J_z \left(1 - \hat{n}_{d\overline{\beta}}\right)} \\
&= -\frac{1}{2} J_z \sum_{q\beta k} V_q \hat{n}_{q\beta} c_{k\beta}^\dagger c_{d\beta} \frac{\left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega^- - \epsilon_q + \epsilon_d - \frac{1}{2} J_z}
\end{aligned} \tag{1.84}$$

3.

$$\Delta_3^- \mathcal{H}_N = \sum_{q\beta k} V_q c_{q\beta}^\dagger c_{d\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_t c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{q\beta} \tag{1.85}$$

The intermediate $(\hat{n}_{q\beta} = \hat{n}_{d\overline{\beta}} = 0, \hat{n}_{d\beta} = 1)$ energy is

$$H_1 = \epsilon_d - \epsilon_q - J_z \beta S_d^z = \epsilon_d - \epsilon_q - \frac{1}{2} J_z \tag{1.86}$$

$$\begin{aligned}
\Delta_3^- \mathcal{H}_N &= \sum_{q\beta k} J_t V_q c_{q\beta}^\dagger c_{d\beta} c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{q\beta} \frac{1}{\omega^- + H_1} \\
&= \sum_{q\beta k} J_t V_q \hat{n}_{q\beta} \left(1 - \hat{n}_{d\beta}\right) c_{k\overline{\beta}}^\dagger c_{d\overline{\beta}} \frac{-1}{\omega^- - \epsilon_q + \epsilon_d - \frac{1}{2} J_z} \\
&= -J_t \sum_{q\beta k} V_q c_{k\beta}^\dagger c_{d\beta} \frac{1 - \hat{n}_{d\overline{\beta}}}{\omega^- - \epsilon_q + \epsilon_d - \frac{1}{2} J_z}
\end{aligned} \tag{1.87}$$

4.

$$\Delta_4^- \mathcal{H}_N = \sum_{q\beta k} \frac{1}{2} J_z \beta S_d^z c_{q\beta}^\dagger c_{k\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} V_q^* c_{d\beta}^\dagger c_{q\beta} \tag{1.88}$$

There is a simplification:

$$\frac{1}{2} J_z \beta S_d^z c_{d\beta}^\dagger = \frac{1}{2} J_z \left(1 - \hat{n}_{d\overline{\beta}}\right) c_{d\beta}^\dagger \tag{1.89}$$

The intermediate $(\hat{n}_{q\beta}=0, \hat{n}_{d\beta}=1)$ energy is

$$H_1 = -\epsilon_q + \epsilon_d + (\epsilon_d + U)\,\hat{n}_{d\bar{\beta}} - \frac{1}{2}J_z\left(1-\hat{n}_{d\bar{\beta}}\right) \tag{1.90}$$

$$\begin{aligned}
\Delta_4^-\mathcal{H}_N &= \sum_{q\beta k} V_q^* c_{q\beta}^\dagger c_{k\beta} c_{d\beta}^\dagger c_{q\beta} \frac{\frac{1}{2}J_z\left(1-\hat{n}_{d\bar{\beta}}\right)}{\omega^- - H_1} \\
&= \sum_{q\beta k} \hat{n}_{q\beta} V_q^* c_{k\beta} c_{d\beta}^\dagger \frac{\frac{1}{2}J_z\left(1-\hat{n}_{d\bar{\beta}}\right)}{\omega^- - \epsilon_q + \epsilon_d + (\epsilon_d+U)\,\hat{n}_{d\bar{\beta}} - \frac{1}{2}J_z\left(1-\hat{n}_{d\bar{\beta}}\right)} \\
&= -\frac{1}{2}J_z \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{k\beta} \frac{1-\hat{n}_{d\bar{\beta}}}{\omega^- - \epsilon_q + \epsilon_d - \frac{1}{2}J_z}
\end{aligned} \tag{1.91}$$

5.

$$\Delta_5^-\mathcal{H}_N = \sum_{q\beta k} J_t c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\bar{\beta}} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} V_q^* c_{d\beta}^\dagger c_{q\beta} \tag{1.92}$$

The intermediate $(\hat{n}_{q\beta}=\hat{n}_{d\bar{\beta}}=0, \hat{n}_{d\beta}=1)$ energy is

$$H_1 = -\epsilon_q + \epsilon_d - \frac{1}{2}J_z \tag{1.93}$$

$$\begin{aligned}
\Delta_5^-\mathcal{H}_N &= \sum_{q\beta k} J_t V_q^* c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\bar{\beta}} c_{d\beta}^\dagger c_{q\beta} \frac{1}{\hat{\omega}^- + H_1} \\
&= -J_t \sum_{q\beta k} V_q^* \hat{n}_{q\beta}\left(1-\hat{n}_{d\beta}\right) c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}} \frac{1}{\omega^- - \epsilon_q + \epsilon_d - \frac{1}{2}J_z} \\
&= -J_t \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{k\beta} \frac{1-\hat{n}_{d\bar{\beta}}}{\omega^- - \epsilon_q + \epsilon_d - \frac{1}{2}J_z}
\end{aligned} \tag{1.94}$$

6.

$$\Delta_6^-\mathcal{H}_N = \sum_{q\beta kk'} J_z \beta S_d^z c_{q\beta}^\dagger c_{k'\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_z \beta S_d^z c_{k\beta}^\dagger c_{q\beta} \tag{1.95}$$

From eq. 1.59,

$$\left(\beta S_d^z\right)^2 = \frac{1}{4}\left(\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right) \tag{1.96}$$

The intermediate $(\hat{n}_{q\beta}=0)$ energy is

$$H_1 = H_{\mathrm{imp}} - \epsilon_q - \beta J_z S_d^z \tag{1.97}$$

$$
\begin{aligned}
\Delta_6^- \mathcal{H}_N &= \sum_{q\beta kk'} \frac{J_z^2}{4} \left(\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right) c^\dagger_{q\beta} c_{k'\beta} c^\dagger_{k\beta} c_{q\beta} \frac{1}{\omega^- + H_1} \\
&= \frac{J_z^2}{4} \sum_{q\beta kk'} \hat{n}_{q\beta} \left(\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right) c_{k'\beta} c^\dagger_{k\beta} \frac{1}{\omega^- - \epsilon_q + H_{\text{imp}} - \beta J_z S_d^z} \\
&= -\frac{J_z^2}{4} \sum_{q\beta kk'} c^\dagger_{k\beta} c_{k'\beta} \left[\frac{\hat{n}_{d\beta}\left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega^- - \epsilon_q + \epsilon_d - \frac{J_z}{2}} + \frac{\hat{n}_{d\overline{\beta}}\left(1 - \hat{n}_{d\beta}\right)}{\omega^- - \epsilon_q + \epsilon_d + \frac{J_z}{2}} \right] \\
&\quad + \frac{J_z^2}{4} \sum_{q\beta k} \left[\frac{\hat{n}_{d\beta}\left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega^- - \epsilon_q + \epsilon_d - \frac{J_z}{2}} + \frac{\hat{n}_{d\overline{\beta}}\left(1 - \hat{n}_{d\beta}\right)}{\omega^- - \epsilon_q + \epsilon_d + \frac{J_z}{2}} \right]
\end{aligned} \tag{1.98}
$$

7.

$$
\Delta_7^- \mathcal{H}_N = \sum_{q\beta kk'} J_z \beta S_d^z c^\dagger_{q\beta} c_{k'\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_t c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{q\beta} \tag{1.99}
$$

Simplification:

$$
\beta S_d^z c^\dagger_{d\beta} c_{d\overline{\beta}} = \beta S_d^z S^+_{d\beta} = \beta \frac{1}{2} \beta S^+_{d\beta} = \frac{1}{2} c^\dagger_{d\beta} c_{d\overline{\beta}} \tag{1.100}
$$

The intermediate ($\hat{n}_{q\beta} = \hat{n}_{d\overline{\beta}} = 0, \hat{n}_{d\beta} = 1$) energy is

$$
H_1 = \epsilon_d - \epsilon_q - \frac{1}{2} J_z \tag{1.101}
$$

$$
\begin{aligned}
\Delta_7^- \mathcal{H}_N &= \sum_{q\beta kk'} \frac{1}{2} J_z J_t c^\dagger_{q\beta} c_{k'\beta} c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{q\beta} \frac{1}{\omega^- - H_1} \\
&= \sum_{q\beta kk'} \frac{1}{2} J_z J_t \hat{n}_{q\beta} c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{k'\beta} \frac{-1}{\omega^- - \epsilon_q + \epsilon_d - \frac{1}{2} J_z} \\
&= -\frac{1}{2} J_z J_t \sum_{q\beta kk'} c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{k'\beta} \frac{1}{\omega^- - \epsilon_q + \epsilon_d - \frac{1}{2} J_z} \\
&= -\frac{1}{2} J_z J_t \sum_{q\beta kk'} c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{k\beta} c_{k'\overline{\beta}} \frac{1}{\omega^- - \epsilon_q + \epsilon_d - \frac{1}{2} J_z}
\end{aligned} \tag{1.102}
$$

8.

$$
\Delta_8^- \mathcal{H}_N = \sum_{q\beta kk'} J_t c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k'\overline{\beta}} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_z \beta S_d^z c^\dagger_{k\beta} c_{q\beta} \tag{1.103}
$$

Simplification:

$$
c^\dagger_{d\overline{\beta}} c_{d\beta} \beta S_d^z = S^+_{d\overline{\beta}} S_d^z \beta = \beta \frac{1}{2} S^+_{d\overline{\beta}} \beta = \frac{1}{2} c^\dagger_{d\overline{\beta}} c_{d\beta} \tag{1.104}
$$

The intermediate ($\hat{n}_{q\beta} = \hat{n}_{d\overline{\beta}} = 0, \hat{n}_{d\beta} = 1$) energy is

$$
H_1 = -\epsilon_q - \frac{J_z}{2} + \epsilon_d \tag{1.105}
$$

$$
\begin{aligned}
\Delta_8^-\mathcal{H}_N &= \sum_{q\beta kk'} \frac{1}{2} J_z J_t c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k'\overline{\beta}} c^\dagger_{k\beta} c_{q\beta} \frac{1}{\omega^- - H_1} \\
&= \sum_{q\beta kk'} \frac{1}{2} J_z J_t \hat{n}_{q\beta} c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{k\beta} c_{k'\overline{\beta}} \frac{-1}{\omega^- - \epsilon_q + \epsilon_d - \frac{J_z}{2}} \\
&= -\frac{1}{2} J_z J_t \sum_{q\beta kk'} c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{k\beta} c_{k'\overline{\beta}} \frac{1}{\omega^- - \epsilon_q + \epsilon_d - \frac{1}{2} J_z}
\end{aligned} \tag{1.106}
$$

9.

$$
\Delta_9^-\mathcal{H}_N = \sum_{q\beta kk'} J_t c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k'\overline{\beta}} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_t c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{q\beta} \tag{1.107}
$$

The intermediate ($\hat{n}_{q\beta} = \hat{n}_{d\overline{\beta}} = 0, \hat{n}_{d\beta} = 1$) energy is

$$
H_1 = -\epsilon_q - \frac{J_z}{2} + \epsilon_d \tag{1.108}
$$

$$
\begin{aligned}
\Delta_9^-\mathcal{H}_N &= \sum_{q\beta kk'} J_t^2 c^\dagger_{d\overline{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k'\overline{\beta}} c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} c_{q\beta} \frac{1}{\omega^- - H_1} \\
&= \sum_{q\beta kk'} J_t^2 \hat{n}_{q\beta} c^\dagger_{d\overline{\beta}} c_{d\beta} c_{k'\overline{\beta}} c^\dagger_{d\beta} c_{d\overline{\beta}} c^\dagger_{k\overline{\beta}} \frac{1}{\omega^- - H_1} \\
&= -\sum_{q\beta kk'} J_t^2 \hat{n}_{q\beta} \hat{n}_{d\overline{\beta}} c_{d\beta} c_{k'\overline{\beta}} c^\dagger_{d\beta} c^\dagger_{k\overline{\beta}} \frac{1}{\omega^- - H_1} \\
&= \sum_{q\beta kk'} J_t^2 \hat{n}_{q\beta} \hat{n}_{d\overline{\beta}} \left(1 - \hat{n}_{d\beta}\right) c_{k'\overline{\beta}} c^\dagger_{k\overline{\beta}} \frac{1}{\omega^- - \epsilon_q^- + \epsilon_d - \frac{1}{2} J_z} \\
&= -J_t^2 \sum_{q\beta kk'} c^\dagger_{k\beta} c_{k'\beta} \frac{\hat{n}_{d\beta} \left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega^- - \epsilon_q^- + \epsilon_d - \frac{1}{2} J_z} + J_t^2 \sum_{qk\beta} \frac{\hat{n}_{d\overline{\beta}} \left(1 - \hat{n}_{d\beta}\right)}{\omega^- - \epsilon_q^- + \epsilon_d - \frac{1}{2} J_z}
\end{aligned} \tag{1.109}
$$

Scaling equations for hole sector

The scaling equations are obtained similarly as in the particle sector. The important things to note are the following. The first two terms in term 6 here cancel the term 6 of the particle sector. The last two terms in term 6 and the last term in term 9 renormalize U and ϵ_d.

$$
\begin{aligned}
\Delta^-\epsilon_d = &\sum_q |V(q)|^2 \left(\frac{1}{\omega^- - \epsilon_q + 2\epsilon_d + U} - \frac{2}{\omega^- - \epsilon_q + \epsilon_d - \frac{1}{2} J_z} \right) + \\
&\sum_{qk} \left[\frac{\frac{1}{4} J_z^2}{\omega^- - \epsilon_q + \epsilon_d - \frac{J_z}{2}} + \frac{J_t^2 + \frac{1}{4} J_z^2}{\omega^- - \epsilon_q + \epsilon_d + \frac{J_z}{2}} \right] \\
\Delta^- U = 2 &\sum_q |V(q)|^2 \left(\frac{1}{\omega^- - \epsilon_q + \epsilon_d - \frac{1}{2} J_z} - \frac{1}{\omega^- - \epsilon_q + 2\epsilon_d + U} \right) -
\end{aligned}
$$

$$2\sum_{qk}\left[\frac{\frac{1}{4}J_z^2}{\omega^- - \epsilon_q + \epsilon_d - \frac{J_z}{2}} + \frac{J_t^2 + \frac{1}{4}J_z^2}{\omega^- - \epsilon_q + \epsilon_d + \frac{J_z}{2}}\right]$$

$$\Delta^- V = -\left(\frac{1}{2}J_z + J_t\right)\sum_q V_q^* \frac{1}{\omega^- - \epsilon_q + \epsilon_d - \frac{1}{2}J_z}$$

$$\Delta^- J_t = -J_z J_t \sum_q \frac{1}{\omega^- - \epsilon_q + \epsilon_d - \frac{1}{2}J_z}$$

$$\Delta^- J_z = -J_t^2 \sum_q \frac{1}{\omega^- - \epsilon_q + \epsilon_d - \frac{1}{2}J_z}$$

1.5 Particle-Hole symmetry

The Anderson model Hamiltonian, eq. 1.33, has an impurity particle-hole symmetry for a certain condition of the couplings. To see this, we apply the particle-hole transformation $c_k \to c_k^\dagger, c_d \to -c_d^\dagger$ to the Hamiltonian. Since we are looking at the impurity symmetry, we will only look at the terms involving the impurity. The particle-hole symmetry of the conduction bath is a separate thing and that requires a specific lattice. Hence we will not consider kinetic energy term in this discussion. The rest of the terms transform as

$$\epsilon_d \sum_\sigma \hat{n}_{d\sigma} \to 2\epsilon_d - \epsilon_d \sum_\sigma \hat{n}_{d\sigma} \tag{1.110}$$

$$U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} \to U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} - U\sum_\sigma \hat{n}_{d\sigma} + U \tag{1.111}$$

$$\sum_{k\sigma} V(k)c_{k\sigma}^\dagger c_{d\sigma} + hc \to \sum_{k\sigma} -V(k)c_{k\sigma}c_{d\sigma}^\dagger + hc = \sum_{k\sigma} V^*(k)c_{k\sigma}^\dagger c_{d\sigma} + hc \tag{1.112}$$

$$S^z \sum_{kq} s_{kq}^z \to (-S^z)\sum_{kq}\left(-s_{kq}^z\right) = S^z \sum_{kq} s_{kq}^z \tag{1.113}$$

$$S^\pm \sum_{kq} s_{kq}^\mp \to \left(-S^\pm\right)\sum_{kq}\left(-s_{kq}^\mp\right) = S^\pm \sum_{kq} s_{kq}^\mp \tag{1.114}$$

The transformation of the spin terms, eqs. 1.113 and 1.114, can be understood from the fact that since a spin degree of freedom can be written in terms of the number operator as $\hat{S} = \hat{n} - \frac{1}{2}$, it must transform by flipping its sign: $\hat{S} = \hat{n} - \frac{1}{2} \to \frac{1}{2} - \hat{n} = -\hat{S}$. The spin terms are thus invariant under the particle-hole transformation. The impurity-bath hopping term can be made symmetric by making $V(k)$ real; then we would have, from eq. 1.112,

$$V(k)\left(c_{k\sigma}^\dagger c_{d\sigma} + c_{d\sigma}^\dagger c_{k\sigma}\right) \to V(k)\left(c_{d\sigma}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger c_{d\sigma}\right) \tag{1.115}$$

The impurity diagonal terms, ϵ_d and U, require a specific condition. Combining eqs. 1.110 and 1.111,

$$\epsilon_d \hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} \to \left(-\epsilon_d - U\right)\hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} \tag{1.116}$$

We dropped some constant terms in the transformed Hamiltonian. For particle-hole symmetry, the left and right hand sides must be same. The required condition is thus

$$\epsilon_d = -\epsilon_d - U \implies \epsilon_d + \frac{1}{2}U = 0 \tag{1.117}$$

This same condition can be obtained in a more physical way. If we consider the singly-occupied state of the impurity as the reference state, the doubly-occupied state is the particle-excitation and the vacant state is the hole excitation. If we measure the energies with w.r.t this singly occupied state, the energy of the particle state is $E_p = 2\epsilon_d + U - \epsilon_d = \epsilon_d + U$ and that of the hole state is $E_h = 0 - \epsilon_d = -\epsilon_d$. Particle-hole symmetry then requires the particle and hole levels to be degenerate, which means $E_p = E_h$, and we recover the condition eq. 1.117.

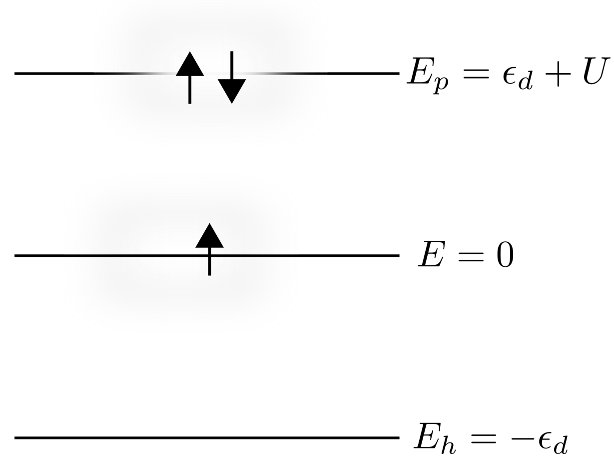

Figure 1: Particle and hole excitations of the impurity

Since the URG is unitary, if we start from a model that is particle-hole symmetric, the RG equations should uphold that symmetry. What this means is that if we have $\epsilon_d + \frac{1}{2}U = 0$ in the bare model, the new couplings should also satisfy $\epsilon_d' + \frac{1}{2}U' = 0$. This means we must have

$$\Delta\left(\epsilon_d + \frac{1}{2}U\right) = 0 \tag{1.118}$$

The quantity $\eta = \epsilon_d + \frac{1}{2}U$ is thus an RG-invariant for the particle-hole symmetric model; it does not change under the RG flow. It is often referred to as the asymmetry parameter; it quantifies the asymmetry in the model. We need to check if our equations satisfy this. Looking at both the particle and hole equations, we can find the RG equation for the asymmetry parameter

$$\begin{aligned} \Delta^+\eta = \Delta^+\left(\epsilon_d + \frac{1}{2}U\right) &= \sum_q |V(q)|^2 \frac{1}{\omega^+ - \epsilon_q - \epsilon_d + \frac{1}{2}J_z} \\ \Delta^-\eta = \Delta^-\left(\epsilon_d + \frac{1}{2}U\right) &= -\sum_q |V(q)|^2 \frac{1}{\omega^- - \epsilon_q + \epsilon_d - \frac{1}{2}J_z} \end{aligned} \tag{1.119}$$

At this point, we must note that ω^+ and ω^-, the quantum fluctuation energy scales, for the particle and hole sectors are not entirely independent. Recall that if we require the RG to be unitary, we must have $\eta(\omega^-) = \left(\eta^\dagger(\omega^+)\right)^\dagger$. This condition constrains the relation between $\omega^\pm$. To see what the relation is, we can demand $\Delta\eta \equiv \Delta^+\eta + \Delta^-\eta = 0$. That gives

$$\omega^+ - \epsilon_d + \frac{1}{2}J_z = \omega^- + \epsilon_d - \frac{1}{2}J_z \tag{1.120}$$

If we apply this condition to the term 6 in hole sector, we see that it cancels the term 6 in particle sector.

1.6 Final scaling equations

If we apply this equation the scaling equations of the hole sector, we can immediately see that

$$
\begin{aligned}
\Delta\epsilon_d \equiv& \Delta^+\epsilon_d + \Delta^-\epsilon_d = \sum_q |V(q)|^2 \left[\frac{1}{\omega^+ - \epsilon_q} + \frac{1}{\omega^+ - \epsilon_q + U + J_z} - \frac{2}{\omega^+ - \epsilon_q - \epsilon_d + \frac{1}{2}J_z}\right] \\
&+ \frac{1}{4}\sum_{qk}\left[\frac{J_z^2}{\omega^+ - \epsilon_q - \epsilon_d + \frac{1}{2}J_z} + \frac{4J_t^2 + J_z^2}{\omega^+ - \epsilon_q - \epsilon_d + \frac{3}{2}J_z}\right] \\
\Delta U \equiv& \Delta^+ U + \Delta^- U = 2\sum_q |V(q)|^2 \left[\frac{2}{\omega^+ - \epsilon_q - \epsilon_d + \frac{1}{2}J_z} - \frac{1}{\omega^+ - \epsilon_q} - \frac{1}{\omega^+ - \epsilon_q + U + J_z}\right] \\
&+ \frac{1}{2}\sum_{qk}\left[\frac{J_z^2}{\omega^+ - \epsilon_q - \epsilon_d + \frac{1}{2}J_z} + \frac{4J_t^2 + J_z^2}{\omega^+ - \epsilon_q - \epsilon_d + \frac{3}{2}J_z}\right] \\
\Delta V \equiv& \Delta^+ V + \Delta^- V = 2\Delta^+ V = -2\left(\frac{1}{2}J_z + J_t\right)\sum_q V_q^* \frac{1}{\omega^+ - \epsilon_q - \epsilon_d + \frac{1}{2}J_z} \\
\Delta J_z \equiv& \Delta^+ J_z + \Delta^- J_z = 2\Delta^+ J_z = -2J_t^2 \sum_q \frac{1}{\omega^+ - \epsilon_q - \epsilon_d + \frac{1}{2}J_z} \\
\Delta J_t \equiv& \Delta^+ J_t + \Delta^- J_t = 2\Delta^+ J_t = -2J_z J_t \sum_q \frac{1}{\omega^+ - \epsilon_q - \epsilon_d + \frac{1}{2}J_z}
\end{aligned}
\tag{1.121}
$$

1.7 "Poor Man's" one-loop form for asymmetric Anderson model

In the limit of $\epsilon_d, J \ll D \ll U$, the equation for ϵ_d becomes, up to lowest order in J,

$$
\delta\epsilon_d = -\sum_q \frac{|V_q|^2}{\omega^+ - \epsilon_q} \tag{1.122}
$$

If we assume an isotropic dispersion ($\epsilon_q = D$), where D is the current(running) bandwidth and a momentum-independent hopping potential V,

$$
\delta\epsilon_d = -\frac{1}{\omega^+ - D}\sum_q |V_q|^2 = -\frac{1}{\omega^+ - D}\rho(D)|\delta D||V|^2
$$

There we used

$$
\sum_q = \sum_{\epsilon_q \in [D - |\delta D|, D]} = \rho(D)|\delta D| \tag{1.123}
$$

where $\rho(D)$ is the single-spin density of states at the energy D and $|\Delta D|$ is the thickness of the band that we disentangled at this step. In the literature, we usually define a quantity that denotes the amount of hybridisation between the impurity and the bath: $\Delta \equiv \pi\rho(D)|V|^2$. In terms of this Δ, we get

$$\delta\epsilon_d = -\frac{\Delta|\delta D|}{\omega^+ - D} \tag{1.124}$$

For low energy excitations, we can use $\omega^+ \ll D$. Further, since we have defined $\delta\epsilon_d = \epsilon_d(D - |\delta D|) - \epsilon_d(D)$, we must have $\delta D = D - |\delta D| - D = -|\delta D|$.

$$\frac{\mathrm{d}\epsilon_d}{\mathrm{d}D} = -\frac{\Delta}{D} \tag{1.125}$$

This is the form obtained from Poor Man's scaling of the asymmetric Anderson model.

1.8 SU(2) invariance and Kondo model one-loop form

Setting $J_z = J_t = \frac{1}{2}J$ makes the interaction $SU(2)$ symmetric; the last two RG equations can then be written in the common form:

$$2\Delta J_z = 2\Delta J_t = \Delta J = -J^2 \sum_q \frac{1}{\omega^+ - \epsilon_q - \epsilon_d + \frac{1}{4}J} \tag{1.126}$$

In order to reach the Kondo RG equations, we need to make the appropriate physical change; the difference between the Anderson model and the Kondo model is that the impurity charge fluctuations are frozen at single occupation in the latter. This means that the ground state of the impurity is now at ϵ_d. We can take account of this change by now measuring ω^+ from the single occupation energy itself, ϵ_d. Hence we should redefine $\omega^+ - \epsilon_d \to \tilde{\omega}^+$.

$$2\Delta J_z = 2\Delta J_t = \Delta J = -J^2 \sum_q \frac{1}{\tilde{\omega}^+ - \epsilon_q + \frac{1}{4}J} \tag{1.127}$$

If we now consider low energy excitations ($\tilde{\omega}^+ - \epsilon_q \approx -\epsilon_q$) and expand the denominator in powers of J and keep only the lowest order, we get

$$\Delta J = -J^2 \sum_q \frac{1}{-\epsilon_q} \tag{1.128}$$

For an isotropic dispersion, we can use $\epsilon_q = D$. The sum can then be evaluated as

$$\sum_q = \rho(D)\Delta D \tag{1.129}$$

The flow equation of J becomes

$$\Delta J = J^2\rho(D)\frac{|\Delta D|}{D} \tag{1.130}$$

This is the familiar one-loop Kondo flow equation obtained from Poor man's scaling. To get the continuum version, we must note that since we are decreasing the bandwidth, we have to set $\Delta D = -|\Delta D|$. Therefore,

$$\frac{\mathrm{d}J}{\mathrm{d}\ln D} = -J^2\rho(D) \tag{1.131}$$

1.9 Connection with Kondo URG result

Recall eq. 1.127.

$$\Delta J = -J^2 \sum_q \frac{1}{\tilde{\omega}^+ - \epsilon_q + \frac{1}{4}J} \tag{1.132}$$

For $\tilde{\omega}^+ = \frac{1}{2}D$, we get

$$\Delta J = 2J^2 \sum_q \frac{1}{D - \frac{1}{2}J} \tag{1.133}$$

This has the same fixed point structure as the Kondo URG scaling equation.

1.10 Fixed points for the symmetric Anderson model with $J_z = J_t$

We first consider the simpler case where $\epsilon_d + \frac{1}{2}U = 0$ and $J_z = J_t = \frac{1}{2}J$. The scaling equations become

$$\begin{aligned}
\Delta U &= \left(U + \frac{1}{2}J\right)\sum_q |V(q)|^2 \frac{1}{(\omega^+ - \epsilon_q)\left(\omega^+ - \epsilon_q + \frac{1}{2}U + \frac{1}{4}J\right)\left(\omega^+ - \epsilon_q + U + \frac{1}{2}J\right)} \\
&\quad + \frac{1}{8}J^2 \sum_{qk} \frac{6\left(\omega^+ - \epsilon_q\right) + 3U + 4J}{\left(\omega^+ - \epsilon_q + \frac{1}{2}U + \frac{1}{4}J\right)\left(\omega^+ - \epsilon_q + \frac{1}{2}U + \frac{3}{4}J\right)} \\
\Delta V &= -\frac{3}{2}J\sum_q V_q^* \frac{1}{\omega^+ - \epsilon_q + \frac{1}{2}U + \frac{1}{4}J} \\
\Delta J &= -J^2 \sum_q \frac{1}{\omega^+ - \epsilon_q + \frac{1}{2}U + \frac{1}{4}J}
\end{aligned} \tag{1.134}$$

In absence of Kondo-type interaction ($J = 0$)

We first consider the case where $J = 0$. The only relevant equation is then that of U, because V and J will then not flow.

$$\Delta U = U \sum_q |V(q)|^2 \frac{1}{(\omega^+ - \epsilon_q)\left(\omega^+ - \epsilon_q + \frac{1}{2}U\right)(\omega^+ - \epsilon_q + U)} \tag{1.135}$$

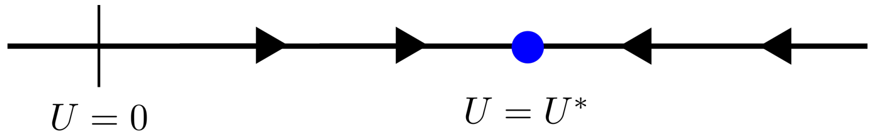

Figure 2: Flows towards local moment for $J = 0$

To get a feel for this equation, we look at a specific value of $\omega^+ = 2\epsilon_q - \frac{1}{2}U$. For this value,

$$\Delta U = U \sum_q |V(q)|^2 \frac{1}{\left(\epsilon_q^2 - \frac{1}{4}U^2\right)\epsilon_q} \tag{1.136}$$

If we start with bare values U and ϵ_q such that $U < 2\epsilon_q$, then U is relevant, and it will increase. Meanwhile, the bandwidth will decrease as we go to lower energies. The fixed point is achieved when the denominator becomes zero.

$$U^* = 2D^* \tag{1.137}$$

The opposite thing happens if we start with bare values such that $U > 2\epsilon_q$. Then, U is irrelevant and it will decrease until it reaches the same fixed point condition. This fixed point, characterized by $U^* = 2\epsilon_q^*, J = 0$, is the local moment fixed point. It is stable along both directions in the $U-$axis. It is however unstable to perturbations in J, as we will see later.

There is another fixed point in this picture, the free orbital fixed point at $U = V = 0$. It is unstable in all directions. The two fixed points and the flows are schematically shown in fig. 2.

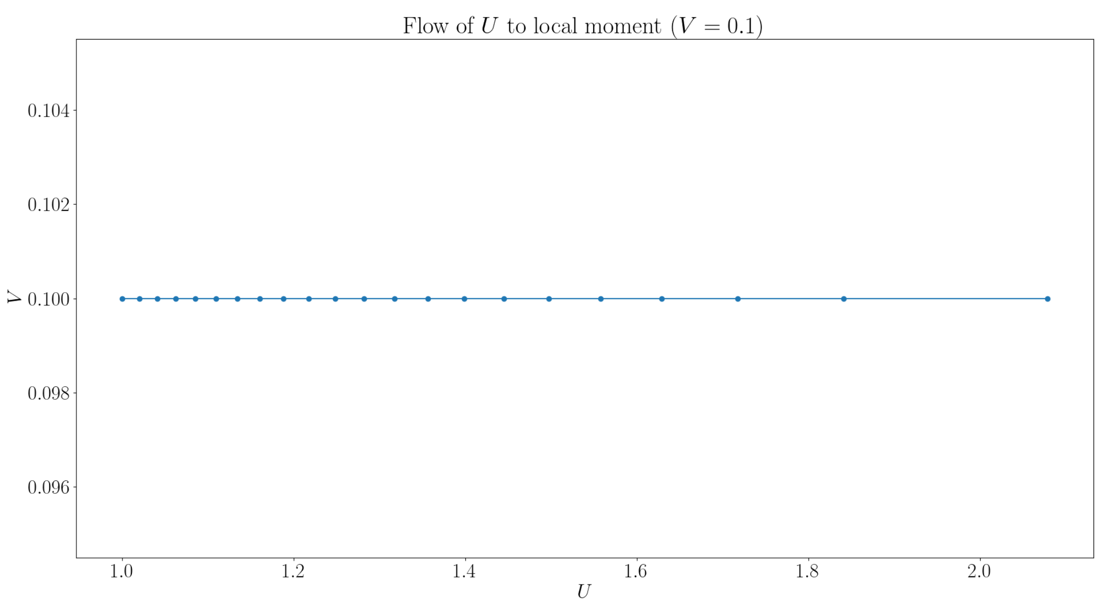

Figure 3: Plot of a particular flow from free orbital (leftmost) to local moment (rightmost)

With the Kondo-type interaction ($J > 0$)

In this case, all three equations will come into play. Using the value $\omega^+ = 0$, the equations become

$$\begin{aligned}
\Delta U &= \sum_q |V(q)|^2 \frac{-\left(U + \frac{1}{2}J\right)}{(\epsilon_q)\left(\epsilon_q - \frac{1}{2}U - \frac{1}{4}J\right)\left(\epsilon_q - U - \frac{1}{2}J\right)} + \frac{1}{8}J^2 \sum_{qk} \frac{-6\epsilon_q + 3U + 4J}{\left(\epsilon_q - \frac{1}{2}U - \frac{1}{4}J\right)\left(\epsilon_q - \frac{1}{2}U - \frac{3}{4}J\right)} \\
\Delta V &= \frac{3}{2}J \sum_q V_q^* \frac{1}{\epsilon_q - \frac{1}{2}U - \frac{1}{4}J} \\
\Delta J &= J^2 \sum_q \frac{1}{\epsilon_q - \frac{1}{2}U - \frac{1}{4}J}
\end{aligned} \tag{1.138}$$

We can now see how the couplings will flow if we start at the local moment fixed point and add a small perturbation J.

$$\begin{aligned}
\Delta U &= \sum_q |V(q)|^2 \frac{-\left(2\epsilon_q + \frac{1}{2}J\right)}{(\epsilon_q)\left(-\frac{1}{4}J\right)\left(-\epsilon_q - \frac{1}{2}J\right)} + \frac{1}{8}J^2 \sum_{qk} \frac{4J}{\left(-\frac{1}{4}J\right)\left(-\frac{3}{4}J\right)} \\
\Delta V &= \frac{3}{2}J \sum_q V_q^* \frac{1}{\epsilon_q - \frac{1}{2}U - \frac{1}{4}J} \\
\Delta J &= J^2 \sum_q \frac{1}{\epsilon_q - \frac{1}{2}U - \frac{1}{4}J}
\end{aligned} \tag{1.139}$$