Unitary Renormalization Group Approach to Single-Impurity Anderson Model

Abhirup Mukherjee

Supervisor: Dr. Siddhartha Lal

Department of Physics, IISER Kolkata

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1 Unitary Renormalization Group Method

This section is adapted from ref.[1].

1.1 Description of the problem

We are given a Hamiltonian $\mathcal{H}$ which is not completely diagonal in the occupation number basis of the electrons, $\hat{n}_k$: $[\mathcal{H}, n_k] \neq 0$. k labels any set of quantum numbers depending on the system. For spin-less Fermions it can be the momentum of the particle, while for spin-full Fermions it can be the set of momentum and spin. There are terms that scatter electrons from one quantum number k to another quantum number k'.

We take a general Hamiltonian,

$$\mathcal{H} = H_e \hat{n}_{q\beta} + H_h \left(1 - \hat{n}_{q\beta}\right) + c^\dagger_{q\beta} T + T^\dagger c_{q\beta} \tag{1.1}$$

Formally, we can decompose the entire Hamiltonian in the subspace of the electron we want to decouple ($q\beta$).

$$\mathcal{H} = \begin{array}{c} \begin{matrix} |1\rangle & |0\rangle \end{matrix} \\ \begin{pmatrix} H_1 & T \\ T^\dagger & H_0 \end{pmatrix} \end{array} \tag{1.2}$$

The basis in which this matrix is written is $\{|1\rangle, |0\rangle\}$ where $|i\rangle$ is the set of all states where $\hat{n}_{q\beta} = i$. The aim of one step of the URG is to find a unitary transformation U such that the new Hamiltonian $U\mathcal{H}U^\dagger$ is diagonal in this already-chosen basis.

$$\tilde{\mathcal{H}} \equiv U\mathcal{H}U^\dagger = \begin{array}{c} \begin{matrix} |1\rangle & |0\rangle \end{matrix} \\ \begin{pmatrix} \tilde{H}_1 & 0 \\ 0 & \tilde{H}_0 \end{pmatrix} \end{array} \tag{1.3}$$

U_q is defined by

$$\tilde{\mathcal{H}} = U_q \mathcal{H} U_q^\dagger \text{ such that } \left[\tilde{\mathcal{H}}, n_q\right] = 0 \tag{1.4}$$

It is clear that U is the diagonalizing matrix for $\mathcal{H}$. Hence we can frame this problem as an eigenvalue equation as well. Let $|\psi_1\rangle, |\psi_0\rangle$ be the basis in which the original Hamiltonian $\mathcal{H}$ has no off-diagonal terms corresponding to $q\beta$. Hence, we can write

$$\mathcal{H} |\psi_i\rangle = \tilde{H}_i |\psi_i\rangle, i \in \{0, 1\} \tag{1.5}$$

Since $|\psi_i\rangle$ is the set of eigenstates of $\mathcal{H}$ and $|i\rangle$ is the set of eigenstates in which $U\mathcal{H}U^\dagger$ has no off-diagonal terms corresponding to $q\beta$, we can relate $|\psi_i\rangle$ and $|i\rangle$ by the same transformation : $|\psi_i\rangle = U^\dagger |i\rangle$. We can expand the state $|\psi_i\rangle$ in the subspace of $q\beta$:

$$|\psi_i\rangle = \sum_{j=0,1} |j\rangle \langle j| |\psi_i\rangle \equiv |1\rangle |\phi^i_1\rangle + |0\rangle |\phi^i_0\rangle \tag{1.6}$$

where $|\phi^i_j\rangle = \langle j| |\psi_i\rangle$. If we substitute the expansion 1.2 into the eigenvalue equation 1.5, we get

$$\left[H_e \hat{n}_{q\beta} + H_h \left(1 - \hat{n}_{q\beta}\right) + c^\dagger_{q\beta} T + T^\dagger c_{q\beta}\right] |\psi_i\rangle = \tilde{H}_i |\psi_i\rangle \tag{1.7}$$

The diagonal parts $H_e = \text{tr}\left[\mathcal{H}\hat{n}_{q\beta}\right]$ and $H_e = \text{tr}\left[\mathcal{H}\left(1-\hat{n}_{q\beta}\right)\right]$ can be separated into a purely diagonal part $\mathcal{H}^d$ that contains the single-particle energies and the multi-particle correlation energies or Hartree-like contributions, and an off-diagonal part $\mathcal{H}^i$ that scatters between the remaining degrees of freedom $k\sigma \neq q\beta$. That is,

$$H_e\hat{n}_{q\beta} + H_h\left(1-\hat{n}_{q\beta}\right) = \mathcal{H}^d + \mathcal{H}^i$$

This gives

$$\left[c^\dagger_{q\beta}T + T^\dagger c_{q\beta}\right]|\psi_i\rangle = \left(\tilde{H}_i - \mathcal{H}^i - \mathcal{H}^d\right)|\psi_i\rangle \tag{1.8}$$

1.2 Obtaining the decoupling transformation

We now define a new operator $\hat{\omega}_i = \tilde{H}_i - \mathcal{H}^i$, such that

$$\left[c^\dagger_{q\beta}T + T^\dagger c_{q\beta}\right]|\psi_i\rangle = \left(\hat{\omega}_i - \mathcal{H}^d\right)|\psi_i\rangle \tag{1.9}$$

From the definition of $\hat{\omega}_i$, we can see that it is Hermitian and has no term that scatters in the subspace of $q\beta$, so it is diagonal in $q\beta$ and we can expand it as $\hat{\omega}_i = \hat{\omega}^1_i\hat{n}_{q\beta} + \hat{\omega}^0_i\left(1-\hat{n}_{q\beta}\right)$. Using the expansion 1.6, we can write

$$\hat{\omega}_i|\psi_i\rangle = \hat{\omega}^1_i|1\rangle|\phi^i_1\rangle + \hat{\omega}^0_i|0\rangle|\phi^i_0\rangle \tag{1.10}$$

Since the only requirement on $|\psi_i\rangle$ is that it diagonalize the Hamiltonian in the subspace of $q\beta$, there is freedom in the choice of this state. We can exploit this freedom and choose the $|\phi^i_{0,}\rangle$ to be an eigenstates of $\hat{\omega}^{1,0}_i$ corresponding to real eigenvalues $\omega^{1,0}_i$:

$$\left[\mathcal{H}^d + c^\dagger_{q\beta}T + T^\dagger c_{q\beta}\right]|\psi_i(\omega_i)\rangle = \left(\omega^1_i - \mathcal{H}^d\right)|1\rangle|\phi^i_1\rangle + \left(\omega^0_i - \mathcal{H}^d\right)|0\rangle|\phi^i_0\rangle \tag{1.11}$$

If we now substitue the expansion 1.6 and gather the terms that result in $\hat{n}_{q\beta} = 1$, we get

$$c^\dagger_{q\beta}T|0\rangle|\phi^i_0\rangle = \left(\omega^1_i - \mathcal{H}^d\right)|1\rangle|\phi^i_1\rangle \tag{1.12}$$

Similarly, gathering the terms that result in $\hat{n}_{q\beta} = 0$ gives

$$T^\dagger c_{q\beta}|1\rangle|\phi^i_1\rangle = \left(\omega^0_i - \mathcal{H}^d\right)|0\rangle|\phi^i_0\rangle \tag{1.13}$$

We now define two many-particle transition operators:

$$\begin{aligned}\eta^\dagger(\omega^1_i) &= \frac{1}{\omega^1_i - \mathcal{H}^d}c^\dagger_{q\beta}T \\ \eta(\omega^0_i) &= \frac{1}{\omega^0_i - \mathcal{H}^d}T^\dagger c_{q\beta}\end{aligned} \tag{1.14}$$

We can write this compactly as

$$\eta(\hat{\omega}) = \frac{1}{\hat{\omega}_i - \mathcal{H}^d}T^\dagger c_{q\beta} \tag{1.15}$$

where $\hat{\omega}_i = \omega^0_i\left(1-\hat{n}_{q\beta}\right) + \omega^1_i\hat{n}_{q\beta} = \begin{pmatrix}\omega^1_i & \\ & \omega^0_i\end{pmatrix}$ is a 2x2 matrix and $\mathcal{H}^d = \mathcal{H}^d_0\left(1-\hat{n}_{q\beta}\right) + \mathcal{H}^d_1\hat{n}_{q\beta}$. It is easy to check that this reproduces the previous forms of η_0 and $\eta^\dagger_1$. We will

later find that it is important to demand that these two be Hermitian conjugates of each other; that constraint is imposed on the denominators:

$$\eta^\dagger(\omega_i^0) = \eta^\dagger(\omega_i^1) \implies \frac{1}{\omega_i^1 - \mathcal{H}^d} c_{q\beta}^\dagger T = c_{q\beta}^\dagger T \frac{1}{\omega_i^0 - \mathcal{H}^d} \tag{1.16}$$

Henceforth we will assume that this constraint has been imposed.

In terms of these operators, eq. 1.13 becomes

$$\begin{aligned} |1\rangle |\phi_1^i\rangle &= \eta^\dagger |0\rangle |\phi_0^i\rangle \\ |0\rangle |\phi_0^i\rangle &= \eta |1\rangle |\phi_1^i\rangle \end{aligned} \tag{1.17}$$

These allow us to write

$$\begin{aligned} |\psi_1\rangle &= |1\rangle |\phi_1^i\rangle + |0\rangle |\phi_0^i\rangle = (1+\eta) |1\rangle |\phi_1^i\rangle \\ |\psi_0\rangle &= \left(1+\eta^\dagger\right) |0\rangle |\phi_0^i\rangle \end{aligned} \tag{1.18}$$

Recalling that $|\psi_i\rangle = U^\dagger |i\rangle$, we can read off the required transformation:

$$U_1 = 1 + \eta \tag{1.19}$$

1.3 Properties of the many-body transition operator η

The operators η have some important properties. First is the Fermionic nature:

$$\eta^2 = \eta^{\dagger 2} = 0 \quad \left[c^{\dagger 2} = c^2 = 0\right] \tag{1.20}$$

Second is:

$$\begin{aligned} |1\rangle |\phi_1^i\rangle = \eta^\dagger |0\rangle |\phi_0^i\rangle = \eta^\dagger \eta |1\rangle |\phi_1^i\rangle &\implies \eta^\dagger \eta = \hat{n}_{q\beta} \\ |0\rangle |\phi_0^i\rangle = \eta |1\rangle |\phi_1^i\rangle = \eta\eta^\dagger |\phi_0^i\rangle &\implies \eta\eta^\dagger = 1 - \hat{n}_{q\beta} \end{aligned} \tag{1.21}$$

and hence the anticommutator

$$\implies \left\{\eta, \eta^\dagger\right\} = 1 \tag{1.22}$$

Note that the three equations in 1.21 work only when applied on the eigenstate $|\psi_i\rangle$ and not any arbitrary state.

$$\begin{gathered} \eta^\dagger \eta |\psi_i\rangle = |1\rangle |\phi_1^i\rangle = \hat{n}_{q\beta} |\psi_i\rangle \\ \eta\eta^\dagger |\psi_i\rangle = |0\rangle |\phi_0^i\rangle = (1 - \hat{n}_{q\beta}) |\psi_i\rangle \\ \left\{\eta^\dagger, \eta\right\} |\psi_i\rangle = |\psi_i\rangle \end{gathered}$$

1.4 Form of the unitary operators

Although we have found the correct similarity transformations U_i (eqs. 1.19), we need to convert them into a unitary transformation. Say we are trying to rotate the eigenstate $|\psi_1\rangle$ into the state $|1\rangle$. We can then work with the transformation

$$U_1 = 1 + \eta \tag{1.23}$$

In this form, this transformation is not unitary. It can however be written in an exponential form:

$$U_1 = e^{\eta} \tag{1.24}$$

using the fact that $\eta^2 = 0$. It is shown in ref. [2] that corresponding to a similarity transformation e^{ω},there exists a unitary transformation e^{G} where

$$G = \tanh^{-1}\left(\omega - \omega^{\dagger}\right) \tag{1.25}$$

Applying that to the problem at hand gives

$$\begin{aligned} U_1^{\dagger} &= \exp\left(\tanh^{-1}\left(\eta - \eta^{\dagger}\right)\right) \\ &= \frac{1 + \eta - \eta^{\dagger}}{1 + \{\eta, \eta^{\dagger}\}} \\ &= \frac{1}{\sqrt{2}}\left(1 + \eta - \eta^{\dagger}\right) \end{aligned} \tag{1.26}$$

The *unitary* operator that transforms the entangled eigenstate $|\psi_1\rangle$ to the state $|1\rangle$ is thus

$$U_1 = \frac{1}{\sqrt{2}}\left(1 + \eta^{\dagger} - \eta\right) \tag{1.27}$$

It can also be written as $\exp\left(\frac{\pi}{4}\left(\eta^{\dagger} - \eta\right)\right)$ because

$$\begin{aligned} \exp\left(\frac{\pi}{4}\left(\eta^{\dagger} - \eta\right)\right) &= 1 + \left(\eta^{\dagger} - \eta\right)\frac{\pi}{4} + \frac{1}{2!}\left(\eta^{\dagger} - \eta\right)^2\left(\frac{\pi}{4}\right)^2 + \frac{1}{3!}\left(\eta^{\dagger} - \eta\right)^3\left(\frac{\pi}{4}\right)^3 + \ldots \\ &= 1 + \left(\eta^{\dagger} - \eta\right)\frac{\pi}{4} - \frac{1}{2!}\left(\frac{\pi}{4}\right)^2 - \frac{1}{3!}\left(\eta^{\dagger} - \eta\right)\left(\frac{\pi}{4}\right)^3 + \frac{1}{4!}\left(\frac{\pi}{4}\right)^4 + \ldots \\ &= \cos\frac{\pi}{4} + \left(\eta^{\dagger} - \eta\right)\sin\frac{\pi}{4} \\ &= 1 + \eta^{\dagger} - \eta \end{aligned} \tag{1.28}$$

There we used

$$\left(\eta^{\dagger} - \eta\right)^2 = {\eta^{\dagger}}^2 + \eta^2 - \left\{\eta^{\dagger}, \eta\right\} = -1 \quad \left[\because \eta^2 = {\eta^{\dagger}}^2 = 0\right] \tag{1.29}$$

and hence

$$\left(\eta^{\dagger} - \eta\right)^3 = -1\left(\eta^{\dagger} - \eta\right) \tag{1.30}$$

and so on.

1.5 Effective Hamiltonian

We can now compute the form of the effective Hamiltonian that comes about when we apply U_1 - that is - when we rotate one exact eigenstate $|\psi_1\rangle$ into the occupied Fock space

basis $|1\rangle$. From eq. 1.27,

$$\begin{aligned} U_1\mathcal{H}U_1^\dagger &= \frac{1}{2}\left(1+\eta^\dagger-\eta\right)\mathcal{H}\left(1+\eta-\eta^\dagger\right) \\ &= \frac{1}{2}\left(1+\eta^\dagger-\eta\right)\left(\mathcal{H}+\mathcal{H}\eta-\mathcal{H}\eta^\dagger\right) \\ &= \frac{1}{2}\left(\mathcal{H}+\mathcal{H}\eta-\mathcal{H}\eta^\dagger+\eta^\dagger\mathcal{H}+\eta^\dagger\mathcal{H}\eta-\eta^\dagger\mathcal{H}\eta^\dagger-\eta\mathcal{H}-\eta\mathcal{H}\eta+\eta\mathcal{H}\eta^\dagger\right) \\ &= \frac{1}{2}\left(\mathcal{H}^d+\mathcal{H}^i+\mathcal{H}^I+\mathcal{H}\eta-\mathcal{H}\eta^\dagger+\eta^\dagger\mathcal{H}+\eta^\dagger\mathcal{H}\eta-\eta^\dagger\mathcal{H}\eta^\dagger-\eta\mathcal{H}-\eta\mathcal{H}\eta+\eta\mathcal{H}\eta^\dagger\right) \\ &= \frac{1}{2}\left(\mathcal{H}^d+\mathcal{H}^i+\mathcal{H}^I+\left[\eta^\dagger-\eta,\mathcal{H}\right]+\eta^\dagger\mathcal{H}\eta-\eta^\dagger\mathcal{H}\eta^\dagger-\eta\mathcal{H}\eta+\eta\mathcal{H}\eta^\dagger\right) \end{aligned} \tag{1.31}$$

In the last two lines, we expanded the Hamiltonian into the three parts $\mathcal{H}^d, \mathcal{H}^i$ and a third piece $\mathcal{H}^I \equiv c_{q\beta}^\dagger T + T^\dagger c_{q\beta}$.

For reasons that will become apparent, we will split the terms into two groups:

$$\tilde{\mathcal{H}} = \frac{1}{2}\left(\underbrace{\mathcal{H}^d+\mathcal{H}^i+\left[\eta^\dagger-\eta,\mathcal{H}\right]+\eta^\dagger\mathcal{H}\eta+\eta\mathcal{H}\eta^\dagger}_{\text{group 1}}+\overbrace{\mathcal{H}^I-\eta^\dagger\mathcal{H}\eta^\dagger-\eta\mathcal{H}\eta}^{\text{group 2}}\right) \tag{1.32}$$

Group 2 can be easily shown to be 0. Note that terms that have two η or two $\eta^\dagger$ sandwiching a $\mathcal{H}$ can only be nonzero if the intervening $\mathcal{H}$ has an odd number of creation or destruction operators.

$$\eta\mathcal{H}\eta = \eta c_q^\dagger T\eta \tag{1.33}$$

and

$$\eta^\dagger\mathcal{H}\eta^\dagger = \eta^\dagger T^\dagger c_q\eta^\dagger \tag{1.34}$$

Group 2 becomes

$$\text{group 2} = \mathcal{H}^I-\eta^\dagger T^\dagger c_q\eta^\dagger-\eta c_q^\dagger T\eta = c_q^\dagger T+T^\dagger c_q-\eta^\dagger T^\dagger c_q\eta^\dagger-\eta c_q^\dagger T\eta \tag{1.35}$$

To simplify this, we use the relation

$$\begin{aligned} \eta c_q^\dagger T\eta &= \frac{1}{\omega_i^0-\mathcal{H}^d}T^\dagger c_q c_q^\dagger T\eta \\ &= T^\dagger c_q\frac{1}{\omega_i^1-\mathcal{H}^d}c_q^\dagger T\eta \quad [\text{eq. 1.16}] \\ &= T^\dagger c_q\eta^\dagger\eta \quad [\text{eq. 1.15}] \\ &= T^\dagger c_q\hat{n}_q \quad [\text{eq. 1.21}] \end{aligned} \tag{1.36}$$

which gives

$$\eta c_q^\dagger T\eta = T^\dagger c_q \tag{1.37}$$

Taking the Hermitian conjugate of eq. 1.37 gives

$$\eta^\dagger T^\dagger c_q\eta^\dagger = c_q^\dagger T \tag{1.38}$$

Substituting the expressions 1.37 and 1.38 into the expression for group 2, 1.35, shows that is vanishes. This leaves us only with group 1:

$$\widetilde{\mathcal{H}} = \frac{1}{2}\left(\mathcal{H}^d + \mathcal{H}^i + \overbrace{\eta^\dagger \mathcal{H}\eta + \eta\mathcal{H}\eta^\dagger}^{\text{group A}} + \underbrace{\left[\eta^\dagger - \eta, \mathcal{H}\right]}_{groupB}\right) \tag{1.39}$$

Group A simplifies in the following way. First note that $\eta^\dagger \mathcal{H}^I \eta = \eta^\dagger \mathcal{H}^I \eta = 0$ must be 0 because it will involve consecutive $c_{q\beta}$ or consecutive $c^\dagger_{q\beta}$. We are therefore left with the diagonal part of $\mathcal{H}$, which is $H_e \hat{n}_{q\beta} + H_h\left(1 - \hat{n}_{q\beta}\right)$.

$$\eta^\dagger \left[H_e \hat{n}_{q\beta} + H_h\left(1 - \hat{n}_{q\beta}\right)\right]\eta + \eta\left[H_e \hat{n}_{q\beta} + H_h\left(1 - \hat{n}_{q\beta}\right)\right]\eta^\dagger = \eta^\dagger H_h \eta + \eta H_e \eta^\dagger \tag{1.40}$$

This can be shown (**clear with AM**) to be equal to the diagonal part:

$$\text{group A} = \eta^\dagger H_h \eta + \eta H_e \eta^\dagger = H_e \hat{n}_{q\beta} + H_h\left(1 - \hat{n}_{q\beta}\right) = \mathcal{H}^d + \mathcal{H}^i \tag{1.41}$$

It can also be shown (**clear with AM**) that

$$\text{group B} = \left[\eta^\dagger - \eta, \mathcal{H}\right] = 2\left[c^\dagger_{q\beta} T, \eta\right] \tag{1.42}$$

Putting it all together,

$$\tilde{\mathcal{H}} = \mathcal{H}^d + \mathcal{H}^i + \left[c^\dagger_{q\beta} T, \eta\right] \tag{1.43}$$

To check that this indeed commutes with $\hat{n}_{q\beta}$,

$$\begin{aligned}
\left[\widetilde{\mathcal{H}}, \hat{n}_{q\beta}\right] &= \left[\left[c^\dagger_{q\beta} T, \eta\right], \hat{n}_{q\beta}\right] \\
&= \left[c^\dagger_{q\beta} T\eta, \hat{n}_{q\beta}\right] - \left[\eta c^\dagger_{q\beta} T, \hat{n}_{q\beta}\right] \\
&= c^\dagger_{q\beta} T\eta \hat{n}_{q\beta} - \hat{n}_{q\beta} c^\dagger_{q\beta} T\eta \qquad \left[2^{\text{nd}}\ [\ .\ ] \text{ is 0, } \because c^\dagger_{q\beta}\hat{n}_{q\beta} = \hat{n}_{q\beta}\eta = 0\right] \\
&= c^\dagger_{q\beta} T\eta - c^\dagger_{q\beta} T\eta \\
&= 0
\end{aligned} \tag{1.44}$$

1.6 Fixed point condition

Within the URG, it is a prescription that the fixed point is reached when the denominator of the RG equation vanishes. This is equivalent to either $\omega^1_i = \mathcal{H}^d_1$ or $\omega^0_i = \mathcal{H}^d_0$. This shows that at the fixed point, one of the eigenvalues of $\hat{\omega}_i$ matches the corresponding eigenvalue of the diagonal blocks. This also leads to the vanishing of the off-diagonal block, because eqs. 1.12 and 1.13 gives

$$c^\dagger_{q\beta} T\left|0\right\rangle\left|\phi^i_0\right\rangle = \left(\omega^1_i - \mathcal{H}^d_1\right)\left|1\right\rangle\left|\phi^i_1\right\rangle = 0 \implies c^\dagger_{q\beta} T = 0 \tag{1.45}$$

1.7 Equivalence of the two unitaries and preservation of partial trace

In the subsection 1.4, we determined the form of the operator U_1 that unitarily decouples the node $q\beta$ from the other degrees of freedom. Eq. 1.27 was derived by reading off the

transformation of $|1\rangle$ to $|\psi_1\rangle$, the first equation in 1.18. We could easily have chosen the other equation in the same equation set,

$$|\psi_0\rangle = \left(1+\eta^\dagger\right)|0\rangle\,|\phi_0^i\rangle$$

which gives a similarity transformation $1+\eta^\dagger$ and hence a unitary

$$U_0 = \frac{1}{\sqrt{2}}\left(1+\eta-\eta^\dagger\right) \tag{1.46}$$

This η will however be different from the η in eq. 1.27. The reason is, in order to get U_1, we must start from the eigenvalue equation $\mathcal{H}\,|\psi_1\rangle = \tilde{H}_1\,|\psi_1\rangle$. This means that the corresponding $\hat{\omega}$ will be defined as $\hat{\omega}_1 = \tilde{H}_1 - \mathcal{H}^i$. On the other hand, in order to get U_0 we must start with $\mathcal{H}\,|\psi_0\rangle = \tilde{H}_0\,|\psi_0\rangle$, and hence this $\hat{\omega}$ will be $\hat{\omega}_0 = \tilde{H}_0 - \mathcal{H}^i$. This difference in the $\hat{\omega}$ will define two different sets of η:

$$\begin{aligned}
&\text{Starting from } |\psi_1\rangle\text{: } \eta_1 = \frac{1}{\omega_1^0 - \mathcal{H}^d}T^\dagger c_{q\beta} \quad \text{and } \eta_1^\dagger = \frac{1}{\omega_1^1 - \mathcal{H}^d}T^\dagger c_{q\beta} \\
&\text{Starting from } |\psi_0\rangle\text{: } \eta_0 = \frac{1}{\omega_0^0 - \mathcal{H}^d}T^\dagger c_{q\beta} \quad \text{and } \eta_0^\dagger = \frac{1}{\omega_0^1 - \mathcal{H}^d}T^\dagger c_{q\beta}
\end{aligned} \tag{1.47}$$

The ω_j^i eigenvalues have both upper and lower indices. The upper index i signifies which eigenstate it relates to - $\omega_j\,|i\rangle = \omega_j^i\,|i\rangle$. The lower index refers to the exact eigenstate we started with - starting with $\mathcal{H}\,|\psi_j\rangle = \tilde{H}_j\,|\psi_j\rangle$ leads to ω_j. The two unitaries are

$$\begin{aligned}
U_1 &= \frac{1}{\sqrt{2}}\left(1+\eta_1^\dagger-\eta_1\right) \\
U_0 &= \frac{1}{\sqrt{2}}\left(1+\eta_0-\eta_0^\dagger\right)
\end{aligned} \tag{1.48}$$

Since the two unitaries should give the same effective Hamiltonian, we require $U_1 = U_0$. That requires $\eta_1 = -\eta_0$. Comparing the expressions of the ηs, we get

$$\omega_1^0 - \mathcal{H}_0^d = -\left(\omega_0^0 - \mathcal{H}_0^d\right) \tag{1.49}$$

This is the constraint that ensures that both unitaries give the same effective Hamiltonian. The condition $\eta_1 + \eta_0 = 0$, when expressed without resolving $\hat{\omega}$ into its eigenvalues can also be shown to be a statement of the preservation of the partial trace under the RG flow.

$$\begin{aligned}
\eta_1 &= \frac{1}{\tilde{H}_1 - \mathcal{H}^i - \mathcal{H}^d}T^\dagger c_{q\beta} \\
\eta_0 &= \frac{1}{\tilde{H}_0 - \mathcal{H}^i - \mathcal{H}^d}T^\dagger c_{q\beta} \\
\implies \eta_1 + \eta_0 &= \left[\frac{1}{\tilde{H}_1 - \mathcal{H}^i - \mathcal{H}^d} + \frac{1}{\tilde{H}_0 - \mathcal{H}^i - \mathcal{H}^d}\right]T^\dagger c_{q\beta} = 0 \\
\implies \tilde{H}_1 - \mathcal{H}^i - \mathcal{H}^d &= -\left[\tilde{H}_0 - \mathcal{H}^i - \mathcal{H}^d\right] \\
\implies \tilde{H}_1 + \tilde{H}_0 &= 2\mathcal{H}_0
\end{aligned} \tag{1.50}$$

$\mathcal{H}_0 = \mathcal{H}^i + \mathcal{H}^d$ is the total diagonal part of the bare model. To match the dimensions, we must take $\tilde{H}_1 = E_1 \otimes I$ and similarly $\tilde{H}_0 = E_0 \otimes I$, where the rotated Hamiltonian is

$$\tilde{H} = \begin{pmatrix} E_1 & 0 \\ 0 & E_0 \end{pmatrix} \tag{1.51}$$

Therefore, the trace of the rotated Hamiltonian is $t_{\text{new}} = E_1 + E_0$. The trace of the LHS in the final equation of 1.50 is $\text{tr}\left(\tilde{H}_1 + \tilde{H}_0\right) = \text{tr}\left(E_1 \otimes I + E_0 \otimes I\right) = 2\left(E_1 + E_0\right) = 2t_{\text{new}}$. The trace of the RHS in final equation of 1.50 is $2 \times \text{tr}\left(\mathcal{H}_0\right) = 2t_{\text{old}}$ where $t_{\text{old}} = \text{tr}\left(\mathcal{H}_0\right)$ is the trace of the old Hamiltonian. Equating the LHS and RHS gives $t_{\text{new}} = t_{\text{old}}$.

1.8 Prescription

Given a Hamiltonian

$$\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_0 + c^\dagger T + T^\dagger c \tag{1.52}$$

the goal is to look at the renormalization of the various couplings in the Hamiltonian as we decouple high energy electron states. Typically we have a shell of electrons at some energy D. During the process, we make one simplification. We assume that there is only one electron on that shell at a time, say with quantum numbers q, σ, and calculate the renormalization of the various couplings due to this electron. We then sum the momentum q over the shell and the spin β, and this gives the total renormalization due to decoupling the entire shell.

From eq. 1.43, the first two terms in the rotated Hamiltonian are just the diagonal parts of the bare Hamiltonian; they are unchanged in that part. The renormalization comes from the third term. For one electron $q\beta$ on the shell, the renormalization is

$$\Delta\mathcal{H} = \left[c^\dagger_{q\beta}\text{Tr}\left(\mathcal{H}c_{q\beta}\right), \eta\right] = c^\dagger_{q\beta}\text{Tr}\left(\mathcal{H}c_{q\beta}\right)\eta - \eta c^\dagger_{q\beta}\text{Tr}\left(\mathcal{H}c_{q\beta}\right) \tag{1.53}$$

Since this assumes we have obtained this from U_1, it is fair to tag the η with a suitable label:

$$\Delta\mathcal{H} = c^\dagger_{q\beta}\text{Tr}\left(\mathcal{H}c_{q\beta}\right)\eta_1 - \eta_1 c^\dagger_{q\beta}\text{Tr}\left(\mathcal{H}c_{q\beta}\right) \tag{1.54}$$

It is clear that the first term takes into account virtual excitations that start from a filled state ($\hat{n}_{q\beta} = 1$ initially) - such a term is said to be a part of the *particle sector*.

$$\Delta_1\mathcal{H} = c^\dagger_{q\beta}\text{Tr}\left(\mathcal{H}c_{q\beta}\right)\eta_1 \tag{1.55}$$

The second term, on the other hand, considers excitations that start from an empty state. They constitute the *hole sector*.

$$\Delta_0\mathcal{H} = -\eta_1 c^\dagger_{q\beta}\text{Tr}\left(\mathcal{H}c_{q\beta}\right) \tag{1.56}$$

To write the total renormalization in a particle-hole symmetric form, we can use the relation $\eta_0 = -\eta_1$, such that both the terms will now come with a positive sign:

$$\Delta\mathcal{H} = c^\dagger_{q\beta}\text{Tr}\left(\mathcal{H}c_{q\beta}\right)\eta_1 + \eta_0 c^\dagger_{q\beta}\text{Tr}\left(\mathcal{H}c_{q\beta}\right) \tag{1.57}$$

We can make one more manipulation: using eq. 1.16, we get

$$\Delta\mathcal{H} = c^\dagger_{q\beta}\text{Tr}\left(\mathcal{H}c_{q\beta}\right)\eta_1 + \text{Tr}\left(c^\dagger_{q\beta}\mathcal{H}\right)c_{q\beta}\eta^\dagger_0 \tag{1.58}$$

This form of the total renormalization is identical to the one we use in the "Poor Man's scaling"-type of renormalization that was used to get the scaling equations in the Kondo and Anderson models [3],[4]. Writing down the forms of η and $\eta^\dagger$ explicitly, we get

$$\Delta\mathcal{H} = c^\dagger_{q\beta}\text{Tr}\left(\mathcal{H}c_{q\beta}\right)\frac{1}{\omega^0_1 - \mathcal{H}^d_0}\text{Tr}\left(c^\dagger_{q\beta}\mathcal{H}\right)c_{q\beta} + \text{Tr}\left(c^\dagger_{q\beta}\mathcal{H}\right)c_{q\beta}\frac{1}{\omega^1_0 - \mathcal{H}^d_1}c^\dagger_{q\beta}\text{Tr}\left(\mathcal{H}c_{q\beta}\right) \tag{1.59}$$

The renormalization due to the entire shell is obtained by summing over all states on the shell.

$$\Delta\mathcal{H} = \sum_{q\beta}\left[c^\dagger_{q\beta}\text{Tr}\left(\mathcal{H}c_{q\beta}\right)\frac{1}{\omega^0_1 - \mathcal{H}^d_0}\text{Tr}\left(c^\dagger_{q\beta}\mathcal{H}\right)c_{q\beta} + \text{Tr}\left(c^\dagger_{q\beta}\mathcal{H}\right)c_{q\beta}\frac{1}{\omega^1_0 - \mathcal{H}^d_1}c^\dagger_{q\beta}\text{Tr}\left(\mathcal{H}c_{q\beta}\right)\right] \tag{1.60}$$

These equations will now need to be simplified. For example, in the particle sector, we can set $\hat{n}_{q\beta} = 0$ in the numerator, because there is no such excitation in the initial state. Similarly, in the hole sector, we can set $\hat{n}_{q\beta} = 1$ because that state was occupied in the initial state. Another simplification we typically employ is that $\mathcal{H}^d_{0,1}$ will, in general, have the energies of all the electrons. But we consider only the energy of the on-shell electrons in the denominator. After integrating out these electrons, we can rearrange the remaining operators to determine which term in the Hamiltonian it renormalizes and what is the renormalization.

At first sight, one might think that we must evaluate lots of traces to obtain the terms in $\Delta\mathcal{H}$. A little thought reveals that the terms in the numerator are simply the off-diagonal terms in the Hamiltonian; $\text{Tr}\left(c^\dagger_{q\beta}\mathcal{H}\right)c_{q\beta}$ is the off-diagonal term that has $c_{q\beta}$ in it, and $c^\dagger_{q\beta}\text{Tr}\left(\mathcal{H}c_{q\beta}\right)$ is the off-diagonal term that has $c^\dagger_{q\beta}$ in it. $\mathcal{H}^D$ is just the diagonal part of the Hamiltonian.

2 Anderson Model URG

2.1 Without spin-spin interaction

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

$$\mathcal{H} = \sum_{k\sigma}\epsilon_k\hat{n}_{k\sigma} + \sum_{k\sigma}\left(V_k c^\dagger_{k\sigma}c_{d\sigma} + h.c.\right) + \epsilon_d\sum_\sigma\hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} \tag{2.1}$$

To allow the calculation of both particle and hole kinetic energies, we will write the kinetic energy part as $\sum_{k\sigma}\epsilon_k\tau_{k\sigma}$ and drop the extra constant part.

$$\mathcal{H} = \sum_{k\sigma}\epsilon_k\tau_{k\sigma} + \sum_{k\sigma}\left(V_k c^\dagger_{k\sigma}c_{d\sigma} + h.c.\right) + \epsilon_d\sum_\sigma\hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} \tag{2.2}$$

From eq. 1.60, the renormalized Hamiltonian is

$$\tilde{\mathcal{H}} = \mathcal{H}_0 + \sum_{q\beta}\left[c^\dagger_{q\beta}\mathrm{Tr}\left(\mathcal{H}c_{q\beta}\right)\frac{1}{\omega^0_1-\mathcal{H}^d_0}\mathrm{Tr}\left(c^\dagger_{q\beta}\mathcal{H}\right)c_{q\beta} + \mathrm{Tr}\left(c^\dagger_{q\beta}\mathcal{H}\right)c_{q\beta}\frac{1}{\omega^1_0-\mathcal{H}^d_1}c^\dagger_{q\beta}\mathrm{Tr}\left(\mathcal{H}c_{q\beta}\right)\right] \tag{2.3}$$

$\mathcal{H}_0$ is the part of the Hamiltonian that conserves the operator $\hat{n}_{q\beta}$.

$$\mathcal{H}_0 = \sum_{k\sigma}\epsilon_k\tau_{k\sigma} + \sum_{k<\Lambda_N,\sigma}\left(V_k c^\dagger_{k\sigma}c_{d\sigma} + h.c.\right) + \epsilon_d\sum_\sigma \hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} \tag{2.4}$$

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 means that the state must be vacant in the initial state, so we must have $\epsilon_q > 0$. This contribution will be given by the second term inside the summation of eq. 2.3.

$$\Delta^+\mathcal{H} = \sum_{q\beta}\mathrm{Tr}\left(c^\dagger_{q\beta}\mathcal{H}\right)c_{q\beta}\frac{1}{\omega_e-\mathcal{H}^d_1}c^\dagger_{q\beta}\mathrm{Tr}\left(\mathcal{H}c_{q\beta}\right) \tag{2.5}$$

We have labeled $\omega^1_0 = \omega_e$. We now compute this term.

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

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

$$\mathcal{H}^d = \sum_{k\sigma}\epsilon_k\tau_{k\sigma} + \epsilon_d\sum_\sigma\hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} \tag{2.6}$$

$$\mathcal{H}^d_1 = \mathrm{Tr}_{q\beta}\left(\mathcal{H}^D\hat{n}_{q\beta}\right) = \sum_{k<\Lambda_N,\sigma}\epsilon_k\tau_{k\sigma} + \epsilon_d\sum_\sigma\hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + \frac{1}{2}\epsilon_q \tag{2.7}$$

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.

Substituting these into the expression for $\Delta^+\mathcal{H}$ gives

$$\begin{aligned}\Delta^+\mathcal{H} &= \sum_{q\beta} \mathrm{Tr}_{q\beta}\left(c_{q\beta}^\dagger \mathcal{H}\right) c_{q\beta} \frac{1}{\omega_e - \mathrm{Tr}_{q\beta}\left(\mathcal{H}^D \hat{n}_{q\beta}\right)\hat{n}_{q\beta}} c_{q\beta}^\dagger \mathrm{Tr}\left(\mathcal{H} c_{q\beta}\right) \\ &= \sum_{q\beta} V_q^* c_{d\beta}^\dagger c_{q\beta} \frac{1}{\omega_e - \left(\sum_{k<\Lambda_N,\sigma} \epsilon_k \tau_{k\sigma} + \epsilon_d \sum_\sigma \hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + \frac{1}{2}\epsilon_q\right)\hat{n}_{q\beta}} V_q c_{q\beta}^\dagger c_{d\beta} \\ &= \sum_{q\beta} |V_q|^2 c_{d\beta}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{d\beta} \frac{1}{\omega_e - \left(\epsilon_d \sum_\sigma \hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + \frac{1}{2}\epsilon_q\right)}\end{aligned} \tag{2.8}$$

At the last step, I dropped the lower shell electrons from the denominator to simplify the calculation. I also replaced $\hat{n}_{q\beta}$ with 1 because the propagator has a $c_{q\beta}$ to the left. Note that since this term has a $c_{d\beta}^\dagger$, it will survive 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.

$$\begin{aligned}\Delta^+\mathcal{H} &= \sum_{q\beta} |V_q|^2 c_{d\beta}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{d\beta} \frac{1}{\omega_e - \frac{1}{2}\epsilon_q - \epsilon_d \hat{n}_{d\bar{\beta}}} \\ &= \sum_{q\beta} |V_q|^2 \hat{n}_{d\beta}\left(1 - \hat{n}_{q\beta}\right) \frac{1}{\omega_e - \frac{1}{2}\epsilon_q - \epsilon_d \hat{n}_{d\bar{\beta}}} \\ &= \sum_{q\beta} |V_q|^2 \hat{n}_{d\beta}\left[\frac{\hat{n}_{d\bar{\beta}}}{\omega_e - \frac{1}{2}\epsilon_q - \epsilon_d} + \frac{1 - \hat{n}_{d\bar{\beta}}}{\omega_e - \frac{1}{2}\epsilon_q}\right]\end{aligned} \tag{2.9}$$

In the last step, we replaced $\hat{n}_{q\beta} = 0$ because we are working with $\epsilon_q > 0$. Also, we used

$$\frac{1}{\omega_e - \frac{1}{2}\epsilon_q - \epsilon_d \hat{n}_{d\bar{\beta}}} = \frac{\hat{n}_{d\bar{\beta}}}{\omega_e - \frac{1}{2}\epsilon_q - \epsilon_d} + \frac{1 - \hat{n}_{d\bar{\beta}}}{\omega_e - \frac{1}{2}\epsilon_q} \tag{2.10}$$

From the expression of $\Delta^+\mathcal{H}$, we see two terms: the first term renormalizes the energy of the doubly-occupied state E_2, while the other term renormalizes the singly-occupied state E_1:

$$\begin{aligned}\Delta^+ E_1 &= \sum_{q,\epsilon_q=+D} \frac{|V_q|^2}{\omega_e - \frac{1}{2}\epsilon_q} \\ \Delta^+ E_2 &= 2\sum_{q,\epsilon_q=+D} \frac{|V_q|^2}{\omega_e - \frac{1}{2}\epsilon_q - \epsilon_d}\end{aligned} \tag{2.11}$$

Hole Sector

The hole sector consists of those excitations where the state is occupied in the initial state but vacant in the final state ($\epsilon_q < 0$). Again from the prescription, we have

$$\begin{aligned}\Delta^-\mathcal{H} &= \sum_{q\beta} c_{q\beta}^\dagger \mathrm{Tr}\left(\mathcal{H} c_{q\beta}\right)\eta_{q\beta} \\ &= \sum_{q\beta} c_{q\beta}^\dagger \mathrm{Tr}\left(\mathcal{H} c_{q\beta}\right) \frac{1}{\omega_h - \mathcal{H}_0^d} \mathrm{Tr}\left(c_{q\beta}^\dagger \mathcal{H}\right) c_{q\beta}\end{aligned} \tag{2.12}$$

where we have labeled $\omega_1^0 = \omega_h$. In this sector, the diagonal part $\mathcal{H}_0^d$ is obtained by changing eq. 2.6: $\epsilon_q \to -\epsilon_q$ and $\tau_{q\beta} = -\frac{1}{2}$:

$$\mathcal{H}_0^d = \frac{1}{2}\epsilon_q + \epsilon_d \sum_\sigma \hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} \tag{2.13}$$

Therefore,

$$\begin{aligned}
\Delta^-\mathcal{H} &= \sum_{q\beta} V_q c_{q\beta}^\dagger c_{d\beta} \frac{1}{\omega_h - \frac{1}{2}\epsilon_q - \sum_\sigma \epsilon_d \hat{n}_{d\sigma} - U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}} V_q^* c_{d\beta}^\dagger c_{q\beta} \\
&= \sum_{q\beta} |V_q|^2 c_{q\beta}^\dagger c_{d\beta} \frac{1}{\omega_h - \frac{1}{2}\epsilon_q - \epsilon_d - (\epsilon_d + U)\hat{n}_{d\bar{\beta}}} c_{d\beta}^\dagger c_{q\beta} \\
&= \sum_{q\beta} |V_q|^2 (1 - \hat{n}_{d\beta}) \left[\frac{\hat{n}_{d\bar{\beta}}}{\omega_h - \frac{1}{2}\epsilon_q - 2\epsilon_d - U} + \frac{1 - \hat{n}_{d\bar{\beta}}}{\omega_h - \frac{1}{2}\epsilon_q - \epsilon_d} \right]
\end{aligned} \tag{2.14}$$

We replaced $\hat{n}_{q\beta} = 1$ because $\epsilon_q < 0$. The renormalizations in this sector are

$$\begin{aligned}
\Delta^- E_0 &= 2 \sum_{q,\epsilon_q = -D} \frac{|V_q|^2}{\omega_h - \frac{1}{2}\epsilon_q - \epsilon_d} \\
\Delta^- E_1 &= \sum_{q,\epsilon_q = -D} \frac{|V_q|^2}{\omega_h - \frac{1}{2}\epsilon_q - 2\epsilon_d - U}
\end{aligned} \tag{2.15}$$

E_0 is the energy of the vacant state.

Flow Equations

The ω have to be determined self-consistently or numerically by searching for fixed points where they become identical to the energy eigenvalues. As a simplification, we set $\omega_e = \omega_h$.

$$\begin{aligned}
\Delta E_2 &= 2 \sum_{q,\epsilon_q = +D} \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d} \\
\Delta E_0 &= 2 \sum_{q,\epsilon_q = -D} \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d} \\
\Delta E_1 &= \sum_{q,\epsilon_q = -D} \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - 2\epsilon_d - U} + \sum_{q,\epsilon_q = +D} \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q}
\end{aligned} \tag{2.16}$$

The above equations are just the total renormalizations obtained by adding the particle and hole sector contributions. This is the total change in the Hamiltonian on decoupling the states at the upper and lower edges of the bandwidth. They can be translated into the renormalizations of the quantities ϵ_d and U by using the relations $\epsilon_d = E_1 - E_0$ and $U = E_2 + E_0 - 2E_1$.

$$\begin{aligned}
\Delta\epsilon_d &= \sum_{q,\epsilon_q = -D} \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - 2\epsilon_d - U} + \sum_{q,\epsilon_q = +D} \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} - 2 \sum_{q,\epsilon_q = -D} \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d} \\
\Delta U &= 2 \sum_{q,|\epsilon_q| = D} \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d} - \sum_{q,\epsilon_q = -D} \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - 2\epsilon_d - U} - \sum_{q,\epsilon_q = +D} \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q}
\end{aligned} \tag{2.17}$$

Connection to Poor Man's scaling

To obtain the results of Poor Man's scaling [4][**?**], we can look at various regimes. First, for $U, \epsilon_d \ll \epsilon_q$, we get

$$\begin{aligned}\Delta\epsilon_d &= \sum_{q,|\epsilon_q|=D} \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} - 2\sum_{q,\epsilon_q=-D} \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} \\ \Delta U &= 2\sum_{q,|\epsilon_q|=D} \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} - \sum_{q,\epsilon_q=-D} \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} - \sum_{q,\epsilon_q=+D} \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q}\end{aligned} \tag{2.18}$$

Assuming the upper and lower band edges are symmetrical such that $\sum_{-D} = \sum_D$, we get $\Delta\epsilon_d = \Delta U = 0$.

In the regime $U \gg \epsilon_q \gg \epsilon_d$, we get

$$\begin{aligned}\Delta\epsilon_d &= \sum_{q,\epsilon_q=+D} \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} - 2\sum_{q,\epsilon_q=-D} \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} \\ \Delta U &= 2\sum_{q,|\epsilon_q|=D} \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} - \sum_{q,\epsilon_q=+D} \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q}\end{aligned} \tag{2.19}$$

Again assuming symmetrical upper and lower edges and $|\epsilon_q| = D$ and $\sum_q |V|^2 = \frac{\Delta}{\pi}|\delta D|$, we get

$$\begin{aligned}\Delta U &= 0 \\ \delta\epsilon_d &= -\frac{\Delta}{\pi}\frac{1}{\omega - \frac{1}{2}D}\end{aligned} \tag{2.20}$$

There we replaced the change symbol Δ for δ to avoid confusion with the hybridisation $\Delta \sim \sum V^2$. If we recall that ω was defined as $\tilde{\mathcal{H}} - \mathcal{H}^i$, we can make a crude estimate of ω by ignoring the off-diagonal part and replace it with the renormalized diagonal part of the initial state from which the particle excitations arise ($\epsilon_q \tau_{q\beta} = -\frac{1}{2}D$:

$$\delta\epsilon_d = \frac{\Delta}{\pi}\frac{\delta D}{D} \tag{2.21}$$

This is the one-loop scaling equation.

2.1.1 Particle-Hole symmetry

For a particle-hole symmetric model, we can substitute $\omega_e = \omega_h = \omega$. This gives

$$\Delta^- E_0 = 2\sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d} = \Delta^+ E_2 \tag{2.22}$$

This shows that the doublon and holon states remain equidistant from the single-particle level, thus maintaining particle-hole symmetry along the flow.

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