The total Hamiltonian can be written in the form

$$\begin{aligned} H_{\text{eff}} = \sum_{k\sigma} \epsilon_{k\sigma} n_{k\sigma} + \left(\epsilon_d + \delta\epsilon_d\right) n_d \\ + \sum_{k\sigma} \left\{ \left(V_k^- + \delta V_k^-\right) c_{k\sigma}^\dagger c_{d\sigma} + \left(V_k^+ + \delta V_k^+\right) c_{d\sigma}^\dagger c_{k\sigma} \right\} \end{aligned} \tag{2.9.108}$$

We now evaluate the changes:

$$\begin{aligned} \delta\epsilon_d &= \left(\sum_q{}^+ \frac{|V_q|^2}{\epsilon_d - \epsilon_q} + 2\sum_q{}^- \frac{|V_q|^2}{\epsilon_d - \epsilon_q} \right) \\ &\approx |V|^2 \rho |\delta D| \left(\frac{1}{\epsilon_d - D} + \frac{2}{\epsilon_d + D} \right) \\ &= |V|^2 \rho |\delta D| \frac{D - 3\epsilon_d}{D^2 - \epsilon_d^2} \end{aligned} \tag{2.9.109}$$

I used the approximation

$$\sum_{q=D-\delta D}^{D} f(q) = \int_{D-\delta D}^{D} dE \rho(E) f(E) \approx \rho f(D) \delta D \tag{2.9.110}$$

Also,

$$\begin{aligned} \delta V_k^+ &= \sum_q{}^+ \frac{|V_q|^2}{(\epsilon_q - \epsilon_d)(\epsilon_k - \epsilon_q)} \\ &\approx |V|^2 \rho |\delta D| \frac{1}{(D - \epsilon_d)(\epsilon_k - D)} \\ \delta V_k^- &= 2\sum_q{}^- \frac{|V_q|^2}{(\epsilon_q - \epsilon_d)(\epsilon_k - \epsilon_q)} \\ &\approx -|V|^2 \rho |\delta D| \frac{2}{(D + \epsilon_d)(\epsilon_k + D)} \end{aligned} \tag{2.9.111}$$

We now make the following assumptions:

- k is close to the Fermi level ($\epsilon_k \approx 0$)
- Because k is close to the Fermi surface, we assume the potential is independent of momenta: $V_k^+ \equiv v^+, V_k^- \equiv v^-$
- Since we truncated at third order, we need $D - |\epsilon_d| \gg v^\pm$. This gives us $D \gg |\epsilon_d|$.

With these assumptions, we get the scaling equations similar to the ones obtained previously.

2.10 Numerical Renormalization Group Calculation of the symmetric SIAM

NRG calculations of the symmetric SIAM were carried out by H. R. Krishnamurthy, Wilkins and Wilson in ref. [1]. They identified three fixed points in the phase diagram. Two of them, the free-orbital and the local moment, are unstable while the strong-coupling fixed point is stable. These fixed points along with typical RG flows are marked in fig. 2.5. The

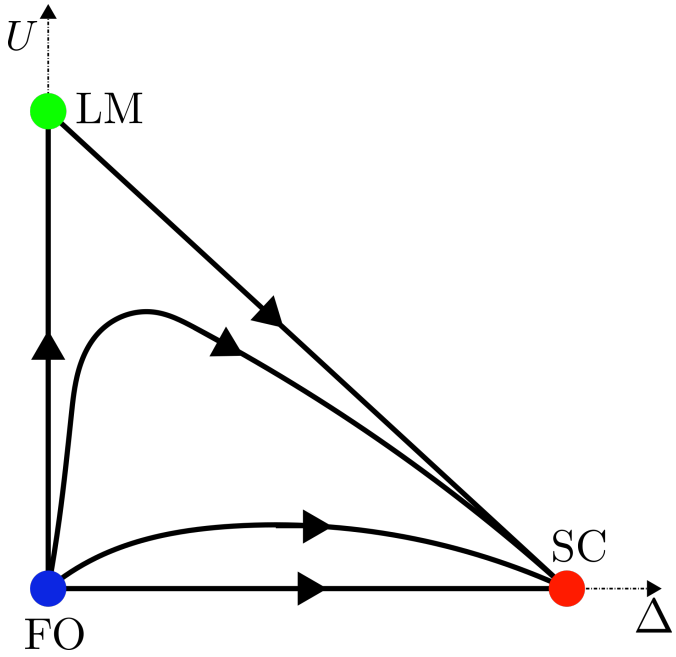

Figure 2.5: Schematic diagram of RG flows and fixed points of the symmetric SIAM, as obtained by ref.[1]. The y-axis is the impurity site repulsion $U = -\frac{1}{2}\epsilon_d$ while the x-axis is the hybridisation parameter $\Delta \sim \rho V^2$. The abbreviations mark the three fixed-points: FO is free-orbital, LM is local moment and SC is strong-coupling. The fixed-points are described in the text.

free-orbital fixed point is described by $U = V = 0$. The local moment fixed point is described by $U \to \infty, V = 0$. The strong-coupling fixed point is described by $U =$ finite, $V \to \infty$. The temperature-dependent susceptibility is found to be very similar to that obtained from the Kondo model, with a suitably-defined T_K. It starts from a constant value at low-temperatures to a Curie-Weiss like form at high temperatures, with the Curie-Weiss constant at very large temperatures being equal to $\frac{1}{8}$.

Chapter 3

Unitary Renormalization Group Method

3.1 Formalism and Results

3.1.1 Description of the problem

We are given a Hamiltonian $\mathcal{H}$ which is not completely diagonal in the occupation number basis of the electrons, $\hat{n}_k$: $\left[\mathcal{H}, n_k\right] \neq 0$. 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,

$$\mathcal{H} = H_e \hat{n}_{q\beta} + H_h \left(1 - \hat{n}_{q\beta}\right) + c^\dagger_{q\beta} T + T^\dagger c_{q\beta} \tag{3.1.1}$$

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

$$\mathcal{H} = \begin{array}{c} \begin{array}{cc} |1\rangle & |0\rangle \end{array} \\ \begin{pmatrix} H_1 & T \\ T^\dagger & H_0 \end{pmatrix} \end{array} \tag{3.1.2}$$

The basis in which this matrix is written is $\left\{|1\rangle, |0\rangle\right\}$ 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.

$$\tilde{\mathcal{H}} \equiv U\mathcal{H}U^\dagger = \begin{array}{c} \begin{array}{cc} |1\rangle & |0\rangle \end{array} \\ \begin{pmatrix} \tilde{H}_1 & 0 \\ 0 & \tilde{H}_0 \end{pmatrix} \end{array} \tag{3.1.3}$$

U_q is defined by

$$\tilde{\mathcal{H}} = U_q \mathcal{H} U_q^\dagger \text{ such that } \left[\tilde{\mathcal{H}}, n_q\right] = 0 \tag{3.1.4}$$

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

$$\mathcal{H}|\psi_i\rangle = \tilde{H}_i|\psi_i\rangle, i \in \{0,1\} \tag{3.1.5}$$

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 $q\beta$:

$$|\psi_i\rangle = \sum_{j=0,1} |j\rangle\langle j||\psi_i\rangle \equiv |1\rangle|\phi_1^i\rangle + |0\rangle|\phi_0^i\rangle \tag{3.1.6}$$

where $|\phi_j^i\rangle = \langle j||\psi_i\rangle$. If we substitute the expansion 3.1.2 into the eigenvalue equation 3.1.5, we get

$$\left[H_e\hat{n}_{q\beta} + H_h\left(1-\hat{n}_{q\beta}\right) + c_{q\beta}^\dagger T + T^\dagger c_{q\beta}\right]|\psi_i\rangle = \tilde{H}_i|\psi_i\rangle \tag{3.1.7}$$

The diagonal parts $H_e = \mathrm{tr}\left[\mathcal{H}\hat{n}_{q\beta}\right]$ and $H_e = \mathrm{tr}\left[\mathcal{H}\left(1-\hat{n}_{q\beta}\right)\right]$ 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

$$\left[c_{q\beta}^\dagger T + T^\dagger c_{q\beta}\right]|\psi_i\rangle = \left(\tilde{H}_i - \mathcal{H}^i - \mathcal{H}^d\right)|\psi_i\rangle \tag{3.1.8}$$

3.1.2 Obtaining the decoupling transformation

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

$$\left[c_{q\beta}^\dagger T + T^\dagger c_{q\beta}\right]|\psi_i\rangle = \left(\hat{\omega}_i - \mathcal{H}^d\right)|\psi_i\rangle \tag{3.1.9}$$

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 $\hat{\omega}_i = \hat{\omega}_i^1\hat{n}_{q\beta} + \hat{\omega}_i^0\left(1-\hat{n}_{q\beta}\right)$. Using the expansion 3.1.6, we can write

$$\hat{\omega}_i|\psi_i\rangle = \hat{\omega}_i^1|1\rangle|\phi_1^i\rangle + \hat{\omega}_i^0|0\rangle|\phi_0^i\rangle \tag{3.1.10}$$

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 $|\phi_{0,}^i\rangle$ to be an eigenstates of $\hat{\omega}_i^{1,0}$ corresponding to real eigenvalues $\omega_i^{1,0}$:

$$\left[\mathcal{H}^d + c_{q\beta}^\dagger T + T^\dagger c_{q\beta}\right]|\psi_i(\omega_i)\rangle = \left(\omega_i^1 - \mathcal{H}^d\right)|1\rangle|\phi_1^i\rangle + \left(\omega_i^0 - \mathcal{H}^d\right)|0\rangle|\phi_0^i\rangle \tag{3.1.11}$$

If we now substitue the expansion 3.1.6 and gather the terms that result in $\hat{n}_{q\beta} = 1$, we get

$$c^\dagger_{q\beta} T \left|0\right\rangle \left|\phi^i_0\right\rangle = \left(\omega^1_i - \mathcal{H}^d\right) \left|1\right\rangle \left|\phi^i_1\right\rangle \tag{3.1.12}$$

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

$$T^\dagger c_{q\beta} \left|1\right\rangle \left|\phi^i_1\right\rangle = \left(\omega^0_i - \mathcal{H}^d\right) \left|0\right\rangle \left|\phi^i_0\right\rangle \tag{3.1.13}$$

We now define two many-particle transition operators:

$$\begin{aligned} \eta^\dagger(\omega^1_i) &= \frac{1}{\omega^1_i - \mathcal{H}^d} c^\dagger_{q\beta} T \equiv G_1 c^\dagger_{q\beta} T \\ \eta(\omega^0_i) &= \frac{1}{\omega^0_i - \mathcal{H}^d} T^\dagger c_{q\beta} \equiv G_0 T^\dagger c_{q\beta} \end{aligned} \tag{3.1.14}$$

wher G_j is the propagator $\frac{1}{\omega^j_i - \mathcal{H}^d}$. We can write this compactly as

$$\eta(\hat{\omega}) = G T^\dagger c_{q\beta} = \frac{1}{\hat{\omega}_i - \mathcal{H}^d} T^\dagger c_{q\beta} \tag{3.1.15}$$

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 $\mathcal{H}^d = \mathcal{H}^d_0 \left(1 - \hat{n}_{q\beta}\right) + \mathcal{H}^d_1 \hat{n}_{q\beta}$ and $G = \left(\hat{\omega} - \mathcal{H}^d\right)^{-1}$. 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:

$$\eta^\dagger(\omega^0_i) = \eta^\dagger(\omega^1_i) \implies \frac{1}{\omega^1_i - \mathcal{H}^d} c^\dagger_{q\beta} T = c^\dagger_{q\beta} T \frac{1}{\omega^0_i - \mathcal{H}^d} \tag{3.1.16}$$

Henceforth we will assume that this constraint has been imposed.

In terms of these operators, eq. 3.1.13 becomes

$$\begin{aligned} \left|1\right\rangle \left|\phi^i_1\right\rangle &= \eta^\dagger \left|0\right\rangle \left|\phi^i_0\right\rangle \\ \left|0\right\rangle \left|\phi^i_0\right\rangle &= \eta \left|1\right\rangle \left|\phi^i_1\right\rangle \end{aligned} \tag{3.1.17}$$

These allow us to write

$$\begin{aligned} \left|\psi_1\right\rangle &= \left|1\right\rangle \left|\phi^i_1\right\rangle + \left|0\right\rangle \left|\phi^i_0\right\rangle = \left(1 + \eta\right) \left|1\right\rangle \left|\phi^i_1\right\rangle \\ \left|\psi_0\right\rangle &= \left(1 + \eta^\dagger\right) \left|0\right\rangle \left|\phi^i_0\right\rangle \end{aligned} \tag{3.1.18}$$

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

$$U_1 = 1 + \eta \tag{3.1.19}$$

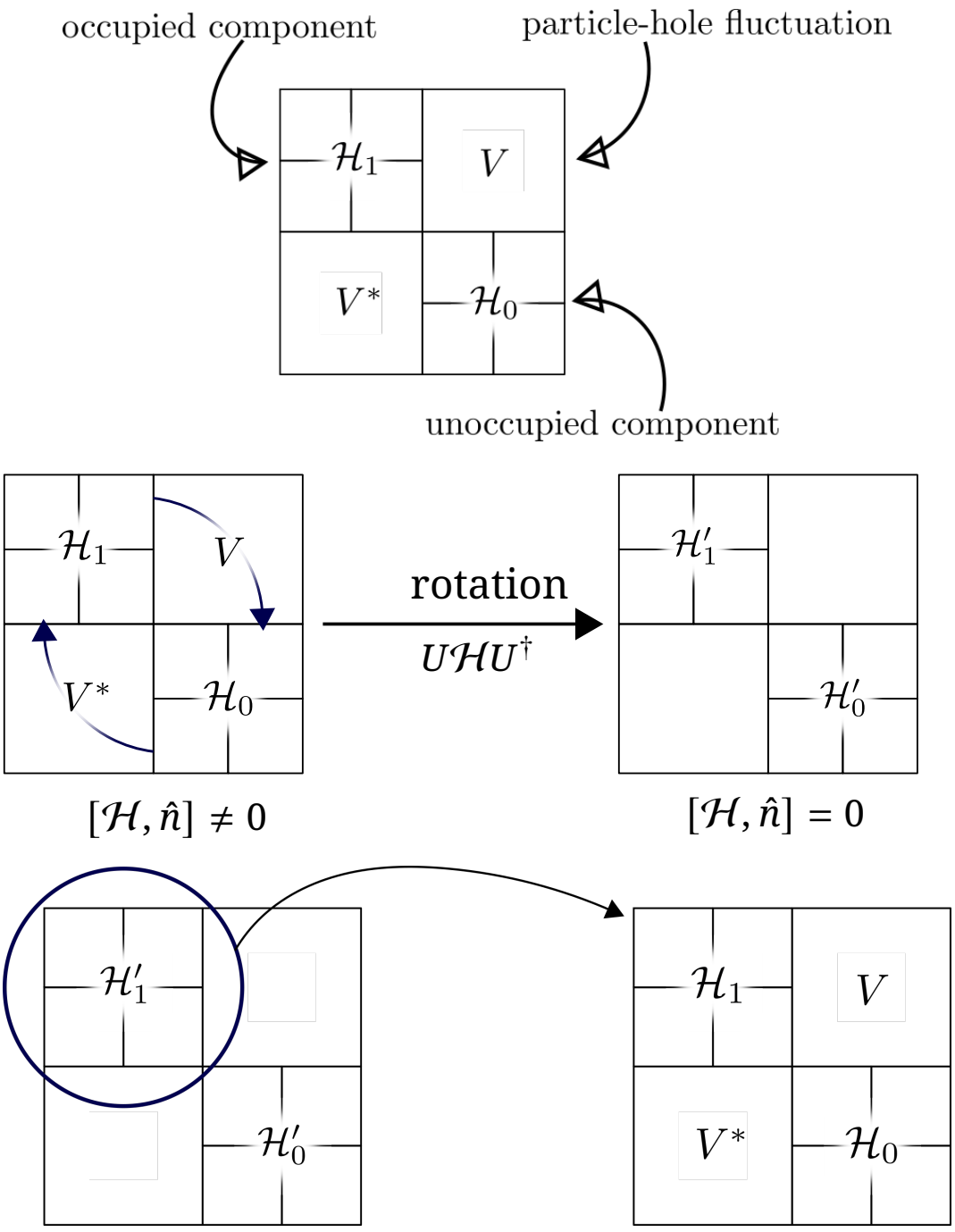

Figure 3.1: Three steps of the URG: Decompose the Hamiltonian in a 2×2 matrix, apply the unitary operator to rotate it, then repeat these steps with one of the rotated blocks.

kinetic energy

3.1.3 Properties of the many-body transition operators

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

$$\eta^2 = {\eta^\dagger}^2 = 0 \quad \left[{c^\dagger}^2 = c^2 = 0 \right] \tag{3.1.20}$$

Second is:

$$\begin{aligned} |1\rangle |\phi_1^i\rangle = \eta^\dagger |0\rangle |\phi_0^i\rangle = \eta^\dagger \eta |1\rangle |\phi_1^i\rangle \implies \eta^\dagger \eta = \hat{n}_{q\beta} \\ |0\rangle |\phi_0^i\rangle = \eta |1\rangle |\phi_1^i\rangle = \eta\eta^\dagger |\phi_0^i\rangle \implies \eta\eta^\dagger = 1 - \hat{n}_{q\beta} \end{aligned} \tag{3.1.21}$$

and hence the anticommutator

$$\implies \left\{ \eta, \eta^\dagger \right\} = 1 \tag{3.1.22}$$

Note that the three equations in 3.1.21 work only when applied on the eigenstate $|\psi_i\rangle$ and not any arbitrary state.

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

3.1.4 Form of the unitary operators

Although we have found the correct similarity transformations U_i (eqs. 3.1.19), 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

$$U_1 = 1 + \eta \tag{3.1.23}$$

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

$$U_1 = e^\eta \tag{3.1.24}$$

using the fact that $\eta^2 = 0$. It is shown in ref. [25] that corresponding to a similarity transformation e^ω,there exists a unitary transformation e^G where

$$G = \tanh^{-1}\left(\omega - \omega^\dagger\right) \tag{3.1.25}$$

Applying that to the problem at hand gives

$$U_1^\dagger = \exp\left(\tanh^{-1}\left(\eta - \eta^\dagger\right)\right) \tag{3.1.26}$$

Let $x = \tanh y$. Then,

$$x = \frac{e^{2y}+1}{e^{2y}-1} \implies y = \frac{1}{2}\log\frac{1+x}{1-x} \implies e^y = e^{\tanh^{-1} x} = \sqrt{\frac{1+x}{1-x}} \tag{3.1.27}$$

Therefore,

$$\begin{aligned}\exp\left(\tanh^{-1}\left(\eta-\eta^\dagger\right)\right) &= \frac{1+\eta-\eta^\dagger}{\sqrt{\left(1+\eta^\dagger-\eta\right)\left(1-\eta^\dagger+\eta\right)}} \\ &= \frac{1+\eta-\eta^\dagger}{\sqrt{1+\left\{\eta,\eta^\dagger\right\}}} \\ &= \frac{1}{\sqrt{2}}\left(1+\eta-\eta^\dagger\right)\end{aligned} \tag{3.1.28}$$

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

$$U_1 = \frac{1}{\sqrt{2}}\left(1+\eta^\dagger-\eta\right) \tag{3.1.29}$$

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

$$\begin{aligned}\exp\left(\frac{\pi}{4}\left(\eta^\dagger-\eta\right)\right) &= 1+\left(\eta^\dagger-\eta\right)\frac{\pi}{4}+\frac{1}{2!}\left(\eta^\dagger-\eta\right)^2\left(\frac{\pi}{4}\right)^2+\frac{1}{3!}\left(\eta^\dagger-\eta\right)^3\left(\frac{\pi}{4}\right)^3+\ldots \\ &= 1+\left(\eta^\dagger-\eta\right)\frac{\pi}{4}-\frac{1}{2!}\left(\frac{\pi}{4}\right)^2-\frac{1}{3!}\left(\eta^\dagger-\eta\right)\left(\frac{\pi}{4}\right)^3+\frac{1}{4!}\left(\frac{\pi}{4}\right)^4+\ldots \\ &= \cos\frac{\pi}{4}+\left(\eta^\dagger-\eta\right)\sin\frac{\pi}{4} \\ &= \frac{1}{\sqrt{2}}\left(1+\eta^\dagger-\eta\right)\end{aligned} \tag{3.1.30}$$

There we used

$$\left(\eta^\dagger-\eta\right)^2 = \eta^{\dagger 2}+\eta^2-\left\{\eta^\dagger,\eta\right\} = -1 \quad \left[\because \eta^2=\eta^{\dagger 2}=0\right] \tag{3.1.31}$$

and hence

$$\left(\eta^\dagger-\eta\right)^3 = -1\left(\eta^\dagger-\eta\right) \tag{3.1.32}$$

and so on.

3.1.5 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. 3.1.29,

$$\begin{aligned} U_1 \mathcal{H} U_1^\dagger &= \frac{1}{2}\left(1+\eta^\dagger-\eta\right)\mathcal{H}\left(1+\eta-\eta^\dagger\right) \\ &= \frac{1}{2}\left(1+\eta^\dagger-\eta\right)\left(\mathcal{H}+\mathcal{H}\eta-\mathcal{H}\eta^\dagger\right) \\ &= \frac{1}{2}\left(\mathcal{H}+\mathcal{H}\eta-\mathcal{H}\eta^\dagger+\eta^\dagger\mathcal{H}+\eta^\dagger\mathcal{H}\eta-\eta^\dagger\mathcal{H}\eta^\dagger-\eta\mathcal{H}-\eta\mathcal{H}\eta+\eta\mathcal{H}\eta^\dagger\right) \\ &= \frac{1}{2}\left(\mathcal{H}^d+\mathcal{H}^i+\mathcal{H}^I+\mathcal{H}\eta-\mathcal{H}\eta^\dagger+\eta^\dagger\mathcal{H}+\eta^\dagger\mathcal{H}\eta-\eta^\dagger\mathcal{H}\eta^\dagger-\eta\mathcal{H}-\eta\mathcal{H}\eta+\eta\mathcal{H}\eta^\dagger\right) \\ &= \frac{1}{2}\left(\mathcal{H}^d+\mathcal{H}^i+\mathcal{H}^I+\left[\eta^\dagger-\eta,\mathcal{H}\right]+\eta^\dagger\mathcal{H}\eta-\eta^\dagger\mathcal{H}\eta^\dagger-\eta\mathcal{H}\eta+\eta\mathcal{H}\eta^\dagger\right) \end{aligned} \tag{3.1.33}$$

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

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

$$\tilde{\mathcal{H}} = \frac{1}{2}\left(\underbrace{\mathcal{H}^d+\mathcal{H}^i+\left[\eta^\dagger-\eta,\mathcal{H}\right]+\eta^\dagger\mathcal{H}\eta+\eta\mathcal{H}\eta^\dagger}_{\text{group 1}}+\overbrace{\mathcal{H}^I-\eta^\dagger\mathcal{H}\eta^\dagger-\eta\mathcal{H}\eta}^{\text{group 2}}\right) \tag{3.1.34}$$

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.

$$\eta\mathcal{H}\eta = \eta c_q^\dagger T\eta \tag{3.1.35}$$

and

$$\eta^\dagger\mathcal{H}\eta^\dagger = \eta^\dagger T^\dagger c_q\eta^\dagger \tag{3.1.36}$$

Group 2 becomes

$$\text{group 2} = \mathcal{H}^I-\eta^\dagger T^\dagger c_q\eta^\dagger-\eta c_q^\dagger T\eta = c_q^\dagger T+T^\dagger c_q-\eta^\dagger T^\dagger c_q\eta^\dagger-\eta c_q^\dagger T\eta \tag{3.1.37}$$

To simplify this, we use the relation

$$\begin{aligned} \eta c_q^\dagger T\eta &= \frac{1}{\omega_i^0-\mathcal{H}^d}T^\dagger c_q c_q^\dagger T\eta \\ &= T^\dagger c_q\frac{1}{\omega_i^1-\mathcal{H}^d}c_q^\dagger T\eta \quad &\left[\text{eq. 3.1.16}\right] \\ &= T^\dagger c_q\eta^\dagger\eta \quad &\left[\text{eq. 3.1.15}\right] \\ &= T^\dagger c_q\hat{n}_q \quad &\left[\text{eq. 3.1.21}\right] \end{aligned} \tag{3.1.38}$$

which gives

$$\eta c_q^\dagger T\eta = T^\dagger c_q \tag{3.1.39}$$

Taking the Hermitian conjugate of eq. 3.1.39 gives

$$\eta^\dagger T^\dagger c_q \eta^\dagger = c_q^\dagger T \tag{3.1.40}$$

Substituting the expressions 3.1.39 and 3.1.40 into the expression for group 2, 3.1.37, shows that is vanishes. This leaves us only with group 1:

$$\widetilde{\mathcal{H}} = \frac{1}{2}\left(\mathcal{H}^d + \mathcal{H}^i + \overbrace{\eta^\dagger \mathcal{H}\eta + \eta\mathcal{H}\eta^\dagger}^{\text{group A}} + \underbrace{\left[\eta^\dagger - \eta, \mathcal{H}\right]}_{groupB}\right) \tag{3.1.41}$$

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 $c_{q\beta}^\dagger$. We are therefore left with the diagonal part of $\mathcal{H}$, which is $H_e \hat{n}_{q\beta} + H_h\left(1 - \hat{n}_{q\beta}\right)$.

$$\eta^\dagger\left[H_e\hat{n}_{q\beta} + H_h\left(1-\hat{n}_{q\beta}\right)\right]\eta + \eta\left[H_e\hat{n}_{q\beta} + H_h\left(1-\hat{n}_{q\beta}\right)\right]\eta^\dagger = \eta^\dagger H_h\eta + \eta H_e\eta^\dagger \tag{3.1.42}$$

This can be shown to be equal to the diagonal part:

$$\text{group A} = \eta^\dagger H_h\eta + \eta H_e\eta^\dagger = H_e\hat{n}_{q\beta} + H_h\left(1-\hat{n}_{q\beta}\right) = \mathcal{H}^d + \mathcal{H}^i \tag{3.1.43}$$

It can also be shown that

$$\text{group B} = \left[\eta^\dagger - \eta, \mathcal{H}\right] = 2\left[c_{q\beta}^\dagger T, \eta\right] \tag{3.1.44}$$

Putting it all together,

$$\tilde{\mathcal{H}} = \mathcal{H}^d + \mathcal{H}^i + \left[c_{q\beta}^\dagger T, \eta\right] \tag{3.1.45}$$

The renormalizing in the Hamiltonian is

$$\Delta\mathcal{H} = \tilde{\mathcal{H}} - \mathcal{H}^d - \mathcal{H}^i = \left[c_{q\beta}^\dagger T, \eta\right] \tag{3.1.46}$$

Because of eq. 3.1.44, it can also be written as

$$\Delta\mathcal{H} = \frac{1}{2}\left[\eta^\dagger - \eta, \mathcal{H}_X\right] = \frac{1}{2}\left[\eta^\dagger - \eta, \mathcal{H}\right] \tag{3.1.47}$$

This form will be useful later when we make the connection with one-shot Schrieffer-Wolff transformation and CUT RG.

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

$$\begin{aligned}
\left[\widetilde{\mathcal{H}}, \hat{n}_{q\beta}\right] &= \left[\left[c_{q\beta}^\dagger T, \eta\right], \hat{n}_{q\beta}\right] \\
&= \left[c_{q\beta}^\dagger T\eta, \hat{n}_{q\beta}\right] - \left[\eta c_{q\beta}^\dagger T, \hat{n}_{q\beta}\right] \\
&= c_{q\beta}^\dagger T\eta\hat{n}_{q\beta} - \hat{n}_{q\beta}c_{q\beta}^\dagger T\eta \qquad \left[2^{\text{nd}}\ [\ .\ ] \text{ is 0},\ \because c_{q\beta}^\dagger\hat{n}_{q\beta} = \hat{n}_{q\beta}\eta = 0\right] \\
&= c_{q\beta}^\dagger T\eta - c_{q\beta}^\dagger T\eta \\
&= 0
\end{aligned} \tag{3.1.48}$$

3.1.6 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 $\omega_i^1 = \mathcal{H}_1^d$ or $\omega_i^0 = \mathcal{H}_0^d$. 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. 3.1.12 and 3.1.13 gives

$$c_{q\beta}^\dagger T \left|0\right\rangle \left|\phi_0^i\right\rangle = \left(\omega_i^1 - \mathcal{H}_1^d\right) \left|1\right\rangle \left|\phi_1^i\right\rangle = 0 \implies c_{q\beta}^\dagger T = 0 \tag{3.1.49}$$

3.1.7 Multiple off-diagonal terms

There is a subtle assumption in the definitions eq. 3.1.14. In order for η to be the Hermitian conjugate of $\eta^\dagger$, $\mathcal{H}_d$ cannot have any information that relates to the structure of T. To see why, say the total off-diagonal term is composed of two parts: $T = T_1 + T_2$.

$$\begin{aligned} \eta &= \frac{1}{\omega_0 - \mathcal{H}_d}\left(T_1^\dagger + T_2^\dagger\right) c = \left[\frac{1}{\omega^0 - E_1^0} T_1^\dagger c + \frac{1}{\omega^0 - E_2^0} T_2^\dagger c\right] \\ \eta^\dagger &= \frac{1}{\omega^1 - \mathcal{H}_d} c^\dagger \left(T_1 + T_2\right) = \left[\frac{1}{\omega^1 - E_1^1} c^\dagger T_1 + \frac{1}{\omega^1 - E_2^1} c^\dagger T_2\right] \end{aligned} \tag{3.1.50}$$

where $\mathcal{H}_d T_i^\dagger c = E_i^0 T_i^\dagger c$ and $\mathcal{H}_d c^\dagger T_i = E_i^1 c^\dagger T_i$. We can now see that in order for $\eta = \left(\eta^\dagger\right)^\dagger$ to hold, two conditions must be met:

$$\omega^0 - E_1^0 = \omega^1 - E_1^1, \quad \omega^0 - E_2^0 = \omega^1 - E_2^1 \tag{3.1.51}$$

This will not hold generally. The correct solution is to realize that each such off-diagonal term T_i will come with its own quantum fluctuation scale ω_i.

$$\begin{aligned} \eta &= \sum_i \frac{1}{\omega_i^0 - E_i^0} T_i^\dagger c \\ \eta^\dagger &= \sum_i \frac{1}{\omega_i^1 - E_1^1} c^\dagger T_i \end{aligned} \tag{3.1.52}$$

If we now impose the condition that $\eta = \left(\eta^\dagger\right)^\dagger$, we get the relations

$$\omega_i^0 - \omega_i^1 = E_i^0 - E_1^1 \tag{3.1.53}$$

and so

$$\eta^\dagger - \eta = \sum_i \frac{1}{\omega_i^0 - E_i^0}\left(c^\dagger T_i - T_i^\dagger c\right) \tag{3.1.54}$$

The expression for the renormalization will not be just $\left[c^\dagger T, \eta\right]$ in this case. That form will be non-Hermitian. The correct form is obtained from the more general form $\left[\eta^\dagger - \eta, \mathcal{H}_X\right]$:

$$\begin{aligned}
\Delta\mathcal{H} &= \frac{1}{2}\left[\eta^\dagger - \eta, c^\dagger T + T^\dagger c\right] \\
&= \frac{1}{2}\sum_{ij}\frac{1}{\omega_i^0 - E_i^0}\left[c^\dagger T_i - T_i^\dagger c, c^\dagger T_j + T_j^\dagger c\right] \\
&= \frac{1}{2}\sum_{ij}\frac{1}{\omega_i^0 - E_i^0}\left[\hat{n}\left(T_i T_j^\dagger + T_j T_i^\dagger\right) - \left(1-\hat{n}\right)\left(T_i^\dagger T_j + T_j^\dagger T_i\right)\right] \\
&= \frac{1}{2}\sum_{ij}\left(\frac{1}{\omega_i^0 - E_i^0} + \frac{1}{\omega_j^0 - E_j^0}\right)\left[\hat{n}T_i T_j^\dagger - \left(1-\hat{n}\right)T_i^\dagger T_j\right]
\end{aligned} \tag{3.1.55}$$

3.1.8 Equivalence of the two unitaries and preservation of partial trace

In the subsection 3.1.4, we determined the form of the operator U_1 that unitarily decouples the node $q\beta$ from the other degrees of freedom. Eq. 3.1.29 was derived by reading off the transformation of $|1\rangle$ to $|\psi_1\rangle$, the first equation in 3.1.18. 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

$$U_0 = \frac{1}{\sqrt{2}}\left(1 + \eta - \eta^\dagger\right) \tag{3.1.56}$$

This η will however be different from the η in eq. 3.1.29. 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:

$$\begin{aligned}
&\text{Starting from } |\psi_1\rangle\text{: } \eta_1 = \frac{1}{\omega_1^0 - \mathcal{H}^d}T^\dagger c_{q\beta} \quad \text{and } \eta_1^\dagger = \frac{1}{\omega_1^1 - \mathcal{H}^d}T^\dagger c_{q\beta} \\
&\text{Starting from } |\psi_0\rangle\text{: } \eta_0 = \frac{1}{\omega_0^0 - \mathcal{H}^d}T^\dagger c_{q\beta} \quad \text{and } \eta_0^\dagger = \frac{1}{\omega_0^1 - \mathcal{H}^d}T^\dagger c_{q\beta}
\end{aligned} \tag{3.1.57}$$

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

$$\begin{aligned} U_1 &= \frac{1}{\sqrt{2}}\left(1 + \eta_1^\dagger - \eta_1\right) \\ U_0 &= \frac{1}{\sqrt{2}}\left(1 + \eta_0 - \eta_0^\dagger\right) \end{aligned} \tag{3.1.58}$$

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

$$\omega_1^0 - \mathcal{H}_0^d = -\left(\omega_0^0 - \mathcal{H}_0^d\right) \tag{3.1.59}$$

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.

$$\begin{aligned} \eta_1 &= \frac{1}{\tilde{H}_1 - \mathcal{H}^i - \mathcal{H}^d} T^\dagger c_{q\beta} \\ \eta_0 &= \frac{1}{\tilde{H}_0 - \mathcal{H}^i - \mathcal{H}^d} T^\dagger c_{q\beta} \\ \implies \eta_1 + \eta_0 &= \left[\frac{1}{\tilde{H}_1 - \mathcal{H}^i - \mathcal{H}^d} + \frac{1}{\tilde{H}_0 - \mathcal{H}^i - \mathcal{H}^d}\right] T^\dagger c_{q\beta} = 0 \\ \implies \tilde{H}_1 - \mathcal{H}^i - \mathcal{H}^d &= -\left[\tilde{H}_0 - \mathcal{H}^i - \mathcal{H}^d\right] \\ \implies \tilde{H}_1 + \tilde{H}_0 &= 2\mathcal{H}_0 \end{aligned} \tag{3.1.60}$$

$\mathcal{H}_0 = \mathcal{H}^i + \mathcal{H}^d$ 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

$$\tilde{H} = \begin{pmatrix} E_1 & 0 \\ 0 & E_0 \end{pmatrix} \tag{3.1.61}$$

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 3.1.60 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 3.1.60 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 $t_{\text{new}} = t_{\text{old}}$.

3.1.9 A note on the various quantum fluctuation scales ω_i^j

At a particular step of the URG, there are two quantum fluctuation energy scales associated with each sector. If we rotate $|\psi_1\rangle$ to $|1\rangle$ (particle/occupied sector), the corresponding unitary will be a function of $\omega_1^{0,1}$. If we, on the other hand, rotate $|\psi_0\rangle$ to $|0\rangle$

(hole/unoccupied sector), the unitary will be a function of $\omega_0^{0,1}$. The superscript j signifies whether this particular ω_i^j is an eigenvalue corresponding to $|1,\phi_i\rangle$ or $|0,\phi_i\rangle$. ω_i^0 occurs in the many-body transition operator η, because η is preceded by c and hence it picks out the eigenstate $|0,\phi_i\rangle$. On the other hand, ω_i^1 occurs in the many-body transition operator $\eta^\dagger$, because that is preceded by $c^\dagger$. This constrains these two values, because we must have $\eta(\omega_i^0) = \left(\eta^\dagger(\omega_i^1)\right)^\dagger$ (eq. 3.1.16), for each value of i, giving us two constraints in total. The subscript i signifies whether ω_i^j is a part of the particle sector unitary $U_1(\omega_1^j)$ or the hole sector unitary $U_0(\omega_0^j)$. As mentioned in the previous section, since both ways are equivalent, we must have $U_1 = U_0$ which leads to the constraints $\eta(\omega_0^j) = -\eta(\omega_1^j)$. All the independent constraints are listed below.

$$\begin{aligned}\omega_1^0 - \omega_1^1 &= \mathcal{H}_d^0 - \mathcal{H}_d^1 \\ \omega_0^0 - \omega_0^1 &= \mathcal{H}_d^0 - \mathcal{H}_d^1 \\ \omega_1^0 + \omega_0^0 &= 2\mathcal{H}_d^0\end{aligned} \tag{3.1.62}$$

The first two come from $\eta(\omega_i^0) = \left(\eta^\dagger(\omega_i^1)\right)^\dagger$ while the last comes from $\eta(\omega_0^j) = -\eta(\omega_1^j)$. These are the only independent relations. Other relations like the one between ω_1^0 and ω_0^1 can be derived from these. This means that we have four ω and three constraints, such that each step of the URG is characterized by just a single independent quantum fluctuation scale.

3.2 Prescription

Given a Hamiltonian

$$\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_0 + c^\dagger T + T^\dagger c \tag{3.2.1}$$

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. 3.1.45, 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

$$\Delta\mathcal{H} = \left[c_{q\beta}^\dagger \mathrm{Tr}\left(\mathcal{H}c_{q\beta}\right), \eta\right] = c_{q\beta}^\dagger \mathrm{Tr}\left(\mathcal{H}c_{q\beta}\right)\eta - \eta c_{q\beta}^\dagger \mathrm{Tr}\left(\mathcal{H}c_{q\beta}\right) \tag{3.2.2}$$

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

$$\Delta\mathcal{H} = c_{q\beta}^\dagger \mathrm{Tr}\left(\mathcal{H}c_{q\beta}\right)\eta_1 - \eta_1 c_{q\beta}^\dagger \mathrm{Tr}\left(\mathcal{H}c_{q\beta}\right) \tag{3.2.3}$$

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*.

$$\Delta_1 \mathcal{H} = c^\dagger_{q\beta} \mathrm{Tr}\left(\mathcal{H} c_{q\beta}\right) \eta_1 \tag{3.2.4}$$

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

$$\Delta_0 \mathcal{H} = -\eta_1 c^\dagger_{q\beta} \mathrm{Tr}\left(\mathcal{H} c_{q\beta}\right) \tag{3.2.5}$$

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:

$$\Delta \mathcal{H} = c^\dagger_{q\beta} \mathrm{Tr}\left(\mathcal{H} c_{q\beta}\right) \eta_1 + \eta_0 c^\dagger_{q\beta} \mathrm{Tr}\left(\mathcal{H} c_{q\beta}\right) \tag{3.2.6}$$

We can make one more manipulation: using eq. 3.1.16, we get

$$\Delta \mathcal{H} = c^\dagger_{q\beta} \mathrm{Tr}\left(\mathcal{H} c_{q\beta}\right) \eta_1 + \mathrm{Tr}\left(c^\dagger_{q\beta} \mathcal{H}\right) c_{q\beta} \eta^\dagger_0 \tag{3.2.7}$$

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, 26]. Writing down the forms of η and $\eta^\dagger$ explicitly, we get

$$\Delta \mathcal{H} = c^\dagger_{q\beta} \mathrm{Tr}\left(\mathcal{H} c_{q\beta}\right) \frac{1}{\omega^0_1 - \mathcal{H}^d_0} \mathrm{Tr}\left(c^\dagger_{q\beta} \mathcal{H}\right) c_{q\beta} + \mathrm{Tr}\left(c^\dagger_{q\beta} \mathcal{H}\right) c_{q\beta} \frac{1}{\omega^1_0 - \mathcal{H}^d_1} c^\dagger_{q\beta} \mathrm{Tr}\left(\mathcal{H} c_{q\beta}\right) \tag{3.2.8}$$

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

$$\Delta \mathcal{H} = \sum_{q\beta} \left[c^\dagger_{q\beta} \mathrm{Tr}\left(\mathcal{H} c_{q\beta}\right) \frac{1}{\omega^0_1 - \mathcal{H}^d_0} \mathrm{Tr}\left(c^\dagger_{q\beta} \mathcal{H}\right) c_{q\beta} + \mathrm{Tr}\left(c^\dagger_{q\beta} \mathcal{H}\right) c_{q\beta} \frac{1}{\omega^1_0 - \mathcal{H}^d_1} c^\dagger_{q\beta} \mathrm{Tr}\left(\mathcal{H} c_{q\beta}\right) \right] \tag{3.2.9}$$

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; $\mathrm{Tr}\left(c^\dagger_{q\beta} \mathcal{H}\right) c_{q\beta}$ is the off-diagonal term that has $c_{q\beta}$ in it, and $c^\dagger_{q\beta} \mathrm{Tr}\left(\mathcal{H} c_{q\beta}\right)$ is the off-diagonal term that has $c^\dagger_{q\beta}$ in it. $\mathcal{H}^D$ is just the diagonal part of the Hamiltonian.

3.3 Star Graph URG

The first URG solution of the star graph problem is in ref. [27]. The system consists of N spin-like degrees of freedom (labeled 1 through N) individually talking to a spin at the center (labeled 0). Each spin i ($\in [0, N]$) has an on-site energy ϵ_i. The coupling strength between 0 and i ($\in [1, N]$) is J_i. We choose the on-site energies such that $\epsilon_{i+1} > \epsilon_i, i \in [N-1, 1]$. In this way, ϵ_1 is the infrared limit and ϵ_N is the ultraviolet limit.

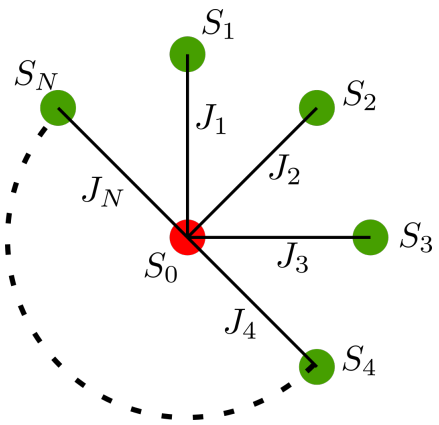

Figure 3.2: Star Graph model

$$\mathcal{H} = \epsilon_0 S_0^z + \sum_{i=1}^{N} \left[\epsilon_i S_i^z + J_i \vec{S}_0 \cdot \vec{S}_i \right] \tag{3.3.1}$$

By converting the last term into S^z and $S^{\pm}$, we can write the Hamiltonian as

$$\mathcal{H} = \epsilon_0 S_0^z + \sum_{i=1}^{N} \left[\epsilon_i S_i^z + J_i \left(S_0^z S_i^z + \frac{1}{2} \left(S_0^+ S_i^- + S_0^- S_i^+ \right) \right) \right] \tag{3.3.2}$$

The diagonal terms are the ones that preserve the number or (in this case) spin.

$$\mathcal{H}^d = \sum_{i=0}^{N} \epsilon_i S_i^z + \sum_{i=1}^{N} J_i S_0^z S_i^z \tag{3.3.3}$$

This is the piece that comes in the denominator. The off-diagonal terms are the ones that change the number or spin. For this problem, they are the last two terms, $S_0^+ S_i^-$ and $S_0^- S_i^+$.

The RG involves decoupling the nodes N through 1, and looking at the resultant renormalization in ϵ_i and J_i. As a simplification, we will ignore the lower nodes in the denominator and keep only the node currently being decoupled, ie node N. Since node 0 is connected to node N, we will keep node 0 in the denominator as well. Making this simplification gives

$$\mathcal{H}^D = \epsilon_0 S_0^z + \epsilon_N S_N^z + J_N S_0^z S_N^z \tag{3.3.4}$$

The off-diagonal part in the subspace of the node N is

$$\mathcal{H}_X = \frac{1}{2} J_N \left(S_N^+ S_0^- + S_N^- S_0^+ \right) \tag{3.3.5}$$

3.3.1 Calculation of Renormalization

The renormalization on doing one step of the URG is given by

$$\Delta\mathcal{H} = c_{q\beta}^\dagger T \eta + T^\dagger c_{q\beta} \eta_0^\dagger \tag{3.3.6}$$

There, $q\beta$ refers to the electron being decoupled. Here, since we are decoupling the spin N, the formula becomes

$$\Delta\mathcal{H} = \left[S_N^+ T, \eta\right] \tag{3.3.7}$$

where $S_N^+ T$ is the off-diagonal term in the Hamiltonian and hence T is S_0^-. η is of course given by

$$\eta = \frac{1}{\omega - \mathcal{H}^d} T^\dagger c_{q\beta} \to \frac{1}{\omega - \mathcal{H}^d} \frac{1}{2} J_N S_0^+ S_N^- \tag{3.3.8}$$

and

$$\eta_0^\dagger = \frac{1}{\omega' - \mathcal{H}^d} \frac{1}{2} J_N S_N^+ S_0^- \tag{3.3.9}$$

Substituting the expression for the diagonal part $\mathcal{H}_d$, we get

$$\eta = \frac{1}{\omega - \epsilon_0 S_0^z - \epsilon_N S_N^z - J_N S_0^z S_N^z} \frac{1}{2} J_N S_0^+ S_N^- = \frac{1}{\omega - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \frac{1}{2} J_N S_0^+ S_N^- \tag{3.3.10}$$

and

$$\eta_0^\dagger = \frac{1}{\omega' - \epsilon_0 S_0^z - \epsilon_N S_N^z - J_N S_0^z S_N^z} \frac{1}{2} J_N S_N^+ S_0^- = \frac{1}{\omega + \frac{1}{2}\epsilon_0 - \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \frac{1}{2} J_N S_N^+ S_0^- \tag{3.3.11}$$

In the final steps, I substituted $S_N^z = -\frac{1}{2}$ and $S_0^z = \frac{1}{2}$ in the denominator of η, and the opposite values in the denominator of $\eta_0^\dagger$, because there is $S_0^+ S_N^- (S_N^+ S_0^-)$ in front of the Greens function of η ($\eta_0^\dagger$). The renormalization thus becomes

$$\Delta\mathcal{H} = \frac{1}{4} J_N^2 S_N^+ S_0^- \frac{1}{\omega - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} S_0^+ S_N^- + \frac{1}{4} J_N^2 S_0^+ S_N^- \frac{1}{\omega' + \frac{1}{2}\epsilon_0 - \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} S_N^+ S_0^- \tag{3.3.12}$$

To compare ω and ω', we will write down their Poor Man' Scaling counterparts.

$$\begin{aligned} \omega &= \frac{1}{2}\epsilon_N - \frac{1}{2}\epsilon_0 - \frac{1}{4}J_N \\ \omega' &= \frac{1}{2}\epsilon_0 - \frac{1}{2}\epsilon_N - \frac{1}{4}J_N = -\omega - \frac{1}{2}J_N \end{aligned} \tag{3.3.13}$$

So, the renormalization becomes

$$\Delta\mathcal{H} = \frac{1}{4} J_N^2 \frac{1}{\omega - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \left[S_N^+ S_0^- S_0^+ S_N^- + S_0^+ S_N^- S_N^+ S_0^-\right] \tag{3.3.14}$$

Using the relations $S^+ S^- = \frac{1}{2} + S^z$ and $S^- S^+ = \frac{1}{2} - S^z$, we can write this as

$$\begin{aligned} \Delta\mathcal{H} &= \frac{1}{4} J_N^2 \frac{1}{\omega - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \left[\left(\frac{1}{2} + S_N^z\right)\left(\frac{1}{2} - S_0^z\right) - \left(\frac{1}{2} - S_N^z\right)\left(\frac{1}{2} + S_0^z\right)\right] \\ &= \frac{1}{4} J_N^2 \frac{1}{\omega - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \left[S_N^z - S_0^z\right] \end{aligned} \tag{3.3.15}$$

We can now read off the renormalizations in ϵ_N and ϵ_0.

$$\begin{aligned} \Delta\epsilon_N &= \frac{1}{4} J_N^2 \frac{1}{\omega - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \\ \Delta\epsilon_0 &= -\frac{1}{4} J_N^2 \frac{1}{\omega - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \end{aligned} \tag{3.3.16}$$

3.3.2 Nature of flows

We are interested in looking at the renormalization of the central node energy ϵ_0, upon removing the nodes N through 1. We will hence concentrate on the second RG equation. We first make some simplifying assumptions: $J_i = J, \epsilon_i = \epsilon$ for all $i \in \{1, N\}$.

$$\Delta\epsilon_0 = -\frac{1}{4}J^2 \frac{1}{\omega - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon + \frac{1}{4}J} \tag{3.3.17}$$

Define $\tilde{\omega} = \omega + \frac{1}{2}\epsilon + \frac{1}{4}J$.

$$\Delta\epsilon_0 = -\frac{1}{4}J^2 \frac{1}{\tilde{\omega} - \frac{1}{2}\epsilon_0} \tag{3.3.18}$$

Our goal here is to look for a fixed-point condition such that the denominator vanishes at some point of the RG. If we start with a bare of ϵ_0 such that $\tilde{\omega} - \frac{1}{2}\epsilon_0 > 0$, the denominator will be positive and the RG equation will be irrelevant. This means that ϵ_0 will keep on decreasing, and the denominator will keep on becoming more and more positive, meaning there cannot be a fixed point in this situation.

If, on other hand, we start with a bare of ϵ_0 such that $\tilde{\omega} - \frac{1}{2}\epsilon_0 < 0$, the denominator will be negative and the RG equation will be relevant. This means that ϵ_0 will keep on increasing, and the denominator will keep on becoming more and more negative, meaning there cannot be a fixed point in this situation either. These situations are depicted in figure 3.3.

Since we cannot find a fixed point, we will use the other ω in the URG formalism. Recall that η and $\eta^\dagger$ will, in general, have different ω, eq. 3.1.14.

$$\eta^\dagger = \frac{1}{\omega' - \mathcal{H}_d} S_N^+ S_0^- = \frac{1}{\omega' - \frac{1}{2}\epsilon + \frac{1}{2}\epsilon_0 + \frac{1}{4}J} S_N^+ S_0^- \tag{3.3.19}$$

Comparing with eq. 3.3.10, and requiring $(\eta)^\dagger = \eta^\dagger$, we get the following equation relating ω and ω':

$$\omega' - \frac{1}{2}\epsilon + \frac{1}{2}\epsilon_0 + \frac{1}{4}J = \omega + \frac{1}{2}\epsilon - \frac{1}{2}\epsilon_0 + \frac{1}{4}J \implies \omega = \omega' - \epsilon + \epsilon_0 \tag{3.3.20}$$

Substituting this in eq. 3.3.17 gives

$$\Delta\epsilon_0 = -\frac{1}{4}J^2 \frac{1}{\omega' - \frac{1}{2}\epsilon + \frac{1}{2}\epsilon_0 + \frac{1}{4}J} \tag{3.3.21}$$

We again define $-\tilde{\omega} = \omega' - \frac{1}{2}\epsilon + \frac{1}{4}J$.

$$\Delta\epsilon_0 = \frac{1}{4}J^2 \frac{1}{\tilde{\omega} - \frac{1}{2}\epsilon_0} \tag{3.3.22}$$

We now repeat the exercise of determining the relevance of the flows under various regime. If we start with a bare ϵ_0 such that $\tilde{\omega} + \frac{1}{2}\epsilon_0 > 0$, then the denominator is positive

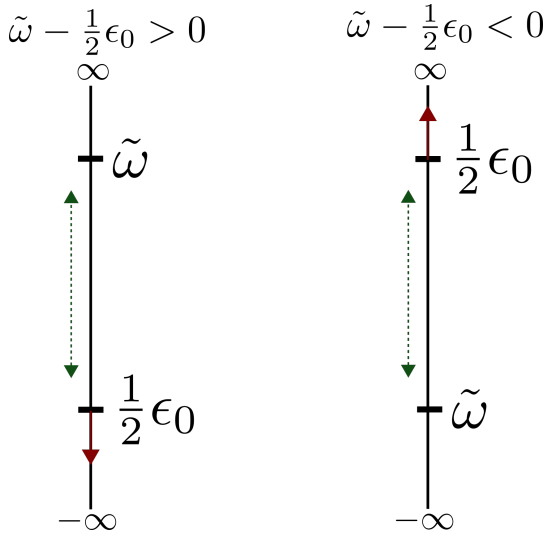

Figure 3.3: RG flow for the two cases. The green line is the distance between the bare values of the two couplings, and hence also the magnitude of the denominator. The red arrow denotes the direction in which ϵ_0 will flow. Upward flow is increase. In both cases, the flow is such that the distance between the two quantities (and hence the magnitude of the denominator) increases. The RG fixed point occurs when the magnitude of the denominator goes to 0. This happens if the distance vanishes. Since the distance necessarily increases, we cannot get a fixed point in this way.

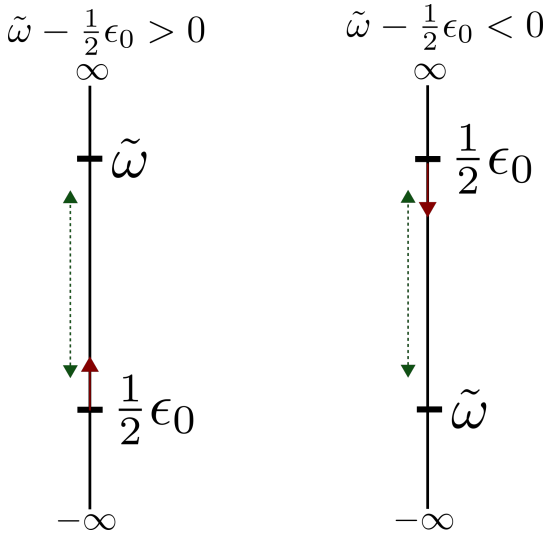

Figure 3.4: RG flow for the two cases with the new $-\tilde{\omega} = \omega' - \frac{1}{2}\epsilon + \frac{1}{4}J$. Now we can see that in both cases, the flow is such that the distance (green dotted line) between the couplings decreases. A fixed point is reached when this distance vanishes.

so the renormalization will be irrelevant. ϵ_0 will decrease until we reach $\tilde{\omega} + \frac{1}{2}\epsilon_0 = 0$. This will be a fixed point. However, if we start with a bare ϵ_0 such that $\tilde{\omega} + \frac{1}{2}\epsilon_0 < 0$, then the denominator is negative so the renormalization will be relevant. ϵ_0 will increase until we reach $\tilde{\omega} + \frac{1}{2}\epsilon_0 = 0$. This will again be a fixed point. This new situation is depicted in figure 3.3.

3.3.3 Effective Hamiltonians

If $\tilde{\omega}$ and ϵ_0 are of the same sign at the bare level, then it is easy to see that since the fixed point is defined by $\tilde{\omega} = \frac{1}{2}\epsilon_0^*$ (* denotes value at fixed point), the effective Hamiltonian at the fixed point will be

$$\mathcal{H}^* = 2\tilde{\omega} S_0^z + \epsilon \sum_i S_i^z + J \sum_i \vec{S}_i \cdot \vec{S}_0, \quad \text{if } \tilde{\omega}\epsilon_0 > 0 \tag{3.3.23}$$

If, at the bare level, ϵ_0 and $\tilde{\omega}$ are of opposite signs, then ϵ_0 would undergo a change in sign at some point as it flows towards $\tilde{\omega}$. Since we do not expect a coupling to change sign under RG, we will restrict it to 0 in such cases.

$$\mathcal{H}^* = \epsilon \sum_i S_i^z + J \sum_i \vec{S}_i \cdot \vec{S}_0, \quad \text{if } \tilde{\omega}\epsilon_0 < 0 \tag{3.3.24}$$

Things get much more simpler if we assume the onsite energies of the surrounding nodes are zero.

$$\begin{aligned} \mathcal{H}^* &= 2\tilde{\omega} S_0^z + J \sum_i \vec{S}_i \cdot \vec{S}_0, && \text{if } \tilde{\omega}\epsilon_0 > 0 \\ \mathcal{H}^* &= J \sum_i \vec{S}_i \cdot \vec{S}_0, && \text{if } \tilde{\omega}\epsilon_0 < 0 \end{aligned} \tag{3.3.25}$$

3.3.4 Fixed points

The fixed points are obtained numerically by solving the RG equation. As mentioned before, there are two types of solutions: The first kind is those in which ϵ_0 and $\tilde{\omega}$ are of the same sign, and the former flows to the latter without crossing the 0 axis. These flows are shown (obtained numerically) in fig. 3.5. The second kind are those where the two couplings have different signs, and so ϵ_0 flows to 0. These are shown in fig. 3.6.

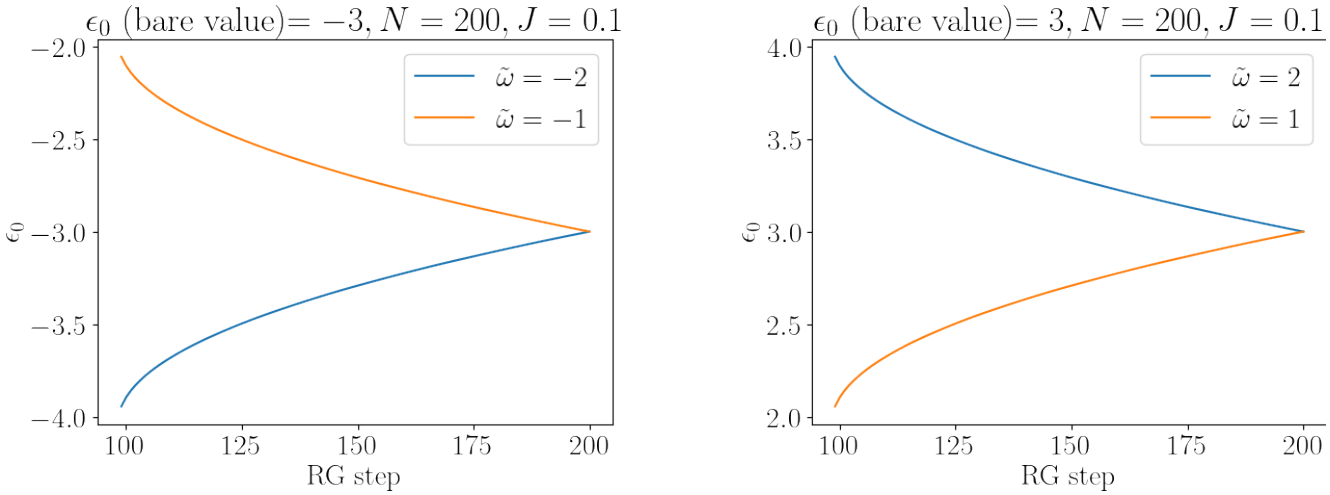

Figure 3.5: Flows where ϵ_0 and $\tilde{\omega}$ have same sign. The left and right panels show flows starting from negative and positive values respectively. The two plots in each panel correspond to different values of $\tilde{\omega}$, one greater than the bare ϵ_0, the other less than that. The fixed point value is $2\tilde{\omega}$.

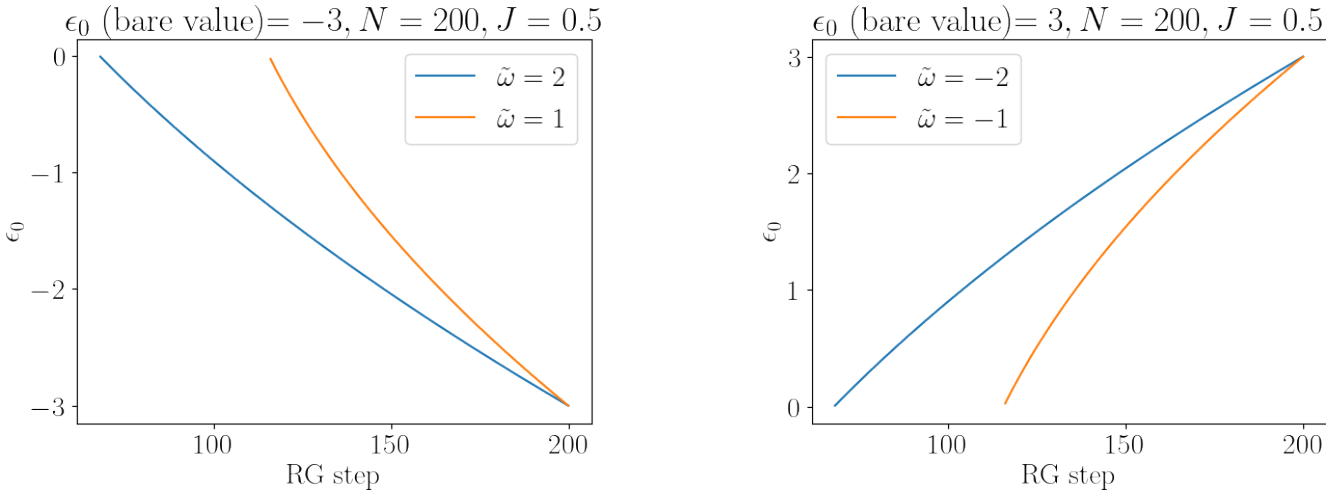

Figure 3.6: Flows where ϵ_0 and $\tilde{\omega}$ have opposite sign. The left and right panels show flows starting from negative and positive values respectively. The two plots in each panel correspond to different values of $\tilde{\omega}$, one greater than the bare ϵ_0, the other less than that. The fixed point value is 0.

3.4 Kondo Model URG

The Kondo model URG analysis is first carried out in ref. [9]. The model is of course described by the Hamiltonian

$$\mathcal{H} = \sum_{k\alpha} \epsilon_k \hat{n}_{k\alpha} + J_z \sum_{k,k'} S^z_d \left(c^\dagger_{k\uparrow} c_{k'\uparrow} - c^\dagger_{k\downarrow} c_{k'\downarrow} \right) + J_t \sum_{k,k'} \left(S^+_d c^\dagger_{k\downarrow} c_{k'\uparrow} + S^-_d c^\dagger_{k\uparrow} c_{k'\downarrow} \right) \tag{3.4.1}$$

The goal is to disentangle an electron $q\beta$ from the Hamiltonian, q being the momentum and β the spin. The diagonal part of the Hamiltonian is

$$\mathcal{H}_d = \epsilon_q \hat{n}_{q\beta} + J_z S^z_d \beta \left(\hat{n}_{q\beta} - \hat{n}_{q\bar{\beta}}\right) \tag{3.4.2}$$

Note that we keep only those terms in the diagonal part that relate to either the impurity or the electron we are disentangling-$q\beta$. This piece $\mathcal{H}_d$ is the one that comes in the denominator. Note that in this form, the hole energy comes out to be zero, because the Hamiltonian is written only in terms of $\hat{n}_{q\beta}$. To remedy this, we write the Hamiltonian in terms of $\tau_{q\beta} = \hat{n}_{q\beta} - \frac{1}{2}$.

$$\mathcal{H}_d = \epsilon_q \tau_{q\beta} + J_z S^z_d \beta \hat{n}_{q\beta} \tag{3.4.3}$$

A constant $\frac{1}{2}\epsilon_q$ has been dropped while transforming the first term.

The off-diagonal part involving the electron on the shell is

$$\mathcal{H}^I = J_z \sum_k S^z_d \beta \left(c^\dagger_{k\beta} c_{q\beta} + c^\dagger_{q\beta} c_{k\beta}\right) + J_t \sum_k \left(c^\dagger_{d\beta} c_{d\bar{\beta}} c^\dagger_{k\bar{\beta}} c_{q\beta} + c^\dagger_{b\bar{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k\bar{\beta}}\right) \tag{3.4.4}$$

These are the terms that come in the numerator.

3.4.1 Particle sector

The particle sector involves integrating out those states which are occupied ($\hat{n}_{q\beta} = 1$). We will work at a shell with energy $-\epsilon_q$.

$$c^\dagger_{q\beta} T \eta \tag{3.4.5}$$

where

$$\begin{aligned} \eta &= \frac{1}{\omega - \mathcal{H}_d} \left[J_z \sum_k \beta S^z_d c^\dagger_{k\beta} c_{q\beta} + J_t \sum_k c^\dagger_{d\beta} c_{d\bar{\beta}} c^\dagger_{k\bar{\beta}} c_{q\beta} \right] \\ &= \sum_k \left[\frac{1}{\hat{\omega}_1 - \hat{E}_1} J_z S^z_d \beta c^\dagger_{k\beta} c_{q\beta} + \frac{1}{\omega_3 - E_3} J_t c^\dagger_{d\beta} c_{d\bar{\beta}} c^\dagger_{k\bar{\beta}} c_{q\beta} \right] \end{aligned} \tag{3.4.6}$$

Noting that $\beta S^z_d = \frac{1}{2}\left(\hat{n}_{d\beta} - \hat{n}_{d\bar{\beta}}\right) = \frac{1}{2}\hat{n}_{d\beta}\left(1 - \hat{n}_{d\bar{\beta}}\right) - \frac{1}{2}\hat{n}_{d\bar{\beta}}\left(1 - \hat{n}_{d\beta}\right)$, we can write the η as

$$\sum_k \left[\frac{J_z \frac{1}{2}\hat{n}_{d\beta}\left(1 - \hat{n}_{d\bar{\beta}}\right) c^\dagger_{k\beta} c_{q\beta}}{\omega_1 - E_1} - \frac{J_z \frac{1}{2}\hat{n}_{d\bar{\beta}}\left(1 - \hat{n}_{d\beta}\right) c^\dagger_{k\beta} c_{q\beta}}{\omega_2 - E_2} + \frac{J_t c^\dagger_{d\beta} c_{d\bar{\beta}} c^\dagger_{k\bar{\beta}} c_{q\beta}}{\omega_3 - E_3} \right] \tag{3.4.7}$$

The energies E_i now need to be determined. For the last term, it is obvious:

$$E_3 = \frac{1}{2}\epsilon_q - \frac{1}{2}J_z \tag{3.4.8}$$

For the first two term, note that these terms do not flip the spin; hence, the denominator should reflect that. The total magnetization for the spin β in the initial state is $\hat{n}_\beta = \hat{n}_{q\beta} = 1$,

because of the $q\beta$. It is also 1 in the intermediate state, because of the spin $k\beta$: $\hat{n}_\beta = \hat{n}_{k\beta} = 1$. This holds for both E_1 and E_2. The impurity magnetization is however 1 in the first term but -1 in the second term. Hence,

$$\begin{aligned} E_1 &= \frac{1}{2}\epsilon_q + \frac{1}{2}J_z \\ E_2 &= \frac{1}{2}\epsilon_q - \frac{1}{2}J_z = E_3 \end{aligned} \tag{3.4.9}$$

To relate the ω_i, we will use their diagonal values. By replacing them with the initial state energies, we can write

$$\begin{aligned} \omega_1 &= -\frac{1}{2}\epsilon_q + \frac{1}{2}J_z \\ \omega_2 = \omega_3 &= -\frac{1}{2}\epsilon_q - \frac{1}{2}J_z \end{aligned} \tag{3.4.10}$$

Defining $\omega \equiv \omega_3$, we can write $\omega_1 = \omega + J_z$ and $\omega_2 = \omega$. Therefore,

$$\eta = \sum_k \left[\frac{J_z \frac{1}{2}\hat{n}_{d\beta}\left(1 - \hat{n}_{d\bar{\beta}}\right) c^\dagger_{k\beta} c_{q\beta}}{\xi_1} - \frac{J_z \frac{1}{2}\hat{n}_{d\bar{\beta}}\left(1 - \hat{n}_{d\beta}\right) c^\dagger_{k\beta} c_{q\beta}}{\xi_2} + \frac{J_t c^\dagger_{d\beta} c_{d\bar{\beta}} c^\dagger_{k\bar{\beta}} c_{q\beta}}{\xi_3} \right] \tag{3.4.11}$$

where $\xi_i \equiv \omega_i - E_i$, hence

$$\xi_1 = \xi_2 = \xi_3 = \omega - \frac{1}{2}\epsilon_q + \frac{1}{2}J_z \equiv \xi \tag{3.4.12}$$

Therefore,

$$\begin{aligned} \eta &= \frac{1}{\xi}\sum_k \left[J_z \frac{1}{2}\hat{n}_{d\beta}\left(1 - \hat{n}_{d\bar{\beta}}\right) c^\dagger_{k\beta} c_{q\beta} - J_z \frac{1}{2}\hat{n}_{d\bar{\beta}}\left(1 - \hat{n}_{d\beta}\right) c^\dagger_{k\beta} c_{q\beta} + J_t c^\dagger_{d\beta} c_{d\bar{\beta}} c^\dagger_{k\bar{\beta}} c_{q\beta} \right] \\ &= \frac{1}{\xi}\sum_k \left[J_z \frac{1}{2}\left(\hat{n}_{d\beta} - \hat{n}_{d\bar{\beta}}\right) c^\dagger_{k\beta} c_{q\beta} + J_t c^\dagger_{d\beta} c_{d\bar{\beta}} c^\dagger_{k\bar{\beta}} c_{q\beta} \right] \\ &= \frac{1}{\xi}\sum_k \left[J_z \beta S^z_d c^\dagger_{k\beta} c_{q\beta} + J_t c^\dagger_{d\beta} c_{d\bar{\beta}} c^\dagger_{k\bar{\beta}} c_{q\beta} \right] \end{aligned} \tag{3.4.13}$$

The renormalization is therefore

$$\begin{aligned} \frac{1}{\xi}\sum_{kk'} \Big[& J_z \beta S^z_d c^\dagger_{q\beta} c_{k'\beta} \times J_z \beta S^z_d c^\dagger_{k\beta} c_{q\beta} + J_t c^\dagger_{d\bar{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k'\bar{\beta}} \times J_t c^\dagger_{d\beta} c_{d\bar{\beta}} c^\dagger_{k\bar{\beta}} c_{q\beta} \\ & + J_t c^\dagger_{d\bar{\beta}} c_{d\beta} c^\dagger_{q\beta} c_{k'\bar{\beta}} \times J_z \beta S^z_d c^\dagger_{k\beta} c_{q\beta} + J_z \beta S^z_d c^\dagger_{q\beta} c_{k'\beta} \times J_t c^\dagger_{d\beta} c_{d\bar{\beta}} c^\dagger_{k\bar{\beta}} c_{q\beta} \Big] \end{aligned} \tag{3.4.14}$$

We can see that the total renormalization will have three types of terms: J_z^2, J_t^2 and $J_z J_t$. We can ignore the J_z^2 term because it has no impurity operator ($S_d^{z\,2} = \frac{1}{4}$). The remaining terms give

$$\frac{1}{\xi}\sum_{kk'} \left[\frac{1}{2} J_z J_t \left(c^\dagger_{d\bar{\beta}} c_{d\beta} c_{k'\bar{\beta}} c^\dagger_{k\beta} + \text{h.c.} \right) + J_t^2 \hat{n}_{d\bar{\beta}}\left(1 - \hat{n}_{d\beta}\right) c_{k'\bar{\beta}} c^\dagger_{k\bar{\beta}} \right] \tag{3.4.15}$$

For the Kondo problem, we are in the subspace of $\hat{n}_d = 1$, so we can write

$$\hat{n}_{d\overline{\beta}}\left(1-\hat{n}_{d\beta}\right) = \left(\frac{1}{2}+\overline{\beta}S_d^z\right) \tag{3.4.16}$$

and

$$\sum_{kk'}\left(c_{d\overline{\beta}}^\dagger c_{d\beta}c_{k'\overline{\beta}}c_{k\beta}^\dagger + \text{h.c.}\right) = -\sum_{kk'}\left(c_{d\overline{\beta}}^\dagger c_{d\beta}c_{k\beta}^\dagger c_{k'\overline{\beta}} + \text{h.c.}\right) = -\left(S_d^+ s^- + S_d^- s^+\right) \tag{3.4.17}$$

The renormalization then becomes

$$\frac{1}{\xi}\left[-\frac{1}{2}J_zJ_t\left(S_d^+s^- + S_d^-s^+\right) + J_t^2\left(\frac{1}{2}+\overline{\beta}S_d^z\right)\sum_{kk'}c_{k'\overline{\beta}}c_{k\overline{\beta}}^\dagger\right] \tag{3.4.18}$$

3.4.2 Hole sector

For the hole sector, we will take the configuration where $\hat{n}_{q\beta} = 0$ and hence the energy ϵ_q. The renormalization here is

$$T^\dagger c_{q\beta}\eta_0^\dagger = T^\dagger c_{q\beta}\frac{1}{\omega' - \mathcal{H}_d}c_{q\beta}^\dagger T \tag{3.4.19}$$

where η_0 is defined in eq. 3.1.57.

$$\eta_0^\dagger = \frac{1}{\hat{\omega}' - \hat{E}_1}\frac{1}{2}J_z\beta S_d^z c_{q\beta}^\dagger c_{k\beta} + \frac{1}{\omega' - E_3}J_t c_{d\overline{\beta}}^\dagger c_{d\beta}c_{q\beta}^\dagger c_{k\overline{\beta}} \tag{3.4.20}$$

We once again split the S_d^z term into two parts, and get

$$\eta_0^\dagger = \sum_k\left[\frac{J_z\frac{1}{2}\hat{n}_{d\beta}\left(1-\hat{n}_{d\overline{\beta}}\right)c_{q\beta}^\dagger c_{k\beta}}{\xi_1'} - \frac{J_z\frac{1}{2}\hat{n}_{d\overline{\beta}}\left(1-\hat{n}_{d\beta}\right)c_{q\beta}^\dagger c_{k\beta}}{\xi_2'} + \frac{J_t c_{d\overline{\beta}}^\dagger c_{d\beta}c_{q\beta}^\dagger c_{k\overline{\beta}}}{\xi_3'}\right] \tag{3.4.21}$$

Calculating the energies gives

$$\begin{aligned} E_1' &= \frac{1}{2}\epsilon_q + \frac{1}{2}J_z \\ E_2' &= \frac{1}{2}\epsilon_q - \frac{1}{2}J_z = E_3' \\ \omega_1' &= -\frac{1}{2}\epsilon_q + \frac{1}{2}J_z = \omega + J_z \\ \omega_2' = \omega_3' &= -\frac{1}{2}\epsilon_q - \frac{1}{2}J_z = \omega \\ \xi_i' &= \omega - \frac{1}{2}\epsilon_q + \frac{1}{2}J_z = \xi \end{aligned} \tag{3.4.22}$$

Evaluating the terms similar to the particle sector gives

$$\frac{1}{\xi}\sum_{kk'}\left[-\frac{1}{2}J_zJ_t\left(c_{d\overline{\beta}}^\dagger c_{d\beta}c_{k\beta}^\dagger c_{k'\overline{\beta}} + \text{h.c.}\right) + J_t^2\hat{n}_{d\beta}\left(1-\hat{n}_{d\overline{\beta}}\right)c_{k\overline{\beta}}^\dagger c_{k'\overline{\beta}}\right] \tag{3.4.23}$$

3.4.3 Scaling equations

Adding the two sectors (eqs. 3.4.15 and 3.4.23) gives

$$\begin{aligned}\Delta\mathcal{H} &= \frac{1}{\xi}\sum_{kk'}\left[-J_zJ_t\left(c^\dagger_{d\overline{\beta}}c_{d\beta}c^\dagger_{k\beta}c_{k'\overline{\beta}}+\text{h.c.}\right)+J_t^2\left(\hat{n}_{d\beta}-\hat{n}_{d\overline{\beta}}\right)c^\dagger_{k\overline{\beta}}c_{k'\overline{\beta}}+J_t^2\hat{n}_{d\overline{\beta}}\left(1-\hat{n}_{d\beta}\right)\delta_{kk'}\right]\\ &= -\frac{1}{\xi}\left[J_zJ_t\left(S_d^+s^-+S_d^-s^+\right)+\sum_{kk'}J_t^2S_d^z\overline{\beta}c^\dagger_{k\overline{\beta}}c_{k'\overline{\beta}}-J_t^2\hat{n}_{d\overline{\beta}}\left(1-\hat{n}_{d\beta}\right)\sum_k\right]\end{aligned} \tag{3.4.24}$$

Summing over β and q gives

$$\sum_{q,\beta}\Delta\mathcal{H} = -\sum_q\frac{1}{\xi}\left[2J_zJ_t\left(S_d^+s^-+S_d^-s^+\right)+2J_t^2S_d^zs^z\right]+\hat{O} \tag{3.4.25}$$

There we used $\sum_\beta\overline{\beta}\sum_{kk'}c^\dagger_{k\overline{\beta}}c_{k'\overline{\beta}}=\sum_{kk'}\left(c^\dagger_{k\uparrow}c_{k'\uparrow}-c^\dagger_{k\downarrow}c_{k'\downarrow}\right)=2s^z$. The operator $\hat{O}$ is

$$\sum_{q\beta}\frac{1}{\xi}J_t^2\hat{n}_{d\overline{\beta}}\left(1-\hat{n}_{d\beta}\right)\sum_k=\sum_q\frac{1}{\xi}J_t^2\left(\hat{n}_d-\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right)\sum_k=\sum_q\frac{1}{\xi}J_t^2\sum_k \tag{3.4.26}$$

where we used $\hat{n}_d=1$ and $\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}=0$ in the singly-occupied subspace. This is a spin-independent impurity-independent potential scattering within the bath, and we will not consider it further, because it will be irrelevant at low ω, where the J is relevant and there is a flow to a strong-coupling fixed point.

We can now write down the flow equations for J_z and J_t:

$$\begin{aligned}\Delta J_z &= -2J_t^2\sum_q\frac{1}{\omega-\frac{1}{2}\epsilon_q+\frac{1}{2}J_z}\\ \Delta J_t &= -2J_zJ_t\sum_q\frac{1}{\omega-\frac{1}{2}\epsilon_q+\frac{1}{2}J_z}\end{aligned} \tag{3.4.27}$$

If we set $J_z=J_t=\frac{J}{2}$, we end up with an SU(2)-symmetric model $J\vec{S}_d\cdot\vec{s}$.

$$\Delta J = -J^2\sum_q\frac{1}{\omega-\frac{1}{2}\epsilon_q+\frac{1}{4}J} \tag{3.4.28}$$

To recover the one-loop form, we can replace ω with the bare value $-\frac{1}{2}\epsilon_q$ and ignore the J in the denominator (small J).

$$\Delta J \approx J^2\sum_q\frac{1}{\epsilon_q} \tag{3.4.29}$$

3.4.4 Numerical Solutions

The symmetric scaling equation 3.4.28 was solved numerically with the choice $\omega = -\frac{\epsilon_q}{2}$, for both positive and negative bare values of J. For sufficiently low values of ω, the Kondo coupling J flows to the strong-coupling limit. This limit, as obtained from the URG, is of course finite. This can be reconciled with the NRG result $J^* = \infty$ by noting the fact that increasing the bare bandwidth D does increase the value of URG J^*, such that in the thermodynamic limit $D \to \infty$, URG should give $J^* \to \infty$. This is shown in fig. 3.8

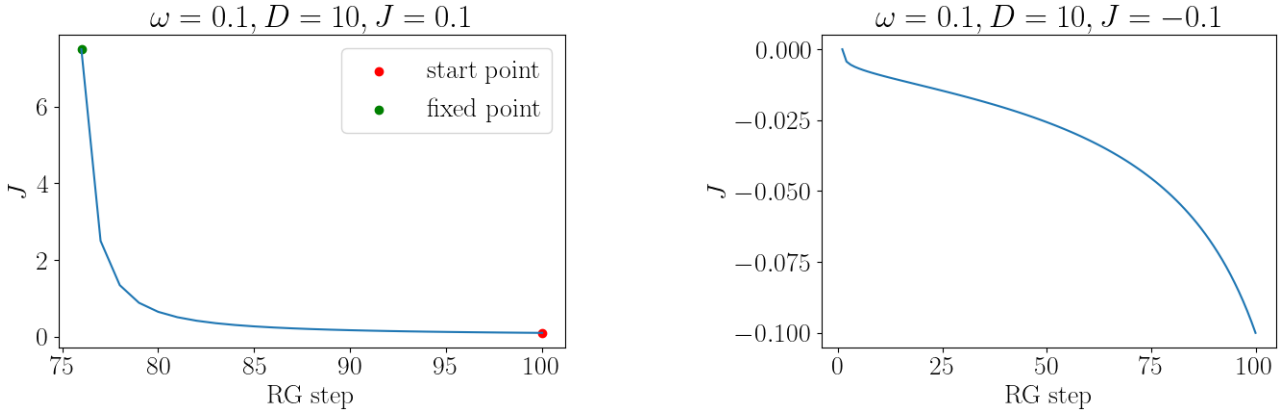

Figure 3.7: Flow of J towards the strong-coupling fixed point (right) and the weak coupling saddle-point (left). The x-axis indicates the index of the energy shell being decoupled. The largest value (UV) is the first step, and we go towards the left (IR).

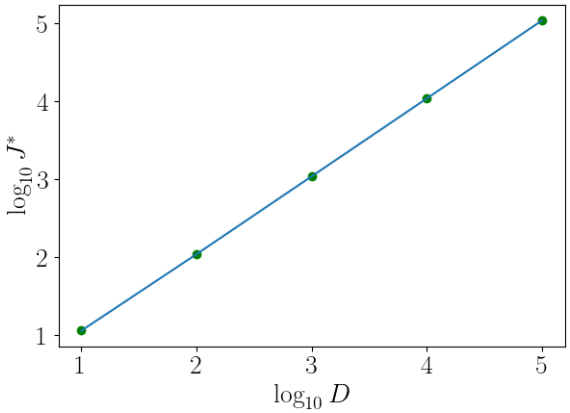

Figure 3.8: Variation of the fixed point value J^* against the bare bandwidth, in log scale.