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

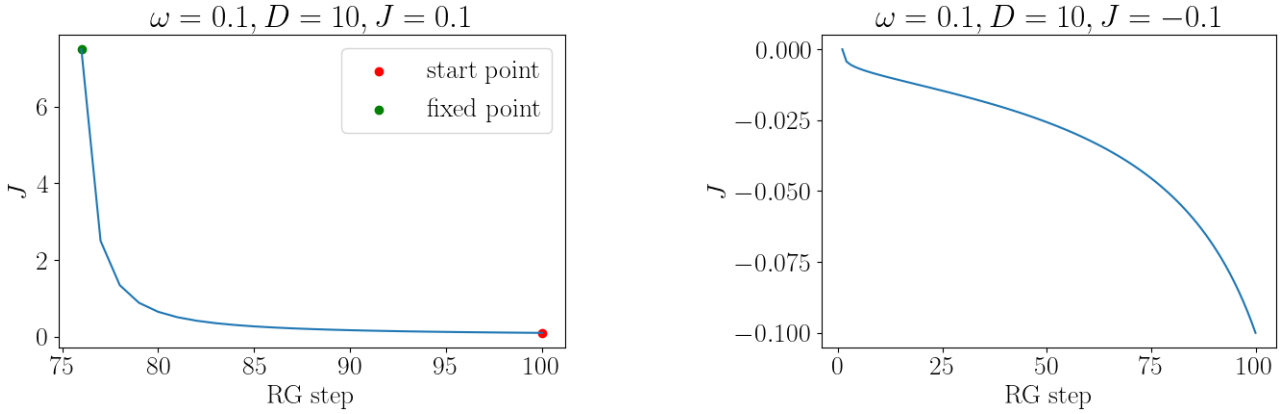

Figure 3.7: Flow of J towards the strong-coupling fixed point (right) and the weak coupling saddle-point (left). The x-axis indicates the index of the energy shell being decoupled. The largest value (UV) is the first step, and we go towards the left (IR).

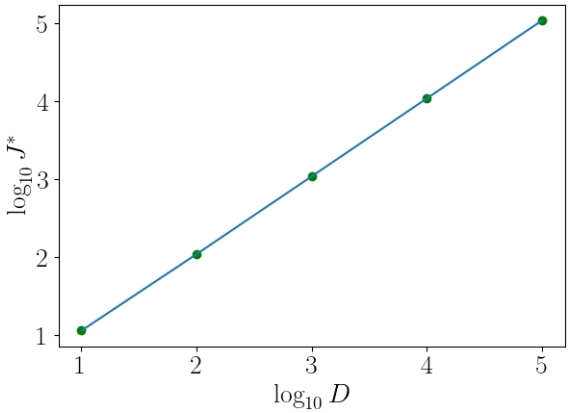

Figure 3.8: Variation of the fixed point value J^* against the bare bandwidth, in log scale.

Chapter 4

Connection between URG and Other Canonical Transformations

4.1 Poor Man's Scaling

We first motivate the formalism of PMS method. The problem is defined as

$$\mathcal{H}\,|\Psi\rangle = E\,|\Psi\rangle \tag{4.1.1}$$

$\mathcal{H}$ is the total Hamiltonian and $|\Psi\rangle$ and E are the exact eigenstate and eigenvalue of $\mathcal{H}$. We imagine a separation of the total Hilbert space into two set of states, and we call these two states $|0\rangle$ and $|1\rangle$. This separation depends on which scattering term we want to kill by this transformation. For example, in the URG, we typically select a particular electron $q\beta$ and then kill the scattering terms that change the number of this state. In that case, $|0\rangle$ will refer to the set of states $\left\{|\hat{n}_{q\beta}=0\rangle\otimes|\phi_0\rangle\right\}$ and $|1\rangle$ will refer to the set of states $\left\{|\hat{n}_{q\beta}=1\rangle\otimes|\phi_1\rangle\right\}$. $|\phi_{0,1}\rangle$ refer to the states of all the other electrons. As another example, if we wanted to separate the charge-Kondo and the spin-Kondo from the SIAM, we would want to kill the terms that scatter between the spin-full subspace $\hat{n}_d = 1$ to the spin-less subspace $\hat{n_d} = 0, 2$. These two will then be the $|0\rangle$ and $|1\rangle$ sets.

Keeping this separation in mind, the exact eigenstate $|\Psi\rangle$ can be split as

$$|\Psi\rangle = \sum_i |\phi_0^i\rangle + \sum |\phi_1^i\rangle \tag{4.1.2}$$

The Hamiltonian can also be split as

$$\mathcal{H} = H_0 + V_+ + V_- \tag{4.1.3}$$

H_0 does not scatter between $\left\{|0\rangle\right\}$ and $\left\{|1\rangle\right\}$. It contains the diagonal parts as well as scatterings inside the subspaces. $V_\pm$ scatter between the subspaces:

$$\begin{aligned} V_+\left\{|0\rangle\right\} &\mapsto \left\{|1\rangle\right\}, \quad V_+\,|1\rangle \to 0 \\ V_-\left\{|1\rangle\right\} &\mapsto \left\{|0\rangle\right\}, \quad V_-\,|0\rangle \to 0 \end{aligned} \tag{4.1.4}$$

The Schrodinger equation can thus be split into

$$\begin{aligned} H_0 \sum_i |\phi_0^i\rangle + V_- \sum_i |\phi_1^i\rangle &= E \sum_i |\phi_0^i\rangle \\ H_0 \sum_i |\phi_1^i\rangle + V_+ \sum_i |\phi_0^i\rangle &= E \sum_i |\phi_1^i\rangle \end{aligned} \tag{4.1.5}$$

Eliminating $\sum_i |\phi_1^i\rangle$ gives

$$H_0 \sum_i |\phi_0^i\rangle + V_- \frac{1}{E_1 - H_0} V_+ \sum_i |\phi_0^i\rangle = E \sum_i |\phi_0^i\rangle \tag{4.1.6}$$

The effective Hamiltonian in this subspace is therefore

$$\tilde{\mathcal{H}}_0 = H_0 + V_- \frac{1}{E - H_0} V_+ \tag{4.1.7}$$

Similarly, eliminating $\sum_i |\phi_0^i\rangle$ gives the effective Hamiltonian in the other subspace,

$$\tilde{\mathcal{H}}_1 = H_0 + V_+ \frac{1}{E - H_0} V_- \tag{4.1.8}$$

The total effective Hamiltonian that does not scatter between the two subspaces is

$$\tilde{\mathcal{H}}(E) = H_0 + \underbrace{V_- \frac{1}{E - H_0} V_+ + V_+ \frac{1}{E - H_0} V_-}_{\text{renormalization}} \tag{4.1.9}$$

This is of course a function of whatever exact energy eigenvalue we chose, E. Different choices will give different effective Hamiltonians. The renormalization will now be written in terms of the matrix elements. Since the entire $\mathcal{H}_X$ must be Hermitian, we must have $V_- = V_+^\dagger \equiv V$.

$$\Delta\mathcal{H}(E) = V \frac{1}{E - H_0} V^\dagger + V^\dagger \frac{1}{E - H_0} V \tag{4.1.10}$$

Now take the first term and insert complete bases on both sides of V and $V^\dagger$.

$$\begin{aligned} V \frac{1}{E - H_0} V^\dagger &= \sum_{ijk} |\phi_0^i\rangle \langle\phi_0^i| V |\phi_1^j\rangle \langle\phi_1^j| \frac{1}{E - H_0} |\phi_1^j\rangle \langle\phi_1^j| V^\dagger |\phi_0^k\rangle \langle\phi_0^k| \\ &= \sum_{ijk} |\phi_0^i\rangle V_{ij} \langle\phi_1^j| \frac{1}{E - H_0} |\phi_1^j\rangle V_{kj}^\dagger \langle\phi_0^k| \end{aligned} \tag{4.1.11}$$

where we defined $\langle\phi_0^i| V |\phi_1^j\rangle = V_{ij}$. We now approximate H_0 by keeping just the diagonal part, and allowing the balance to redefine E into ω. Then, $(E - H_0) |\phi_{0,1}^j\rangle \equiv \left(\omega_{0,1} - E_{0,1}^j\right) |\phi_{0,1}^j\rangle$. That gives

$$V \frac{1}{E - H_0} V^\dagger = \sum_{ijk} |\phi_0^i\rangle \langle\phi_0^k| \frac{V_{ij} V_{kj}^\dagger}{\omega_1 - E_1^j} \tag{4.1.12}$$

The second term similarly gives

$$V^\dagger \frac{1}{E - H_0} V = \sum_{ijk} |\phi_1^i\rangle \langle\phi_1^k| \frac{V_{ji}^\dagger V_{jk}}{\omega_0 - E_0^j} \tag{4.1.13}$$

The total renormalization becomes

$$\Delta\mathcal{H}(E) = \sum_{ijk} \left(\frac{1}{\omega_1 - E_1^j} |\phi_0^i\rangle \langle\phi_0^k| V_{ij} V_{kj}^\dagger + \frac{1}{\omega_0 - E_0^j} |\phi_1^i\rangle \langle\phi_1^k| V_{ji}^\dagger V_{jk} \right) \tag{4.1.14}$$

This is a general expression that would work irrespective of whether you are decoupling multiple electrons or a single electron. However, the ω are unknown and we need some prescription for replacing them. Since the E is the eigenstate of the initial state on which the scattering terms act, it makes sense to replace them with the initial state energy.

$$\Delta\mathcal{H}(E) = \sum_{ijk} \left(\frac{1}{E_0^k - E_1^j} |\phi_0^i\rangle \langle\phi_0^k| V_{ij} V_{kj}^\dagger + \frac{1}{E_1^k - E_0^j} |\phi_1^i\rangle \langle\phi_1^k| V_{ji}^\dagger V_{jk} \right) \tag{4.1.15}$$

However, closer inspection reveals that this choice makes the renormalization non-Hermitian. So the correct choice is to keep both the initial and final energies.

$$\begin{aligned}
\Delta\mathcal{H} &= \frac{1}{2} \sum_{ijk} \frac{1}{\omega_1 - E_1^j} \left(|\phi_0^i\rangle \langle\phi_0^k| V_{ij} V_{kj}^\dagger + |\phi_0^k\rangle \langle\phi_0^i| V_{kj} V_{ij}^\dagger \right) \\
&+ \frac{1}{2} \sum_{ijk} \frac{1}{\omega_0 - E_0^j} \left(|\phi_1^i\rangle \langle\phi_1^k| V_{ji}^\dagger V_{jk} + |\phi_1^k\rangle \langle\phi_1^i| V_{jk}^\dagger V_{ji} \right) \\
&= \frac{1}{2} \sum_{ijk} \left(\frac{1}{E_0^k - E_1^j} |\phi_0^i\rangle \langle\phi_0^k| V_{ij} V_{kj}^\dagger + \frac{1}{E_0^k - E_1^j} |\phi_0^k\rangle \langle\phi_0^i| V_{kj} V_{ij}^\dagger \right) \\
&+ \frac{1}{2} \sum_{ijk} \left(\frac{1}{E_1^k - E_0^j} |\phi_1^i\rangle \langle\phi_1^k| V_{ji}^\dagger V_{jk} + \frac{1}{E_1^k - E_0^j} |\phi_1^k\rangle \langle\phi_1^i| V_{jk}^\dagger V_{ji} \right)
\end{aligned} \tag{4.1.16}$$

Therefore,

$$\begin{aligned}
\Delta\mathcal{H} &= \frac{1}{2} \sum_{ijk} \left(\frac{1}{E_0^k - E_1^j} + \frac{1}{E_0^i - E_1^j} \right) |\phi_0^i\rangle \langle\phi_0^k| V_{ij} V_{kj}^\dagger \\
&+ \frac{1}{2} \sum_{ijk} \left(\frac{1}{E_1^k - E_0^j} + \frac{1}{E_1^i - E_0^j} \right) |\phi_1^i\rangle \langle\phi_1^k| V_{ji}^\dagger V_{jk}
\end{aligned} \tag{4.1.17}$$

In summary, the prescription of replacing all ω with the initial state energy will be correct only if the initial and final states are the same. This happens when we are decoupling a single-electron state - then the total renormalization is of the form $c^\dagger T^\dagger c$ such that we start from an initial state, scatter to an intermediate state and then go back to the initial

state so that the final state is the same as the initial state. However, if we are using PMS to decouple states in one-shot, each subspace will have multiple states and there might be terms where we do not end up at the initial state we started with. Then the correct prescription would be to use the mean of the initial and final state denominators.

To make a better connection with URG, we next show how the PMS formalism works out for a single-electron decoupling.

We want to decouple one electron at momentum q. We can split the exact wavefunction as

$$|\Psi\rangle = |\Psi_0\rangle + |\Psi_1\rangle \tag{4.1.18}$$

where $|\Psi_0\rangle = \left(1 - \hat{n}_q\right)|\Psi^N\rangle$ is that part of the wavefunction where the state q is occupied. $|\Psi_1^N\rangle = \hat{n}_q|\Psi\rangle$ is that part of the wavefunction where the state q is occupied. We can also split the Hamiltonian as

$$\mathcal{H} = \mathcal{H}^d + V_0 + V_+ + V_- \tag{4.1.19}$$

$\mathcal{H}^d$ is the diagonal part; it has the purely energy terms as well as self-energies that may arise from the diagonal parts of interactions; V_0 is the purely off-diagonal term that does not change $\hat{n}_q$; it is the scattering *inside* the low energy subspace. V_+ and V_- are the purely off-diagonal terms that *do* change $\hat{n}_q$; V_+ takes you from $\hat{n}_q = 0$ to $\hat{n}_q = 1$ and V_- does the opposite.

Substituting eqs. 4.1.19 and 4.1.18 in eq. 4.1.1 gives

$$\left(\mathcal{H}^d + V_0 + V_+ + V_-\right)\left(|\Psi_0\rangle + |\Psi_1\rangle\right) = E\left(|\Psi_0\rangle + |\Psi_1\rangle\right) \tag{4.1.20}$$

Gathering the kets with $\hat{n}_q = 0, 1$ gives

$$\begin{aligned}\left(\mathcal{H}_0^d + V_0\right)|\Psi_0\rangle + V_-|\Psi_1\rangle &= E|\Psi_0\rangle \\ \left(\mathcal{H}_1^d + V_0\right)|\Psi_1\rangle + V_+|\Psi_0\rangle &= E|\Psi_1\rangle\end{aligned} \tag{4.1.21}$$

The second equation can be written as

$$|\Psi_1\rangle = \eta^\dagger|\Psi_0\rangle \tag{4.1.22}$$

where

$$\left(\eta^\dagger\right)_{\text{PMS}} = \frac{1}{E - \mathcal{H}_1^d - V_0}V_+ \tag{4.1.23}$$

Substituting this in the first equation gives

$$\left(\mathcal{H}_0^d + V_0 + V_-\eta^\dagger\right)|\Psi_0\rangle = E|\Psi_0\rangle \tag{4.1.24}$$

This new Hamiltonian,

$$\tilde{\mathcal{H}}_0 = \mathcal{H}_0^d + V_0 + V_-\eta^\dagger \tag{4.1.25}$$

has the high energy mode removed; the scattering terms start from the low energy subspace and end at the low energy subspace as well. The renormalization in the low energy subspace scatterings is

$$\Delta V_0 = V_- \eta^\dagger \tag{4.1.26}$$

If we eliminate $|\Psi_0\rangle$ instead of $|\Psi_1\rangle$, we get the renormalized equation in the high energy subspace:

$$|\Psi_0\rangle = \eta\,|\Psi_1\rangle \tag{4.1.27}$$

where

$$(\eta)_{\text{PMS}} = \frac{1}{E - \mathcal{H}_0^d - V_0} V_- \tag{4.1.28}$$

,so

$$\left(\mathcal{H}_1^d + V_0 + V_+\eta\right)|\Psi_1\rangle = E\,|\Psi_1\rangle \tag{4.1.29}$$

The renormalized Hamiltonian in the high energy subspace is thus

$$\tilde{\mathcal{H}}_1 = \mathcal{H}_1^d + V_0 + V_+\eta \tag{4.1.30}$$

If we want to keep both the high energy and low energy parts of the Hamiltonian, the new Hamiltonian is

$$\begin{aligned}\tilde{\mathcal{H}} &= \tilde{\mathcal{H}}_1\hat{n} + \tilde{\mathcal{H}}_0\left(1-\hat{n}\right)\\ &= \mathcal{H}_0^d + \mathcal{H}_1^d + V_0 + V_+\eta + V_-\eta^\dagger\end{aligned} \tag{4.1.31}$$

The total renormalization is

$$(\Delta\mathcal{H})_{\text{PMS}} = V_+\,(\eta)_{\text{PMS}} + V_-\left(\eta^\dagger\right)_{\text{PMS}} \tag{4.1.32}$$

It can be shown that if we define a unitary operator $U = 1 - \eta + \eta^\dagger$, the transformed Hamiltonian $U\mathcal{H}U^\dagger$ is the same as eq. 4.1.31. This, along with the properties of η, have been shown in section 3. The important feature of eq. 4.1.31 is that there is no term in the transformed Hamiltonian which scatters between $|\Psi_0\rangle$ and $|\Psi_0\rangle$- the two subspaces have been truly decoupled.

$$\left[U\mathcal{H}U^\dagger, n_q\right] = 0 \tag{4.1.33}$$

We can write down the renormalized Schrodinger equation in the low energy subspace, from eq. 4.1.24,

$$\tilde{\mathcal{H}}_0\,|\Psi_0\rangle = E\,|\Psi_0\rangle \tag{4.1.34}$$

and again repeat the entire process. $\tilde{\mathcal{H}}_0$ now takes the place of $\mathcal{H}$ and $|\Psi_0\rangle$ takes the place of $|\Psi\rangle$ in eq. 4.1.1.

The expression for URG is obtained in an almost identical way. The only difference is that instead of starting with the exact eigenpair $(E, |\Psi\rangle)$, we start with a more general pair $(\tilde{\mathcal{H}}, |\Phi\rangle)$ where $|\Phi\rangle$ is not necessarily an exact eigenstate of $\mathcal{H}$. It is defined by $\mathcal{H}'$, which is in turn defined as $\hat{n}_q\mathcal{H}'\left(1-\hat{n}_q\right) = 0$. $|\Phi\rangle$ is then defined by

$$\mathcal{H}\,|\Phi\rangle = \mathcal{H}'\,|\Phi\rangle \tag{4.1.35}$$

This definition of $\mathcal{H}'$ is the very minimum that we must have in order to fulfill our goal (decouple q).

The operators η and its conjugate change accordingly:

$$\begin{aligned}(\eta)_{\text{URG}} &= \frac{1}{\tilde{\mathcal{H}} - \mathcal{H}_0^d - V_0} V_- \\ &= \frac{1}{\hat{\omega} - \mathcal{H}_0^d} V_-\end{aligned} \tag{4.1.36}$$

where $\hat{\omega} \equiv \mathcal{H}' - V_0$ now embodies the quantum fluctuations inherent in the Hamiltonian through the scattering term V_0. Similarly,

$$\left(\eta^\dagger\right)_{\text{URG}} = \frac{1}{\hat{\omega} - \mathcal{H}_1^d} V_+ \tag{4.1.37}$$

The renormalization is again

$$(\Delta\mathcal{H})_{\text{URG}} = V_+ (\eta)_{\text{URG}} + V_- \left(\eta^\dagger\right)_{\text{URG}} \tag{4.1.38}$$

This again allows us to write down a unitary operator that decouples the entangled state:

$$U = 1 - \eta + \eta^\dagger, \left[\hat{n}_q, U\mathcal{H}U^\dagger\right] = 0 \tag{4.1.39}$$

where $\tilde{\mathcal{H}} = U^\dagger \mathcal{H} U$. We can now write down a new problem in this decoupled space with the rotated items and attempt to decouple another electron q'. We will again choose some general eigenpair $(\mathcal{H}', |\Phi\rangle)$ such that $\tilde{\mathcal{H}} |\Phi\rangle = \mathcal{H}' |\Phi\rangle$ and $\left[\mathcal{H}', \hat{n}_{q'}\right] = 0$.

Summarizing, the general Hamiltonian is not diagonal in the Fock space basis. URG, in order to proceed, selects one non-Fock basis of states $|\Phi\rangle$ such that q is decoupled in that Hamiltonian. Since there can be lots of such basis, there is a freedom in this choice. With this basis in mind, URG then finds a unitary operator which when operated on the Hamiltonian takes us to the form in which it is diagonal in the Fock space basis. Note that this form is a function of the chosen $|\Phi\rangle$. We then select the second degree of freedom and repeat the process. What PMS does is, it exploits the freedom of choice and selects the exact eigenstate $|\Psi\rangle$ of the Hamiltonian as the non-Fock basis $|\Phi\rangle$. Doing that returns a rotated Hamiltonian which is diagonal in q, and is a function of the chosen state, same as URG. The conclusion is that depending on which state we choose as our diagonal non-Fock basis, URG and PMS will cause flows along different lines in general.

As the couplings flow, V_0 will also flow, leading to a flow of $\hat{\omega}$. Just at the fixed point, the denominator of URG vanishes, giving the equation

$$\left(\hat{\omega} - \mathcal{H}_1^d\right) V_+ |\Psi_0\rangle \text{ or } \left(\hat{\omega} - \mathcal{H}_1^d\right) V_- |\Psi_1\rangle \tag{4.1.40}$$

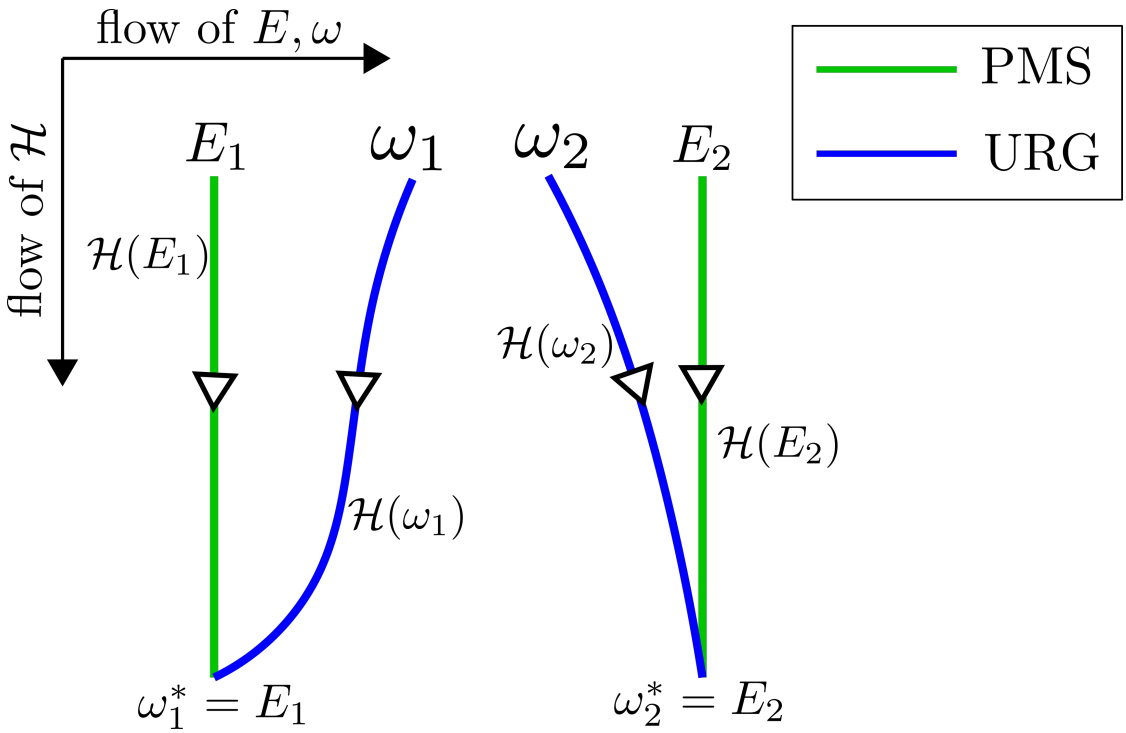

Figure 4.1: Flows of PMS(green) and URG(blue)

This means that one of the eigenvalues of $\hat{\omega}$ matches with the eigenvalue of the diagonal part $\mathcal{H}^d$, either in the occupied sector ($\mathcal{H}_1^d$) or unoccupied sector ($\mathcal{H}_1^d$). Since the eigenvalues are unchanged during the unitary renormalization, this implies that ω takes up one of the eigenvalues of the whole Hamiltonian $\mathcal{H}$. This will correspond to the fixed point obtained from PMS if we had started PMS with that eigenvalue.

In short, while the PMS flow is parametrised by one of the exact energy eigenvalues E, the URG flow is parametrised by a non-trivial operator $\hat{\omega}$ which incorporates both a diagonal part and an off-diagonal part and itself flows under the URG. At the fixed point, the off-diagonal part cancels out and the $\hat{\omega}$ finally flows to one of the energy eigenvalues and the URG fixed point matches with one of the PMS fixed points.

To demonstrate the implementation, we can look at a specific model. For the SIAM,

$$\mathcal{H} = \sum_{k\sigma} \left(\epsilon_k \tau_{k\sigma} + V c_{k\sigma}^\dagger c_{d\sigma} + \text{h.c.} \right) \tag{4.1.41}$$

where $\tau = \hat{n} - \frac{1}{2}$. We want to decouple the state $q\beta$ from the rest of the electrons. We have $\hat{\mathcal{H}}_0 = \epsilon_d \hat{n}_d + U \hat{n}_{d\uparrow} n_{d\downarrow} + \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma}$, $V_0 = \sum_{k<q,\sigma} c_{k\sigma}^\dagger c_{d\sigma} + \text{h.c.}$, $V_+ = V c_{q\beta}^\dagger c_{d\beta}$ and $V_- = V c_{d\beta}^\dagger c_{q\beta}$. The renormalization in particle sector

$$\Delta V_0 = c_{d\beta}^\dagger c_{q\beta} \frac{1}{(E - V_0) - \hat{\mathcal{H}}_0^d} c_{q\beta}^\dagger c_{d\beta} \tag{4.1.42}$$

The intermediate energy (at the propagator) is

$$\hat{\mathcal{H}}_0^d = \sum_{k,\sigma} \epsilon_k \tau_{k\sigma} + \epsilon_d \hat{n}_{d\bar{\beta}} \tag{4.1.43}$$

This is because the $c_{d\beta}$ at the right of the propagator ensures that we must have $\hat{n}_{d\beta} = 0$ at the propagator.

$$\Delta V_0 = c_{d\beta}^\dagger c_{q\beta} \frac{1}{(E - V_0) - \sum_{k,\sigma} \epsilon_k \tau_{k\sigma} - \epsilon_d \hat{n}_{d\bar{\beta}}} c_{q\beta}^\dagger c_{d\beta} \tag{4.1.44}$$

Since E is the exact eigenvalue, we do not have an expression for it. Instead, we approximate $E - V_0$ by substituting it with the current diagonal part corresponding to the initial state on which this entire term will act. The intial state is characterized by $\hat{n}_{q\beta} = 0$ and $\hat{n}_{d\beta} = 1$, so

$$E - V_0 = \sum_{k<q,\sigma} \epsilon_k \tau_{k\sigma} - \frac{1}{2}\epsilon_q + \epsilon_d + \left(\epsilon_d + U\right) \hat{n}_{d\bar{\beta}} \tag{4.1.45}$$

The $-\frac{1}{2}\epsilon_q$ comes from substituting $\hat{n}_{q\beta} = 0$ in $\epsilon_q \tau_{q\beta}$.

Substituting this in ΔV_0 gives

$$\begin{aligned}
\Delta V_0 &= c_{d\beta}^\dagger c_{q\beta} \frac{1}{-\frac{1}{2}\epsilon_q - \epsilon_q \tau_{q\beta} + \epsilon_d + U\hat{n}_{d\bar{\beta}}} c_{q\beta}^\dagger c_{d\beta} \\
&= c_{d\beta}^\dagger c_{q\beta} \frac{1}{-\epsilon_q + \epsilon_d + U\hat{n}_{d\bar{\beta}}} c_{q\beta}^\dagger c_{d\beta} \\
&= c_{d\beta}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{d\beta} \frac{1}{-\epsilon_q + \epsilon_d + U\hat{n}_{d\bar{\beta}}} \\
&= -c_{d\beta}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{d\beta} \frac{1}{\epsilon_q - \epsilon_d - U\hat{n}_{d\bar{\beta}}} \\
&= \left(1 - \hat{n}_{q\beta}\right) \left(\frac{-\hat{n}_{d\beta}\hat{n}_{d\bar{\beta}}}{\epsilon_q - \epsilon_d - U} + \frac{-\hat{n}_{d\beta}\left(1 - \hat{n}_{d\bar{\beta}}\right)}{\epsilon_q - \epsilon_d} \right)
\end{aligned} \tag{4.1.46}$$

On the second line, we substituted $\tau_{q\beta} = \frac{1}{2}$ in the denominator, which is ensured by the $c_{q\beta}^\dagger$ to the right of the propagator. The first term renormalizes the energy of the doublon state and the second term renormalizes that of the singly-occupied state:

$$\begin{aligned}
\Delta E_2 &= \frac{-1}{\epsilon_q - \epsilon_d - U} \\
\Delta E_1 &= \frac{-1}{\epsilon_q - \epsilon_d}
\end{aligned} \tag{4.1.47}$$

The renormalization in the hole sector is

$$\begin{aligned}\Delta V_0 &= c^\dagger_{q\beta} c_{d\beta} \frac{1}{\left(E - V_0\right) - \hat{\mathcal{H}}^d_0} c^\dagger_{d\beta} c_{q\beta} \\ &= c^\dagger_{q\beta} c_{d\beta} \frac{1}{\left(E - V_0\right) - \sum_{k,\sigma} \epsilon_k \tau_{k\sigma} - \epsilon_d - \left(\epsilon_d + U\right) \hat{n}_{d\bar{\beta}}} c^\dagger_{d\beta} c_{q\beta}\end{aligned} \tag{4.1.48}$$

This time we substitute

$$\begin{aligned}E - V_0 &= \sum_{k<q,\sigma} \epsilon_k \tau_{k\sigma} + \tau_{q\beta} \epsilon^-_q + \epsilon_d \hat{n}_{d\bar{\beta}} \\ &= \sum_{k<q,\sigma} \epsilon_k \tau_{k\sigma} + \frac{1}{2} \epsilon^-_q + \epsilon_d \hat{n}_{d\bar{\beta}}\end{aligned} \tag{4.1.49}$$

In the last step we put $\tau_{q\beta} = \frac{1}{2}$ because the state is occupied in the initial configuratin. Note that since the electron $q\beta$ was occupied in the intial state, the energy ϵ^-_q in this sector must be opposite to that of the particle sector, ϵ_q. Hence $\epsilon^-_q = -\epsilon_q$, which gives

$$\begin{aligned}\Delta V_0 &= c^\dagger_{q\beta} c_{d\beta} \frac{1}{-\frac{1}{2}\epsilon_q - \epsilon^-_q \tau_{q\beta} - \epsilon_d - U \hat{n}_{d\bar{\beta}}} c^\dagger_{d\beta} c_{q\beta} \\ &= c^\dagger_{q\beta} c_{d\beta} c^\dagger_{d\beta} c_{q\beta} \frac{1}{-\epsilon_q - \epsilon_d - U \hat{n}_{d\bar{\beta}}} \\ &= \hat{n}_{q\beta} \left(\frac{-\left(1 - \hat{n}_{d\beta}\right) \hat{n}_{d\bar{\beta}}}{\epsilon_q + \epsilon_d + U} + \frac{-\left(1 - \hat{n}_{d\beta}\right)\left(1 - \hat{n}_{d\bar{\beta}}\right)}{\epsilon_q + \epsilon_d} \right)\end{aligned} \tag{4.1.50}$$

In the second line, we put $\epsilon^-_q = -\epsilon_q$ and $\tau_{q\beta} = -\frac{1}{2}$. The first term renormalizes the singly-occupied state while the second term renormalizes the holon state. Combining with the particle sector results, the total renormalization in all the three impurity states (holon, single and doublon) are

$$\begin{aligned}\Delta E_0 &= -\frac{1}{\epsilon_q + \epsilon_d} \\ \Delta E_1 &= -\frac{1}{\epsilon_q + \epsilon_d + U} - \frac{1}{\epsilon_q - \epsilon_d} \\ \Delta E_2 &= -\frac{1}{\epsilon_q - \epsilon_d - U}\end{aligned} \tag{4.1.51}$$

These results are also obtained in ref. [12]. The complete process is depicted in fig. 4.2.

Some conclusions:

- The *only* difference in the formalism of PMS and URG is that while PMS uses the exact energy eigenvalue E to parameterise the flow, URG uses a general intermediate decoupled Hamiltonian to do the same. Since the E is also, technically, an intermediate decoupled Hamiltonian (it is the final Hamiltonian), PMS can be seen as an URG but with a specific choice for the paramter.

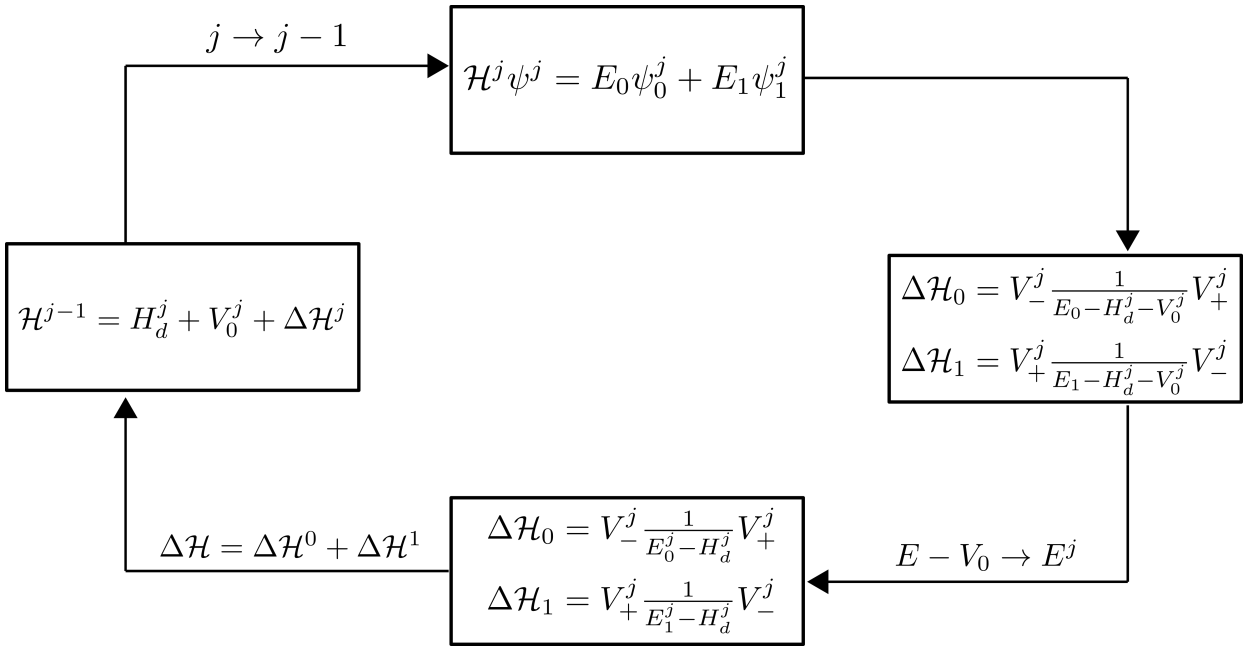

Figure 4.2: Flow chart of "Poor Man's" scaling algorithm

- In practise, PMS replaces $E - V_0$ with the diagonal part of the initial state at the current step of the RG. We are talking about the energy of the initial state, not the intermediate state. This is because, from eq. 4.1.1, E is the energy of the initial state on which $V_\pm$ act.
- The ideal solution would have been to substitute the exact energy and the total scattering term V, but since we do not know E and keeping the V would make the thing untractable, we use our current best guess (renormalised diagonal part). As the RG flows, both E_j and V flow, such that at the fixed point, V becomes zero (scattering terms get removed) and E_j morphs into the exact E.
- In practise, URG replaces the $\hat{\omega}$ with a guess for the final energy E. This however ignores the renormalization of $\hat{\omega}$. A better approach would be to replace it with E_j, following PMS. That would act like the one-particle renormalization of $\hat{\omega}$.
- PMS usually drops any diagonal component of the scattering from the denominator. For example, in the PMS of the Kondo model by Anderson [3] or that of the anisotropic power law Kondo model by Chenge et.al [28], they do not keep the term $J_z S_d^z s^z$ in the denominator although it is number(spin) conserving. Such terms are kept in the denominator of the URG though. It must be mentioned however that ref. [29] *does* bring a diagonal charge-charge interaction in the denominator in the PMS of the extended Anderson model.

4.2 Schrieffer-Wolff transformation

Formal Differences

We have a general Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_X \tag{4.2.1}$$

$\mathcal{H}_0$ is diagonal w.r.t a particular degree of freedom. V is off-diagonal w.r.t that same degree of freedom. Let S be an *anti-Hermitian* and *off-diagonal* operator. $U = e^S$ is then a unitary transformation.

$$\begin{aligned} U\mathcal{H}U^\dagger &= e^S \left(\mathcal{H}_0 + \mathcal{H}_X\right) e^{-S} \\ &= \Big(\cosh\left(S\right) + \sinh\left(S\right)\Big) \left(\mathcal{H}_0 + \mathcal{H}_X\right) \Big(\cosh\left(S\right) - \sinh\left(S\right)\Big) \\ &= H_1 + H_2 \end{aligned} \tag{4.2.2}$$

where H_1 is diagonal and H_2 is off-diagonal.

$$\begin{aligned} H_1 = \cosh\left(S\right)\mathcal{H}_0\cosh\left(S\right) - \sinh\left(S\right)\mathcal{H}_0\sinh\left(S\right) - \cosh\left(S\right)\mathcal{H}_X\sinh\left(S\right) \\ + \sinh\left(S\right)\mathcal{H}_X\cosh\left(S\right) \\ H_2 = -\cosh\left(S\right)\mathcal{H}_0\sinh\left(S\right) + \sinh\left(S\right)\mathcal{H}_0\cosh\left(S\right) + \cosh\left(S\right)\mathcal{H}_X\cosh\left(S\right) \\ - \sinh\left(S\right)\mathcal{H}_X\sinh\left(S\right) \end{aligned} \tag{4.2.3}$$

The decoupling condition is $H_2 = 0$.

For small S, we have $\sinh S \sim S$ and $\cosh S \sim 1 + \frac{1}{2}S^2$. Therefore, the off-diagonal part, up to second order, is

$$H_2 = -\mathcal{H}_0 S + S\mathcal{H}_0 + \mathcal{H}_X + O(S^3) = \left[S, \mathcal{H}_0\right] + \mathcal{H}_X \tag{4.2.4}$$

The second order decoupling condition is thus

$$\left[S, \mathcal{H}_0\right] = -\mathcal{H}_X \tag{4.2.5}$$

The effective Hamiltonian is what remains, H_1. That becomes, at second order,

$$\begin{aligned} H_1 &= \left(1 + \frac{1}{2}S^2\right)\mathcal{H}_0\left(1 + \frac{1}{2}S^2\right) - S\mathcal{H}_0 S - \left(1 + \frac{1}{2}S^2\right)\mathcal{H}_X S + S\mathcal{H}_X\left(1 + \frac{1}{2}S^2\right) \\ &= \mathcal{H}_0 + \frac{1}{2}\left\{S^2, \mathcal{H}_0\right\} - S\mathcal{H}_0 S - \mathcal{H}_X S + S\mathcal{H}_X + O(S^3) \\ &= \mathcal{H}_0 + \frac{1}{2}S\left[S, \mathcal{H}_0\right] - \frac{1}{2}\left[S, \mathcal{H}_0\right]S + \left[S, \mathcal{H}_X\right] + O(S^3) \\ &= \mathcal{H}_0 + \frac{1}{2}\left[S, \left[S, \mathcal{H}_0\right]\right] + \left[S, \mathcal{H}_X\right] + O(S^3) \\ &= \mathcal{H}_0 + \frac{1}{2}\left[S, -\mathcal{H}_X\right] + \left[S, \mathcal{H}_X\right] + O(S^3) \\ &= \mathcal{H}_0 + \frac{1}{2}\left[S, \mathcal{H}_X\right] + O(S^3) \end{aligned} \tag{4.2.6}$$

Avoiding the perturbative route, we can take $S = \frac{\pi}{4}\left(\eta^\dagger - \eta\right)$, where η and its conjugate are non-perturbative and Fermionic - they satisfy $\eta^2 = \eta^{\dagger 2} = 0$ and $\left\{\eta, \eta^\dagger\right\} = 1$. We can then write

$$\begin{aligned} e^S &= \exp\left(\frac{\pi}{4}\left(\eta^\dagger - \eta\right)\right) \\ &= 1 + \left(\eta^\dagger - \eta\right)\frac{\pi}{4} + \frac{1}{2!}\left(\eta^\dagger - \eta\right)^2\left(\frac{\pi}{4}\right)^2 + \frac{1}{3!}\left(\eta^\dagger - \eta\right)^3\left(\frac{\pi}{4}\right)^3 + \ldots \\ &= 1 + \left(\eta^\dagger - \eta\right)\frac{\pi}{4} - \frac{1}{2!}\left(\frac{\pi}{4}\right)^2 - \frac{1}{3!}\left(\eta^\dagger - \eta\right)\left(\frac{\pi}{4}\right)^3 + \frac{1}{4!}\left(\frac{\pi}{4}\right)^4 + \ldots \\ &= \cos\frac{\pi}{4} + \left(\eta^\dagger - \eta\right)\sin\frac{\pi}{4} \\ &= \frac{1}{\sqrt{2}}\left(1 + \eta^\dagger - \eta\right) \end{aligned} \tag{4.2.7}$$

There we used

$$\left(\eta^\dagger - \eta\right)^2 = \eta^{\dagger 2} + \eta^2 - \left\{\eta^\dagger, \eta\right\} = -1 \quad \left[\because \eta^2 = \eta^{\dagger 2} = 0\right] \tag{4.2.8}$$

and hence

$$\left(\eta^\dagger - \eta\right)^3 = -1\left(\eta^\dagger - \eta\right) \tag{4.2.9}$$

and so on. This simplification allows us to write

$$\cosh S = \frac{1}{2}\left[e^S + e^{-S}\right] = \frac{1}{2\sqrt{2}}\left(1 + \eta^\dagger - \eta + 1 - \eta^\dagger + \eta\right) = \frac{1}{\sqrt{2}} \tag{4.2.10}$$

and

$$\sinh S = \frac{1}{2}\left[e^S - e^{-S}\right] = \frac{1}{2\sqrt{2}}\left(1 + \eta^\dagger - \eta - 1 + \eta^\dagger - \eta\right) = \frac{1}{\sqrt{2}}\left(\eta^\dagger - \eta\right) \tag{4.2.11}$$

The off-diagonal part now becomes

$$H_2 = \frac{1}{2}\left(\mathcal{H}_X - \eta^\dagger \mathcal{H}_X \eta^\dagger - \eta \mathcal{H}_X \eta + \left[\eta^\dagger - \eta, \mathcal{H}_0\right]\right) \tag{4.2.12}$$

The vanishing of this quantity is now the decoupling condition, and is also given in eq 16 of ref. [22].

To look for a decoupling condition similar to eq. 4.2.5, we can re-express the cosh and sinh in eq. 4.2.10 in terms of S, by substituting $\eta^\dagger - \eta = \frac{4}{\pi}S$:

$$\cosh S = \frac{1}{\sqrt{2}}, \text{ and } \sinh S = \frac{4}{\sqrt{2}\pi}S \tag{4.2.13}$$

That gives

$$H_2 = \frac{1}{2}\left(\frac{4}{\pi}\left[S, \mathcal{H}_0\right] + \mathcal{H}_X - \frac{16}{\pi^2}S\mathcal{H}_X S\right) \tag{4.2.14}$$

	renormalization	decoupling condition
SWT	$\frac{1}{2}\left[S, \mathcal{H}_X\right]$	$\left[S, \mathcal{H}_0\right] = -\mathcal{H}_X$
URG	$\frac{2}{\pi}\left[S, \mathcal{H}_X\right]$	$\left[S, \mathcal{H}_0\right] = -\frac{\pi}{4}\mathcal{H}_X + \frac{4}{\pi}S\mathcal{H}_X S$

Table 4.1: Comparison of perturbative and non-perturbative canonical transformations

The decoupling condition becomes

$$\left[S, \mathcal{H}_0\right] = -\frac{\pi}{4}\mathcal{H}_X + \frac{4}{\pi}S\mathcal{H}_X S \tag{4.2.15}$$

This can be compared to the second order condition: $\left[S, \mathcal{H}_0\right] = -\mathcal{H}_X$. We can also write the effective Hamiltonian for this non-perturbative case.

$$U\mathcal{H}U^\dagger = H_1 = \frac{1}{2}\mathcal{H}_0 - \frac{4}{\pi^2}S\mathcal{H}_0 S + \frac{2}{\pi}\left[S, \mathcal{H}_X\right] \tag{4.2.16}$$

The differences between the perturbative and non-perturbative ways are summarized in table 4.1. There appear to be two differences between these decoupling conditions: (a) a pre-factor of $\frac{\pi}{4}$ for the first term on the right hand side, and (b) the altogether new second term on the right hand side. Both are outcomes of the non-perturbative nature of URG. This offers evidence that the physics captured by the effective Hamiltonian (and its associated low-energy many-particle Hilbert space) obtained from URG lies well beyond that obtained from SWT. Further, it shows that the SWT can only be justified as an expansion in a small parameter (say, $\frac{1}{U}$) in the Anderson impurity problem), followed by a truncation of the BCH expansion and a projection onto a particular low-energy subspace. The truncation and projection are adopted simultaneously, and appear to impose the limit of $U = \infty$ by hand. The URG flow never attains such a limit, thus suggesting that there exists a lot of interesting physics that could potentially be lost in the SWT procedure. Further, the projection finally applied within SWT means that we can never recover what is thrown away. This is again not the case with URG.

Renormalization due to SWT and Comparison with PMS and URG

Similar to the situation in Poor Man's scaling, one can visualize two set of states and let $\mathcal{H}_X = V_+ + V_-$ be the scattering that connects them and hence the one we want to kill. Let S be of the form

$$S = \sum_{ij}\left[s\left|\phi_1^i\right\rangle\left\langle\phi_0^j\right| - s^\dagger\left|\phi_0^j\right\rangle\left\langle\phi_1^i\right|\right] \tag{4.2.17}$$

This form is of course chosen to make S anti-Hermitian and off-diagonal. The part s can be determined from the decoupling condition:

$$-\mathcal{H}_X = \left[S, H_0\right] = SH_0 - H_0 S \tag{4.2.18}$$

Multiplying with $\langle\phi_0^a|$ and $|\phi_1^b\rangle$ from the left and right respectively gives

$$-\langle\phi_0^a| V + V^\dagger |\phi_1^b\rangle = \langle\phi_0^a| SH_0 - H_0 S |\phi_1^b\rangle \tag{4.2.19}$$

Since $V^\dagger$ acts on $|0\rangle$, it will not affect the LHS. Also, $\langle\phi_0^a| V |\phi_1^b\rangle = V_{ab}$. If we now consider only the diagonal part of H_0, we can write $H_0(|\phi_0^a\rangle, |\phi_1^b\rangle) = (E_{0,a}|\phi_0^a\rangle, E_{1,b}|\phi_1^b\rangle))$. We then get

$$\begin{aligned} -V_{ab} &= \langle\phi_0^a| \sum_i \left[S|\phi_1^i\rangle\langle\phi_1^i| H_0 - H_0 |\phi_0^i\rangle\langle\phi_0^i| S \right] |\phi_1^b\rangle \\ &= \sum_i \left[S_{ai} E_1^i \delta_{bi} - E_0^i \delta_{ai} S_{ib} \right] \\ &= S_{ab} E_1^b - E_0^a S_{ab} \\ \implies S_{ab} &= \frac{V_{ab}}{E_0^a - E_1^b} \end{aligned} \tag{4.2.20}$$

where we defined $\langle\phi_0^x| S |\phi_1^y\rangle = S_{xy}$. The total generator is

$$\begin{aligned} S &= \sum_{ij} \left[S_{ij} |\phi_0^i\rangle\langle\phi_1^j| - S_{ij}^\dagger |\phi_1^j\rangle\langle\phi_0^i| \right] \\ &= \sum_{ij} \frac{1}{E_0^i - E_1^j} \left[V_{ij} |\phi_0^i\rangle\langle\phi_1^j| - V_{ij}^\dagger |\phi_1^j\rangle\langle\phi_0^i| \right] \end{aligned} \tag{4.2.21}$$

The renormalization is thus

$$\begin{aligned} \Delta\mathcal{H} &= \frac{1}{2}\left[S, \mathcal{H}_X\right] \\ &= \frac{1}{2}\sum_{ij,kl}\left[\frac{1}{E_0^i - E_1^j}\left(V_{ij}|\phi_0^i\rangle\langle\phi_1^j| - V_{ij}^\dagger|\phi_1^j\rangle\langle\phi_0^i|\right), V_{kl}|\phi_0^k\rangle\langle\phi_1^l| + V_{kl}^\dagger|\phi_1^l\rangle\langle\phi_0^k|\right] \\ &= \frac{1}{2}\sum_{ij,kl}\left[\frac{1}{E_0^i - E_1^j}\left(V_{ij}V_{kl}^\dagger|\phi_0^i\rangle\langle\phi_0^k|\delta_{jl} - V_{ij}^\dagger V_{kl}|\phi_1^j\rangle\langle\phi_1^l|\delta_{ik}\right.\right. \\ &\quad \left.\left. - V_{kl}^\dagger V_{ij}|\phi_1^l\rangle\langle\phi_1^j|\delta_{ki} + V_{kl}V_{ij}^\dagger|\phi_0^k\rangle\langle\phi_0^i|\delta_{lj}\right)\right] \\ &= \frac{1}{2}\sum_{ijk}\left[\frac{1}{E_0^i - E_1^j}\left(V_{ij}V_{kj}^\dagger|\phi_0^i\rangle\langle\phi_0^k| - V_{ij}^\dagger V_{ik}|\phi_1^j\rangle\langle\phi_1^k| - V_{ik}^\dagger V_{ij}|\phi_1^k\rangle\langle\phi_1^j| + V_{kj}V_{ij}^\dagger|\phi_0^k\rangle\langle\phi_0^i|\right)\right] \\ &= \frac{1}{2}\sum_{ijk}\left[\left(\frac{1}{E_0^i - E_1^j} + \frac{1}{E_0^k - E_1^j}\right)V_{ij}V_{kj}^\dagger|\phi_0^i\rangle\langle\phi_0^k| - \left(\frac{1}{E_0^i - E_1^j} + \frac{1}{E_0^i - E_1^k}\right)V_{ij}^\dagger V_{ik}|\phi_1^j\rangle\langle\phi_1^k|\right] \end{aligned} \tag{4.2.22}$$

This is the same as the PMS result eq. 4.1.17. It is easy to see that since this transformation is unitary, it has zero trace so as to preserve the trace of the Hamiltonian:

$$\begin{aligned}\mathrm{Tr}\left[\mathcal{H}\right] &= \sum_l \left(\langle\phi_0^l| + \langle\phi_1^l|\right) \Delta\mathcal{H} \left(|\phi_0^l\rangle + |\phi_1^l\rangle\right) \\ &= \frac{1}{2}\sum_{jl} \frac{2}{E_0^l - E_1^j} V_{lj} V_{lj}^\dagger - \frac{1}{2}\sum_{ji} \frac{2}{E_0^i - E_1^l} V_{il}^\dagger V_{il} \\ &= 0\end{aligned} \tag{4.2.23}$$

We can also make a comparison to the renormalization obtained from URG.

$$\Delta\mathcal{H} = \frac{1}{2}\left[\eta^\dagger - \eta, \mathcal{H}\right] \tag{4.2.24}$$

where

$$\begin{aligned}\eta &= \frac{1}{\omega - \mathcal{H}^d} \sum_{ij} V_{ij} |\phi_0^i\rangle \langle\phi_1^j| = \sum_{ij} \frac{1}{\omega_1^j - E_0^i} V_{ij} |\phi_0^i\rangle \langle\phi_1^j| \\ \implies \eta^\dagger &= \sum_{ij} \frac{1}{\omega_1^j - E_0^i} V_{ij}^\dagger |\phi_1^j\rangle \langle\phi_0^i| \\ \implies \eta^\dagger - \eta &= \sum_{ij} \frac{1}{\omega_1^j - E_0^i} \left(V_{ij}^\dagger |\phi_1^j\rangle \langle\phi_0^i| - V_{ij} |\phi_0^i\rangle \langle\phi_1^j|\right)\end{aligned} \tag{4.2.25}$$

This can be thought of as the generator for the unitary transformations of URG. Comparing with the generator S of eq. 4.2.21, the prescription to go from URG to SWT is to replace $\omega_1^j \to E_1^j$. Doing a similar calculation gives

$$\begin{aligned}\Delta\mathcal{H}_{URG} = \frac{1}{2}\sum_{ijk} \Bigg[&\left(\frac{1}{E_0^i - \omega_1^j} + \frac{1}{E_0^k - \omega_1^j}\right) V_{ij} V_{kj}^\dagger |\phi_0^i\rangle \langle\phi_0^k| \\ &- \left(\frac{1}{E_0^i - \omega_1^j} + \frac{1}{E_0^i - \omega_1^k}\right) V_{ij}^\dagger V_{ik} |\phi_1^j\rangle \langle\phi_1^k| \Bigg]\end{aligned} \tag{4.2.26}$$

SIAM URG vs SIAM SWT

The SWT for the single-impurity Anderson model is briefly sketched below. In order to decouple a state $q\beta$ from the SIAM ($\epsilon_q > 0$) , we take an ansatz $S = (A + B\hat{n}_{d\bar{\beta}})(c_{q\beta}^\dagger c_{d\beta} - \text{h.c.})$. Plugging this into the decoupling condition gives

$$-\epsilon_q \left(A + B\hat{n}_{d\bar{\beta}}\right) + \epsilon_d \left(A + B\hat{n}_{d\bar{\beta}}\right) + U\left(A + B\right)\hat{n}_{d\bar{\beta}} = -V \tag{4.2.27}$$

which gives

$$S = V\left[\frac{1-\hat{n}_{d\bar{\beta}}}{\epsilon_q-\epsilon_d}+\frac{\hat{n}_{d\bar{\beta}}}{\epsilon_q-\epsilon_d-U}\right](c^\dagger_{q\beta}c_{d\beta}-\text{h.c.}) \tag{4.2.28}$$

The remaining diagonal part constitutes the effective Hamiltonian.

$$\begin{aligned} U\mathcal{H}U^\dagger = H_1 &= \mathcal{H}_0+\frac{1}{2}\left\{\mathcal{H}_0,S^2\right\}-S\mathcal{H}_0S+\left[S,\mathcal{H}_X\right] \\ &= \mathcal{H}_0+\frac{1}{2}\left[\left[\mathcal{H}_0,S\right],S\right]+\left[S,\mathcal{H}_X\right] \\ &= \mathcal{H}_0+\frac{1}{2}\left[\mathcal{H}_X,S\right]+\left[S,\mathcal{H}_X\right] \\ &= \mathcal{H}_0+\frac{1}{2}\left[S,\mathcal{H}_X\right] \end{aligned} \tag{4.2.29}$$

For the SIAM (and noting that we are decoupling $q\beta$), the two parts are

$$\begin{aligned} \mathcal{H}_0 &= \sum_{k\sigma}\epsilon_k\hat{n}_{k\sigma}+\epsilon_d\hat{n}_d+U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}+\sum_{k\sigma\neq q\beta}\left(c^\dagger_{k\sigma}c_{d\sigma}+\text{h.c.}\right) \\ \mathcal{H}_X &= c^\dagger_{q\beta}c_{d\beta}+\text{h.c.} \end{aligned} \tag{4.2.30}$$

The renormalization in the effective Hamiltonian from decoupling a high energy particle state is thus

$$\begin{aligned} \frac{1}{2}\left[S,\mathcal{H}_X\right]\Big|_{\hat{n}_{q\beta}=0} &= |V|^2\left[\frac{1-\hat{n}_{d\bar{\beta}}}{\epsilon_q-\epsilon_d}+\frac{\hat{n}_{d\bar{\beta}}}{\epsilon_q-\epsilon_d-U}\right]\left[\hat{n}_{q\beta}\left(1-\hat{n}_{d\beta}\right)-\hat{n}_{d\beta}\left(1-\hat{n}_{q\beta}\right)\right]\Big|_{\hat{n}_{q\beta}=0} \\ &= -\hat{n}_{d\beta}|V|^2\left[\frac{1-\hat{n}_{d\bar{\beta}}}{\epsilon_q-\epsilon_d}+\frac{\hat{n}_{d\bar{\beta}}}{\epsilon_q-\epsilon_d-U}\right] \end{aligned} \tag{4.2.31}$$

In the last step, we put $\hat{n}_{q\beta}=0$ because previously we assumed $\epsilon_q>0$ and high energy virtual excitations above the Fermi surface must necessarily be vacant in the initial state (at $T=0$). We can obtain the renormalization from decoupling a high energy *hole* state directly from this expression, just by choosing $\hat{n}_{q\beta}=1$ and setting $\epsilon_q\to-\epsilon_q$.

$$\frac{1}{2}\left[S,\mathcal{H}_X\right]\Big|_{\hat{n}_{q\beta}=1} = -\left(1-\hat{n}_{d\beta}\right)|V|^2\left[\frac{1-\hat{n}_{d\bar{\beta}}}{\epsilon_q+\epsilon_d}+\frac{\hat{n}_{d\bar{\beta}}}{\epsilon_q+\epsilon_d+U}\right] \tag{4.2.32}$$

These two results - the renormalization in the particle and hole sectors - is identical to the result (see [12]) obtained from PMS of the SIAM. The renormalizations in the various energy levels of the impurity can be read off now, after summing over all states in the

interval we are decoupling.

$$\begin{aligned}\Delta E_2 &= -2\sum_q \frac{|V_q|^2}{\epsilon_q - \epsilon_d - U}\\ \Delta E_1 &= -\sum_q \frac{|V_q|^2}{\epsilon_q - \epsilon_d} - \sum_q \frac{|V_q|^2}{\epsilon_q + \epsilon_d + U}\\ \Delta E_0 &= -2\sum_q \frac{|V_q|^2}{\epsilon_q + \epsilon_d}\end{aligned} \tag{4.2.33}$$

This can be compared with the URG result, eq. 5.1.12,

$$\begin{aligned}\Delta E_2 &= 2\sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d + U}\\ \Delta E_1 &= \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d - U} + \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d}\\ \Delta E_0 &= 2\sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d}\end{aligned} \tag{4.2.34}$$

We can transform the URG result to the SWT result if we ignore the effect of the quantum fluctuations in ω (arising from the presence of the off-diagonal term $\mathcal{H}^i$) and replace it with the renormalised diagonal value of $-\frac{1}{2}\epsilon_q$. This means that SWT tracks the effect of the off-diagonal terms only in the numerator. Of course, all this assumes we are doing an iterative SWT instead of a one-shot SWT; the latter is the conventional way. A second difference is that URG has a Green's function like structure in the renormalization such that a fixed point is reached when the diagonal part $\mathcal{H}^d$ matches one of the eigenvalues of ω (see 3.1.6). SWT does not have such a fixed point structure.

Another point to note is that decoupling a single electron does not generate all the charge-charge or spin-spin interactions that come out when one performs a one-shot SWT. This implies that such terms are a result of decoupling the non-local interactions of the impurity (it is talking to all the mobile electrons), and cannot be generated when we remove just the local interactions of the mobile electrons. Instead, if one performs a URG in which we non-perturbatively kill the 2-point vertices in the SIAM, such 4-point vertices are generated. This is shown in the next subsection.

4.2.1 Obtaining the Kondo model from the SIAM via a one-shot URG

Here we will show how we can obtain the spin-spin interaction of the Kondo model by performing a one-shot URG on the SIAM. This should justify that the action of performing an SWT is analogous to decoupling the whole band via URG.

There are three departures from the conventional way of doing URG (or PMS).

- We will be severing the connections of the impurity with all the mobile electrons in one-shot, and not iteratively.
- We will have to trivialize the quantum fluctuation operator $\hat{\omega}$ by replacing it with the diagonal part of the initial state energy.

Since we are decoupling the whole band, the off-diagonal part that we want to remove is

$$\mathcal{H}^I = \sum_{k\sigma} \left[V_k c^\dagger_{k\sigma} c_{d\sigma} + \text{h.c.} \right] \tag{4.2.35}$$

The diagonal part is the rest of the Hamiltonian.

$$\begin{aligned} \mathcal{H}^d &= \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \epsilon_d \hat{n}_d + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \\ &= \sum_{k\sigma} \epsilon_k \tau_{k\sigma} + \epsilon_d \hat{n}_d + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \end{aligned} \tag{4.2.36}$$

Following eq. 3.1.47, the renormalization is

$$\Delta\mathcal{H} = \frac{1}{2} \left[\eta^\dagger - \eta, \mathcal{H}_X \right] \tag{4.2.37}$$

The transition operator η is

$$\begin{aligned} \eta &= \frac{1}{\omega - \mathcal{H}^d} \sum_{k\sigma} V_k^* c^\dagger_{d\sigma} c_{k\sigma} \\ &= \sum_{k\sigma} \frac{1}{\omega + \frac{1}{2}\epsilon_k - \epsilon_d - \left(\epsilon_d + U\right) \hat{n}_{d\bar{\sigma}}} V_k^* c^\dagger_{d\sigma} c_{k\sigma} \\ &= \sum_{k\sigma} \left[\frac{\hat{n}_{d\bar{\sigma}}}{\omega_1 + \frac{1}{2}\epsilon_k - 2\epsilon_d - U} + \frac{1 - \hat{n}_{d\bar{\sigma}}}{\omega_0 + \frac{1}{2}\epsilon_k - \epsilon_d} \right] V_k^* c^\dagger_{d\sigma} c_{k\sigma} \\ &= \sum_{k\sigma} \left[\frac{\hat{n}_{d\bar{\sigma}}}{E_k^1} + \frac{1 - \hat{n}_{d\bar{\sigma}}}{E_k^0} \right] V_k^* c^\dagger_{d\sigma} c_{k\sigma} \end{aligned} \tag{4.2.38}$$

where $E_k^1 = \omega_1 + \frac{1}{2}\epsilon_k - 2\epsilon_d - U$ and $E_k^0 = \omega_0 + \frac{1}{2}\epsilon_k - \epsilon_d$. The total generator is therefore

$$\eta^\dagger - \eta = \sum_{k\sigma} \left[\frac{\hat{n}_{d\bar{\sigma}}}{E_k^1} + \frac{1 - \hat{n}_{d\bar{\sigma}}}{E_k^0} \right] \left(V_k c^\dagger_{k\sigma} c_{d\sigma} - V_k^* c^\dagger_{d\sigma} c_{k\sigma} \right) \tag{4.2.39}$$

The renormalization is

$$\Delta\mathcal{H}(\omega_1, \omega_0) = \frac{1}{2} \sum_{kq\sigma\alpha} \left[\left(\frac{\hat{n}_{d\bar{\sigma}}}{E_k^1} + \frac{1 - \hat{n}_{d\bar{\sigma}}}{E_k^0} \right) \left(V_k c^\dagger_{k\sigma} c_{d\sigma} - V_k^* c^\dagger_{d\sigma} c_{k\sigma} \right), V_q c^\dagger_{q\alpha} c_{d\alpha} + V_q^* c^\dagger_{d\alpha} c_{q\alpha} \right] \tag{4.2.40}$$

The summation has two parts, $\Delta_{1,2}$ - one where $\sigma = \alpha$ and another where $\sigma = \overline{\alpha}$. The first part Δ_1 gives

$$\begin{aligned}
\Delta_1 &= \frac{1}{2}\sum_{kq\sigma=\alpha}\left[\left(\frac{\hat{n}_{d\overline{\sigma}}}{E_k^1}+\frac{1-\hat{n}_{d\overline{\sigma}}}{E_k^0}\right)\left(V_k c_{k\sigma}^\dagger c_{d\sigma} - V_k^* c_{d\sigma}^\dagger c_{k\sigma}\right), V_q c_{q\sigma}^\dagger c_{d\sigma} + V_q^* c_{d\sigma}^\dagger c_{q\sigma}\right] \\
&= \frac{1}{2}\sum_{kq\sigma}\left(\frac{\hat{n}_{d\overline{\sigma}}}{E_k^1}+\frac{1-\hat{n}_{d\overline{\sigma}}}{E_k^0}\right)\left[V_k c_{k\sigma}^\dagger c_{d\sigma} - V_k^* c_{d\sigma}^\dagger c_{k\sigma}, V_q c_{q\sigma}^\dagger c_{d\sigma} + V_q^* c_{d\sigma}^\dagger c_{q\sigma}\right] \\
&= \frac{1}{2}\sum_{kq\sigma}\left(\frac{\hat{n}_{d\overline{\sigma}}}{E_k^1}+\frac{1-\hat{n}_{d\overline{\sigma}}}{E_k^0}\right)\left\{V_k V_q^*\left[c_{k\sigma}^\dagger c_{d\sigma}, V_q^* c_{d\sigma}^\dagger c_{q\sigma}\right] - V_k^* V_q\left[c_{d\sigma}^\dagger c_{k\sigma}, c_{q\sigma}^\dagger c_{d\sigma}\right]\right\} \\
&= \frac{1}{2}\sum_{kq\sigma}\left(\frac{\hat{n}_{d\overline{\sigma}}}{E_k^1}+\frac{1-\hat{n}_{d\overline{\sigma}}}{E_k^0}\right)\left\{V_k V_q^*\left[c_{k\sigma}^\dagger c_{d\sigma}, V_q^* c_{d\sigma}^\dagger c_{q\sigma}\right] + V_k^* V_q\left[c_{q\sigma}^\dagger c_{d\sigma}, c_{d\sigma}^\dagger c_{k\sigma}\right]\right\} \\
&= \frac{1}{2}\sum_{kq\sigma}\left[\hat{n}_{d\overline{\sigma}}\left(\frac{1}{E_k^1}+\frac{1}{E_q^1}\right)+\left(1-\hat{n}_{d\overline{\sigma}}\right)\left(\frac{1}{E_k^0}+\frac{1}{E_q^0}\right)\right] V_k V_q^*\left[c_{k\sigma}^\dagger c_{d\sigma}, c_{d\sigma}^\dagger c_{q\sigma}\right] \\
&= \sum_{kq\sigma}\left[\frac{1}{2}V_k V_q^*\left(\frac{1}{E_k^0}+\frac{1}{E_q^0}\right)+\hat{n}_{d\overline{\sigma}}\frac{1}{2}V_k V_q^*\left(\frac{1}{E_k^1}+\frac{1}{E_q^1}-\frac{1}{E_k^0}-\frac{1}{E_q^0}\right)\right]\left(c_{k\sigma}^\dagger c_{q\sigma} - c_{d\sigma}^\dagger c_{d\sigma}\delta_{kq}\right)
\end{aligned} \tag{4.2.41}$$

We can now define two new energy scales:

$$W_{kq} = \frac{1}{2}V_k V_q^*\left(\frac{1}{E_k^0}+\frac{1}{E_q^0}\right), \qquad J_{kq} = \frac{1}{2}V_k V_q^*\left(\frac{1}{E_k^1}+\frac{1}{E_q^1}-\frac{1}{E_k^0}-\frac{1}{E_q^0}\right) \tag{4.2.42}$$

The renormalization Δ_1 becomes

$$\begin{aligned}
\Delta_1 &= \sum_{kq\sigma}\left[W_{kq}+\hat{n}_{d\overline{\sigma}}J_{kq}\right]\left(c_{k\sigma}^\dagger c_{q\sigma} - c_{d\sigma}^\dagger c_{d\sigma}\delta_{kq}\right) \\
&= \sum_{kq\sigma}\left[W_{kq}+\hat{n}_{d\overline{\sigma}}J_{kq}\right]c_{k\sigma}^\dagger c_{q\sigma} - \sum_{k\sigma}\left[W_{kk}+\hat{n}_{d\overline{\sigma}}J_{kk}\right]\hat{n}_{d\sigma} \\
&= \sum_{kq\sigma}\left[W_{kq}+\frac{1}{2}\hat{n}_d J_{kq}\right]c_{k\sigma}^\dagger c_{q\sigma} - \sum_{kq\sigma}\sigma J_{kq}S_d^z c_{k\sigma}^\dagger c_{q\sigma} - \sum_{k\sigma}\left[W_{kk}+\hat{n}_{d\overline{\sigma}}J_{kk}\right]\hat{n}_{d\sigma}
\end{aligned} \tag{4.2.43}$$

There we exchanged $\hat{n}_{d\overline{\sigma}}$ for S_d^z and $\hat{n}_d$, in the first term, by using the definitions $\hat{n}_{d\sigma}+\hat{n}_{d\overline{\sigma}} = \hat{n}_{d\sigma}$ and $\hat{n}_{d\sigma} - \hat{n}_{d\overline{\sigma}} = 2\sigma S_d^z$.

The second term in the summation comes from the choice $\sigma = \overline{\alpha}$.

$$\begin{aligned}
\Delta_2 &= \frac{1}{2}\sum_{kq\overline{\sigma}=\alpha}\left[\left(\frac{\hat{n}_{d\overline{\sigma}}}{E_k^1}+\frac{1-\hat{n}_{d\overline{\sigma}}}{E_k^0}\right)\left(V_k c_{k\sigma}^\dagger c_{d\sigma}-V_k^* c_{d\sigma}^\dagger c_{k\sigma}\right), V_q c_{q\overline{\sigma}}^\dagger c_{d\overline{\sigma}}+V_q^* c_{d\overline{\sigma}}^\dagger c_{q\overline{\sigma}}\right] \\
&= \frac{1}{2}\sum_{kq\sigma}\left(V_k c_{k\sigma}^\dagger c_{d\sigma}-V_k^* c_{d\sigma}^\dagger c_{k\sigma}\right)\left[\frac{\hat{n}_{d\overline{\sigma}}}{E_k^1}+\frac{1-\hat{n}_{d\overline{\sigma}}}{E_k^0}, V_q c_{q\overline{\sigma}}^\dagger c_{d\overline{\sigma}}+V_q^* c_{d\overline{\sigma}}^\dagger c_{q\overline{\sigma}}\right] \\
&= \frac{1}{2}\sum_{kq\sigma}\left(V_k c_{k\sigma}^\dagger c_{d\sigma}-V_k^* c_{d\sigma}^\dagger c_{k\sigma}\right)\left(V_q^* c_{d\overline{\sigma}}^\dagger c_{q\overline{\sigma}}-V_q c_{q\overline{\sigma}}^\dagger c_{d\overline{\sigma}}\right)\left(\frac{1}{E_k^1}-\frac{1}{E_k^0}\right) \\
&= \frac{1}{2}\sum_{kq\sigma}\left(V_k V_q^* c_{k\sigma}^\dagger c_{d\sigma} c_{d\overline{\sigma}}^\dagger c_{q\overline{\sigma}}-V_k V_q c_{k\sigma}^\dagger c_{d\sigma} c_{q\overline{\sigma}}^\dagger c_{d\overline{\sigma}}-V_k^* V_q^* c_{d\sigma}^\dagger c_{k\sigma} c_{d\overline{\sigma}}^\dagger c_{q\overline{\sigma}}+V_k^* V_q c_{d\sigma}^\dagger c_{k\sigma} c_{q\overline{\sigma}}^\dagger c_{d\overline{\sigma}}\right) \\
&\times\left(\frac{1}{E_k^1}-\frac{1}{E_k^0}\right)
\end{aligned} \tag{4.2.44}$$

We now use the following trick to combine the first and fourth terms:

$$\begin{aligned}
&\frac{1}{2}\sum_{kq\sigma}\left(V_k V_q^* c_{k\sigma}^\dagger c_{d\sigma} c_{d\overline{\sigma}}^\dagger c_{q\overline{\sigma}}+V_k^* V_q c_{d\sigma}^\dagger c_{k\sigma} c_{q\overline{\sigma}}^\dagger c_{d\overline{\sigma}}\right)\times\left(\frac{1}{E_k^1}-\frac{1}{E_k^0}\right) \\
&= \frac{1}{2}\sum_{kq\sigma} V_k V_q^* c_{k\sigma}^\dagger c_{d\sigma} c_{d\overline{\sigma}}^\dagger c_{q\overline{\sigma}}\left(\frac{1}{E_k^1}-\frac{1}{E_k^0}\right)+\frac{1}{2}\sum_{kq\sigma} V_k^* V_q c_{d\sigma}^\dagger c_{k\sigma} c_{q\overline{\sigma}}^\dagger c_{d\overline{\sigma}}\left(\frac{1}{E_k^1}-\frac{1}{E_k^0}\right) \\
&= \frac{1}{2}\sum_{kq\sigma} V_k V_q^* c_{k\sigma}^\dagger c_{d\sigma} c_{d\overline{\sigma}}^\dagger c_{q\overline{\sigma}}\left(\frac{1}{E_k^1}-\frac{1}{E_k^0}\right)+\frac{1}{2}\sum_{qk\sigma} V_q^* V_k c_{d\overline{\sigma}}^\dagger c_{q\overline{\sigma}} c_{k\sigma}^\dagger c_{d\sigma}\left(\frac{1}{E_q^1}-\frac{1}{E_q^0}\right) \\
&= -\sum_{kq\sigma} J_{kq} c_{k\sigma}^\dagger c_{q\overline{\sigma}} c_{d\overline{\sigma}}^\dagger c_{d\sigma}
\end{aligned} \tag{4.2.45}$$

In the penultimate step, we interchanged the dummy indices k and q and changed $\sigma \leftrightarrow \overline{\sigma}$ in the second term.

Similarly, for the second term, we get

$$\begin{aligned}
&\frac{1}{2}\sum_{kq\sigma} V_k V_q c_{k\sigma}^\dagger c_{d\sigma} c_{q\overline{\sigma}}^\dagger c_{d\overline{\sigma}}\left(\frac{1}{E_k^1}-\frac{1}{E_k^0}\right) \\
&= \frac{1}{4}\sum_{kq\sigma}\left[V_k V_q\left(\frac{1}{E_k^1}-\frac{1}{E_k^0}\right) c_{k\sigma}^\dagger c_{d\sigma} c_{q\overline{\sigma}}^\dagger c_{d\overline{\sigma}}+\underbrace{V_k V_q\left(\frac{1}{E_k^1}-\frac{1}{E_k^0}\right) c_{k\overline{\sigma}}^\dagger c_{d\overline{\sigma}} c_{q\sigma}^\dagger c_{d\sigma}}_{\sigma\leftrightarrow\overline{\sigma}}\right]
\end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{4}\sum_{kq\sigma}\left[V_k V_q\left(\frac{1}{E_k^1}-\frac{1}{E_k^0}\right)c_{k\sigma}^\dagger c_{d\sigma}c_{q\bar{\sigma}}^\dagger c_{d\bar{\sigma}} + \underbrace{V_q V_k\left(\frac{1}{E_q^1}-\frac{1}{E_q^0}\right)c_{q\bar{\sigma}}^\dagger c_{d\bar{\sigma}}c_{k\sigma}^\dagger c_{d\sigma}}_{k\leftrightarrow q}\right]\\
&= \sum_{kq\sigma} V_k V_q \frac{1}{4}\left(\frac{1}{E_k^1}-\frac{1}{E_k^0}+\frac{1}{E_q^1}-\frac{1}{E_q^0}\right)c_{k\sigma}^\dagger c_{d\sigma}c_{q\bar{\sigma}}^\dagger c_{d\bar{\sigma}}\\
&= \frac{1}{2}\sum_{kq\sigma} K_{kq}c_{k\sigma}^\dagger c_{d\sigma}c_{q\bar{\sigma}}^\dagger c_{d\bar{\sigma}}
\end{aligned}
$$

where K_{kq} is yet another energy scale.

$$
K_{kq} = \frac{1}{2}V_k V_q\left(\frac{1}{E_k^1}-\frac{1}{E_k^0}+\frac{1}{E_q^1}-\frac{1}{E_q^0}\right) \tag{4.2.46}
$$

The third term gives

$$
\frac{1}{2}\sum_{kq\sigma} V_k^* V_q^* c_{d\sigma}^\dagger c_{k\sigma}c_{d\bar{\sigma}}^\dagger c_{q\bar{\sigma}}\left(\frac{1}{E_k^1}-\frac{1}{E_k^0}\right) = \sum_{kq\sigma} K_{kq}c_{d\sigma}^\dagger c_{k\sigma}c_{d\bar{\sigma}}^\dagger c_{q\bar{\sigma}} \tag{4.2.47}
$$

The total renormalization can thus be written as

$$
\begin{aligned}
\Delta\mathcal{H}(\omega_1,\omega_0) = &-\sum_{k\sigma}\left[W_{kk}+\hat{n}_{d\bar{\sigma}}J_{kk}\right]\hat{n}_{d\sigma} && \left[\text{renormalization in } \epsilon_d, U\right]\\
&+\sum_{kq\sigma}\left[W_{kq}+\frac{1}{2}\hat{n}_d J_{kq}\right]c_{k\sigma}^\dagger c_{q\sigma} && \left[\text{potential scattering}\right]\\
&-\sum_{kq\sigma}J_{kq}\left[S_d^z\sigma c_{k\sigma}^\dagger c_{q\sigma}+\sum_{kq\sigma}J_{kq}c_{k\sigma}^\dagger c_{q\bar{\sigma}}c_{d\bar{\sigma}}^\dagger c_{d\sigma}\right] && \left[\text{spin Kondo}\right]\\
&+\sum_{kq\sigma}K_{kq}c_{k\sigma}^\dagger c_{d\sigma}c_{q\bar{\sigma}}^\dagger c_{d\bar{\sigma}}+\text{h.c.} && \left[\text{charge Kondo}\right]
\end{aligned} \tag{4.2.48}
$$

Note that this renormalization is in a particular eigendirection of the total quantum fluctuation operator $\hat{\omega}$. In other words, the single perturbative J_{kq} has been replaced with 2^N scales, each with its own value of ω. This is where the complexity has been transferred in going from the second-order SWT to the non-perturbative URG. The new energy scales

are thus the non-perturbative variants of the ones generated in SWT.

$$\begin{aligned}
W_{kq}^{SWT} &= \frac{1}{2}V_k V_q^* \left(\frac{1}{\epsilon_k - \epsilon_d} + \frac{1}{\epsilon_q - \epsilon_d}\right) \\
J_{kq}^{SWT} &= \frac{1}{2}V_k V_q^* \left(\frac{1}{\epsilon_k - \epsilon_d - U} + \frac{1}{\epsilon_q - \epsilon_d - U} - \frac{1}{\epsilon_k - \epsilon_d} - \frac{1}{\epsilon_q - \epsilon_d}\right) \\
W_{kq}^{URG}(\omega) &= \frac{1}{2}V_k V_q^* \left(\frac{1}{\omega_0 + \frac{1}{2}\epsilon_k - \epsilon_d} + \frac{1}{\omega_0 + \frac{1}{2}\epsilon_q - \epsilon_d}\right) \\
J_{kq}^{URG}(\omega) &= \frac{1}{2}V_k V_q^* \left(\frac{1}{\omega_1 + \epsilon_k - \epsilon_d - U} + \frac{1}{\omega_1 + \epsilon_q - \epsilon_d - U} - \frac{1}{\omega_0 + \epsilon_k - \epsilon_d} - \frac{1}{\omega_0 + \epsilon_q - \epsilon_d}\right)
\end{aligned} \tag{4.2.49}$$

To recover the SWT scales from the URG ones, we have to substitute each ω_i by the energy of the initial state to which it corresponds. From eq. 4.2.38, we note that ω_1 refers to the initial state in which $\hat{n}_{k\sigma} = \hat{n}_{d\overline{\sigma}} = 1 - \hat{n}_{d\sigma} = 1$. Therefore, $\omega_1 = \frac{1}{2}\epsilon_k + \epsilon_d$. Similarly, ω_0 refers to the initial state in which $\hat{n}_{k\sigma} = 1 - \hat{n}_{d\overline{\sigma}} = 1 - \hat{n}_{d\sigma} = 1$. Therefore, $\omega_0 = \frac{1}{2}\epsilon_k$. Substituting these into the URG energy scales gives back the SWT scales.

4.3 CUT RG

Formalism

The following equation generates a family of unitary Hamiltonians.

$$\frac{\mathrm{d}\mathcal{H}(l)}{\mathrm{d}l} = \left[\mathcal{H}, \eta(l)\right] \tag{4.3.1}$$

To prove the unitarity[30], we construct the unitary operator $U(l)$ that connects the Hamiltonians $\mathcal{H}(l)$ and $\mathcal{H}(l=0)$. Let $\mathcal{H}(l) = U(l)\mathcal{H}(l=0)U^\dagger(l)$, where $U(l)$ is defined by

$$\eta(l) = \frac{\mathrm{d}U}{\mathrm{d}l}U^\dagger = -U\frac{\mathrm{d}U^\dagger}{\mathrm{d}l} \quad \left[UU^\dagger = 1 \implies \frac{\mathrm{d}\left(UU^\dagger\right)}{\mathrm{d}l} = 0\right] \tag{4.3.2}$$

This will give

$$\begin{aligned}
\frac{\mathrm{d}\mathcal{H}(l)}{\mathrm{d}l} &= \frac{\mathrm{d}U}{\mathrm{d}l}\mathcal{H}(0)U^\dagger(l) + U\mathcal{H}(0)\frac{\mathrm{d}U^\dagger}{\mathrm{d}l} \\
&= \frac{\mathrm{d}U}{\mathrm{d}l}U^\dagger\mathcal{H}(l) + \mathcal{H}(l)U\frac{\mathrm{d}U(l)^\dagger}{\mathrm{d}l} \\
&= \eta(l)\mathcal{H}(l) - \mathcal{H}(l)\eta(l) \\
&= \left[\eta(l), \mathcal{H}(l)\right]
\end{aligned} \tag{4.3.3}$$

This proves that the family of Hamiltonians $\mathcal{H}(l)$ satisfy the flow equation eq. 4.3.1. $\eta(l)$ is referred to as the generator of the flow equation. It is chosen so as to reduce the off-diagonal part of the Hamiltonian, either progressively or in one shot. In Schrieffer-Wolff

transformation, the transformation is one-shot, and the η there is the S that sits on top of the exponential in the unitary transformation. In URG, the generator to decouple one electron $q\beta$ is $\eta^\dagger_{q\beta} - \eta_{q\beta}$.

In CUT (Continuous Unitary Transformation) RG [31], we progressively block-diagonalize the Hamiltonian by removing off-diagonal terms that are farthest from the diagonal, through infinitesimal unitary transformations. The change is described as a flow against the parameter l. The canonical choice of the generator is $\eta(l) = \left[\mathcal{H}_d, \mathcal{H}_X\right]$, where $\mathcal{H}_d$ is the diagonal part of the Hamiltonian and $\mathcal{H}_X = \mathcal{H} - \mathcal{H}_d$ is the off-diagonal part of the Hamiltonian. Therefore,

$$\frac{\mathrm{d}\mathcal{H}}{\mathrm{d}l} = \left[\left[\mathcal{H}_d(l), \mathcal{H}_X(l)\right], \mathcal{H}(l)\right] \tag{4.3.4}$$

To see how this choice of the generator results in a decay of the off-diagonal terms, we can consider a simple 2-particle Hamiltonian:

$$\mathcal{H} = \sum_i \epsilon_i \hat{n}_i + \sum_{i\neq j} g_{ij} c_i^\dagger c_j \tag{4.3.5}$$

where $g^*_{ij} = g_j i$. The canonical generator then turns out to be

$$\eta = \left[\sum_i \epsilon_i \hat{n}_i, \sum_{j\neq k} g_{jk} c_j^\dagger c_k\right] = \sum_{k\neq i} \epsilon_i \left[g_{ik} c_i^\dagger c_k - g_{ki} c_k^\dagger c_i\right] = \sum_{k\neq i} g_{ik} c_i^\dagger c_k \left(\epsilon_i - \epsilon_k\right) \tag{4.3.6}$$

and the renormalization in the Hamiltonian is

$$\frac{d\mathcal{H}}{dl} = \left[\eta, \mathcal{H}\right] = \left[\sum_{k\neq i} g_{ik} c_i^\dagger c_k \left(\epsilon_i - \epsilon_k\right), \sum_i \epsilon_i \hat{n}_i + \sum_{i\neq j} g_{ij} c_i^\dagger c_j\right] \tag{4.3.7}$$

The first commutator gives

$$-\sum_{i\neq k} g_{ik} \left(\epsilon_i - \epsilon_k\right)^2 c_i^\dagger c_k \tag{4.3.8}$$

The second commutator gives

$$\sum_{\substack{k\neq i \\ j}} \left[g_{kj} g_{ik} \left(\epsilon_i - \epsilon_k\right) c_i^\dagger c_j + g_{ji} g_{ik} \left(\epsilon_k - \epsilon_i\right) c_j^\dagger c_k\right] = \sum_{\substack{k\neq i \\ j}} g_{ik} g_{kj} \left(\epsilon_i + \epsilon_j - 2\epsilon_k\right) c_i^\dagger c_j \tag{4.3.9}$$

The total renormalization is

$$\frac{d\mathcal{H}}{dl} = -\sum_{i\neq j} g_{ij} \left(\epsilon_i - \epsilon_j\right)^2 c_i^\dagger c_j + \sum_{\substack{k\neq i \\ j}} g_{ik} g_{kj} \left(\epsilon_i + \epsilon_j - 2\epsilon_k\right) c_i^\dagger c_j \tag{4.3.10}$$

The couplings renormalize as

$$\begin{aligned} \frac{\mathrm{d}\epsilon_i}{\mathrm{d}l} &= \sum_{k\neq i} 2|g_{ik}|^2 \left(\epsilon_i - \epsilon_k\right) \\ \frac{\mathrm{d}g_{ij}}{\mathrm{d}l} &= -g_{ij} \left(\epsilon_i - \epsilon_j\right)^2 + \sum_{k\neq i} g_{ik} g_{kj} \left(\epsilon_i + \epsilon_j - 2\epsilon_k\right) \end{aligned} \tag{4.3.11}$$

To see the decay of the off-diagonal terms, first we will relate the off-diagonal flow to the diagonal flow using the invariance of the trace under a unitary transformation:

$$0 = \frac{\mathrm{dTr}\left(\mathcal{H}\right)^2}{\mathrm{d}l} = \frac{\mathrm{dTr}\left(\mathcal{H}\right)^2}{\mathrm{d}l} = \sum_i \frac{\mathrm{d}\epsilon_i^2}{\mathrm{d}l} + \sum_{i\neq j} \frac{\mathrm{d}|g_{ij}|^2}{\mathrm{d}l} \implies \sum_{i\neq j} \frac{\mathrm{d}|g_{ij}|^2}{\mathrm{d}l} = -\sum_i \frac{\mathrm{d}\epsilon_i^2}{\mathrm{d}l} \tag{4.3.12}$$

From the flow equation, we can see that

$$\sum_i \frac{\mathrm{d}\epsilon_i^2}{\mathrm{d}l} = 2\sum_{i\neq k} \epsilon_i \frac{\mathrm{d}\epsilon_i}{\mathrm{d}l} = 2\sum_i |g_{ik}|^2 \left(\epsilon_i - \epsilon_k\right)^2 \geq 0 \tag{4.3.13}$$

Therefore,

$$\sum_{i\neq j} \frac{\mathrm{d}|g_{ij}|^2}{\mathrm{d}l} \leq 0 \tag{4.3.14}$$

This implies that at $l \to \infty$, the only off-diagonal terms that survive are those with g_{ij} that scatter between degenerate states, that is, those with $\epsilon_i - \epsilon_j = 0$.

To get a feel for the method, we will apply it on the Fröhlick Hamiltonian to remove the electron-phonon coupling term.

$$\mathcal{H} = \mathcal{H}_d + \mathcal{H}_X \tag{4.3.15}$$

where $\mathcal{H}_X$ is the electron-phonon coupling term

$$\sum_{kq} g_q b_{-q}^\dagger c_{k+q,\sigma}^\dagger c_{k\sigma} + \mathrm{h.c.} \tag{4.3.16}$$

and-1 $\mathcal{H}_d = \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_q \hbar\omega_q b_q^\dagger b_q$ is the kinetic energy of the electron and phonons. We assume time-reversal invariance such that $\omega_q = \omega_{-q}$. We choose

$$\eta(l) = \left[\mathcal{H}_d, \mathcal{H}\right] = \left[\mathcal{H}_d, \mathcal{H}_X\right] \tag{4.3.17}$$

It is easy to compute the commutators.

$$\begin{aligned} \left[\sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma}, \sum_{kq\sigma} b_{-q}^\dagger c_{k+q,\sigma}^\dagger c_{k\sigma}\right] &= \sum_{kq\sigma} g_q \left(\epsilon_{k+q} - \epsilon_k\right) g_q b_{-q}^\dagger c_{k+q,\sigma}^\dagger c_{k\sigma} \\ \left[\sum_q \hbar\omega_q b_q^\dagger b_q, \sum_{kq} g_q b_{-q}^\dagger c_{k+q,\sigma}^\dagger c_{k\sigma}\right] &= \sum_{kq} g_q \hbar\omega_q b_{-q}^\dagger c_{k+q,\sigma}^\dagger c_{k\sigma} \end{aligned} \tag{4.3.18}$$

Therefore,

$$\eta = \sum_{kq\sigma} g_q \left(\epsilon_{k+q} - \epsilon_k + \hbar\omega_q\right) b_{-q}^\dagger c_{k+q,\sigma}^\dagger c_{k\sigma} - \mathrm{h.c.} \tag{4.3.19}$$

We define $\xi \equiv \epsilon_{k+q} - \epsilon_k + \hbar\omega_q$. The renormalization in the total Hamiltonian becomes

$$\frac{\mathrm{d}\mathcal{H}}{\mathrm{d}l} = \left[\eta, \mathcal{H}\right] \tag{4.3.20}$$

The flow equation for the electron-phonon coupling is

$$\frac{\mathrm{d}g_q}{\mathrm{d}l} = -\xi^2 g_q \implies g_q(l) = g_q(0)\exp\left(-\xi^2 l\right) \tag{4.3.21}$$

A new electron-electron coupling $V_{kk^q} c^\dagger_{k+q} c^\dagger_{k'-q} c_{k'} c_k$ is also generated. For the Cooper channel ($k' = -k$), the flow equation is

$$V_{k,-k,q}(\infty) = V_{k,-k,-q}(0) - \frac{g_q^2 \omega_q}{\omega_q^2 + \left(\epsilon_{k+q} - \epsilon_k\right)^2} \tag{4.3.22}$$

Off-diagonal terms that connect larger energy differences ξ decay the fastest.

CUT RG from URG

We will now see that the renormalization in URG can also be put into a similar form. From eq. 3.1.47, we can write the URG renormalization in the diagonal part as

$$\Delta\mathcal{H}^0 = \frac{1}{2}\left[\eta^\dagger - \eta, \mathcal{H}\right] \tag{4.3.23}$$

where $\mathcal{H}^0 = \mathcal{H}^d + \mathcal{H}^i$. The URG generator can be recast (starting from the definitions of η, eqs. 3.1.14) as

$$\begin{aligned}
\eta^\dagger - \eta &= G_1 c^\dagger T - G_0 T^\dagger c \\
&= \frac{1}{\omega_1 - \omega_0}\left[G_1\left(\omega_1 - \omega_0\right) c^\dagger T - G_0\left(\omega_1 - \omega_0\right) T^\dagger c\right] \\
&= \frac{1}{\omega_1 - \omega_0}\left[G_1\omega_1 c^\dagger T - c^\dagger T\omega_0 G_0 - T^\dagger c\omega_1 G_1 + G_0\omega_0 T^\dagger c\right]
\end{aligned} \tag{4.3.24}$$

In the last step, we changed the second and fourth terms using the constraints $G_1 c^\dagger T = c^\dagger T G_0$ and $G_0 T^\dagger c = T^\dagger c G_1$, eq. 3.1.16. We now add and subtract $G_1 G_1^{-1} c^\dagger T = c^\dagger T$ and $G_0 G_0^{-1} T^\dagger c = T^\dagger c$ for each term.

$$\begin{aligned}
\eta^\dagger - \eta = \frac{1}{\omega_1 - \omega_0}\Bigg[&G_1\left(\omega_1 - G_1^{-1}\right) c^\dagger T + c^\dagger T - c^\dagger T\left(\omega_0 - G_0^{-1}\right) G_0 - c^\dagger T \\
&- T^\dagger c\left(\omega_1 - G_1^{-1}\right) G_1 - T^\dagger c + G_0\left(\omega_0 - G_0^{-1}\right) T^\dagger c + T^\dagger c\Bigg] \\
= \frac{1}{\omega_1 - \omega_0}\Bigg[&G_1\left(\omega_1 - G_1^{-1}\right) c^\dagger T - c^\dagger T\left(\omega_0 - G_0^{-1}\right) G_0 \\
&- T^\dagger c\left(\omega_1 - G_1^{-1}\right) G_1 + G_0\left(\omega_0 - G_0^{-1}\right) T^\dagger c\Bigg]
\end{aligned} \tag{4.3.25}$$