
Unitary Renormalization Group Solution of The Single-Impurity Anderson Model

MS Project Report

submitted in partial fulfillment of the requirements for the degree of

Master of Science

by

Abhirup Mukherjee
(18IP014)

under the supervision of

Dr. Siddhartha Lal

November 13, 2021

Emergent Phenomena and Quantum Matter Group

Department of Physical Sciences

Indian Institute of Science Education and Research Kolkata



Acknowledgments

I express my heartfelt gratitude to my supervisor Dr. Siddhartha Lal for providing very useful guidance and very crucial insights into the tough problems. This project would not have been possible without the help of my group senior Siddhartha Patra and former group member Dr. Anirban Mukherjee. Their experience with the method as well as work on similar projects paved the entire journey for me. A special shout out to my friend Mounica Mahankali for all the useful discussions. The support of IISER Kolkata in the form of a junior research fellowship is gratefully acknowledged.

To you, 5 years from now

Abstract

This thesis reports a renormalization group analysis of the single impurity Anderson model (SIAM). The analysis includes a derivation of RG equations for the couplings as well as computation of physical properties. The renormalization group method (URG) is based on unitary transformations that decouple high energy nodes from the Hamiltonian, rendering them integrals of motion. It has been introduced and formalised in refs. [1, 2, 3, 4]. Some chapters have been devoted to deriving and explaining the method in detail and as well as applying it on some simpler models like the star graph model and the single-channel Kondo model. To give a clearer view of what the URG does, we connect this method to other unitary transformations in the literature, like the Schrieffer-Wolff transformation, poor man's scaling and continuous unitary transformation renormalization group. Having set up the method, we apply it on a generalized version of the SIAM with explicit spin-exchange and charge isospin-exchange couplings. We find strong-coupling fixed points for both the spin and isospin couplings. From the zero mode, we then calculate the ground state wavefunctions, which turn out to be spin singlet and isospin singlet. We then calculate thermodynamic quantities like the magnetic susceptibility and the specific heat. We then extract an effective Hamiltonian for the cloud of electrons that screen the impurity. This is done by integrating out the impurity from the fixed point Hamiltonian. This process of integrating out generates interactions among the members of the Kondo cloud. This effective Hamiltonian is found to contain both Fermi liquid as well as four-Fermion off-diagonal interaction terms. We calculate the zero temperature Wilson ratio from the local Fermi liquid formulation of Nozières, which turns out to be 2 for the Kondo regime of the SIAM. We also calculate the change in Luttinger's volume as we move from the high energy fixed point to the low energy fixed point, by tracking the changes in the number of poles of the impurity and conduction bath Green's functions. We find that the total Luttinger volume increases by 1, because the impurity state also gets added to the Fermi volume. We also compute the impurity spectral across the RG flow, and it is seen that the three peak structure at the local moment fixed point evolves into a single peak structure at the strong-coupling fixed point, demonstrating the transfer of spectral weight to zero frequency in the low energy theory. We finally calculate the mutual information and correlations along the RG flow between impurity and a Kondo cloud electron, as well as between two members of the Kondo cloud. Both the measures increase towards the strong-coupling fixed point, showing that the flow towards low energies is accompanied by a substantial increase in the entanglement content.

List of Figures

1.1	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.	4
1.2	Star Graph model	14
1.3	Left: 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. Right: 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.	16
1.4	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 $2\tilde{\omega}$	17
1.5	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. . .	17
1.6	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).	20
1.7	Variation of the fixed point value J^* against the bare bandwidth, in log scale.	20
1.8	Attractive finite J fixed point of poor man scaling RG equation	24
1.9	24
1.10	Red curve shows variation of ρ_{\min} against D_0 . It vanishes at large D_0 . Blue curve shows variation of the ratio J_1^*/D_0 with D_0 . That shrinks as well, showing that the fixed point J_1^* remains finite in the thermodynamic limit, and the distance between J_1^* and J_2^* keeps growing. . . .	25
2.1	Particle and hole excitations of the impurity	29
2.2	Left: Irrelevant flow towards $ \epsilon_d = 0$, at low ω . Right: Relevant flow towards large $ \epsilon_d $, at large ω . The former can be thought of as the projection of the strong-coupling flow on to the $\epsilon_d - D$ plane. The latter is the flow towards the local moment fixed point, if we start from a negative ϵ_d	30
2.3	Change in fixed point value of $ \epsilon_d $ with system size.	31

List of Tables

Contents

List of Figures	iv
List of Tables	v
Contents	vi
I Unitary Renormalization Group Method	I
I.1 Formalism and Results	I
I.1.1 Description of the problem	I
I.1.2 Obtaining the decoupling transformation	2
I.1.3 Properties of the many-body transition operators	3
I.1.4 Form of the unitary operators	4
I.1.5 Effective Hamiltonian	6
I.1.6 Fixed point condition	8
I.1.7 Multiple off-diagonal terms	8
I.1.8 Equivalence of the two unitaries and preservation of partial trace	9
I.1.9 Complete generator for the unitary transformation	10
I.1.10 A note on the various quantum fluctuation scales ω_i^j	11
I.2 Prescription	12
I.3 URG analysis of the star graph model	14
I.3.1 Calculation of Renormalization	14
I.3.2 Nature of flows	15
I.3.3 Effective Hamiltonians	16
I.3.4 Fixed points	16
I.4 URG analysis of the single-channel Kondo model	17
I.4.1 Particle sector	18
I.4.2 Hole sector	19
I.4.3 Scaling equations	19
I.4.4 Numerical Solutions	19
I.5 URG analysis of the multi-channel Kondo model	19
I.5.1 Introduction	19
I.5.2 Leading order renormalization	21
I.5.3 Next-to-leading order renormalization	21
I.5.4 Total renormalization $\Delta H^{(3)}$	23

2	URG of the SIAM and its Spin and Charge Generalizations	26
2.1	URG of the SIAM	26
2.1.1	Calculation of renormalization	26
2.1.2	Scaling equations	27
2.1.3	Connection to Poor Man's scaling	28
2.1.4	Particle-Hole symmetry	28
2.1.5	Numerical analysis of symmetric SIAM	30
2.2	Anderson-Kondo (spin) model URG	31
2.2.1	Spin-spin interaction	31
2.2.2	Calculation of renormalization in particle sector	33
2.2.3	Calculation of renormalization in hole sector	35
2.2.4	Relating the ω_i and ω'_i	35
2.2.5	Making sense of the various terms	37
2.2.6	Scaling equations	39
2.2.7	Particle-Hole symmetry	39
2.2.8	"Poor Man's" one-loop form for asymmetric Anderson model	39
2.2.9	SU(2) invariance and Kondo model one-loop form	40
2.3	Anderson-Kondo (charge) model URG	40
2.3.1	Calculation of renormalization in particle sector	42
2.3.2	Calculation of renormalization in hole sector	43
2.3.3	Relating the ω	43
2.3.4	Scaling Equations	45
2.3.5	Particle-hole symmetry and charge SU(2) invariance	45
	Bibliography	46

Chapter I

Unitary Renormalization Group Method

The URG method was introduced and formalised in refs. [1, 2, 3, 4]. This section is adapted from those references and expanded wherever required.

I.1 Formalism and Results

I.1.1 Description of the problem

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

We take a general Hamiltonian,

$$\mathcal{H} = H_e \hat{n}_{q\beta} + H_h (1 - \hat{n}_{q\beta}) + c_{q\beta}^\dagger T + T^\dagger c_{q\beta} \quad (\text{I.1.1})$$

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

$$\mathcal{H} = \begin{pmatrix} |1\rangle & |0\rangle \\ H_1 & T \\ T^\dagger & H_0 \end{pmatrix} \quad (\text{I.1.2})$$

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

$$\tilde{\mathcal{H}} \equiv U\mathcal{H}U^\dagger = \begin{pmatrix} |1\rangle & |0\rangle \\ \tilde{H}_1 & 0 \\ 0 & \tilde{H}_0 \end{pmatrix} \quad (\text{I.1.3})$$

U_q is defined by

$$\tilde{\mathcal{H}} = U_q \mathcal{H} U_q^\dagger \text{ such that } [\tilde{\mathcal{H}}, n_q] = 0 \quad (\text{I.1.4})$$

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

$$\mathcal{H} |\psi_i\rangle = \tilde{H}_i |\psi_i\rangle, i \in \{0, 1\} \quad (1.1.5)$$

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 $q\beta$:

$$|\psi_i\rangle = \sum_{j=0,1} |j\rangle \langle j | \psi_i \rangle \equiv |1\rangle |\phi_1^i\rangle + |0\rangle |\phi_0^i\rangle \quad (1.1.6)$$

where $|\phi_j^i\rangle = \langle j | \psi_i \rangle$. If we substitute the expansion 1.1.2 into the eigenvalue equation 1.1.5, we get

$$\left[H_e \hat{n}_{q\beta} + H_h \left(1 - \hat{n}_{q\beta} \right) + c_{q\beta}^\dagger T + T^\dagger c_{q\beta} \right] |\psi_i\rangle = \tilde{H}_i |\psi_i\rangle \quad (1.1.7)$$

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

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

This gives

$$\left[c_{q\beta}^\dagger T + T^\dagger c_{q\beta} \right] |\psi_i\rangle = \left(\tilde{H}_i - \mathcal{H}^i - \mathcal{H}^d \right) |\psi_i\rangle \quad (1.1.8)$$

1.1.2 Obtaining the decoupling transformation

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

$$\left[c_{q\beta}^\dagger T + T^\dagger c_{q\beta} \right] |\psi_i\rangle = \left(\hat{\omega}_i - \mathcal{H}^d \right) |\psi_i\rangle \quad (1.1.9)$$

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 $\hat{\omega}_i = \hat{\omega}_i^1 \hat{n}_{q\beta} + \hat{\omega}_i^0 (1 - \hat{n}_{q\beta})$. Using the expansion 1.1.6, we can write

$$\hat{\omega}_i |\psi_i\rangle = \hat{\omega}_i^1 |1\rangle |\phi_1^i\rangle + \hat{\omega}_i^0 |0\rangle |\phi_0^i\rangle \quad (1.1.10)$$

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

$$\left[\mathcal{H}^d + c_{q\beta}^\dagger T + T^\dagger c_{q\beta} \right] |\psi_i(\omega_i)\rangle = \left(\omega_i^1 - \mathcal{H}^d \right) |1\rangle |\phi_1^i\rangle + \left(\omega_i^0 - \mathcal{H}^d \right) |0\rangle |\phi_0^i\rangle \quad (1.1.11)$$

If we now substitute the expansion 1.1.6 and gather the terms that result in $\hat{n}_{q\beta} = 1$, we get

$$c_{q\beta}^\dagger T |0\rangle |\phi_0^i\rangle = \left(\omega_i^1 - \mathcal{H}^d \right) |1\rangle |\phi_1^i\rangle \quad (1.1.12)$$

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

$$T^\dagger c_{q\beta} |1\rangle |\phi_1^i\rangle = (\omega_i^0 - \mathcal{H}^d) |0\rangle |\phi_0^i\rangle \quad (1.1.13)$$

We now define two many-particle transition operators:

$$\begin{aligned} \eta^\dagger(\omega_i^1) &= \frac{1}{\omega_i^1 - \mathcal{H}^d} c_{q\beta}^\dagger T \equiv G_1 c_{q\beta}^\dagger T \\ \eta(\omega_i^0) &= \frac{1}{\omega_i^0 - \mathcal{H}^d} T^\dagger c_{q\beta} \equiv G_0 T^\dagger c_{q\beta} \end{aligned} \quad (1.1.14)$$

where G_j is the propagator $\frac{1}{\omega_i^j - \mathcal{H}^d}$. We can write this compactly as

$$\eta(\hat{\omega}) = G T^\dagger c_{q\beta} = \frac{1}{\hat{\omega}_i - \mathcal{H}^d} T^\dagger c_{q\beta} \quad (1.1.15)$$

where $\hat{\omega}_i = \omega_i^0 (1 - \hat{n}_{q\beta}) + \omega_i^1 \hat{n}_{q\beta} = \begin{pmatrix} \omega_i^1 \\ \omega_i^0 \end{pmatrix}$ is a 2x2 matrix and $\mathcal{H}^d = \mathcal{H}_0^d (1 - \hat{n}_{q\beta}) + \mathcal{H}_1^d \hat{n}_{q\beta}$ and

$G = (\hat{\omega} - \mathcal{H}^d)^{-1}$. It is easy to check that this reproduces the previous forms of η_0 and η_1^\dagger . We will later find that it is important to demand that these two be Hermitian conjugates of each other; that constraint is imposed on the denominators:

$$\eta^\dagger(\omega_i^0) = \eta^\dagger(\omega_i^1) \implies \frac{1}{\omega_i^1 - \mathcal{H}^d} c_{q\beta}^\dagger T = c_{q\beta}^\dagger T \frac{1}{\omega_i^0 - \mathcal{H}^d} \quad (1.1.16)$$

Henceforth we will assume that this constraint has been imposed.

In terms of these operators, eq. 1.1.13 becomes

$$\begin{aligned} |1\rangle |\phi_1^i\rangle &= \eta^\dagger |0\rangle |\phi_0^i\rangle \\ |0\rangle |\phi_0^i\rangle &= \eta |1\rangle |\phi_1^i\rangle \end{aligned} \quad (1.1.17)$$

These allow us to write

$$\begin{aligned} |\psi_1\rangle &= |1\rangle |\phi_1^i\rangle + |0\rangle |\phi_0^i\rangle = (1 + \eta) |1\rangle |\phi_1^i\rangle \\ |\psi_0\rangle &= (1 + \eta^\dagger) |0\rangle |\phi_0^i\rangle \end{aligned} \quad (1.1.18)$$

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

$$U_1 = 1 + \eta \quad (1.1.19)$$

1.1.3 Properties of the many-body transition operators

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

$$\eta^2 = \eta^{\dagger 2} = 0 \quad [c^{\dagger 2} = c^2 = 0] \quad (1.1.20)$$

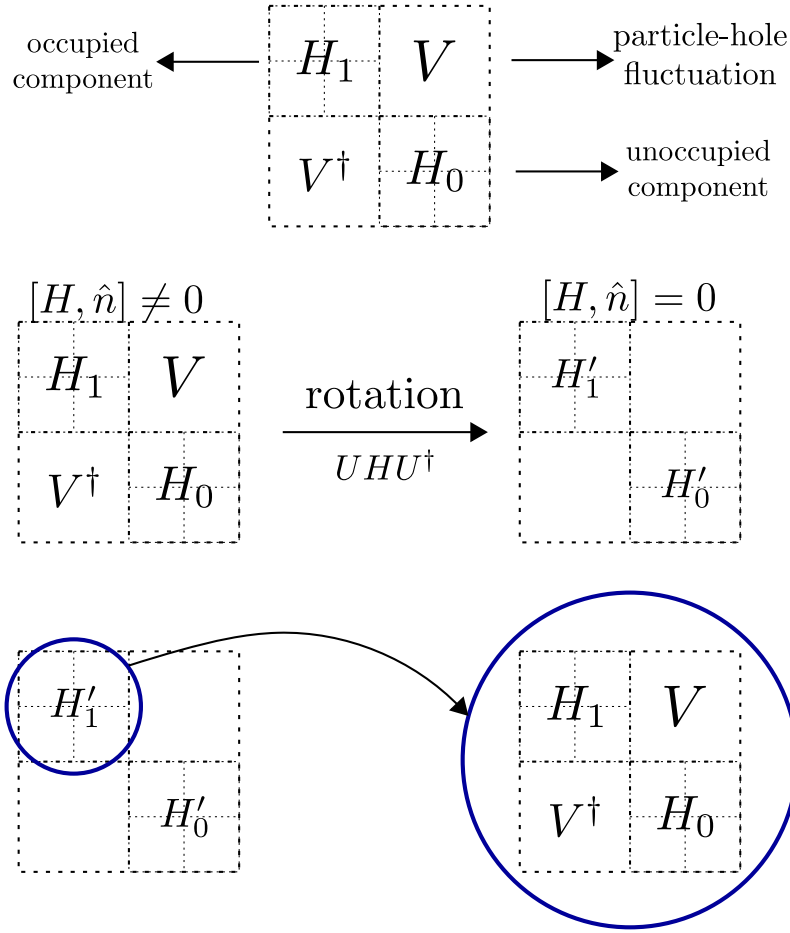


Figure 1.1: Three steps of the URG: Decompose the Hamiltonian in a 2×2 matrix, apply the unitary operator to rotate it, then repeat these steps with one of the rotated blocks.

Second is:

$$\begin{aligned} |1\rangle |\phi_1^i\rangle &= \eta^\dagger |0\rangle |\phi_0^i\rangle = \eta^\dagger \eta |1\rangle |\phi_1^i\rangle \implies \eta^\dagger \eta = \hat{n}_{q\beta} \\ |0\rangle |\phi_0^i\rangle &= \eta |1\rangle |\phi_1^i\rangle = \eta \eta^\dagger |\phi_0^i\rangle \implies \eta \eta^\dagger = 1 - \hat{n}_{q\beta} \end{aligned} \quad (1.1.21)$$

and hence the anticommutator

$$\implies \{\eta, \eta^\dagger\} = 1 \quad (1.1.22)$$

Note that the three equations in 1.1.21 work only when applied on the eigenstate $|\psi_i\rangle$ and not any arbitrary state.

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

1.1.4 Form of the unitary operators

Although we have found the correct similarity transformations U_i (eqs. 1.1.19), 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

$$U_1 = 1 + \eta \quad (\text{I.I.23})$$

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

$$U_1 = e^\eta \quad (\text{I.I.24})$$

using the fact that $\eta^2 = 0$. It is shown in ref. [5] that corresponding to a similarity transformation e^ω , there exists a unitary transformation e^G where

$$G = \tanh^{-1}(\omega - \omega^\dagger) \quad (\text{I.I.25})$$

Applying that to the problem at hand gives

$$U_1^\dagger = \exp \left\{ \tanh^{-1}(\eta - \eta^\dagger) \right\} \quad (\text{I.I.26})$$

Let $x = \tanh y$. Then,

$$x = \frac{e^{2y} + 1}{e^{2y} - 1} \implies y = \frac{1}{2} \log \frac{1+x}{1-x} \implies e^y = e^{\tanh^{-1} x} = \sqrt{\frac{1+x}{1-x}} \quad (\text{I.I.27})$$

Therefore,

$$\begin{aligned} \exp \left\{ \tanh^{-1}(\eta - \eta^\dagger) \right\} &= \frac{1 + \eta - \eta^\dagger}{\sqrt{(1 + \eta^\dagger - \eta)(1 - \eta^\dagger + \eta)}} \\ &= \frac{1 + \eta - \eta^\dagger}{\sqrt{1 + \{\eta, \eta^\dagger\}}} \\ &= \frac{1}{\sqrt{2}} (1 + \eta - \eta^\dagger) \end{aligned} \quad (\text{I.I.28})$$

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

$$U_1 = \frac{1}{\sqrt{2}} (1 + \eta^\dagger - \eta) \quad (\text{I.I.29})$$

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

$$\begin{aligned} \exp \left\{ \frac{\pi}{4} (\eta^\dagger - \eta) \right\} &= 1 + (\eta^\dagger - \eta) \frac{\pi}{4} + \frac{1}{2!} (\eta^\dagger - \eta)^2 \left(\frac{\pi}{4} \right)^2 + \frac{1}{3!} (\eta^\dagger - \eta)^3 \left(\frac{\pi}{4} \right)^3 + \dots \\ &= 1 + (\eta^\dagger - \eta) \frac{\pi}{4} - \frac{1}{2!} \left(\frac{\pi}{4} \right)^2 - \frac{1}{3!} (\eta^\dagger - \eta) \left(\frac{\pi}{4} \right)^3 + \frac{1}{4!} \left(\frac{\pi}{4} \right)^4 + \dots \\ &= \cos \frac{\pi}{4} + (\eta^\dagger - \eta) \sin \frac{\pi}{4} \\ &= \frac{1}{\sqrt{2}} (1 + \eta^\dagger - \eta) \end{aligned} \quad (\text{I.I.30})$$

There we used

$$(\eta^\dagger - \eta)^2 = \eta^{\dagger 2} + \eta^2 - \{\eta^\dagger, \eta\} = -1 \quad [\because \eta^2 = \eta^{\dagger 2} = 0] \quad (\text{I.I.31})$$

and hence

$$(\eta^\dagger - \eta)^3 = -1 (\eta^\dagger - \eta) \quad (\text{I.I.32})$$

and so on.

1.1.5 Effective Hamiltonian

We can now compute the form of the effective Hamiltonian that comes about when we apply U_1 - that is - when we rotate one exact eigenstate $|\psi_1\rangle$ into the occupied Fock space basis $|1\rangle$. From eq. 1.1.29,

$$\begin{aligned}
 U_1 \mathcal{H} U_1^\dagger &= \frac{1}{2} \left(1 + \eta^\dagger - \eta \right) \mathcal{H} \left(1 + \eta - \eta^\dagger \right) \\
 &= \frac{1}{2} \left(1 + \eta^\dagger - \eta \right) \left(\mathcal{H} + \mathcal{H}\eta - \mathcal{H}\eta^\dagger \right) \\
 &= \frac{1}{2} \left(\mathcal{H} + \mathcal{H}\eta - \mathcal{H}\eta^\dagger + \eta^\dagger \mathcal{H} + \eta^\dagger \mathcal{H}\eta - \eta^\dagger \mathcal{H}\eta^\dagger - \eta \mathcal{H} - \eta \mathcal{H}\eta + \eta \mathcal{H}\eta^\dagger \right) \quad (1.1.33) \\
 &= \frac{1}{2} \left(\mathcal{H}^d + \mathcal{H}^i + \mathcal{H}^I + \mathcal{H}\eta - \mathcal{H}\eta^\dagger + \eta^\dagger \mathcal{H} + \eta^\dagger \mathcal{H}\eta - \eta^\dagger \mathcal{H}\eta^\dagger - \eta \mathcal{H} - \eta \mathcal{H}\eta + \eta \mathcal{H}\eta^\dagger \right) \\
 &= \frac{1}{2} \left(\mathcal{H}^d + \mathcal{H}^i + \mathcal{H}^I + \left[\eta^\dagger - \eta, \mathcal{H} \right] + \eta^\dagger \mathcal{H}\eta - \eta^\dagger \mathcal{H}\eta^\dagger - \eta \mathcal{H}\eta + \eta \mathcal{H}\eta^\dagger \right)
 \end{aligned}$$

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

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

$$\tilde{\mathcal{H}} = \frac{1}{2} \left(\underbrace{\mathcal{H}^d + \mathcal{H}^i + \left[\eta^\dagger - \eta, \mathcal{H} \right] + \eta^\dagger \mathcal{H}\eta + \eta \mathcal{H}\eta^\dagger}_{\text{group 1}} + \overbrace{\mathcal{H}^I - \eta^\dagger \mathcal{H}\eta^\dagger - \eta \mathcal{H}\eta}^{\text{group 2}} \right) \quad (1.1.34)$$

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

$$\eta \mathcal{H} \eta = \eta c_q^\dagger T \eta \quad (1.1.35)$$

and

$$\eta^\dagger \mathcal{H} \eta^\dagger = \eta^\dagger T^\dagger c_q \eta^\dagger \quad (1.1.36)$$

Group 2 becomes

$$\text{group 2} = \mathcal{H}^I - \eta^\dagger T^\dagger c_q \eta^\dagger - \eta c_q^\dagger T \eta = c_q^\dagger T + T^\dagger c_q - \eta^\dagger T^\dagger c_q \eta^\dagger - \eta c_q^\dagger T \eta \quad (1.1.37)$$

To simplify this, we use the relation

$$\begin{aligned}
 \eta c_q^\dagger T \eta &= \frac{1}{\omega_i^0 - \mathcal{H}^d} T^\dagger c_q c_q^\dagger T \eta \\
 &= T^\dagger c_q \frac{1}{\omega_i^1 - \mathcal{H}^d} c_q^\dagger T \eta \quad [\text{eq. 1.1.16}] \\
 &= T^\dagger c_q \eta^\dagger \eta \quad [\text{eq. 1.1.15}] \\
 &= T^\dagger c_q \hat{n}_q \quad [\text{eq. 1.1.21}]
 \end{aligned} \quad (1.1.38)$$

which gives

$$\eta c_q^\dagger T \eta = T^\dagger c_q \quad (1.1.39)$$

Taking the Hermitian conjugate of eq. 1.1.39 gives

$$\eta^\dagger T^\dagger c_q \eta^\dagger = c_q^\dagger T \quad (1.1.40)$$

Substituting the expressions 1.1.39 and 1.1.40 into the expression for group 2, 1.1.37, shows that it vanishes. This leaves us only with group 1:

$$\tilde{\mathcal{H}} = \frac{1}{2} \left(\mathcal{H}^d + \mathcal{H}^i + \overbrace{\eta^\dagger \mathcal{H} \eta + \eta \mathcal{H} \eta^\dagger}^{\text{group A}} + \underbrace{[\eta^\dagger - \eta, \mathcal{H}]}_{\text{group B}} \right) \quad (1.1.41)$$

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 $H_e \hat{n}_{q\beta} + H_h (1 - \hat{n}_{q\beta})$.

$$\eta^\dagger \left[H_e \hat{n}_{q\beta} + H_h (1 - \hat{n}_{q\beta}) \right] \eta + \eta \left[H_e \hat{n}_{q\beta} + H_h (1 - \hat{n}_{q\beta}) \right] \eta^\dagger = \eta^\dagger H_h \eta + \eta H_e \eta^\dagger \quad (1.1.42)$$

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

$$\text{group A} = \eta^\dagger H_h \eta + \eta H_e \eta^\dagger = H_e \hat{n}_{q\beta} + H_h (1 - \hat{n}_{q\beta}) = \mathcal{H}^d + \mathcal{H}^i \quad (1.1.43)$$

It can also be shown that

$$\text{group B} = [\eta^\dagger - \eta, \mathcal{H}] = 2 [c_{q\beta}^\dagger T, \eta] \quad (1.1.44)$$

Putting it all together,

$$\tilde{\mathcal{H}} = \mathcal{H}^d + \mathcal{H}^i + [c_{q\beta}^\dagger T, \eta] \quad (1.1.45)$$

The renormalizing in the Hamiltonian is

$$\Delta \mathcal{H} = \tilde{\mathcal{H}} - \mathcal{H}^d - \mathcal{H}^i = [c_{q\beta}^\dagger T, \eta] \quad (1.1.46)$$

Because of eq. 1.1.44, it can also be written as

$$\Delta \mathcal{H} = \frac{1}{2} [\eta^\dagger - \eta, \mathcal{H}_X] = \frac{1}{2} [\eta^\dagger - \eta, \mathcal{H}] \quad (1.1.47)$$

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 $\hat{n}_{q\beta}$,

$$\begin{aligned} [\tilde{\mathcal{H}}, \hat{n}_{q\beta}] &= \left[[c_{q\beta}^\dagger T, \eta], \hat{n}_{q\beta} \right] \\ &= [c_{q\beta}^\dagger T \eta, \hat{n}_{q\beta}] - [\eta c_{q\beta}^\dagger T, \hat{n}_{q\beta}] \\ &= c_{q\beta}^\dagger T \eta \hat{n}_{q\beta} - \hat{n}_{q\beta} c_{q\beta}^\dagger T \eta \quad \left[2^{\text{nd}} [.] \text{ is 0, } \because c_{q\beta}^\dagger \hat{n}_{q\beta} = \hat{n}_{q\beta} \eta = 0 \right] \\ &= c_{q\beta}^\dagger T \eta - c_{q\beta}^\dagger T \eta \\ &= 0 \end{aligned} \quad (1.1.48)$$

1.1.6 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. 1.1.12 and 1.1.13 gives

$$c_{q\beta}^\dagger T |0\rangle |\phi_0^i\rangle = \left(\omega_i^1 - \mathcal{H}_1^d \right) |1\rangle |\phi_1^i\rangle = 0 \implies c_{q\beta}^\dagger T = 0 \quad (1.1.49)$$

1.1.7 Multiple off-diagonal terms

There is a subtle assumption in the definitions eq. 1.1.14. In order for η to be the Hermitian conjugate of η^\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: $T = T_1 + T_2$.

$$\begin{aligned} \eta &= \frac{1}{\omega_0 - \mathcal{H}_d} \left(T_1^\dagger + T_2^\dagger \right) c = \left[\frac{1}{\omega^0 - E_1^0} T_1^\dagger c + \frac{1}{\omega^0 - E_2^0} T_2^\dagger c \right] \\ \eta^\dagger &= \frac{1}{\omega^1 - \mathcal{H}_d} c^\dagger (T_1 + T_2) = \left[\frac{1}{\omega^1 - E_1^1} c^\dagger T_1 + \frac{1}{\omega^1 - E_2^1} c^\dagger T_2 \right] \end{aligned} \quad (1.1.50)$$

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:

$$\omega^0 - E_1^0 = \omega^1 - E_1^1, \quad \omega^0 - E_2^0 = \omega^1 - E_2^1 \quad (1.1.51)$$

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 .

$$\begin{aligned} \eta &= \sum_i \frac{1}{\omega_i^0 - E_i^0} T_i^\dagger c \\ \eta^\dagger &= \sum_i \frac{1}{\omega_i^1 - E_i^1} c^\dagger T_i \end{aligned} \quad (1.1.52)$$

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

$$\omega_i^0 - \omega_i^1 = E_i^0 - E_i^1 \quad (1.1.53)$$

and so

$$\eta^\dagger - \eta = \sum_i \frac{1}{\omega_i^0 - E_i^0} \left(c^\dagger T_i - T_i^\dagger c \right) \quad (1.1.54)$$

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

$$\begin{aligned}
\Delta \mathcal{H} &= \frac{1}{2} [\eta^\dagger - \eta, c^\dagger T + T^\dagger c] \\
&= \frac{1}{2} \sum_{ij} \frac{1}{\omega_i^0 - E_i^0} [c^\dagger T_i - T_i^\dagger c, c^\dagger T_j + T_j^\dagger c] \\
&= \frac{1}{2} \sum_{ij} \frac{1}{\omega_i^0 - E_i^0} \left[\hat{n} (T_i T_j^\dagger + T_j T_i^\dagger) - (1 - \hat{n}) (T_i^\dagger T_j + T_j^\dagger T_i) \right] \\
&= \frac{1}{2} \sum_{ij} \left(\frac{1}{\omega_i^0 - E_i^0} + \frac{1}{\omega_j^0 - E_j^0} \right) [\hat{n} T_i T_j^\dagger - (1 - \hat{n}) T_i^\dagger T_j]
\end{aligned} \tag{1.1.55}$$

1.1.8 Equivalence of the two unitaries and preservation of partial trace

In the subsection 1.1.4, we determined the form of the operator U_1 that unitarily decouples the node $q\beta$ from the other degrees of freedom. Eq. 1.1.29 was derived by reading off the transformation of $|1\rangle$ to $|\psi_1\rangle$, the first equation in 1.1.18. We could easily have chosen the other equation in the same equation set,

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

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

$$U_0 = \frac{1}{\sqrt{2}} (1 + \eta - \eta^\dagger) \tag{1.1.56}$$

This η will however be different from the η in eq. 1.1.29. 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 :

$$\begin{aligned}
\text{Starting from } |\psi_1\rangle: \eta_1 &= \frac{1}{\omega_1^0 - \mathcal{H}^d} T^\dagger c_{q\beta} \quad \text{and } \eta_1^\dagger = \frac{1}{\omega_1^1 - \mathcal{H}^d} T^\dagger c_{q\beta} \\
\text{Starting from } |\psi_0\rangle: \eta_0 &= \frac{1}{\omega_0^0 - \mathcal{H}^d} T^\dagger c_{q\beta} \quad \text{and } \eta_0^\dagger = \frac{1}{\omega_0^1 - \mathcal{H}^d} T^\dagger c_{q\beta}
\end{aligned} \tag{1.1.57}$$

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

$$\begin{aligned}
U_1 &= \frac{1}{\sqrt{2}} (1 + \eta_1^\dagger - \eta_1) \\
U_0 &= \frac{1}{\sqrt{2}} (1 + \eta_0 - \eta_0^\dagger)
\end{aligned} \tag{1.1.58}$$

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 η s, we get

$$\omega_1^0 - \mathcal{H}_0^d = -(\omega_0^0 - \mathcal{H}_0^d) \quad (1.1.59)$$

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.

$$\begin{aligned} \eta_1 &= \frac{1}{\tilde{H}_1 - \mathcal{H}^i - \mathcal{H}^d} T^\dagger c_{q\beta} \\ \eta_0 &= \frac{1}{\tilde{H}_0 - \mathcal{H}^i - \mathcal{H}^d} T^\dagger c_{q\beta} \\ \implies \eta_1 + \eta_0 &= \left[\frac{1}{\tilde{H}_1 - \mathcal{H}^i - \mathcal{H}^d} + \frac{1}{\tilde{H}_0 - \mathcal{H}^i - \mathcal{H}^d} \right] T^\dagger c_{q\beta} = 0 \\ \implies \tilde{H}_1 - \mathcal{H}^i - \mathcal{H}^d &= -[\tilde{H}_0 - \mathcal{H}^i - \mathcal{H}^d] \\ \implies \tilde{H}_1 + \tilde{H}_0 &= 2\mathcal{H}_0 \end{aligned} \quad (1.1.60)$$

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

$$\tilde{H} = \begin{pmatrix} E_1 & 0 \\ 0 & E_0 \end{pmatrix} \quad (1.1.61)$$

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 1.1.60 is $\text{tr}(\tilde{H}_1 + \tilde{H}_0) = \text{tr}(E_1 \otimes I + E_0 \otimes I) = 2(E_1 + E_0) = 2t_{\text{new}}$. The trace of the RHS in final equation of 1.1.60 is $2 \times \text{tr}(\mathcal{H}_0) = 2t_{\text{old}}$ where $t_{\text{old}} = \text{tr}(\mathcal{H}_0)$ is the trace of the old Hamiltonian. Equating the LHS and RHS gives $t_{\text{new}} = t_{\text{old}}$.

1.1.9 Complete generator for the unitary transformation

Given some operator O_0 , we can generate a family of unitarily-connected operators O_j using a unitary operator $U(t)$:

$$O_j = U_j O(0) U_j^\dagger, \quad j = 1, 2, \dots \quad (1.1.62)$$

The discrete change equation for O_j can be represented in the form of a commutator:

$$\Delta O_j \equiv O_{j+1} - O_j = [O_j, S_j] \quad (1.1.63)$$

where

$$S_j = U_j \Delta U_j^\dagger. \quad (1.1.64)$$

Note that because $\Delta(U_j U_j^\dagger) = 0$, we have $(\Delta U_j) U_j^\dagger = -U_j (\Delta U_j^\dagger)$ and so S_j is anti-Hermitian. To verify that eq. 1.1.62 is indeed the solution of eq. 1.1.63, we differentiate eq. 1.1.62:

$$O_{j+1} - O_j = \Delta U_j O(0) U_j^\dagger + U_j O(0) \Delta U_j^\dagger = \Delta U_j U_j^\dagger O_j + O_j U_j \Delta U_j^\dagger = [O_j, S_j] \quad (1.1.65)$$

This shows that given a family of operators eq. 1.1.62 connected through U_j , we can obtain a generator S_j that defines the flow equation of O_j .

Since the URG is unitary, we should be able to obtain such a generator for it as well. From the expression of the unitary transformation of URG:

$$U_j = \frac{1}{\sqrt{2}} \left(1 + \eta_j^\dagger - \eta_j \right) \quad (1.1.66)$$

From the definition of the generator S_j , we then get

$$S_j = \frac{1}{2} \left(1 + \eta_j^\dagger - \eta_j \right) \left(\eta_{j+1} - \eta_{j+1}^\dagger - \eta_j + \eta_j^\dagger \right) \quad (1.1.67)$$

The operators η_j and its hermitean conjugate can be thought of as angular momentum creation and annihilation operators acting on the 2×2 Hilbert space of the occupied and vacant states $|1\rangle |\phi_1\rangle, |0\rangle |\phi_0\rangle$:

$$\eta_j |1\rangle |\phi_1\rangle = |0\rangle |\phi_0\rangle, \quad \eta_j |0\rangle |\phi_0\rangle = 0, \quad \eta_j^\dagger |0\rangle |\phi_0\rangle = |1\rangle |\phi_1\rangle, \quad \eta_j^\dagger |1\rangle |\phi_1\rangle = 0, \quad (1.1.68)$$

$$(1.1.69)$$

To check whether they have the correct algebra, we design the three spin operators $S^i, i = \{x, y, z\}$.

$$\begin{aligned} S^x &= \frac{1}{2} (S^+ + S^-) = \frac{1}{2} (\eta_j^\dagger + \eta_j) \\ S^y &= \frac{1}{2i} (S^+ - S^-) = \frac{1}{2i} (\eta_j^\dagger - \eta_j) \\ S^z &= \hat{n} - \frac{1}{2} \end{aligned} \quad (1.1.70)$$

The commutation relations give

$$\begin{aligned} [S^x, S^y] &= \frac{1}{4i} [\eta_j^\dagger + \eta_j, \eta_j^\dagger - \eta_j] = \frac{1}{2i} [\eta_j, \eta_j^\dagger] = \frac{1}{2i} (1 - \hat{n} - \hat{n}) = \frac{-1}{i} \left(\hat{n} - \frac{1}{2} \right) = iS^z \\ [S^y, S^z] &= \frac{1}{2i} \left[\eta_j^\dagger - \eta_j, \hat{n} - \frac{1}{2} \right] = \frac{1}{2i} [-\eta_j \hat{n} - \hat{n} \eta_j^\dagger] = \frac{1}{2i} (-\eta_j - \eta_j^\dagger) = \frac{i}{2} (\eta_j^\dagger + \eta_j) = iS^x \\ [S^z, S^x] &= \frac{1}{2} \left[\hat{n} - \frac{1}{2}, \eta_j^\dagger + \eta_j \right] = \frac{1}{2} [\hat{n} \eta_j^\dagger - \eta_j \hat{n}] = \frac{1}{2} (\eta_j^\dagger - \eta_j) = i \frac{1}{2i} (\eta_j^\dagger - \eta_j) = iS^y \end{aligned} \quad (1.1.71)$$

These operators therefore satisfy the commutation algebra of angular momentum operators $[S^i, S^j] = i\epsilon^{ijk} S^k$.

1.1.10 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 η^\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. 1.1.16), 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.

$$\begin{aligned}\omega_1^0 - \omega_1^1 &= \mathcal{H}_d^0 - \mathcal{H}_d^1 \\ \omega_0^0 - \omega_0^1 &= \mathcal{H}_d^0 - \mathcal{H}_d^1 \\ \omega_1^0 + \omega_0^0 &= 2\mathcal{H}_d^0\end{aligned}\tag{1.1.72}$$

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.

1.2 Prescription

Given a Hamiltonian

$$\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_0 + c^\dagger T + T^\dagger c\tag{1.2.1}$$

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. 1.1.45, 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

$$\Delta\mathcal{H} = \left[c_{q\beta}^\dagger \text{Tr} \left(\mathcal{H} c_{q\beta} \right), \eta \right] = c_{q\beta}^\dagger \text{Tr} \left(\mathcal{H} c_{q\beta} \right) \eta - \eta c_{q\beta}^\dagger \text{Tr} \left(\mathcal{H} c_{q\beta} \right)\tag{1.2.2}$$

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

$$\Delta\mathcal{H} = c_{q\beta}^\dagger \text{Tr} \left(\mathcal{H} c_{q\beta} \right) \eta_1 - \eta_1 c_{q\beta}^\dagger \text{Tr} \left(\mathcal{H} c_{q\beta} \right)\tag{1.2.3}$$

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*.

$$\Delta_1\mathcal{H} = c_{q\beta}^\dagger \text{Tr} \left(\mathcal{H} c_{q\beta} \right) \eta_1\tag{1.2.4}$$

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

$$\Delta_0 \mathcal{H} = -\eta_1 c_{q\beta}^\dagger \text{Tr} \left(\mathcal{H} c_{q\beta} \right) \quad (1.2.5)$$

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:

$$\Delta \mathcal{H} = c_{q\beta}^\dagger \text{Tr} \left(\mathcal{H} c_{q\beta} \right) \eta_1 + \eta_0 c_{q\beta}^\dagger \text{Tr} \left(\mathcal{H} c_{q\beta} \right) \quad (1.2.6)$$

We can make one more manipulation: using eq. 1.1.16, we get

$$\Delta \mathcal{H} = c_{q\beta}^\dagger \text{Tr} \left(\mathcal{H} c_{q\beta} \right) \eta_1 + \text{Tr} \left(c_{q\beta}^\dagger \mathcal{H} \right) c_{q\beta} \eta_0^\dagger \quad (1.2.7)$$

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 [6, 7]. Writing down the forms of η and η^\dagger explicitly, we get

$$\Delta \mathcal{H} = c_{q\beta}^\dagger \text{Tr} \left(\mathcal{H} c_{q\beta} \right) \frac{1}{\omega_1^0 - \mathcal{H}_0^d} \text{Tr} \left(c_{q\beta}^\dagger \mathcal{H} \right) c_{q\beta} + \text{Tr} \left(c_{q\beta}^\dagger \mathcal{H} \right) c_{q\beta} \frac{1}{\omega_0^1 - \mathcal{H}_1^d} c_{q\beta}^\dagger \text{Tr} \left(\mathcal{H} c_{q\beta} \right) \quad (1.2.8)$$

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

$$\Delta \mathcal{H} = \sum_{q\beta} \left[c_{q\beta}^\dagger \text{Tr} \left(\mathcal{H} c_{q\beta} \right) \frac{1}{\omega_1^0 - \mathcal{H}_0^d} \text{Tr} \left(c_{q\beta}^\dagger \mathcal{H} \right) c_{q\beta} + \text{Tr} \left(c_{q\beta}^\dagger \mathcal{H} \right) c_{q\beta} \frac{1}{\omega_0^1 - \mathcal{H}_1^d} c_{q\beta}^\dagger \text{Tr} \left(\mathcal{H} c_{q\beta} \right) \right] \quad (1.2.9)$$

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 $\mathcal{H}_{0,1}^d$ will, in general, have the energies of all the electrons. But we consider only the energy of the on-shell electrons in the denominator. After integrating out these electrons, we can rearrange the remaining operators to determine which term in the Hamiltonian it renormalizes and what is the renormalization.

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

1.3 URG analysis of the star graph model

The star graph problem has already been analyzed using URG and an extensive study of its entanglement properties has already been carried out, in ref. [8]. Here we focus on just deriving the RG equations. 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.

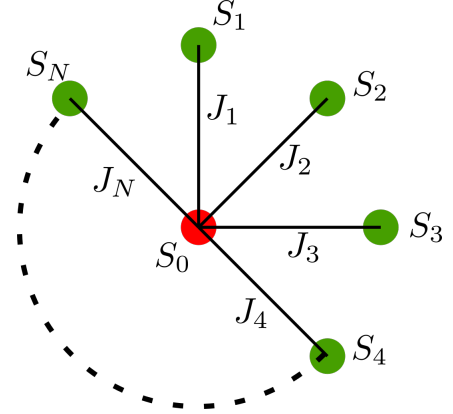


Figure 1.2: Star Graph model

$$\mathcal{H} = \epsilon_0 S_0^z + \sum_{i=1}^N \left[\epsilon_i S_i^z + J_i \vec{S}_0 \cdot \vec{S}_i \right] \quad (1.3.1)$$

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

$$\mathcal{H} = \epsilon_0 S_0^z + \sum_{i=1}^N \left[\epsilon_i S_i^z + J_i \left(S_0^z S_i^z + \frac{1}{2} (S_0^+ S_i^- + S_0^- S_i^+) \right) \right] \quad (1.3.2)$$

1.3.1 Calculation of Renormalization

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

$$\mathcal{H}^D = \epsilon_0 S_0^z + \epsilon_N S_N^z + J_N S_0^z S_N^z \quad (1.3.3)$$

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

$$\mathcal{H}_X = S_N^+ T + T^\dagger S_N^- = \frac{1}{2} J_N (S_N^+ S_0^- + S_N^- S_0^+) \quad (1.3.4)$$

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

$$\begin{aligned} \Delta \mathcal{H} &= S_N^+ T \frac{1}{\omega_1^0 - \mathcal{H}^D} T^\dagger S_N^- + T^\dagger S_N^- \frac{1}{\omega_1^0 - \mathcal{H}^D} S_N^+ T \\ &= \frac{J_N^2}{4} S_N^+ S_0^- \frac{1}{\omega_1^0 - \epsilon_0 S_0^z - \epsilon_N S_N^z - J_N S_0^z S_N^z} S_0^+ S_N^- + \frac{J_N^2}{4} S_0^+ S_N^- \frac{1}{\omega_1^0 - \epsilon_0 S_0^z - \epsilon_N S_N^z - J_N S_0^z S_N^z} S_N^+ S_0^- \end{aligned} \quad (1.3.5)$$

There, N refers to the spin being decoupled. The first Greens function has S_0^+ and S_N^- in front of it, so we substitute $S_0^z = \frac{1}{2}$, $S_N^z = -\frac{1}{2}$ in that Greens function. For the other Greens function we do the opposite.

$$\Delta \mathcal{H} = \frac{J_N^2}{4} S_N^+ S_0^- \frac{1}{\omega_1^0 - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} S_0^+ S_N^- + \frac{J_N^2}{4} S_0^+ S_N^- \frac{1}{\omega_1^0 + \frac{1}{2}\epsilon_0 - \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} S_N^+ S_0^- \quad (1.3.6)$$

To relate ω_1^0 and ω_0^1 , we use eq. 1.1.72:

$$\omega_1^0 + \omega_0^1 = \mathcal{H}_0^D + \mathcal{H}_1^D = -\frac{1}{2} J_N \implies \omega_1^0 \equiv \omega, \quad \omega_0^1 \equiv \omega' = -\frac{1}{2} J_N - \omega \quad (1.3.7)$$

So, the renormalization becomes

$$\Delta\mathcal{H} = \frac{J_N^2}{4} \frac{1}{\omega - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \left(S_N^+ S_0^- S_0^+ S_N^- - S_0^+ S_N^- S_N^+ S_0^- \right) = \frac{J_N^2}{4} \frac{1}{\omega - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} (S_N^z - S_0^z) \quad (1.3.8)$$

There we used $S^+ S^- = \frac{1}{2} + S^z$ and $S^- S^+ = \frac{1}{2} - S^z$.

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

$$\begin{aligned} \Delta\epsilon_N &= \frac{1}{4} J_N^2 \frac{1}{\omega - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \\ \Delta\epsilon_0 &= -\frac{1}{4} J_N^2 \frac{1}{\omega - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \end{aligned} \quad (1.3.9)$$

1.3.2 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 $i \in \{1, N\}$.

$$\Delta\epsilon_0 = -\frac{1}{4} J^2 \frac{1}{\omega - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon + \frac{1}{4}J} \quad (1.3.10)$$

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

$$\Delta\epsilon_0 = -\frac{1}{4} J^2 \frac{1}{\tilde{\omega} - \frac{1}{2}\epsilon_0} \quad (1.3.11)$$

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 1.3.

Since we cannot find a fixed point, we will use a different ω . Instead of ω_1^0 , we will use ω_1^1 . From eq. 1.1.72, we have

$$\omega_1^0 - \omega_1^1 = \mathcal{H}_0^D - \mathcal{H}_1^D = \epsilon_0 - \epsilon_N = \epsilon_0 - \epsilon \quad (1.3.12)$$

Defining $\omega_1^1 = \omega'$ and substituting this in eq. 1.3.10 gives

$$\Delta\epsilon_0 = -\frac{1}{4} J^2 \frac{1}{\omega' - \frac{1}{2}\epsilon + \frac{1}{2}\epsilon_0 + \frac{1}{4}J} \quad (1.3.13)$$

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

$$\Delta\epsilon_0 = \frac{1}{4} J^2 \frac{1}{\tilde{\omega} - \frac{1}{2}\epsilon_0} \quad (1.3.14)$$

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 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 right panel of figure 1.3.

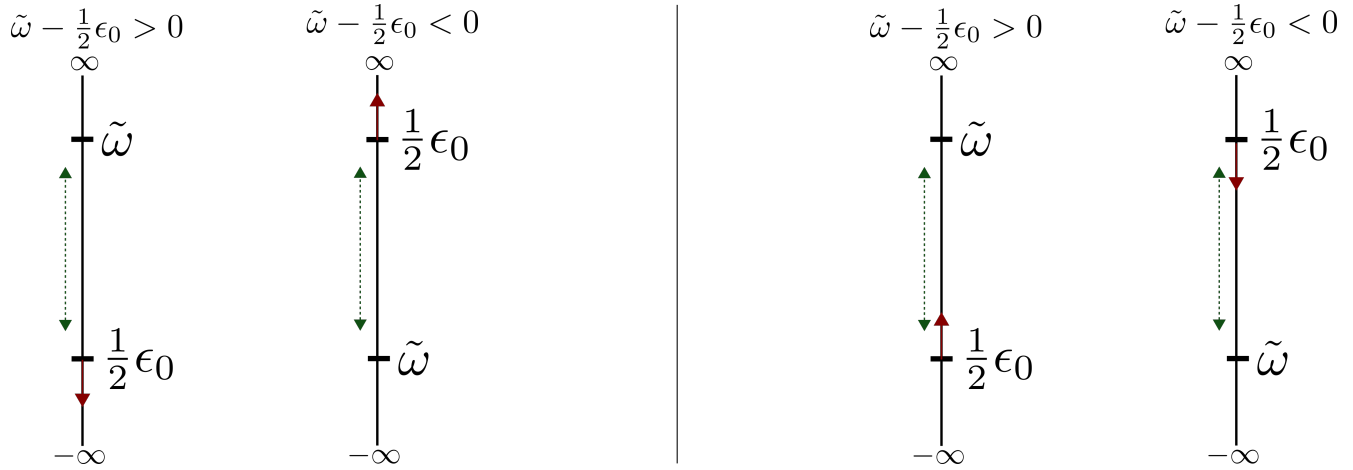


Figure 1.3: Left: RG flow for the two cases. The green line is the distance between the bare values of the two couplings, and hence also the magnitude of the denominator. The red arrow denotes the direction in which ϵ_0 will flow. Upward flow is increase. In both cases, the flow is such that the distance 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. Right: 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.

1.3.3 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

$$\mathcal{H}^* = 2\tilde{\omega}S_0^z + \epsilon \sum_i S_i^z + J \sum_i \vec{S}_i \cdot \vec{S}_0, \quad \text{if } \tilde{\omega}\epsilon_0 > 0 \quad (1.3.15)$$

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.

$$\mathcal{H}^* = \epsilon \sum_i S_i^z + J \sum_i \vec{S}_i \cdot \vec{S}_0, \quad \text{if } \tilde{\omega}\epsilon_0 < 0 \quad (1.3.16)$$

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

$$\begin{aligned} \mathcal{H}^* &= 2\tilde{\omega}S_0^z + J \sum_i \vec{S}_i \cdot \vec{S}_0, & \text{if } \tilde{\omega}\epsilon_0 > 0 \\ \mathcal{H}^* &= J \sum_i \vec{S}_i \cdot \vec{S}_0, & \text{if } \tilde{\omega}\epsilon_0 < 0 \end{aligned} \quad (1.3.17)$$

1.3.4 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. 1.4. The second kind are those where the two couplings have different signs, and so ϵ_0 flows to 0. These are shown in fig. 1.5.

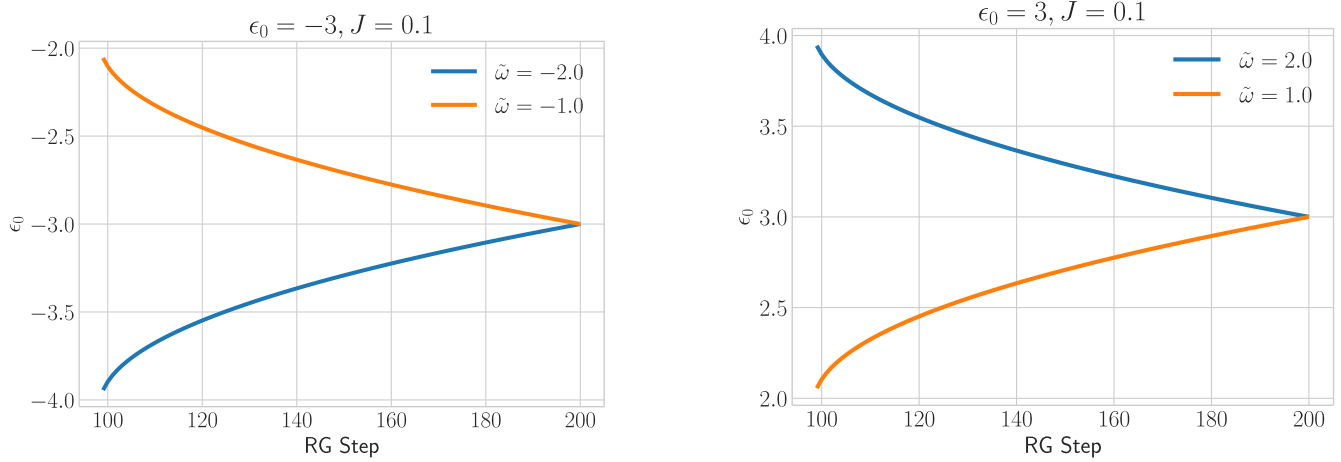


Figure 1.4: Flows where ϵ_0 and $\tilde{\omega}$ have same sign. The left and right panels show flows starting from negative and positive values respectively. The two plots in each panel correspond to different values of $\tilde{\omega}$, one greater than the bare ϵ_0 , the other less than that. The fixed point value is $2\tilde{\omega}$.

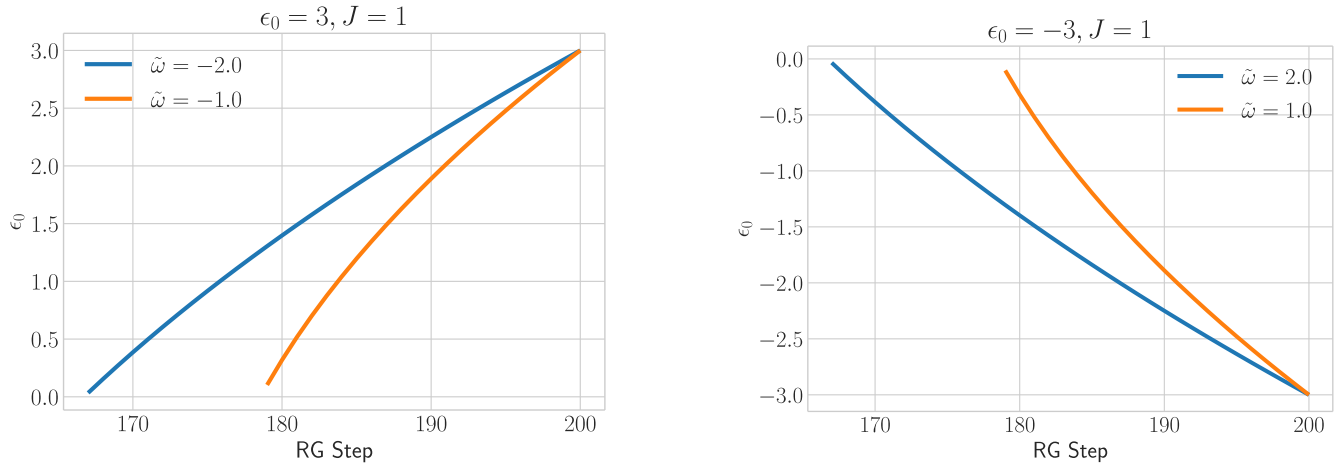


Figure 1.5: Flows where ϵ_0 and $\tilde{\omega}$ have opposite sign. The left and right panels show flows starting from negative and positive values respectively. The two plots in each panel correspond to different values of $\tilde{\omega}$, one greater than the bare ϵ_0 , the other less than that. The fixed point value is 0.

1.4 URG analysis of the single-channel Kondo model

The Kondo model URG analysis was originally carried out in ref. [9]. A specific version of the model is described by the Hamiltonian

$$\mathcal{H} = \sum_{k\sigma} \epsilon_k \tau_{k\sigma} + \sum_{k,l} J^z S_d^z s_{kl}^z + \frac{1}{2} \sum_{k,l} J^t \left(S_d^+ s_{kl}^- + S_d^- s_{kl}^+ \right) \quad (1.4.1)$$

where $s_{kl}^z = \frac{1}{2} (c_{k\uparrow}^\dagger c_{l\uparrow} - c_{k\downarrow}^\dagger c_{l\downarrow})$, $s_{kl}^- = c_{k\downarrow}^\dagger c_{l\uparrow}$ and $s_{kl}^+ = s_{lk}^{-\dagger}$. Also, $\tau = \hat{n} - \frac{1}{2}$. k, l sum over the momentum states. \vec{S}_d is the impurity spin operator.

The scheme is that we will disentangle an electron $q\beta$ from the Hamiltonian, q being the momentum and β the spin. The diagonal part of the Hamiltonian under this scheme is

$$H_{q\beta}^D = \epsilon_q \tau_{q\beta} + J^z S_d^z s_{qq}^z \quad (1.4.2)$$

The off-diagonal parts at a particular RG step H_1^I and H_0^I , that start from particle and hole states respectively, are

$$\begin{aligned} H_1^I &= \sum_{|k| < \Lambda, q} J^z S_d^z s_{kq}^z + \frac{1}{2} \sum_{|k| < \Lambda, q} J^t \left(S_d^+ s_{kq}^- + S_d^- s_{kq}^+ \right) \\ H_0^I &= \sum_{|k| < \Lambda, q} J^z S_d^z s_{qk}^z + \frac{1}{2} \sum_{|k| < \Lambda, q} J^t \left(S_d^+ s_{qk}^- + S_d^- s_{qk}^+ \right) \end{aligned} \quad (1.4.3)$$

H_1^I is the Hamiltonian term that scatters from the occupied configuration of q , H_0^I is the same from the unoccupied configuration. These are the terms that appear in the numerator.

1.4.1 Particle sector

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

$$H_0^I \frac{1}{\omega - H_{q\beta}^D} H_1^I \quad (1.4.4)$$

Both H_0^I and H_1^I have all three operators S_d^z, S_d^\pm . We call S_d^z the spin-keep term and the others spin-flip terms. The entire product will thus have $3 \times 3 = 9$ terms. Not all terms however renormalize the Hamiltonian. Those terms that have identical operators on both sides can be ignored because $S_d^{z2} = \text{constant}$ and $S^\pm{}^2 = 0$. The other six terms will renormalize the Hamiltonian. This brings in one more simplification: all the six terms that *will* renormalize the Hamiltonian have a spin flip operator on at least one side of the Greens function. This means that in the denominator of the Greens function, S_d^z and s_{qq}^z have to be anti-parallel in order to produce a non-zero result for that term. This means we can identically replace $S_d^z s_{qq}^z = -\frac{1}{4}$. Also, in the particle sector, the Greens function always has $c_{q\beta}$ in front of it, so $\epsilon_q \tau_{q\beta} = D/2$. Substituting all this, we get

$$\begin{aligned} \frac{1}{\omega - D/2 + J/4} \sum_{|k, k'| < \Lambda, q} & \left[\frac{1}{2} J^z J^t \left(S_d^z S_d^+ s_{qk'}^- s_{kq}^- + S_d^z S_d^- s_{qk'}^+ s_{kq}^+ \right) + \frac{1}{2} J^t J^z \left(S_d^+ S_d^z s_{qk'}^- s_{kq}^z + S_d^- S_d^z s_{qk'}^+ s_{kq}^z \right) \right. \\ & \left. + \frac{1}{4} J^{t2} \left(S_d^- S_d^+ s_{qk'}^+ s_{kq}^- + S_d^+ S_d^- s_{qk'}^- s_{kq}^+ \right) \right] \end{aligned} \quad (1.4.5)$$

We now simplify the products and keep only terms diagonal in q . For example: $s_{qk'}^z s_{kq}^+ = \frac{1}{2} \hat{n}_{q\downarrow} s_{kk'}^+$ and $s_{qk'}^z s_{kq}^- = -\frac{1}{2} \hat{n}_{q\uparrow} s_{kk'}^-$. The renormalization becomes

$$\frac{1}{\omega - D/2 + J/4} \sum_{|k, k'| < \Lambda, q} \left[\frac{1}{4} J^z J^t \left(-\frac{1}{2} S_d^+ \hat{n}_q s_{kk'}^- - \frac{1}{4} S_d^- \hat{n}_q s_{kk'}^z \right) - \frac{1}{4} J^{t2} S_d^z \left(-\hat{n}_{q\uparrow} c_{k\downarrow}^\dagger c_{k'\downarrow} + \hat{n}_{q\downarrow} c_{k\uparrow}^\dagger c_{k'\uparrow} \right) \right] \quad (1.4.6)$$

We now replace $\sum_q \hat{n}_{q\sigma} = n(D)$. The renormalization due to excitations coming from the particle sector is

$$\Delta H_1 = -\frac{1}{2} \frac{n(D)}{\omega - D/2 + J/4} \sum_{|k, k'| < \Lambda} \left[J^z J^t \frac{1}{2} \left(S_d^+ s_{kk'}^- + S_d^- s_{kk'}^z \right) + J^{t2} S_d^z s_{kk'}^z \right] \quad (1.4.7)$$

The renormalization in the couplings coming from the particle sector is therefore,

$$\Delta J^z = -\frac{1}{2} \frac{J^{t2} n(D)}{\omega - D/2 + J/4}, \quad \Delta J^t = -\frac{1}{2} \frac{J^z J^t n(D)}{\omega - D/2 + J/4} \quad (1.4.8)$$

1.4.2 Hole sector

The hole sector involves integrating out those states which are vacant ($\hat{n}_{q\beta} = 1$). We will work at an energy shell $\epsilon_q = D$. The renormalization is

$$H_1^I \frac{1}{\omega - H_{q\beta}^D} H_0^I \quad (1.4.9)$$

The same considerations as those in the particle sector apply here, and the denominator becomes $\omega - D/2 + J/4$, while the numerator is $H_1^I H_0^I$. Since this is just the Hermitian conjugate of the particle sector form, we do not need to calculate this separately, because the renormalization here will be $\Delta H_0 = \Delta H_1^\dagger = \Delta H_1$.

1.4.3 Scaling equations

Since the renormalization in the hole sector is equal to that in the particle sector, the total renormalization is simply twice that in the particle sector (eqs. 1.4.8):

$$\Delta J^z = -\frac{J^2 n(D)}{\omega - D/2 + J/4}, \quad \Delta J^t = -\frac{J^z J^t n(D)}{\omega - D/2 + J/4} \quad (1.4.10)$$

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

$$\Delta J = -\frac{J^2 n(D)}{\omega - D/2 + \frac{1}{4}J} \quad (1.4.11)$$

To recover the one-loop form, we can replace ω with the bare value $-D/2$ and ignore the J in the denominator (small J).

$$\Delta J \approx \frac{J^2 n(D)}{D} \quad (1.4.12)$$

1.4.4 Numerical Solutions

The symmetric scaling equation 1.4.11 was solved numerically with the choice $\omega = -\frac{\epsilon_a}{2}$, 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 $D \rightarrow \infty$, URG should give $J^* \rightarrow \infty$. This is shown in fig. 1.7

1.5 URG analysis of the multi-channel Kondo model

1.5.1 Introduction

The multi-channel Kondo model is described by the Hamiltonian

$$H = \sum_{k,\alpha,\gamma} \epsilon_k^\gamma \hat{n}_{k\alpha}^\gamma + J \sum_{kk',\gamma} \vec{S}_d \cdot \vec{s}_{\alpha\alpha'} c_{k\alpha}^\gamma \dagger c_{k'\alpha'}^\gamma \quad (1.5.1)$$

It is mostly identical to the single-channel Kondo model: k, k' sum over the momentum states, α, α' sum over the spin indices and γ sums over the various channels. \vec{S}_d, \vec{s} are the impurity and conduction bath spin vectors.

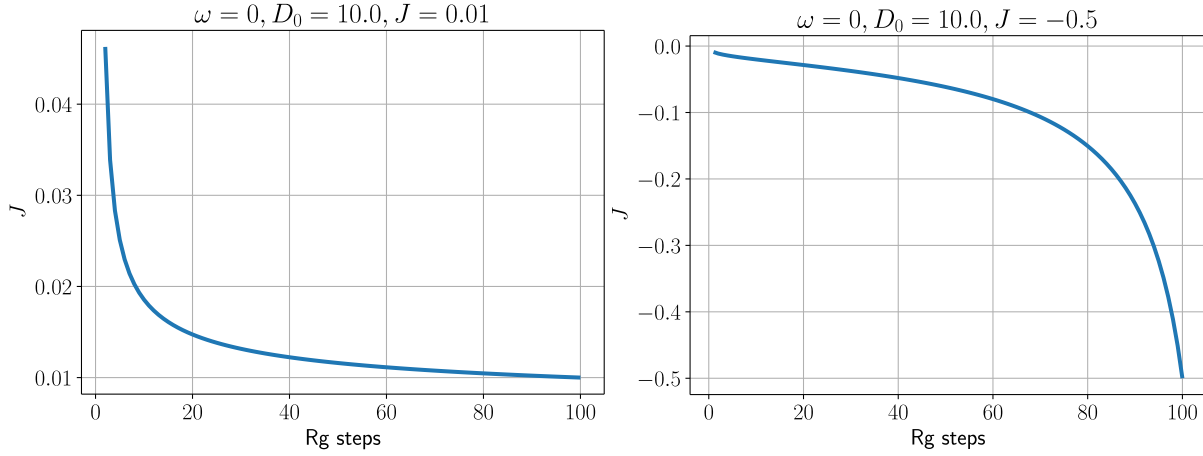


Figure 1.6: Flow of J towards the strong-coupling fixed point (right) and the weak coupling saddle-point (left). The x-axis indicates the index of the energy shell being decoupled. The largest value (UV) is the first step, and we go towards the left (IR).

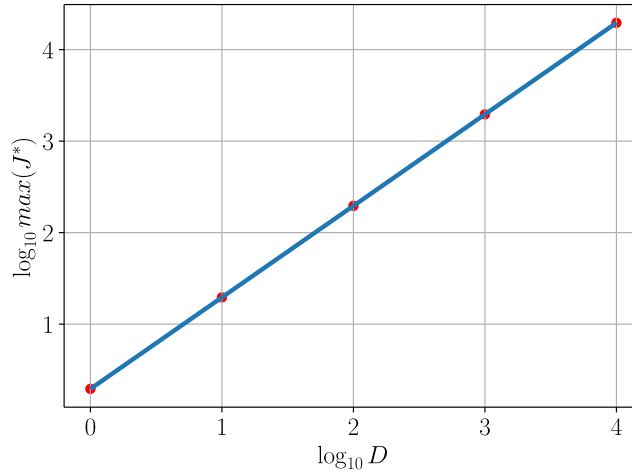


Figure 1.7: Variation of the fixed point value J^* against the bare bandwidth, in log scale.

The renormalization at step j is given by

$$\Delta H_j = \left(c^\dagger T \frac{1}{\hat{\omega} - H_D} T^\dagger c + T^\dagger c \frac{1}{\hat{\omega} - H_D} c^\dagger T \right), \quad c^\dagger T = J \sum_{k < \Lambda_j, \alpha} \vec{S}_d \cdot \vec{s}_{\beta\alpha} c_{q\beta}^\dagger c_{k\alpha}, H_D = \epsilon_q \tau_{q\beta} + J S_d^z s_q^z \quad (1.5.2)$$

Usually we treat the $\hat{\omega}$ as number(s) and study the renormalization in the couplings as functions of the quantum fluctuation scales. Each value of the fluctuation scale defines an eigendirection of $\hat{\omega}$. We have then essentially traded off the complexity in the non-commutation of the diagonal and off-diagonal terms for all the directions in the manifold of $\hat{\omega}$.

Here we will do something different. We will redefine the $\hat{\omega}$ by pulling out the off-diagonal term from it: $\hat{\omega} \rightarrow \hat{\omega} - H_X$, and then study the renormalization at various orders by expanding the denominator in powers of H_X . Such a redefinition essentially amounts to a rotation of the eigendirections of $\hat{\omega}$. This is done in order to extract some information out of $\hat{\omega}$, specifically the dependence of the RG equations on the channel number $K = \sum_\gamma$. This dependence is in principle present even if we do not do such a redefinition and expansion, in the various directions and values of ω , because those values encode the non-perturbative information regarding

scattering at all loops. However, it is difficult to read off this information directly. This step of redefinition followed by expansion is being done with the sole aim of exposing such information.

The expansion we are talking about is

$$\eta = \frac{1}{\hat{\omega} - H_D} T^\dagger c = \frac{1}{\omega' - H_D - H_X} T^\dagger c \simeq \frac{1}{\omega' - H_D} T^\dagger c + \frac{1}{\omega' - H_D} H_X \frac{1}{\omega' - H_D} T^\dagger c \quad (1.5.3)$$

where $H_X = J \sum_{k,k' < \Lambda_j, \alpha, \alpha'} \vec{S}_d \cdot \vec{S}_{\alpha\alpha'} c_{k\alpha}^\dagger c_{k'\alpha'}$ is scattering between the entangled electrons. With this change, the second and third order renormalizations will take the form

$$\Delta H_j^{(2)} = c^\dagger T \frac{1}{\omega' - H_D} T^\dagger c + T^\dagger c \frac{1}{\omega - H_D} c^\dagger T \quad (1.5.4)$$

$$\Delta H_j^{(3)} = c^\dagger T \frac{1}{\omega' - H_D} H_X \frac{1}{\omega' - H_D} T^\dagger c + T^\dagger c \frac{1}{\omega - H_D} H_X \frac{1}{\omega - H_D} c^\dagger T \quad (1.5.5)$$

We will use the identity

$$S_d^a S_d^z S_d^b = \left(\frac{1}{4} \delta^{az} + \frac{i}{2} \sum_c \epsilon^{azc} S_d^c \right) S_d^b = \left(\frac{1}{4} \delta^{az} S_d^b + \frac{i}{8} \epsilon^{azb} - \frac{1}{4} \sum_{c_1, c} \epsilon^{azc_1} \epsilon^{c_1 bc} S_d^c \right) = \frac{1}{4} \left(\delta^{az} S_d^b - \delta^{ab} S_d^z + \delta^{bz} S_d^a \right) \quad (1.5.6)$$

1.5.2 Leading order renormalization

$$\Delta H_j^{(2)} = \underbrace{c^\dagger T \frac{1}{\omega' - H_D} T^\dagger c}_{\text{first term}} + \underbrace{T^\dagger c \frac{1}{\omega - H_D} c^\dagger T}_{\text{second term}} \quad (1.5.7)$$

This renormalization is identical to that in the single channel. There is no additional physics due to the presence of multiple channels at this order.

$$\Delta J^{(2)} = - \frac{J^2 n(D)}{\omega - D/2 + J/4} \quad (1.5.8)$$

For $\omega < D/2$, we get the flow towards the strong-coupling fixed point. That is, there appears a stable fixed point at $J^* = 4|\omega - D/2|$ for all bare $J > 0$. We also get a decay towards the local moment fixed point $J^* = 0$ for $J < 0$. For $\omega = -D/2$ and $J \ll D$, we get the one-loop PMS form.

$$\Delta J^{(2)} = \frac{J^2 n(D)}{D - J/4} \simeq \frac{J^2 n(D)}{D} \quad (1.5.9)$$

1.5.3 Next-to-leading order renormalization

$$\Delta H_j^{(3)} = \underbrace{c^\dagger T \frac{1}{\omega' - H_D} H_X \frac{1}{\omega' - H_D} T^\dagger c}_{\text{first term}} + \underbrace{T^\dagger c \frac{1}{\omega - H_D} H_X \frac{1}{\omega - H_D} c^\dagger T}_{\text{second term}} \quad (1.5.10)$$

A general term of this summation has three sets of spin operators coming from $c^\dagger T$, H_X and $T^\dagger c$. If we had expressed the spin operators in terms of S^z , S^\pm , most of the terms would have atleast one S^+ or S^- , and by the same argument as in the single-channel case, the denominator will have anti-parallel spins and the Ising term will be negative, leading to the form: $\omega - D/2 - \epsilon_k/2 + J/4$. ϵ_k is the energy of the other electron that will be

summed over. The only term that does not have even one S^\pm is the one with three S^z . We can show that this term will also have the same denominator. An instance of this term (in shorthand) is

$$S_d^z c_{q\uparrow}^\dagger \frac{1}{\omega - D/2 - \epsilon_k/2 + J/2 S_d^z} S_d^z \frac{1}{\omega - D/2 - \epsilon_k/2 + J/2 S_d^z} S_d^z c_{q\uparrow} \quad (1.5.11)$$

This can be split into up and down configurations of the impurity spin using the decomposition $S_d^z = \frac{1}{2} \left(\frac{1}{2} + S_d^z \right) - \frac{1}{2} \left(\frac{1}{2} - S_d^z \right)$. These configurations will have different quantum fluctuation scales ω, ω' :

$$\frac{1}{2} S_d^z c_{q\uparrow}^\dagger \left[\frac{\left(\frac{1}{2} + S_d^z \right)}{\left(\omega - D/2 - \epsilon_k/2 + J/4 \right)^2} - \frac{\left(\frac{1}{2} - S_d^z \right)}{\left(\omega' - D/2 - \epsilon_k/2 - J/4 \right)^2} \right] S_d^z c_{q\uparrow} \quad (1.5.12)$$

If we now use poor man's scaling values to relate the two ω s, we get $\omega' - \omega = J/2$. Substituting this will make both the denominators identical: $\omega - D/2 - \epsilon_k/2 + J/4$. This means that the denominator for all non-zero terms that renormalize the Hamiltonian is $\omega - D/2 - \epsilon_k/2 + J/4$.

Calculation of first term

$$c^\dagger T \frac{1}{\omega' - H_D} H_X \frac{1}{\omega' - H_D} T^\dagger c = J^3 \sum_{\substack{q, k, k_1, k_2, \\ \beta, \alpha, \alpha_1, \alpha_2, \\ l_1, l_2, a, b, c}} \frac{c_{q\beta, l_1}^\dagger c_{k\alpha, l_1} S_d^a s_{\beta\alpha}^a S_d^b s_{\alpha_1\alpha_2}^b c_{k_1\alpha_1, l_2}^\dagger c_{k_2\alpha_2, l_2} c_{k\alpha, l_1}^\dagger c_{q\beta, l_1} S_d^c s_{\alpha\beta}^c}{\left(\omega - D/2 - \epsilon_k/2 + J/4 \right)^2} \quad (1.5.13)$$

q sums over the momenta being decoupled. k, k_1, k_2 sum over the momenta not being decoupled. $\beta, \alpha, \alpha_1, \alpha_2$ sum over the spin indices. l_1, l_2 sum over the channels. We will start simplifying this equation by summing over q . $c_{q\beta}^\dagger$ and $c_{q\beta}$ can be easily combined to form $\hat{n}_{q\beta}$, because they anti-commute with the other momenta. The sum gives $\sum_q \hat{n}_{q\beta l_1} = n(D)$. This gives

$$c^\dagger T \frac{1}{\omega' - H_D} H_X \frac{1}{\omega' - H_D} T^\dagger c = J^3 n(D) \sum_{\substack{k, k_1, k_2, \\ \beta, \alpha, \alpha_1, \alpha_2, \\ l_1, l_2, a, b, c}} \frac{c_{k\alpha, l_1} S_d^a s_{\beta\alpha}^a S_d^b s_{\alpha_1\alpha_2}^b c_{k_1\alpha_1, l_2}^\dagger c_{k_2\alpha_2, l_2} c_{k\alpha, l_1}^\dagger S_d^c s_{\alpha\beta}^c}{\left(\omega - D/2 - \epsilon_k/2 + J/4 \right)^2} \quad (1.5.14)$$

The operators $c_{k\alpha}^\dagger$ and its conjugate can be brought together without any change of sign because there will be an even number of flips. The sum over k gives

$$\sum_k \frac{1 - \hat{n}_{k\alpha l_1}}{\left(\omega - D/2 - \epsilon_k/2 + J/4 \right)^2} = \rho \int \frac{d\epsilon [1 - \hat{n}(\epsilon)_{\alpha l_1}]}{\left(\omega - D/2 - \epsilon/2 + J/4 \right)^2} = \rho \int_0^{D-2(\omega+J/4)} \frac{d\epsilon}{\left(\omega - D/2 - \epsilon/2 + J/4 \right)^2} \quad (1.5.15)$$

The integration goes over positive energies only because of the $1 - \hat{n}$ operator; the upper limit of the integration is chosen so as to make the denominator double, because this preserves the symmetry of the denominator and this is what happens in poor man's scaling. Performing the integration gives

$$\sum_k \frac{1 - \hat{n}_{k\alpha l_1}}{\left(\omega - D/2 - \epsilon_k/2 + J/4 \right)^2} = -\frac{1}{2} \frac{\rho}{\omega - D/2 + J/4} \quad (1.5.16)$$

The sum over the channel index l_1 produces a factor of K . $K = \sum_{l_1}$ is the total number of conduction bath channels. The entire expression is now

$$c^\dagger T \frac{1}{\omega' - H_D} H_X \frac{1}{\omega' - H_D} T^\dagger c = -\frac{1}{2} \frac{J^3 n(D) \rho K}{\omega - D/2 + J/4} \sum_{\substack{\beta, \alpha, \alpha_1, \alpha_2, \\ a, b, c}} S_d^a s_{\beta\alpha}^a S_d^b s_{\alpha_1\alpha_2}^b S_d^c s_{\alpha\beta}^c \sum_{k_1, k_2, l_2} c_{k_1\alpha_1, l_2}^\dagger c_{k_2\alpha_2, l_2} \quad (1.5.17)$$

We now need to simplify the spin products. The sum over α, β can be carried out immediately: $\sum_{\alpha, \beta} s_{\beta\alpha}^a s_{\alpha\beta}^c = \text{Trace}(s^a s^c) = \frac{1}{2} \delta^{ac}$. Substituting this gives

$$c^\dagger T \frac{1}{\omega' - H_D} H_X \frac{1}{\omega' - H_D} T^\dagger c = -\frac{1}{2} \frac{J^3 n(D) \rho K}{\omega - D/2 + J/4} \frac{1}{2} \sum_{\alpha_1, \alpha_2, a, b} S_d^a S_d^b S_d^a \sum_{k_1, k_2, l_2} c_{k_1\alpha_1, l_2}^\dagger c_{k_2\alpha_2, l_2} s_{\alpha_1\alpha_2}^b \quad (1.5.18)$$

The spin product can now be carried out:

$$\begin{aligned} \sum_a S_d^a S_d^b S_d^a &= \sum_a S_d^a \left[\frac{1}{4} \delta^{ab} + \frac{i}{2} \sum_c \epsilon^{bac} S_d^c \right] = \frac{1}{4} S_d^b - \frac{1}{4} \sum_{ace} \epsilon^{bac} \epsilon^{ace} S_d^e = \frac{1}{4} S_d^b - \frac{1}{4} S_d^b \sum_{ac} \epsilon^{bac} \epsilon^{acb} \\ &= -\frac{1}{4} S_d^b \end{aligned} \quad (1.5.19)$$

The renormalization becomes

$$\begin{aligned} \Delta H_1 &= c^\dagger T \frac{1}{\omega' - H_D} H_X \frac{1}{\omega' - H_D} T^\dagger c = -\frac{1}{2} \frac{J^3 n(D) \rho K}{\omega - D/2 + J/4} \frac{1}{2} \left(-\frac{1}{4} \right) \sum_{k_1, k_2, \alpha_1, \alpha_2, b} S_d^b s_{\alpha_1\alpha_2}^b c_{k_1\alpha_1, l_2}^\dagger c_{k_2\alpha_2, l_2} \\ &= \frac{1}{16} \frac{J^3 n(D) \rho K}{\omega - D/2 + J/4} \sum_{k_1, k_2, \alpha_1, \alpha_2} \vec{S}_d \cdot \vec{s}_{\alpha_1\alpha_2} c_{k_1\alpha_1, l_2}^\dagger c_{k_2\alpha_2, l_2} \end{aligned} \quad (1.5.20)$$

Calculation of second term

Like the single-channel case, the renormalization coming from the hole excitations is exactly the Hermitian conjugate of that in the particle sector. And since the renormalization ΔH_1 is Hermitian, we have $\Delta H_0 = \Delta H_1$

1.5.4 Total renormalization $\Delta H^{(3)}$

The total renormalization is twice that in the particle sector.

$$\Delta H^{(3)} = \frac{1}{8} \frac{J^3 n(D) \rho K}{\omega - D/2 + J/4} \sum_{k_1, k_2, \alpha_1, \alpha_2} \vec{S}_d \cdot \vec{s}_{\alpha_1\alpha_2} c_{k_1\alpha_1, l_2}^\dagger c_{k_2\alpha_2, l_2} \quad (1.5.21)$$

Combining with $\Delta H^{(2)}$ and replacing $n(D) = \rho |\delta D|$, we get

$$\frac{\Delta J}{|\Delta D|} = -\frac{J^2 \rho}{\omega - D/2 + J/4} + \frac{1}{8} \frac{J^3 \rho^2 K}{\omega - D/2 + J/4} = -\frac{J^2 \rho}{\omega - D/2 + J/4} \left[1 - \frac{1}{8} J \rho K \right] \quad (1.5.22)$$

We choose $\omega = -D/2$ to get a clearer idea of what the equations say.

$$\frac{\Delta J}{|\Delta D|} = \frac{J^2 \rho}{D - J/4} \left[1 - \frac{1}{8} J \rho K \right] \quad (1.5.23)$$

Quantities with zero in the subscript will denote their values in the bare Hamiltonian. Using $\delta D = -|\delta D|$, we can write the continuum form of the equation:

$$\frac{dJ}{dD} = \frac{J^2 \rho}{D - J/4} \left(\frac{1}{8} J \rho K - 1 \right) \quad (1.5.24)$$

For $D \gg J$, we can ignore the J in the denominator, and the equation reduces to the one-loop poor man's scaling form

$$\frac{dJ}{dD} \simeq \frac{J^2 \rho}{D} \left(\frac{1}{8} J \rho K - 1 \right) \quad (1.5.25)$$

This equation has a stable fixed point at $J^* = \frac{8}{\rho K}$.

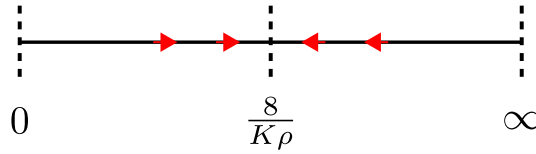


Figure 1.8: Attractive finite J fixed point of poor man scaling RG equation

For D not so large, the denominator also comes into play, and eq.1.5.23 holds. We get the possibility of two fixed points - one from the numerator and the other from the denominator.

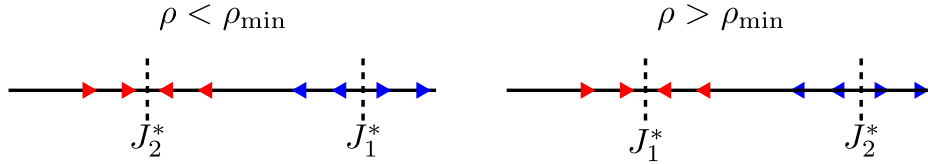


Figure 1.9

The numerator and denominator fixed points, J_1^* and J_2^* respectively, are given by

$$J_1^* = \frac{8}{K\rho}, \quad D^* = \frac{J_2^*}{4} \quad (1.5.26)$$

For a given K , the position of J_1^* will be governed by ρ . In general, for each bare bandwidth D_0 , there exists a minimal ρ , $\rho_{\min}(D_0)$, above which the the lower fixed point is the one from the numerator. That is, for $\rho > \rho_{\min}$, if we start scaling from small J_0 , it grows until it hits J_1^* which acts as the attractive fixed point, and J_2^* lies at a higher value and acts as the repulsive fixed point. For $\rho < \rho_{\min}$, J will grow and hit J_2^* instead, and $J_1^* > J_2^*$ now becomes the repulsive fixed point.

$$\rho_{\min} = \text{minimum} \left\{ \rho, \text{ such that } \frac{8}{K\rho} < 4D^*(\rho) \right\} \quad (1.5.27)$$

This behaviour is shown schematically in fig. 1.9. In fig. 1.10, we plot ρ_{\min} against the bare bandwidth. For large D_0 , it essentially shrinks to zero, and the numerator becomes the first fixed point for essentially all ρ .

If we assume we are at a sufficiently large D_0 and $\rho > \rho_{\min}$, the lower fixed point is J_1^* . As shown in fig. 1.10, we have $J_1^* \ll D_0$. If we start with J_0 in the neighborhood of J_1^* , we can use $J_1^* \ll D_0$ to ignore J in the denominator and the RG equation reduces to the poor man's scaling form eq. 1.5.25. The denominator fixed

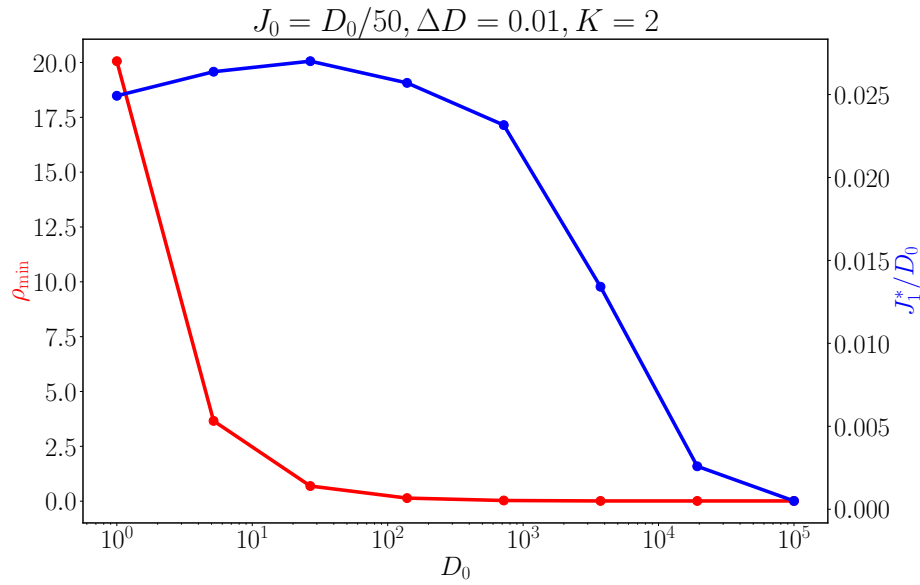


Figure 1.10: Red curve shows variation of ρ_{\min} against D_0 . It vanishes at large D_0 . Blue curve shows variation of the ratio J_1^*/D_0 with D_0 . That shrinks as well, showing that the fixed point J_1^* remains finite in the thermodynamic limit, and the distance between J_1^* and J_2^* keeps growing.

point has effectively moved off to infinity. That this is true can also be argued from the single-channel Kondo model URG results. There, we saw that when the bandwidth is scaled to larger values, the strong-coupling fixed point was stable at successively larger values of J^* . Since the denominator fixed point is identical in structure in both problems, its reasonable that the same thing will happen here.

Chapter 2

URG of the SIAM and its Spin and Charge Generalizations

2.1 URG of the SIAM

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

$$\mathcal{H} = \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{k\sigma} \left(V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right) + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \quad (2.1.1)$$

To allow the calculation of both particle and hole kinetic energies, we will write the kinetic energy part as $\sum_{k\sigma} \epsilon_k \tau_{k\sigma}$, where $\tau = \hat{n} - \frac{1}{2}$ and drop the extra constant part.

$$\mathcal{H} = \sum_{k\sigma} \epsilon_k \tau_{k\sigma} + \sum_{k\sigma} \left(V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right) + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \quad (2.1.2)$$

2.1.1 Calculation of renormalization

The renormalization is

$$c_{q\beta}^\dagger T \frac{1}{\omega - H^D} T^\dagger c_{q\beta} + T^\dagger c_{q\beta} \frac{1}{\omega' - H^D} c_{q\beta}^\dagger T \quad (2.1.3)$$

We will be decoupling an electron $q\beta$ at the energy shell $\epsilon_q = \pm D$. The diagonal part (that comes down in the denominator) is

$$H^D = \epsilon_q \tau_{q\beta} + \epsilon_d \hat{n}_{d\beta} + U \hat{n}_{d\beta} \hat{n}_{d\bar{\beta}} \quad (2.1.4)$$

The off-diagonal part is

$$c_{q\beta}^\dagger T = V_q c_{q\beta}^\dagger c_{d\beta} \quad (2.1.5)$$

The renormalization from a single electron $q\beta$ is

$$\begin{aligned} \Delta H &= c_{q\beta}^\dagger c_{d\beta} \frac{1|V_q|^2}{\omega - H^D} c_{d\beta}^\dagger c_{q\beta} + c_{d\beta}^\dagger c_{q\beta} \frac{1|V_q|^2}{\omega' - H^D} c_{q\beta}^\dagger c_{d\beta} \\ &= c_{q\beta}^\dagger c_{d\beta} \frac{|V_q|^2}{\omega - D/2 - \epsilon_d - U \hat{n}_{d\bar{\beta}}} c_{d\beta}^\dagger c_{q\beta} + c_{d\beta}^\dagger c_{q\beta} \frac{|V_q|^2}{\omega' - D/2} c_{q\beta}^\dagger c_{d\beta} \\ &= \frac{\hat{n}_{q\beta} (1 - \hat{n}_{d\beta}) |V_q|^2}{\omega - D/2 - \epsilon_d - U \hat{n}_{d\bar{\beta}}} + \frac{\hat{n}_{d\beta} (1 - \hat{n}_{q\beta}) |V_q|^2}{\omega' - D/2} \end{aligned} \quad (2.1.6)$$

For comparing the two ω s, we will use the relation eq. 1.1.72: $\omega_0^1 + \omega_0^1 = H_0^D + H_1^D$ where $\omega_0^1 = \omega'$. ω_0^1 however is not ω . This is because the relation assumes the ω s to be calculated at the same energy - while ω' is calculated at energy $-D$, ω is at energy D . The ω_0^1 should hence be the ω at energy $-D$, which is $-\omega$. With this in mind, the relation says

$$\omega' - \omega = D/2 + \epsilon_d + U\hat{n}_{d\beta} - D/2 \quad (2.1.7)$$

This gives an expression of ω' in terms of ω . Substituting this into ΔH gives

$$\Delta H = \frac{\hat{n}_{q\beta} (1 - \hat{n}_{d\beta}) |V_q|^2}{\omega - D/2 - \epsilon_d - U\hat{n}_{d\bar{\beta}}} + \frac{\hat{n}_{d\beta} (1 - \hat{n}_{q\beta}) |V_q|^2}{\omega - D/2 + \epsilon_d + U\hat{n}_{d\bar{\beta}}} \quad (2.1.8)$$

The total renormalization from the entire shell $\pm D$ is

$$\begin{aligned} \Delta H &= \sum_{q\beta} |V_q|^2 \left[\frac{\hat{n}_{q\beta} (1 - \hat{n}_{d\beta})}{\omega - D/2 - \epsilon_d - U\hat{n}_{d\bar{\beta}}} + \frac{\hat{n}_{d\beta} (1 - \hat{n}_{q\beta})}{\omega - D/2 + \epsilon_d + U\hat{n}_{d\bar{\beta}}} \right] \\ &= \sum_q |V_q|^2 \left[\frac{(1 - \hat{n}_{d\beta}) \hat{n}_{d\bar{\beta}}}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d - U} + \frac{(1 - \hat{n}_{d\beta}) (1 - \hat{n}_{d\bar{\beta}})}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d} + \frac{\hat{n}_{d\beta} \hat{n}_{d\bar{\beta}}}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d + U} + \frac{\hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}})}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d} \right] \end{aligned} \quad (2.1.9)$$

2.1.2 Scaling equations

Once we have the renormalization for decoupling one electronic or hole state, we can just sum over the spins and momenta to get the total renormalization upon decoupling the entire shells $\pm\epsilon_q$. From the structure of $\Delta\mathcal{H}$ in eq. 2.1.9, we can see that there are renormalizations to all three configuration energies of the impurity: the doublon energy E_2 corresponding to the state $\hat{n}_{d\beta}\hat{n}_{d\bar{\beta}}$, the single energy E_1 corresponding to $(\hat{n}_{d\beta}(1 - \hat{n}_{d\bar{\beta}}) + \hat{n}_{d\bar{\beta}}(1 - \hat{n}_{d\beta}))$, and the holon energy E_0 corresponding to $(1 - \hat{n}_{d\beta})(1 - \hat{n}_{d\bar{\beta}}) + \hat{n}_{d\bar{\beta}}(1 - \hat{n}_{d\beta})$.

$$\begin{aligned} \Delta E_2 &= +2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d + U} \\ \Delta E_1 &= + \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d} + \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d - U} \\ \Delta E_0 &= +2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d} \end{aligned} \quad (2.1.10)$$

Using the relations $\epsilon_d = E_1 - E_0$ and $U = E_2 + E_0 - 2E_1$, we can write

$$\begin{aligned} \Delta\epsilon_d &= + \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d} + \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d - U} - 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d} \\ \Delta U &= \sum_q \frac{2|V_q|^2}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d + U} + \sum_q \frac{2|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d} - \sum_q \frac{2|V_q|^2}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d} - \sum_q \frac{2|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d - U} \end{aligned} \quad (2.1.11)$$

2.1.3 Connection to Poor Man's scaling

To obtain the results of Poor Man's scaling [7][10], we can look at various regimes. First we look at the case when both ϵ_d and U are small such that both the singly-occupied and doubly-occupied subspaces of the impurity are comfortably inside the bandwidth, $U, \epsilon_d \ll \epsilon_q$. We can then ignore the ϵ_d and U in the denominator compared to the ϵ_q .

$$\begin{aligned}\Delta\epsilon_d &= \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} + \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} - 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} \\ \Delta U &= 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} + 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} - 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} - 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q}\end{aligned}\tag{2.1.12}$$

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

In the regime $U \gg \epsilon_q \gg \epsilon_d$, the doubly-occupied state is far above the bandwidth. We can now ignore the terms that have U in the denominator. We get

$$\begin{aligned}\Delta\epsilon_d &= \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} - 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} \\ \Delta U &= 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} - 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q}\end{aligned}\tag{2.1.13}$$

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

$$\begin{aligned}\Delta U &= 0 \\ \delta\epsilon_d &= -\frac{\Delta}{\pi} \frac{1}{\omega - \frac{1}{2}D}\end{aligned}\tag{2.1.14}$$

There we replaced the difference symbol Δ with δ to avoid confusion with the hybridisation $\Delta \sim \sum V^2$. For low quantum fluctuations, we can ignore the renormalization in the couplings and replace ω with the initial conduction electron energy: $\omega = \epsilon_q \tau_{q\beta} = -\frac{1}{2}D$.

$$\delta\epsilon_d = \frac{\Delta}{\pi} \frac{\delta D}{D}\tag{2.1.15}$$

This is the one-loop scaling equation.

2.1.4 Particle-Hole symmetry

The Anderson model Hamiltonian, eq. 2.2.7, has an impurity particle-hole symmetry for a certain condition of the couplings. To see this, we apply the particle-hole transformation $c_k \rightarrow c_k^\dagger, c_d \rightarrow -c_d^\dagger$ to the Hamiltonian. Since we are looking at the impurity symmetry, we will only look at the terms involving the impurity. The particle-hole symmetry of the conduction bath is a separate thing and that requires a specific lattice. Hence we will not consider kinetic energy term in this discussion. The rest of the terms transform as

$$\epsilon_d \sum_\sigma \hat{n}_{d\sigma} \rightarrow 2\epsilon_d - \epsilon_d \sum_\sigma \hat{n}_{d\sigma}\tag{2.1.16}$$

$$U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \rightarrow U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} - U \sum_\sigma \hat{n}_{d\sigma} + U\tag{2.1.17}$$

$$\sum_{k\sigma} V(k) c_{k\sigma}^\dagger c_{d\sigma} + hc \rightarrow \sum_{k\sigma} -V(k) c_{k\sigma} c_{d\sigma}^\dagger + hc = \sum_{k\sigma} V^*(k) c_{k\sigma}^\dagger c_{d\sigma} + hc \quad (2.1.18)$$

$$S^z \sum_{kq} s_{kq}^z \rightarrow (-S^z) \sum_{kq} (-s_{kq}^z) = S^z \sum_{kq} s_{kq}^z \quad (2.1.19)$$

$$S^\pm \sum_{kq} s_{kq}^\mp \rightarrow (-S^\pm) \sum_{kq} (-s_{kq}^\mp) = S^\pm \sum_{kq} s_{kq}^\mp \quad (2.1.20)$$

The transformation of the spin terms, eqs. 2.1.19 and 2.1.20, can be understood from the fact that since a spin degree of freedom can be written in terms of the number operator as $\hat{S} = \hat{n} - \frac{1}{2}$, it must transform by flipping its sign: $\hat{S} = \hat{n} - \frac{1}{2} \rightarrow \frac{1}{2} - \hat{n} = -\hat{S}$. The spin terms are thus invariant under the particle-hole transformation. The impurity-bath hopping term can be made symmetric by making $V(k)$ real; then we would have, from eq. 2.1.18,

$$V(k) (c_{k\sigma}^\dagger c_{d\sigma} + c_{d\sigma}^\dagger c_{k\sigma}) \rightarrow V(k) (c_{d\sigma}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger c_{d\sigma}) \quad (2.1.21)$$

The impurity diagonal terms, ϵ_d and U , require a specific condition. Combining eqs. 2.1.16 and 2.1.17,

$$\epsilon_d \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \rightarrow (-\epsilon_d - U) \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \quad (2.1.22)$$

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

$$\epsilon_d = -\epsilon_d - U \implies \epsilon_d + \frac{1}{2}U = 0 \quad (2.1.23)$$

This same condition can be obtained in a more physical way. If we consider the singly-occupied state of the impurity as the reference state, the doubly-occupied state is the particle-excitation and the vacant state is the hole excitation. The energy of this particle state is $E_2 = 2\epsilon_d + U$ and that of the hole state is $E_0 = 0$. Particle-hole symmetry then requires the particle and hole levels to be degenerate, which means $E_2 = E_0$, and we recover the condition eq. 2.1.23.

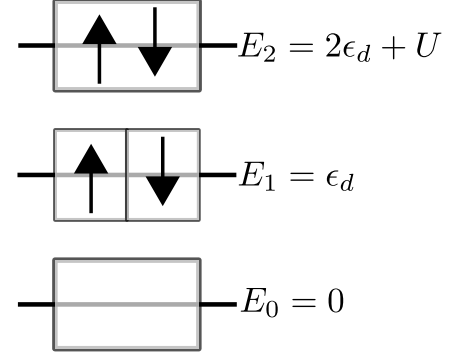


Figure 2.1: Particle and hole excitations of the impurity

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

$$\Delta \left(\epsilon_d + \frac{1}{2}U \right) = 0 \quad (2.1.24)$$

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

equation for the asymmetry parameter. The slightly easier way is to just note that the renormalization in E_2 should be equal to the renormalization in E_0 , in order for p-h symmetry to hold.

$$\Delta E_2 = 2 \frac{\Delta}{\pi} \frac{1}{\omega - D + \epsilon_d + U}, \Delta E_0 = 2 \frac{\Delta}{\pi} \frac{1}{\omega - D - \epsilon_d} \quad (2.1.25)$$

If we start with a particle-hole symmetric model, we will have $-\epsilon_d = \epsilon_d + U$. Substituting that gives $\Delta E_2 = \Delta E_0$. This shows that the doublon and holon states remain equidistant from the single-particle level, thus maintaining particle-hole symmetry along the flow.

2.1.5 Numerical analysis of symmetric SIAM

We will specialize to the particle-hole symmetric case, $2\epsilon_d + U = 0$, and a symmetric energy shell $\epsilon_q = D$, and look at the scaling behavior of ϵ_d .

$$\Delta \epsilon_d = -4|V|^2 \frac{\epsilon_d}{\left(\omega - \frac{1}{2}D\right)^2 - \epsilon_d^2} \quad (2.1.26)$$

Since the equation is symmetric under $\epsilon_d \rightarrow -\epsilon_d$, we might as well work with the magnitude of the onsite energy:

$$\Delta |\epsilon_d| = -4|V|^2 \frac{|\epsilon_d|}{\left(\omega - \frac{1}{2}D\right)^2 - \epsilon_d^2} \quad (2.1.27)$$

Depending on the signature of the denominator, the flows will be either relevant or irrelevant. For the flow to

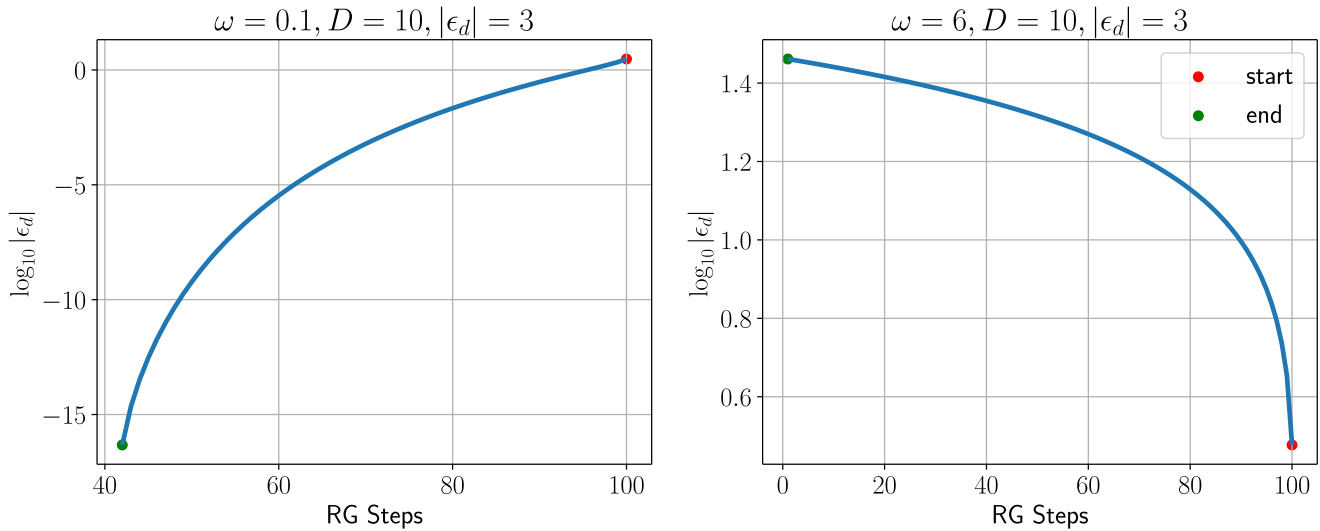
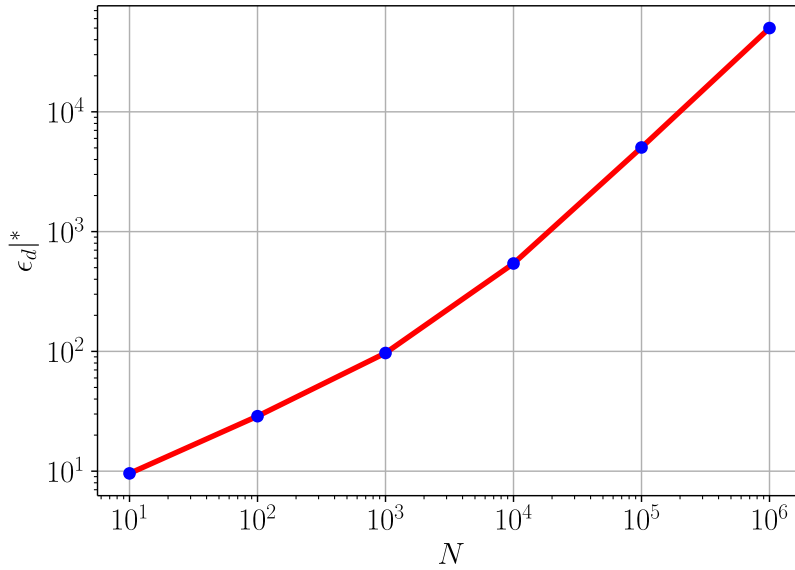


Figure 2.2: Left: Irrelevant flow towards $|\epsilon_d| = 0$, at low ω . Right: Relevant flow towards large $|\epsilon_d|$, at large ω . The former can be thought of as the projection of the strong-coupling flow on to the $\epsilon_d - D$ plane. The latter is the flow towards the local moment fixed point, if we start from a negative ϵ_d .

the local moment fixed point, the fixed point value of $|\epsilon_d|$ grows as we increase the bandwidth. This implies that for a thermodynamically large system, the local moment fixed point will be at $-\epsilon_d \rightarrow \infty$. This behavior is shown in fig. 2.3.


 Figure 2.3: Change in fixed point value of $|\epsilon_d|$ with system size.

2.2 Anderson-Kondo (spin) model URG

In order to obtain a renormalization in V , we will introduce a spin-spin interaction between the impurity and the mobile electrons. Such terms are generated when one does a Schrieffer-Wolff transformation on the SIAM, but we will find it prudent to keep these terms in the bare model itself.

2.2.1 Spin-spin interaction

We first consider a general four-Fermion interaction of the form

$$\mathcal{H}_I = \sum_{k,k',\sigma_i} u c_{d\sigma_2}^\dagger c_{d\sigma_4} c_{k'\sigma_3} c_{k\sigma_1}^\dagger \delta_{(\sigma_1+\sigma_2=\sigma_3+\sigma_4)} \quad (2.2.1)$$

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

$$\mathcal{H}_I = \underbrace{\sum_{k,k',\sigma,\sigma'} u_1 \hat{n}_{d\sigma'} c_{k\sigma}^\dagger c_{k'\sigma}}_{\text{spin-preserving scattering}} + \overbrace{\sum_{k,k',\sigma} u_2 c_{d\bar{\sigma}}^\dagger c_{d\sigma} c_{k\sigma}^\dagger c_{k'\bar{\sigma}}}^{\text{spin-flip scattering}} \quad (2.2.2)$$

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

$$\mathcal{H}_{I,N} = \sum_{k,k',\sigma,\sigma'} u_P \hat{n}_{d\sigma'} c_{k\sigma}^\dagger c_{k'\sigma} + \sum_{k,k',\sigma} u_A c_{d\bar{\sigma}}^\dagger c_{d\sigma} c_{k\sigma}^\dagger c_{k'\bar{\sigma}} \quad (2.2.3)$$

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

$$u_{\uparrow\uparrow} \hat{n}_{d\uparrow} c_{k\uparrow}^\dagger c_{k'\uparrow} + u_{\downarrow\downarrow} \hat{n}_{d\downarrow} c_{k\downarrow}^\dagger c_{k'\downarrow} + u_{\uparrow\downarrow} \hat{n}_{d\uparrow} c_{k\downarrow}^\dagger c_{k'\downarrow} + u_{\downarrow\uparrow} \hat{n}_{d\downarrow} c_{k\uparrow}^\dagger c_{k'\uparrow} \quad (2.2.4)$$

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

$$\begin{aligned}\mathcal{H}_I &= J_z \frac{\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow}}{2} \sum_{kk'} \left(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow} \right) + J_t \sum_{kk'} \left[c_{d\uparrow}^\dagger c_{d\downarrow} c_{k\downarrow}^\dagger c_{k'\uparrow} + c_{d\downarrow}^\dagger c_{d\uparrow} c_{k\uparrow}^\dagger c_{k'\downarrow} \right] \\ &= 2J_z S_d^z s^z + J_t \left(S_d^+ s^- + S_d^- s^+ \right)\end{aligned}\quad (2.2.5)$$

The spin-like operators are defined as

$$\begin{aligned}S_d^z &\equiv \frac{1}{2} \left(\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow} \right) & S_d^+ &\equiv c_{d\uparrow}^\dagger c_{d\downarrow} & S_d^- &\equiv c_{d\downarrow}^\dagger c_{d\uparrow} \\ s_{kk'}^z &\equiv \frac{1}{2} \left(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow} \right) & s_{kk'}^+ &\equiv c_{k\uparrow}^\dagger c_{k'\downarrow} & s_{kk'}^- &\equiv c_{k\downarrow}^\dagger c_{k'\uparrow} \\ s^a &\equiv \sum_{kk'} s_{kk'}^a\end{aligned}\quad (2.2.6)$$

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

$$\mathcal{H} = \sum_{k\sigma} \left(\epsilon_k \hat{n}_{k\sigma} + V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right) + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + 2J_z S_d^z s^z + J_t \left(S_d^+ s^- + S_d^- s^+ \right)\quad (2.2.7)$$

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

$$\mathcal{H}_I = J \left[S_d^z s^z + \frac{1}{2} \left(S_d^+ s^- + S_d^- s^+ \right) \right] = J \mathbf{S}_d \cdot \mathbf{s}\quad (2.2.8)$$

For the URG, we take two electrons on the shell Λ_N , $q\beta$ and $\bar{q}\bar{\beta}$, then decouple the electron $q\beta$. The reason for taking two electrons is to allow the symmetries to be preserved. For simplicity, we will only consider those diagonal terms in the denominator that either have both $q\beta$ and $\bar{q}\bar{\beta}$ or both $q\beta$ and d or both $\bar{q}\bar{\beta}$ and d . Terms that have purely $\bar{q}\bar{\beta}$ will not be considered. Also, the scattering between just d and $\bar{q}\bar{\beta}$ can be ignored since it is diagonal in $q\beta$. The Hamiltonian for such a system is

$$\begin{aligned}\mathcal{H}_N &= H_{N-1} + H_{\text{imp}} + \epsilon_q \hat{n}_{q\beta} + 2J_z S_d^z s_q^z + V_q c_{q\beta}^\dagger c_{d\beta} + h.c. + \\ &\sum_{k < \Lambda_N} \left[J_z S_d^z \beta \left(c_{k\beta}^\dagger c_{q\beta} + c_{q\beta}^\dagger c_{k\beta} \right) + J_t \left(c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} + c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\bar{\beta}} \right) \right] \\ &+ J_t \left(c_{d\beta}^\dagger c_{d\bar{\beta}} c_{q\bar{\beta}}^\dagger c_{q\beta} + c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{q\bar{\beta}} \right)\end{aligned}\quad (2.2.9)$$

where $s_q^z = \frac{1}{2} \left(\hat{n}_{q\uparrow} - \hat{n}_{q\downarrow} \right)$ and H_{imp} is the impurity-diagonal part of the Hamiltonian ($\epsilon_d \hat{n}_d + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow}$) and

$$H_{N-1} = \sum_{k < \Lambda_N, \sigma} \left[\left(\epsilon_k + \sigma J_z S_d^z \right) \hat{n}_{k\sigma} + V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right] + H_{I, N-1}\quad (2.2.10)$$

The diagonal (number-preserving) part is

$$\mathcal{H}_D = H_{N-1}^D + \epsilon_q \left(\hat{n}_{q\beta} + \hat{n}_{q\bar{\beta}} \right) + 2J_z S_d^z s_q^z + H_{\text{imp}}\quad (2.2.11)$$

In line with the simplifications mentioned above, we will work with the following terms:

$$\mathcal{H}_D = \epsilon_q \hat{n}_{q\beta} + 2J_z S_d^z s_q^z + H_{imp} \quad (2.2.12)$$

To allow the calculation of hole and particle energies on an equal footing, we will make a transformation at the bare model itself:

$$\sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} = \sum_{k\sigma} \epsilon_k \hat{\tau}_{k\sigma} + \mathcal{C} \quad (2.2.13)$$

where $\tau \equiv \hat{n} - \frac{1}{2}$ and \mathcal{C} is non-dynamic and will hence be dropped. This transforms the diagonal part \mathcal{H}^D . Eq. 2.2.12 becomes

$$\mathcal{H}_D = \epsilon_q \tau_{q\beta} + 2J_z S_d^z s_q^z + H_{imp} \quad (2.2.14)$$

The entire off-diagonal piece can be split into 6 parts:

$$\begin{aligned} \mathcal{H}_X = & \underbrace{V_1^* c_{d\beta}^\dagger c_{q\beta} \hat{n}_{d\bar{\beta}}}_{T_1^\dagger c_{q\beta}} + \overbrace{V_0^* c_{d\beta}^\dagger c_{q\beta} (1 - \hat{n}_{d\bar{\beta}})}^{T_2^\dagger c_{q\beta}} + \underbrace{\sum_{k < \Lambda_N} J_0^z \hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}}) c_{k\beta}^\dagger c_{q\beta}}_{T_3^\dagger c_{q\beta}} \\ & - \underbrace{\sum_{k < \Lambda_N} J_1^z \hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta}) c_{k\beta}^\dagger c_{q\beta}}_{T_4^\dagger c_{q\beta}} + \underbrace{\sum_{k < \Lambda_N} J^t c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta}}_{T_5^\dagger c_{q\beta}} + \overbrace{J^t c_{d\beta}^\dagger c_{d\bar{\beta}} c_{q\bar{\beta}}^\dagger c_{q\beta}}^{T_6^\dagger c_{q\beta}} + \text{h.c.} \end{aligned} \quad (2.2.15)$$

The various parts of the off-diagonal piece are

$$\begin{aligned} T_1 &= V_1 c_{d\beta} \hat{n}_{d\bar{\beta}} \\ T_2 &= V_0 c_{d\beta} (1 - \hat{n}_{d\bar{\beta}}) \\ T_3 &= \sum_{k < \Lambda_N} J_0^z \hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}}) c_{k\beta} \\ T_4 &= - \sum_{k < \Lambda_N} J_1^z \hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta}) c_{k\beta} \\ T_5 &= \sum_{k < \Lambda_N} J^t c_{d\bar{\beta}}^\dagger c_{d\beta} c_{k\bar{\beta}} \end{aligned} \quad (2.2.16)$$

2.2.2 Calculation of renormalization in particle sector

We will first look at the renormalization of ϵ_d , U and the interaction couplings for the lower shell electrons, so we can ignore T_6 for the time-being. The renormalization in the particle sector ($\hat{n}_{q\beta} = 1$) is of the form

$$c_{q\beta}^\dagger T \eta \quad (2.2.17)$$

Since we have $\hat{n}_{q\beta} = 1$ in the initial state, this will be at energy $-\epsilon_q$. The generator η will have five parts:

$$\eta = \sum_{i=1}^5 \frac{1}{\omega_i - E_i^0} T_i^\dagger c_{q\beta} \quad (2.2.18)$$

We need to compute a quantity of the form

$$\begin{aligned}
& \sum_{ij} \left(\frac{1}{\omega_i - E_i^0} + \frac{1}{\omega - E_j^0} \right) T_i T_j^\dagger \\
&= \frac{1}{\omega_1 - E_1^0} T_1 T_1^\dagger + \frac{1}{\omega_2 - E_2^0} T_2 T_2^\dagger + \frac{1}{\omega_3 - E_3^0} T_3 T_3^\dagger + \frac{1}{\omega_4 - E_4^0} T_4 T_4^\dagger + \frac{1}{\omega_5 - E_5^0} T_5 T_5^\dagger \\
&+ \left(\frac{1}{\omega_2 - E_2^0} + \frac{1}{\omega_5 - E_5^0} \right) (T_2 T_5^\dagger + T_5 T_2^\dagger) + \left(\frac{1}{\omega_2 - E_2^0} + \frac{1}{\omega_3 - E_3^0} \right) (T_2 T_3^\dagger + T_3 T_2^\dagger) \\
&+ \left(\frac{1}{\omega_3 - E_3^0} + \frac{1}{\omega_5 - E_5^0} \right) (T_3 T_5^\dagger + T_5 T_3^\dagger)
\end{aligned}$$

The diagonal parts E_i^0 are

$$\begin{aligned}
E_1^0 &= \frac{\epsilon_q}{2} + 2\epsilon_d + U \\
E_2^0 = E_5^0 = E_4^0 &= \frac{\epsilon_q}{2} + \epsilon_d - \frac{J_z}{2} \\
E_3^0 &= \frac{\epsilon_q}{2} + \epsilon_d + \frac{J_z}{2}
\end{aligned} \tag{2.2.19}$$

Note that in writing these diagonal parts, we have considered the effect of c_k^\dagger on the J_z part. For example, if there is a $\hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}}) c_{k\beta}^\dagger$ in front of the propagator, that means the intermediate state has $\hat{n}_{d\beta} - \hat{n}_{d\bar{\beta}} = 1 = \hat{n}_{k\beta}$ and that will contribute a term $\frac{J_z}{2} (\hat{n}_{d\beta} - \hat{n}_{d\bar{\beta}}) \hat{n}_{k\beta} = \frac{J_z}{2}$ to E^0 . Also, while calculating E_5 , we have ignored the presence of $\hat{n}_{q\bar{\beta}}$, because it violates the spin reversal symmetry for this term.

Defining $\xi_i \equiv \omega_i - E_i^0$ and evaluating the terms $T_i T_j^\dagger$ gives

$$\begin{aligned}
& \sum_{ij} \left(\frac{1}{\omega_i - E_i^0} + \frac{1}{\omega - E_j^0} \right) T_i T_j^\dagger \\
&= \frac{|V_1|^2}{\xi_1} (1 - \hat{n}_{d\beta}) \hat{n}_{d\bar{\beta}} + \frac{|V_0|^2}{\xi_2} (1 - \hat{n}_{d\beta}) (1 - \hat{n}_{d\bar{\beta}}) \\
&+ \frac{1}{4} \left[J_0^{z2} \frac{\hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}})}{\xi_3} + J_1^{z2} \frac{\hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta})}{\xi_4} \right] c_{k'\beta} c_{k\beta}^\dagger + \frac{1}{\xi_5} J_t^2 (1 - \hat{n}_{d\beta}) \hat{n}_{d\bar{\beta}} c_{k'\bar{\beta}} c_{k\bar{\beta}}^\dagger \\
&- \frac{1}{2} \left(\frac{1}{\xi_2} + \frac{1}{\xi_5} \right) J_t (1 - \hat{n}_{d\beta}) (V_0 c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} + \text{h.c.}) - \frac{1}{2} \left(\frac{1}{\xi_2} + \frac{1}{\xi_3} \right) \frac{J_0^z}{2} (1 - \hat{n}_{d\bar{\beta}}) (V_0 c_{k\beta}^\dagger c_{d\beta} + \text{h.c.}) \\
&- \frac{1}{2} \left(\frac{1}{\xi_3} + \frac{1}{\xi_5} \right) \frac{J_t J_0^z}{2} (c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{k'\beta} + \text{h.c.})
\end{aligned} \tag{2.2.20}$$

The indices k and k' are being summed over, wherever they appear.

2.2.3 Calculation of renormalization in hole sector

The renormalization in the particle sector ($\hat{n}_{q\beta} = 0$) is of the form

$$T_{q\beta}^\dagger c \eta_0^\dagger \quad (2.2.21)$$

where η_0^\dagger is of the form

$$\eta_0^\dagger = \sum_{i=1}^5 \frac{1}{\omega'_i - E_i^1} c_{q\beta}^\dagger T_i \quad (2.2.22)$$

This will be at an energy $+\epsilon_q$, because the state is occupied. The scattering terms T_i are already written down in the previous subsection. The diagonal parts are

$$\begin{aligned} E_1^1 &= E_4^1 = E_5^1 = \frac{\epsilon_q}{2} + \epsilon_d - \frac{J_z}{2} \\ E_2^1 &= \frac{\epsilon_q}{2} \\ E_3^1 &= \frac{\epsilon_q}{2} + \epsilon_d + \frac{J_z}{2} \end{aligned} \quad (2.2.23)$$

The renormalization can be computed by calculating $\sum_{ij} T_i^\dagger T_j$.

$$\begin{aligned} & \sum_{ij} \left(\frac{1}{\omega'_i - E_i^1} + \frac{1}{\omega'_j - E_j^1} \right) T_i^\dagger T_j \\ &= \frac{|V_1|^2}{\xi'_1} \hat{n}_{d\bar{\beta}} \hat{n}_{d\beta} + \frac{|V_0|^2}{\xi'_2} \hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}}) \\ &+ \frac{1}{4} \left[J_0^{z2} \frac{\hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}})}{\xi'_3} + J_1^{z2} \frac{\hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta})}{\xi'_4} \right] c_{k\beta}^\dagger c_{k'\beta} + \frac{1}{\xi'_5} J_t^2 (1 - \hat{n}_{d\bar{\beta}}) \hat{n}_{d\beta} c_{k\bar{\beta}}^\dagger c_{k'\bar{\beta}} \\ &- \frac{1}{2} \left(\frac{1}{\xi'_4} + \frac{1}{\xi'_1} \right) \frac{J_1^z}{2} \hat{n}_{d\bar{\beta}} (V_1 c_{k\beta}^\dagger c_{d\beta} + \text{h.c.}) - \frac{1}{2} \left(\frac{1}{\xi'_1} + \frac{1}{\xi'_5} \right) J_t \hat{n}_{d\beta} (V_1 c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} + \text{h.c.}) \\ &- \frac{1}{2} \left(\frac{1}{\xi'_4} + \frac{1}{\xi'_5} \right) \frac{J_t J_1^z}{2} (c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{k'\beta} + \text{h.c.}) \end{aligned}$$

where ξ'_i is defined similar to the particle sector: $\xi'_i = \omega'_i - E_i^1$. The indices k and k' are being summed over, wherever they appear.

2.2.4 Relating the ω_i and ω'_i

To relate the ω_i and their primed counterparts, we will look at their bare non-interacting values:

$$\begin{aligned} \omega_1 &= -\frac{1}{2}\epsilon_q + \epsilon_d \\ \omega_2 &= -\frac{1}{2}\epsilon_q \\ \omega_3 &= -\frac{1}{2}\epsilon_q + \epsilon_d + \frac{J_z}{2} \\ \omega_5 &= \omega_4 = -\frac{1}{2}\epsilon_q + \epsilon_d - \frac{J_z}{2} \end{aligned} \quad (2.2.24)$$

We will *assume* that the relations between these values of ω_i will hold for the URG ω_i along the flow as well. We want to write all the ω_i in terms of a single $\omega = -\frac{\epsilon_q}{2} - \frac{1}{2}J_z$.

$$\begin{aligned}\omega_1 &= \omega + \frac{J_z}{2} + \epsilon_d \\ \omega_2 &= \omega + \frac{J_z}{2} \\ \omega_3 &= \omega + J_z + \epsilon_d \\ \omega_5 &= \omega_4 = \omega + \epsilon_d\end{aligned}\tag{2.2.25}$$

The denominators can now be written in terms of the single ω :

$$\begin{aligned}\xi_1 &= \omega - \frac{\epsilon_q}{2} - \epsilon_d - U + \frac{J_z}{2} \\ \xi_2 &= \omega - \frac{\epsilon_q}{2} - \epsilon_d + J_z \\ \xi_3 &= \xi_4 = \xi_5 = \omega - \frac{\epsilon_q}{2} + \frac{J_z}{2}\end{aligned}\tag{2.2.26}$$

Similarly, for the ω'_i of the hole sector, we have

$$\begin{aligned}\omega'_1 &= -\frac{1}{2}\epsilon_q + 2\epsilon_d + U \\ \omega'_2 &= -\frac{1}{2}\epsilon_q + \epsilon_d \\ \omega'_3 &= -\frac{1}{2}\epsilon_q + \epsilon_d + \frac{J_z}{2} \\ \omega'_4 &= \omega'_5 = -\frac{1}{2}\epsilon_q + \epsilon_d - \frac{J_z}{2}\end{aligned}\tag{2.2.27}$$

Writing these in terms of $\omega = -\frac{\epsilon_q}{2} - \frac{1}{2}J_z$ gives

$$\begin{aligned}\omega'_1 &= \omega + U + \frac{J_z}{2} \\ \omega'_2 &= \omega + \epsilon_d + \frac{J_z}{2} \\ \omega'_3 &= \omega + \epsilon_d + J_z \\ \omega'_4 &= \omega'_5 = \omega + \epsilon_d\end{aligned}\tag{2.2.28}$$

The denominators are therefore

$$\begin{aligned}\xi'_1 &= \omega - \frac{\epsilon_q}{2} + \epsilon_d + U + J_z \\ \xi'_2 &= \omega - \frac{\epsilon_q}{2} + \epsilon_d + \frac{J_z}{2} \\ \xi'_3 &= \xi'_4 = \xi'_5 = \omega - \frac{\epsilon_q}{2} + \frac{J_z}{2} = \xi_3 = \xi_4 = \xi_5\end{aligned}\tag{2.2.29}$$

2.2.5 Making sense of the various terms

We will now look at each of the renormalizations separately. Note that the indices k and k' are being summed over, wherever they appear. The first two terms in each sector form a part of the renormalization in ϵ_d and U .

$$\frac{|V_1|^2}{\xi_1} (1 - \hat{n}_{d\beta}) \hat{n}_{d\bar{\beta}} + \frac{|V_0|^2}{\xi_2} (1 - \hat{n}_{d\beta}) (1 - \hat{n}_{d\bar{\beta}}) + \frac{|V_1|^2}{\xi'_1} \hat{n}_{d\bar{\beta}} \hat{n}_{d\beta} + \frac{|V_0|^2}{\xi'_2} \hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}}) \quad (2.2.30)$$

We can read off the renormalizations in the doublon, spin and holon states. Note that the spin ($\hat{n}_d = 1$) are only renormalized by half, because the other half of the renormalization comes when you decouple the other spin $\bar{\beta}$.

$$\Delta E_2 = \frac{|V_1|^2}{\xi'_1}, \quad \Delta E_1 = \frac{|V_1|^2}{2\xi_1} + \frac{|V_0|^2}{2\xi'_2}, \quad \Delta E_0 = \frac{|V_0|^2}{\xi_2} \quad (2.2.31)$$

Using $\epsilon_d = E_1 - E_0$ and $U = E_2 + E_0 - 2E_1$, we can write

$$\begin{aligned} \Delta \epsilon_d &= \frac{|V_1|^2}{2\xi_1} + \frac{|V_0|^2}{2\xi'_2} - \frac{|V_0|^2}{\xi_2} \\ \Delta U &= \frac{|V_1|^2}{\xi'_1} + \frac{|V_0|^2}{\xi_2} - \frac{|V_1|^2}{\xi_1} - \frac{|V_0|^2}{\xi'_2} \end{aligned} \quad (2.2.32)$$

The J_z^2 terms, together, give

$$\frac{J_z^2}{4} \left[\frac{\hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}})}{\xi_3} + \frac{\hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta})}{\xi_4} \right] c_{k'\beta} c_{k\beta}^\dagger + \frac{1}{4} \left[\frac{\hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}})}{\xi'_3} + \frac{\hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta})}{\xi'_4} \right] c_{k\beta}^\dagger c_{k'\beta} \quad (2.2.33)$$

There we used $J_0^z = J_1^z = J_z$. From the expressions of ξ_i and ξ'_i , we know that $\xi_3 = \xi_4 = \xi'_3 = \xi'_4$. Therefore, the terms in the box brackets are identical, and we can simplify this to

$$\frac{J_z^2}{4\xi_3} \left[\hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}}) + \hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta}) \right] (c_{k'\beta} c_{k\beta}^\dagger + c_{k\beta}^\dagger c_{k'\beta}) = \frac{J_z^2}{4\xi_3} [\hat{n}_d - 2\hat{n}_{d\beta}\hat{n}_{d\bar{\beta}}] \delta_{kk'} \quad (2.2.34)$$

This will further renormalize $\epsilon_d \hat{n}_d$ and $U \hat{n}_{d\beta} \hat{n}_{d\bar{\beta}}$, now at J^2 order:

$$\begin{aligned} \Delta \epsilon_d &= \frac{J_z^2}{4\xi_3} \delta_{kk'} \\ \Delta U &= -2 \frac{J_z^2}{4\xi_3} \delta_{kk'} \end{aligned} \quad (2.2.35)$$

We next look at the $J_z V$ terms:

$$-\frac{J_z}{4} \left[\left(\frac{1}{\xi_2} + \frac{1}{\xi_3} \right) (1 - \hat{n}_{d\bar{\beta}}) V_0 c_{k\beta}^\dagger c_{d\beta} + \left(\frac{1}{\xi'_4} + \frac{1}{\xi'_1} \right) \hat{n}_{d\bar{\beta}} V_1 c_{k\beta}^\dagger c_{d\beta} \right] + \text{h.c.} \quad (2.2.36)$$

The first term in the box bracket renormalizes $V_0 c_{k\beta}^\dagger c_{d\beta} (1 - \hat{n}_{d\bar{\beta}})$, while the second term renormalizes $V_1 c_{k\beta}^\dagger c_{d\beta} \hat{n}_{d\bar{\beta}}$. Because this renormalizes only one spin component (β), the other spin component will get renormalized when

we decouple $\bar{\beta}$, and so we attribute only half of this to the total renormalization.

$$\begin{aligned}\Delta V_0 &= -\frac{1}{2} \frac{J_z}{2} V_0 \left(\frac{1}{\xi_2} + \frac{1}{\xi_3} \right) \\ \Delta V_1 &= -\frac{1}{2} \frac{J_z}{2} V_1 \left(\frac{1}{\xi'_1} + \frac{1}{\xi_3} \right)\end{aligned}\tag{2.2.37}$$

where we used $\xi'_4 = \xi_3$. The terms with $J_t V$ also renormalize the same terms. Combining this with the previous renormalization gives the total renormalization of V_0 and V_1 :

$$\begin{aligned}\Delta V_0 &= -\left(\frac{J_z}{4} V_0 + J_t V_0 \right) \left(\frac{1}{\xi_2} + \frac{1}{\xi_3} \right) \\ \Delta V_1 &= -\left(\frac{J_z}{4} V_1 + J_t V_1 \right) \left(\frac{1}{\xi'_1} + \frac{1}{\xi_3} \right)\end{aligned}\tag{2.2.38}$$

There we used $\xi'_5 = \xi_5 = \xi_3$.

The remaining terms are all of order J^2 . First we look at the J_t^2 terms:

$$\begin{aligned}& \frac{1}{\xi_5} J_t^2 \left(1 - \hat{n}_{d\beta} \right) \hat{n}_{d\bar{\beta}} c_{k'\bar{\beta}} c_{k\bar{\beta}}^\dagger + \frac{1}{\xi'_5} J_t^2 \left(1 - \hat{n}_{d\bar{\beta}} \right) \hat{n}_{d\beta} c_{k\bar{\beta}}^\dagger c_{k'\bar{\beta}} \\ &= \frac{1}{\xi_3} J_t^2 c_{k\bar{\beta}}^\dagger c_{k'\bar{\beta}} \left[\left(1 - \hat{n}_{d\bar{\beta}} \right) \hat{n}_{d\beta} - \left(1 - \hat{n}_{d\beta} \right) \hat{n}_{d\bar{\beta}} \right] + \delta_{kk'} \frac{1}{\xi_3} J_t^2 \left(1 - \hat{n}_{d\beta} \right) \hat{n}_{d\bar{\beta}} \\ &= -\frac{1}{\xi_3} 2 J_t^2 c_{k\bar{\beta}}^\dagger c_{k'\bar{\beta}} \frac{\hat{n}_{d\bar{\beta}} - \hat{n}_{d\beta}}{2} + \delta_{kk'} \frac{1}{\xi_3} J_t^2 \left(1 - \hat{n}_{d\beta} \right) \hat{n}_{d\bar{\beta}}\end{aligned}\tag{2.2.39}$$

In the second step, we used $\xi'_5 = \xi_5 = \xi_3$ and $c_k c_{k'}^\dagger = \delta_{kk'} - c_{k'}^\dagger c_k$. The first term in the final expression renormalizes half of the Ising Kondo coupling $J_z S_d^z s^z$, the other half will be renormalized when we decouple $q\bar{\beta}$.

$$\Delta J_z = -\frac{1}{2\xi_3} 2J_t^2\tag{2.2.40}$$

The other term in the final expression renormalizes U and half of ϵ_d (only $\bar{\beta}$).

$$\begin{aligned}\Delta \epsilon_d &= \frac{1}{2\xi_3} J_t^2 \delta_{kk'} \\ \Delta U &= -\frac{1}{\xi_3} J_t^2 \delta_{kk'}\end{aligned}\tag{2.2.41}$$

The remaining terms are those with $J_z J_t$:

$$\left[-\frac{1}{2} \left(\frac{1}{\xi_3} + \frac{1}{\xi_5} \right) \frac{J_t J_0^z}{2} c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{k'\beta} - \frac{1}{2} \left(\frac{1}{\xi'_4} + \frac{1}{\xi'_5} \right) \frac{J_t J_1^z}{2} c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{k'\beta} \right] + \text{h.c.}\tag{2.2.42}$$

They renormalize the transverse Kondo coupling. Noting that $\xi_5 = \xi'_4 = \xi'_5 = \xi_3$, we get

$$\Delta J_t = -\frac{1}{\xi_3} J_t J_0^z\tag{2.2.43}$$

2.2.6 Scaling equations

Looking at eqs. 2.2.32, 2.2.35, 2.2.41, 2.2.38, 2.2.40 and 2.2.43, and summing over β , we can write down the scaling equations for the Anderson-Kondo model.

$$\begin{aligned}
\Delta\epsilon_d &= \frac{|V_1|^2}{\xi_1} + \frac{|V_0|^2}{\xi'_2} - \frac{2|V_0|^2}{\xi_2} + \sum_k \frac{1}{\xi_3} \left(J_t^2 + \frac{1}{2} J_z^2 \right) \\
\Delta U &= \frac{2|V_1|^2}{\xi'_1} + \frac{2|V_0|^2}{\xi_2} - \frac{2|V_1|^2}{\xi_1} - \frac{2|V_0|^2}{\xi'_2} - \sum_k \frac{1}{\xi_3} \left(2J_t^2 + J_z^2 \right) \\
\Delta V_0 &= -V_0 \left(\frac{J_z}{2} + J_t \right) \left(\frac{1}{\xi_2} + \frac{1}{\xi_3} \right) \\
\Delta V_1 &= -V_1 \left(\frac{J_z}{2} + J_t \right) \left(\frac{1}{\xi'_1} + \frac{1}{\xi_3} \right) \\
\Delta J_z &= -\frac{2}{\xi_3} J_t^2 \\
\Delta J_t &= -\frac{2}{\xi_3} J_t J_0^z
\end{aligned}
\quad
\begin{aligned}
\xi_1 &= \omega - \frac{\epsilon_q}{2} - \epsilon_d - U + \frac{J_z}{2} \\
\xi_2 &= \omega - \frac{\epsilon_q}{2} - \epsilon_d + J_z \\
\xi'_1 &= \omega - \frac{\epsilon_q}{2} + \epsilon_d + U + J_z \\
\xi'_2 &= \omega - \frac{\epsilon_q}{2} + \epsilon_d + \frac{J_z}{2} \\
\xi'_3 &= \xi'_4 = \xi'_5 \\
&= \omega - \frac{\epsilon_q}{2} + \frac{J_z}{2} \\
&= \xi_3 = \xi_4 = \xi_5
\end{aligned}
\tag{2.2.44}$$

2.2.7 Particle-Hole symmetry

As discussed in the previous section, the particle-hole symmetry condition for the basic SIAM ($J = 0$) is $\epsilon_d + U = -\epsilon_d$. With the inclusion of J , we will need to see what the new condition is. We will first write the impurity part of the Hamiltonian and see how it transforms under a particle-hole transformation.

$$\begin{aligned}
&\epsilon_d \hat{n}_d + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + J_z \left(\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow} \right) \left(\hat{n}_{q\uparrow} - \hat{n}_{q\downarrow} \right) \\
&\rightarrow 2\epsilon_d + U - (\epsilon_d + U) \hat{n}_d + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + J_z \left(\hat{n}_{d\downarrow} - \hat{n}_{d\uparrow} \right) \left(\hat{n}_{q\downarrow} - \hat{n}_{q\uparrow} \right)
\end{aligned}
\tag{2.2.45}$$

This gives us the same condition as in the $J = 0$ case. The p-h symmetry condition implies that $2\epsilon_d + U$ must be an RG-invariant. The RG equation for $2\epsilon_d + U$ is

$$\Delta(2\epsilon_d + U) = \frac{|V_1|^2}{\xi'_1} - \frac{|V_1|^2}{\xi_2}
\tag{2.2.46}$$

For $2\epsilon_d + U = 0$ in the bare model, we can write $\xi_2 = \xi'_1$, which means $\Delta(2\epsilon_d + U) = 0$.

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

In the limit of $\epsilon_d, J \ll D \ll U$, we can ignore the J^2 terms in ϵ_d and U , and the remaining terms simplify:

$$\begin{aligned}
\frac{1}{\xi_1} &= \frac{1}{\xi'_1} \approx 0 \\
\xi_2 &= \xi'_2 \approx \omega - \frac{\epsilon_q}{2}
\end{aligned}
\tag{2.2.47}$$

These give

$$\begin{aligned}\Delta U &\approx 0 \\ \Delta\epsilon_d &\approx -\frac{|V_0|^2}{\xi_2} \approx -\frac{|V_0|^2}{\omega - \frac{\epsilon_q}{2}}\end{aligned}\quad (2.2.48)$$

This is the same form that we had in the pure SIAM, and we can again repeat what we did in subsection 2.1.3.

2.2.9 $SU(2)$ invariance and Kondo model one-loop form

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

$$\Delta J = -\frac{1}{\xi_3} J^2 = -J^2 \frac{1}{\omega - \frac{\epsilon_q}{2} + \frac{J_z}{2}} \quad (2.2.49)$$

For low quantum fluctuations we can ignore the renormalization and replace ω with the bare initial energy value $-\frac{1}{2}\epsilon_q$.

$$\Delta J = -J^2 \frac{1}{-\epsilon_q + \frac{1}{4}J} \quad (2.2.50)$$

We can now expand the denominator in powers of J and keep only the lowest order, we get

$$\Delta J = J^2 \frac{1}{\epsilon_q} \quad (2.2.51)$$

This is the Kondo model one-loop form.

2.3 Anderson-Kondo (charge) model URG

Performing the Schrieffer-Wolff transformation on the SIAM generates four types of terms. The simplest terms are ones that renormalize the impurity scales ϵ_d and U . The next are the potential scattering terms that describe interactions between mobile electrons with the impurity simply acting as a stationary potential. The third term is the familiar Kondo model interaction terms that involve a Heisenberg-like interaction between the impurity spin $S_d^z = \frac{1}{2}(\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow})$ and the global spin of the mobile electrons $\frac{1}{2} \sum_{kk'\alpha\beta} c_{k\alpha}^\dagger \vec{\sigma}_{\alpha\beta} c_{k'\beta}$. The fourth term is the interactions that modify the charge of either entity by 2, $c_{k\alpha}^\dagger c_{k'\bar{\alpha}}^\dagger c_{d\alpha} c_{d\bar{\alpha}}$. We will be considering the last kind of terms in this section. For that, we define the Nambu spinor [11, 12].

$$\psi^k = \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow}^\dagger \end{pmatrix} \quad (2.3.1)$$

and the charge isospin [13] for the mobile conduction electrons

$$\vec{C} = \sum_{kk'} \psi^{k\dagger} \vec{S} \psi^{k'} = \frac{1}{2} \sum_{kk'\alpha\beta} \psi_\alpha^{k\dagger} \vec{\sigma}_{\alpha\beta} \psi_\beta^{k'} \quad (2.3.2)$$

The various components of the isospin are

$$\begin{aligned}
C^z &= \sum_{kk'\sigma} \frac{1}{2} \psi_\sigma^{k\dagger} \sigma_{\sigma\sigma}^z \psi_\sigma^{k'} = \frac{1}{2} \sum_{kk'} \left(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k'\downarrow}^\dagger c_{k\downarrow} \right) = \frac{1}{2} \sum_{kk'} \left(c_{k\uparrow}^\dagger c_{k'\uparrow} + c_{k\downarrow}^\dagger c_{k'\downarrow} - \delta_{kk'} \right) \\
&= \frac{1}{2} \sum_{kk'\sigma} \left(c_{k\sigma}^\dagger c_{k'\sigma} - \frac{1}{2} \delta_{kk'} \right) \\
C^x &= \sum_{kk'\sigma} \frac{1}{2} \psi_\sigma^{k\dagger} \sigma_{\sigma\bar{\sigma}}^x \psi_{\bar{\sigma}}^{k'} = \frac{1}{2} \sum_{kk'} \left(c_{k\uparrow}^\dagger c_{k'\downarrow}^\dagger + c_{k\downarrow} c_{k'\uparrow} \right) = \sum_{kk'\sigma} \frac{\sigma}{4} \left(c_{k\sigma}^\dagger c_{k'\bar{\sigma}}^\dagger + \text{h.c.} \right) \\
C^y &= \sum_{kk'\sigma} \frac{1}{2} \psi_\sigma^{k\dagger} \sigma_{\sigma\bar{\sigma}}^y \psi_{\bar{\sigma}}^{k'} = -\frac{i}{2} \sum_{kk'} \left(c_{k\uparrow}^\dagger c_{k'\downarrow}^\dagger - c_{k\downarrow} c_{k'\uparrow} \right) = \sum_{kk'\sigma} -\frac{i\sigma}{4} \left(c_{k\sigma}^\dagger c_{k'\bar{\sigma}}^\dagger - \text{h.c.} \right)
\end{aligned} \tag{2.3.3}$$

It is easy to verify that these operators satisfy the $SU(2)$ commutation algebra. For example, if we write $C^x = A + A^\dagger$ and $C^y = B + B^\dagger$, then $[C^x, C^y] = [A, B^\dagger] - \text{h.c.}$, where

$$[A, B^\dagger] = \frac{1}{4} \sum_{kk', qq'} \left[c_{k\uparrow}^\dagger c_{k'\downarrow}^\dagger, i c_{q'\downarrow} c_{q\uparrow} \right] = \frac{i}{4} \sum_{kq} \left(c_{k\uparrow}^\dagger c_{q\uparrow} - c_{k\downarrow} c_{q\downarrow}^\dagger \right) \tag{2.3.4}$$

and therefore

$$\Rightarrow [C^x, C^y] = \frac{i}{2} \sum_{kq} \left(c_{k\uparrow}^\dagger c_{q\uparrow} - c_{k\downarrow} c_{q\downarrow}^\dagger \right) = iC^z \tag{2.3.5}$$

There are similar operators for the impurity electron:

$$\begin{aligned}
\psi_d &= \begin{pmatrix} c_{d\uparrow} \\ c_{d\downarrow}^\dagger \end{pmatrix} \\
C_d^z &= \frac{1}{2} \left(c_{d\uparrow}^\dagger c_{d\uparrow} + c_{d\downarrow}^\dagger c_{d\downarrow} - 1 \right) = \frac{1}{2} (\hat{n}_d - 1) \\
C_d^x &= \frac{1}{2} \left(c_{d\uparrow}^\dagger c_{d\downarrow}^\dagger + c_{d\downarrow} c_{d\uparrow} \right) = \sum_{\sigma} \frac{\sigma}{4} \left(c_{d\sigma}^\dagger c_{d\bar{\sigma}}^\dagger + \text{h.c.} \right) \\
C_d^y &= -i \frac{1}{2} \left(c_{d\uparrow}^\dagger c_{d\downarrow}^\dagger - c_{d\downarrow} c_{d\uparrow} \right) = -i \sum_{\sigma} \frac{\sigma}{4} \left(c_{d\sigma}^\dagger c_{d\bar{\sigma}}^\dagger - \text{h.c.} \right)
\end{aligned} \tag{2.3.6}$$

The full charge-Kondo interaction can now be written down in terms of these isospins:

$$4K_z C_d^z C^z + K_t \left(C_d^+ C^- + C_d^- C^+ \right) \tag{2.3.7}$$

where $C^\pm \equiv C^x \pm iC^y$.

$$C^+ = \sum_{kk'} c_{k\uparrow}^\dagger c_{k'\downarrow}^\dagger, \quad C^- = \sum_{kk'} c_{k'\downarrow} c_{k\uparrow} \tag{2.3.8}$$

For $4K_z = 2K_t = K$, we get an $SU(2)$ -charge symmetric model:

$$KC_d^z C^z + \frac{1}{2} K \left(C_d^+ C^- + C_d^- C^+ \right) = K \vec{C}_d \cdot \vec{C} \tag{2.3.9}$$

To proceed with the URG, we start with the outermost shell Λ_N and consider an electron $q\beta$ on that shell. The URG then involves decoupling this electron. In the subspace of $q\beta$, the diagonal and off-diagonal parts are

$$\begin{aligned}\mathcal{H}_d &= \epsilon_q \tau_{q\beta} + H_{imp} + K_z (\hat{n}_d - 1) \tau_{q\beta} \\ \mathcal{H}_X &= V_q c_{q\beta}^\dagger c_{d\beta} + \text{h.c.} + K_z (\hat{n}_d - 1) \sum_k \left(c_{q\beta}^\dagger c_{k\beta} + \text{h.c.} \right) + K_t \sum_k \left(c_{d\beta}^\dagger c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}} c_{q\beta} + \text{h.c.} \right)\end{aligned}\quad (2.3.10)$$

As usual, we have considered only one mobile electron on the shell we are decoupling, and we keep only the energy of that electron and the impurity in the diagonal part which comes down in the denominator. Note that the factors of half in C^z are cancelled by the factor of 4 in $4K_z$. The last term in \mathcal{H}_d is obtained by setting $k = k' = q$ and $\sigma = \beta$ in eq. 2.3.3, and then recognizing that $\hat{n}_{q\beta} - \frac{1}{2} = \tau_{q\beta}$. The K_z part of \mathcal{H}_X is obtained by noting:

$$\begin{aligned}C_{q \neq k}^z &= \frac{1}{2} \left(c_{q\uparrow}^\dagger c_{k\uparrow} + c_{k\uparrow}^\dagger c_{q\uparrow} - c_{k\downarrow} c_{q\downarrow}^\dagger - c_{q\downarrow} c_{k\downarrow}^\dagger \right) \\ &= \frac{1}{2} \left(c_{q\uparrow}^\dagger c_{k\uparrow} + c_{k\uparrow}^\dagger c_{q\uparrow} + c_{q\downarrow}^\dagger c_{k\downarrow} + c_{k\downarrow}^\dagger c_{q\downarrow} \right) \\ &= \frac{1}{2} \sum_\sigma \left(c_{q\sigma}^\dagger c_{k\sigma} + \text{h.c.} \right)\end{aligned}\quad (2.3.11)$$

The calculation of renormalization will proceed similar to the spin-Kondo Anderson URG. We will again separate the off-diagonal piece \mathcal{H}_d^X into separate parts T_i , calculate the renormalization in particle and hole sectors, and then finally relate the ω_i using their bare values. The off-diagonal parts for this problem are

$$\begin{aligned}T_1 &= V_1 c_{d\beta} \hat{n}_{d\bar{\beta}} \\ T_2 &= V_0 c_{d\beta} \left(1 - \hat{n}_{d\bar{\beta}} \right) \\ T_3 &= K_z^1 \hat{n}_{d\beta} \hat{n}_{d\bar{\beta}} c_{k\beta} \\ T_4 &= -K_z^0 \left(1 - \hat{n}_{d\beta} \right) \left(1 - \hat{n}_{d\bar{\beta}} \right) c_{k\beta} \\ T_5 &= K_t c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} c_{d\beta}\end{aligned}\quad (2.3.12)$$

2.3.1 Calculation of renormalization in particle sector

The renormalization in this sector is

$$c_{q\beta}^\dagger T \eta \quad (2.3.13)$$

This is at energy $-\epsilon_q$. Using the expressions of the T_i , this becomes

$$\begin{aligned}& \left(1 - \hat{n}_{d\beta} \right) \left[\hat{n}_{d\bar{\beta}} \frac{|V_1|^2}{\xi_1} + \left(1 - \hat{n}_{d\bar{\beta}} \right) \frac{|V_0|^2}{\xi_2} \right] + \left[\frac{K_z^1}{\xi_3} \hat{n}_{d\beta} \hat{n}_{d\bar{\beta}} + \frac{K_z^0}{\xi_4} \left(1 - \hat{n}_{d\beta} \right) \left(1 - \hat{n}_{d\bar{\beta}} \right) \right] c_{k'\beta} c_{k\beta}^\dagger \\ & + \frac{K_t^2}{\xi_5} \left(1 - \hat{n}_{d\beta} \right) \left(1 - \hat{n}_{d\bar{\beta}} \right) c_{k\bar{\beta}}^\dagger c_{k'\bar{\beta}} - \frac{1}{2} \left(\frac{1}{\xi_1} + \frac{1}{\xi_3} \right) V_1 K_z^1 \hat{n}_{d\bar{\beta}} \left(c_{k\beta}^\dagger c_{d\beta} + \text{h.c.} \right) \\ & + \frac{1}{2} \left(\frac{1}{\xi_1} + \frac{1}{\xi_5} \right) V_1 K_t \left(1 - \hat{n}_{d\beta} \right) \left(c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} + \text{h.c.} \right) - \frac{1}{2} \left(\frac{1}{\xi_3} + \frac{1}{\xi_5} \right) K_z^1 K_t \left(c_{d\beta}^\dagger c_{d\bar{\beta}}^\dagger c_{k'\bar{\beta}} c_{k\beta} + \text{h.c.} \right)\end{aligned}\quad (2.3.14)$$

The indices k, k' are summed over. ξ_i is defined exactly as before, $\omega_i = E_i^0$.

The intermediate energies, E_i^0 , are

$$\begin{aligned} E_1^0 &= E_3^0 = \frac{\epsilon_q}{2} + 2\epsilon_d + U \\ E_2^0 &= \frac{\epsilon_q}{2} + \epsilon_d \\ E_4^0 &= \frac{\epsilon_q}{2} \\ E_5^0 &= \frac{\epsilon_q}{2} + 2\epsilon_d + U - K_z \end{aligned} \tag{2.3.15}$$

The contribution of $k\bar{\beta}$ in the denominators of $E_{3,4,5}^0$ has been considered.

2.3.2 Calculation of renormalization in hole sector

The renormalization in the hole sector is given by

$$T^\dagger c_{q\beta} \eta_0^\dagger \tag{2.3.16}$$

at energy ϵ_q . That comes out to be

$$\begin{aligned} & \frac{|V_1|^2}{\xi_1'} \hat{n}_{d\beta} \hat{n}_{d\bar{\beta}} + \frac{|V_0|^2}{\xi_2'} \hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}}) + \left[\frac{K_z^2}{\xi_3'} \hat{n}_{d\beta} \hat{n}_{d\bar{\beta}} + \frac{K_z^2}{\xi_4'} (1 - \hat{n}_{d\beta}) (1 - \hat{n}_{d\bar{\beta}}) \right] c_{k\beta}^\dagger c_{k'\beta} \\ & + \frac{K_t^2}{\xi_5'} \hat{n}_{d\beta} \hat{n}_{d\bar{\beta}} c_{k'\bar{\beta}} c_{k\beta}^\dagger - \frac{1}{2} \left(\frac{1}{\xi_2'} + \frac{1}{\xi_4'} \right) V_0 K_z^0 (1 - \hat{n}_{d\bar{\beta}}) (c_{k\beta}^\dagger c_{d\beta} + \text{h.c.}) \\ & + \frac{1}{2} \left(\frac{1}{\xi_2'} + \frac{1}{\xi_5'} \right) V_0 K_t \hat{n}_{d\beta} (c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} + \text{h.c.}) - \frac{1}{2} \left(\frac{1}{\xi_4'} + \frac{1}{\xi_5'} \right) K_z^0 K_t (c_{d\beta}^\dagger c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}} c_{k'\beta} + \text{h.c.}) \end{aligned} \tag{2.3.17}$$

where $\xi' = \omega' = E_i^1$. The intermediate energies in this sector are

$$\begin{aligned} E_1^1 &= \frac{\epsilon_q}{2} + \epsilon_d \\ E_2^1 &= E_4^1 = \frac{\epsilon_q}{2} \\ E_3^1 &= \frac{\epsilon_q}{2} + 2\epsilon_d + U \\ E_5^1 &= \frac{\epsilon_q}{2} - K_z \end{aligned} \tag{2.3.18}$$

2.3.3 Relating the ω

Just as in the previous subsection, we relate the ω_i using their diagonal values.

First the particle sector ω_i :

$$\begin{aligned} \omega_1 &= -\frac{\epsilon_q}{2} + \epsilon_d \\ \omega_2 &= \omega_5 = -\frac{\epsilon_q}{2} - K_z \\ \omega_3 &= -\frac{\epsilon_q}{2} + 2\epsilon_d + U \\ \omega_4 &= -\frac{\epsilon_q}{2} \end{aligned} \tag{2.3.19}$$

Rewriting everything in terms of $\omega = -\frac{\epsilon_q}{2} - K_z$ gives

$$\begin{aligned}\omega_1 &= \omega + \epsilon_d + K_z \\ \omega_2 &= \omega_5 = \omega \\ \omega_3 &= \omega + 2\epsilon_d + U + K_z \\ \omega_4 &= \omega + K_z\end{aligned}\tag{2.3.20}$$

For the hole sector, we get

$$\begin{aligned}\omega'_1 &= \omega'_5 = -\frac{\epsilon_q}{2} + 2\epsilon_d + U - K_z \\ \omega'_2 &= -\frac{\epsilon_q}{2} + \epsilon_d \\ \omega'_3 &= -\frac{\epsilon_q}{2} + 2\epsilon_d + U \\ \omega'_4 &= -\frac{\epsilon_q}{2}\end{aligned}\tag{2.3.21}$$

and, in terms of ω ,

$$\begin{aligned}\omega'_1 &= \omega'_5 = \omega + 2\epsilon_d + U \\ \omega'_2 &= \omega + \epsilon_d + K_z \\ \omega'_3 &= \omega + 2\epsilon_d + U + K_z \\ \omega'_4 &= \omega + K_z\end{aligned}\tag{2.3.22}$$

The denominators can thus be written as

$$\begin{aligned}\xi_1 &= \omega - \frac{\epsilon_q}{2} - \epsilon_d - U + K_z, & \xi'_1 &= \omega - \frac{\epsilon_q}{2} + \epsilon_d + U \\ \xi_2 &= \omega - \frac{\epsilon_q}{2} - \epsilon_d, & \xi'_2 &= \omega - \frac{\epsilon_q}{2} + \epsilon_d + K_z \\ \xi_3 &= \xi_4 = \omega - \frac{\epsilon_q}{2} + K_z, & \xi'_3 &= \xi'_4 = \omega - \frac{\epsilon_q}{2} + K_z \\ \xi_5 &= \omega - \frac{\epsilon_q}{2} - 2\epsilon_d - U + K_z, & \xi'_5 &= \omega - \frac{\epsilon_q}{2} + 2\epsilon_d + U + K_z\end{aligned}\tag{2.3.23}$$

2.3.4 Scaling Equations

$$\begin{aligned}
\Delta\epsilon_d &= \frac{|V_1|^2}{\xi_1} + \frac{|V_0|^2}{\xi'_2} - \frac{2|V_0|^2}{\xi_2} - \sum_k \left(2\frac{K_z^2}{\xi_3} + \frac{K_t^2}{\xi_5} \right) \\
\Delta U &= \frac{2|V_1|^2}{\xi'_1} + \frac{2|V_0|^2}{\xi_2} - \frac{2|V_1|^2}{\xi_1} - \frac{2|V_0|^2}{\xi'_2} + 2 \sum_k \left(2\frac{K_z^2}{\xi_3} + \frac{K_t^2}{\xi_5} \right) \\
\Delta V_1 &= -\frac{1}{4} \left[V_1 K_z \left(\frac{1}{\xi_1} + \frac{1}{\xi_3} \right) - V_0 K_t \left(\frac{1}{\xi'_2} + \frac{1}{\xi'_5} \right) \right] \\
\Delta V_0 &= -\frac{1}{4} \left[V_0 K_z \left(\frac{1}{\xi'_2} + \frac{1}{\xi'_4} \right) - V_1 K_t \left(\frac{1}{\xi_1} + \frac{1}{\xi_5} \right) \right] \\
\Delta K_z &= -K_t^2 \frac{1}{\xi_5} \\
\Delta K_t &= -K_z K_t \left(\frac{1}{\xi_3} + \frac{1}{\xi_5} + \frac{1}{\xi'_4} + \frac{1}{\xi'_5} \right)
\end{aligned} \tag{2.3.24}$$

2.3.5 Particle-hole symmetry and charge SU(2) invariance

An important distinction between the SIAM charge Kondo and the SIAM spin-Kondo models is that, unlike the charge Kondo model where we had independent spin-rotation invariance (obtained by setting $J_z = J_t$) and impurity particle-hole symmetry (obtained by setting $\epsilon_d = -\epsilon_d - U$), this model has a composite particle-hole symmetry and SU(2)-charge symmetry. To see this, consider the impurity part of the model:

$$\epsilon_d \hat{n}_d + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + K_z (\hat{n}_d - 1) \left(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k'\downarrow} c_{k\downarrow}^\dagger \right) + \frac{K_t}{2} \left(c_{d\beta}^\dagger c_{d\bar{\beta}}^\dagger c_{k\beta} c_{k'\bar{\beta}} + \text{h.c.} \right) \tag{2.3.25}$$

The charge isospin reversal here corresponds to the transformation $c_d \rightarrow c_d^\dagger$ and $c_k \rightarrow c_k^\dagger$, because then $2C_d^z = \hat{n}_d - 1 \rightarrow 1 - \hat{n}_d = -2C_d^z$. But this transformation is just the impurity particle-hole transformation we encountered earlier. As a result, the total constraint for SU(2)-charge symmetry and impurity particle-hole symmetry is

$$\epsilon_d = -\epsilon_d - U, \quad V_1 = V_0, \& \quad 2K_z = K_t = \frac{K}{2} \tag{2.3.26}$$

With these conditions, we get $\xi_1 = \xi'_2, \xi'_1 = \xi_2$, and $\xi_3 = \xi_4 = \xi_5 = \xi'_3 = \xi'_4 = \xi'_5$, and

$$\begin{aligned}
\Delta\epsilon_d &= -\frac{1}{2} \Delta U \\
\Delta V_1 &= \Delta V_0 = \frac{V_1 K}{8} \left(\frac{1}{\xi_1} + \frac{1}{\xi_6} \right) \\
\Delta K &= K^2 \frac{1}{\xi_5}
\end{aligned} \tag{2.3.27}$$

Bibliography

- [1] Anirban Mukherjee and Siddhartha Lal. Unitary renormalisation group for correlated electrons-i: a tensor network approach. *Nuclear Physics B*, 960:115170, 2020.
- [2] Anirban Mukherjee and Siddhartha Lal. Unitary renormalisation group for correlated electrons-ii: insights on fermionic criticality. *Nuclear Physics B*, 960:115163, 2020.
- [3] Anirban Mukherjee and Siddhartha Lal. Scaling theory for mott–hubbard transitions: I. $t = 0$ phase diagram of the $1/2$ -filled hubbard model. *New Journal of Physics*, 22(6):063007, jun 2020.
- [4] Anirban Mukherjee and Siddhartha Lal. Scaling theory for mott–hubbard transitions-II: quantum criticality of the doped mott insulator. *New Journal of Physics*, 22(6):063008, jun 2020.
- [5] Kenji Suzuki. Construction of Hermitian Effective Interaction in Nuclei: — General Relation between Hermitian and Non-Hermitian Forms —. *Progress of Theoretical Physics*, 68, 1982.
- [6] P W Anderson. A poor man's derivation of scaling laws for the kondo problem. *Journal of Physics C: Solid State Physics*, 3(12):2436–2441, dec 1970.
- [7] F. D. M. Haldane. Scaling theory of the asymmetric anderson model. *Phys. Rev. Lett.*, 40:416–419, Feb 1978.
- [8] Siddhartha Patra. *unpublished*, 2021.
- [9] Anirban Mukherjee. *Unitary renormalization group for correlated electrons*. PhD thesis, Indian Institute of Science Education and Research Kolkata, 2020.
- [10] J H Jefferson. A renormalisation group approach to the mixed valence problem. *Journal of Physics C: Solid State Physics*, 10(18):3589–3599, sep 1977.
- [11] Yoichiro Nambu. Quasi-particles and gauge invariance in the theory of superconductivity. *Phys. Rev.*, 117:648–663, Feb 1960.
- [12] P. W. Anderson. Random-phase approximation in the theory of superconductivity. *Phys. Rev.*, 112:1900–1916, Dec 1958.
- [13] Rok Zitko and Janez Bonca. Spin-charge separation and simultaneous spin and charge kondo effect. *Phys. Rev. B*, 74:224411, Dec 2006.