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# Unitary Renormalization Group Solution of the Generalised Anderson Impurity Model

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## MS Project Report

*submitted in partial fulfillment of the requirements for the degree of*

## Master of Science

*by*

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*under the supervision of*

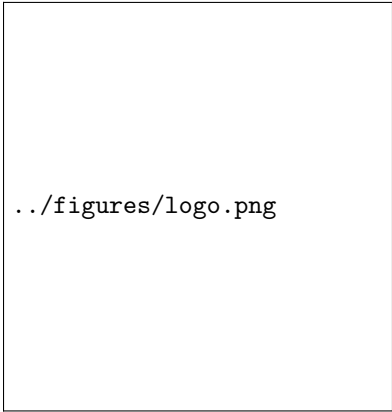
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*To you, 5 years from now*

# 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 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 Greens 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.

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# Chapter 1

## Introduction

### 1.1 Summary of the problem

The single-impurity Anderson model (SIAM) is one of the most well-studied models in condensed matter physics and is the prototypical model for magnetism. It shows how strong correlations between electrons give rise to a residual local moment. Friedel[5], in 1958, gave a phenomenological theory in which a local impurity developed an effective repulsion which forced the formation of bound states; those bound states where the up and down states became non-degenerate would correspond to the local moment. Taking inspiration from this, P.W.Anderson[6] in 1961 designed a model for the formation of local moment in second quantization. The model consisted of a bath of mobile electrons which interacted with the local impurity. The engine of magnetism was the local onsite Coulomb repulsion on the impurity site. This repulsion favours the formation of local moments because it makes it harder for the impurity to be doubly-occupied. Mean-field calculations of the impurity occupation reveal a criterion for the formation of local moments; this criterion is similar to the Stoner criterion for ferromagnetism. This mean-field analysis is of course only valid at high temperatures where electron-correlations are not so important. At low temperatures, it was found that the resistivity of the material reaches a minimum at some temperature, and then increases as  $\ln T$  as we further reduce the temperature. This is in contrast to the previous results. And that was not all; at a sufficiently low temperature, it was found that the  $\ln T$ -dependence disappears and the susceptibility became constant, implying the formation of a singlet state.

The fact that this logarithmic dependence vanishes once the singlet is formed suggests that it arises from the local moment on the impurity; once the local moment disappears (singlet), the log dependence vanishes as well. This led people to design a model in which the impurity interacted with the conduction bath through a Heisenberg-like spin-spin interaction. This model can be related to the SIAM through a canonical transformation followed by a projection to the low energy subspace. In 1964, Jun Kondo[7] found that a perturbative calculation of the transition probability of electrons from scattering via the impurity, up to second order in the exchange coupling  $J$ , revealed a logarithmic dependence of the resistivity on temperature. The crucial scattering process was that in which the spin of the incoming electron flipped (the  $S^+s^-$  and  $S^-s^+$  terms). This explained the mystery of the resistivity minimum and the logarithmic dependence. But the mystery of the singlet state at very low temperatures still remained. The perturbative analysis would break down at low temperatures, so it was unreliable. The log term showed that the physics of the singlet involved all energy scales; one could not hope to capture it simply by taking the first few terms of a perturbative expansion. This problem came to be known as the Kondo problem. In 1970, Anderson attacked this problem by a renormalization group approach to account for all energy scales. In his "Poor Man's Scaling" approach, he progressively reduced the bandwidth while taking account of the eliminated states into the couplings via second order perturbation theory. This showed how the couplings would flow as we went to low temperatures, but it still could not remove the divergence as it was perturbative.

Anderson found that the exchange coupling increased as we go to lower temperatures, so he surmised that the low energy theory was one where  $J = \infty$ . In 1975, Kenneth Wilson solved the problem by using his numerical renormalization group method in which he iteratively diagonalized chains of increasing length to go to the low energy physics. He proved that Anderson's guess was right and the low energy Hamiltonian was the same as that with  $J = \infty$ . Later calculations with Bethe ansatz in 1980 by Andrei and Wiegmann [8, 9] corroborated Wilson's findings. A similar sequence of events also happened in the context of the Anderson model. In 1977 and 1978, Jefferson and Haldane independently calculated the "Poor Man's" scaling equations for the asymmetric SIAM, in the limit of infinitely large onsite repulsion. They were unable to access the strong-coupling fixed point (analogous to

the  $J = \infty$  fixed point in Kondo model), but their equations revealed which were the important regimes to consider. Later, in 1975, Krishnamurthy, Wilkins and Wilson applied the NRG method to the symmetric Anderson model and obtained the non-perturbative fixed points and susceptibility [10]. Their calculations were again supported by later Bethe ansatz calculations by Wiegmann and Tsvetick[11]. The physics of the Anderson model and the Kondo model has connotations with quantum field theory. The numerical renormalization group methods ushered in a revolution. The idea that physics on all length scales affect the low energy physics was very deep and has far-reaching consequences. The phenomenon in which the impurity electron strongly couples to one real space lattice site at low temperatures resulting in the screening of the local moment via spin-flip scatterings with the mobile electrons at that site is analogous to the phenomenon of quark confinement in which the quarks become bound at low energies. The high energy fixed point,  $J = 0$ , corresponds to the phenomenon of asymptotic freedom in which the interactions between particles become asymptotically weaker at high temperatures.

## 1.2 Some outstanding questions

Even though the problem of the SIAM has been essentially solved, some questions and clarifications still remain. In this work, we explore some of these questions.

- *Is it possible to get **non-perturbative scaling equations** for the whole journey?*

Neither NRG nor Bethe ansatz gives us scaling equations for the RG flows. Poor Man's scaling only gives perturbative ones which are valid close to the high energy theories. In the absence of scaling equations that show the complete crossover from the high energy to the low energy theory, it is difficult to visualize how the Hamiltonian is precisely changing.

- *Is it possible to show the **transfer of spectral weight** along the flow, possibly by tracking the spectral function?*

Such an exercise will require the entire spectrum to be preserved along the flow. NRG, being projective will not work here. If the entire spectrum is available, computing the spectral function along the flow should indicate how the spectral weight is being distributed between the impurity and the conduction bath, or between various states of the impurity. It can also shed light on which terms or processes in the Hamiltonian contribute to which parts of the spectral function.

- *How does NRG obtain the local moment in the **absence of hybridisation**?* For the symmetric mode, NRG results show that in the absence of any interaction between the bath and the impurity, the value of the onsite repulsion flows to a large value and we end up with a local moment. The obvious question is, how does the impurity coupling renormalize when there is no term connecting the bath with the impurity?
- *Are there any interesting **topological aspects** of the fixed points?* We also intend to search for the existence of and possible changes in topological quantities at the fixed points. Since this is a zero-dimensional phenomenon, there will not be any gapping out of the Fermi surface, but there might be changes in topological quantities related to the Fermi surface or in the analyticity of the Green's function due to the presence of the coupling between the bath and the impurity. A strong indication of this is the change in the Wilson ratio from the non-interacting value of  $R = 1$  to the local-Fermi liquid fixed point value of  $R = 2$  obtained by Nozières[12].
- *What is the nature of the Kondo cloud that screens the spin(charge) of the impurity?* We do not yet have a theory for the excitations of the cloud of electrons at the zeroth site that couple to the impurity at the fixed point. The local Fermi liquid sits just outside the cloud and is able to "feel" its effects and gauge certain gross quantities like the Wilson ratio, but it does not have the excitations of the cloud because that part, along with the impurity, has been assumed to be "frozen" into the singlet configuration. A recent result in this context [13] is the effective Hamiltonian of the Kondo model cloud, also obtained using the same method that has been used in this thesis. The goal here is to do something similar for the SIAM as well.
- *How do entanglement measures respond to the RG flow?* Can we find a reflection of the screening mechanism in something like the mutual information or correlations? This requires a knowledge of the wavefunctions at the fixed point. Does the enhanced scattering of the electrons off the impurity lead to an increase in the entanglement between various electrons of the bath? It will also be interesting to check how various correlation functions vary across the RG flow.

## 1.3 Salient features of the method

The method employed in this work is a unitary renormalization group (URG) technique which progressively block-diagonalizes the Hamiltonian in the space of single high energy electrons. At each step of the process, the highest electron is decoupled from the system and it becomes an integral of motion, and the lower electronic system gets rotated to account for the decoupled electron. In this way, the RG goes on resolving the number fluctuations of the electrons. A fixed point is reached when the off-diagonal terms can no longer be removed. Since the method is unitary, it preserves the spectrum and allows calculating effective eigenvalues and eigenstates. It has some characteristic features:

- *Presence of a quantum fluctuation energy scale  $\omega$* : The URG process involves a parameter  $\omega$  which contains the off-diagonal terms in the Hamiltonian. It quantifies the quantum fluctuation still unresolved in the system. Exactly at the fixed point, when the fluctuations are resolved, it assumes the value of one of the energies of the Hamiltonian. By probing the values of  $\omega$ , all regions of the spectrum can, at least in principle, be accessed.
- *Presence of finite-valued fixed points*: The URG has a definite prescription for reaching the fixed point and it terminates after a finite number of steps (for a finite system). This leads to finite values of the fixed point couplings. This is also in accordance with our intuition that finite systems should not have diverging couplings.
- *Spectrum-preserving transformations*: Since the RG transformations are unitary, all eigenvalues and eigenstates are kept track of the in the process. This allows us to calculate exact quantities for simple systems like the Kondo model.
- *Tractable low-energy effective Hamiltonians*: The final Hamiltonians obtained at the fixed point are usually tractable and allow us to extract information.

## 1.4 Layout of the thesis

Chapter 2 goes over the available work on the single-impurity Anderson model and its derivative - Kondo model. We go over the mean-field calculation of the Anderson model which gives a criteria for magnetism in terms of the onsite repulsion parameter  $U$  and the hybridisation parameter  $\Delta$ . We then derive the Kondo model from the SIAM by way of a Schrieffer-Wolff transformation, which we solve using NRG. We also spend some time on the Poor Man's scaling approaches of both the SIAM and the Kondo model, and end the chapter with some discussions on the local Fermi liquid aspects of the fixed point theory.

Chapter 3 lays out the URG formalism and prescription. We derive the URG effective Hamiltonian and the unitaries that perform the RG transformations. We discuss several important features of the method and provide a prescription for applying it on models. We also perform the URG explicitly on two models - the star graph model and the Kondo model. We discuss various subtleties, especially the quantum fluctuation parameter  $\omega$  and show that the URG actually diagonalizes the Hamiltonian. We derive many-body creation and annihilation operators  $\eta^\dagger$  and  $\eta$  which rotate the full Hamiltonian into successively more block-diagonal form.

Chapter 4 is closely tied to the formalism chapter and develops the connections between URG and other canonical transformations in the literature. We first define and setup each of the other transformations - the Schrieffer-Wolff transformation (SWT), Poor Man's scaling (PMS) and the Continuous Unitary Transformation (CUT) RG. We show that all of these are in some sense perturbative derivatives of URG. A byproduct of the discussion is a demonstration of the fact that PMS and SWT are exactly identical and differ only in the contexts in which they are applied. We also discuss the differences between URG and CUT-RG, and show that URG behaves like a generalized double-bracket flow [14].

Chapter 5 contains the URG analysis of the SIAM and its generalization, obtained by adding spin-spin and charge-charge interactions to the SIAM. The RG equations are derived in detail. We focus mostly on the generalised version. We discuss both the positive and the negative regimes of the impurity correlation  $U$ . From the RG fixed point, we write down the fixed point Hamiltonian, and then discuss the spectrum of this Hamiltonian.

Chapter 6 computes some important quantities from the fixed point theory like the specific heat, magnetic susceptibility, charge susceptibility, Wilson ratio, Kondo cloud Hamiltonian, entanglement and correlation measures of the Kondo cloud electrons and change in the Luttinger's count of the bath. The Kondo cloud Hamiltonian is

obtained by tracing out the impurity operators from the fixed point Hamiltonian. We compute the mutual information between various members of the fixed point Hamiltonian, as well as some off-diagonal correlations. We extract a low temperature local Fermi liquid from the Hamiltonian which we then use to calculate the zero temperature Wilson ratio for the Kondo regime of the SIAM. We also calculate the change in Luttinger's volume between the fixed points.

## 1.5 Summary of main results

The first of the main results in this work is the connection between URG and other canonical transformations. It is shown that URG is a non-perturbative variation of the most general unitary transformation. Other unitary transformations like the Schrieffer-Wolff transformation and Poor Man's scaling are simpler forms of URG, obtained by trivializing one of the terms in the Green's function that comes up in the URG formalism. CUT-RG is still more different from URG, since it is not only perturbative but also philosophically different in that it gradually suppresses the off-diagonal terms rather than killing more and more terms progressively. URG is thus different in two major ways - it provides non-perturbative equations because of the specific denominator structure as well as accommodates, at least in principle, the feedback effects of the off-diagonal terms through a quantum fluctuation operator in the denominator. We next look at the results concerning the SIAM. In the absence of any spin-exchange or charge isospin-exchange scattering, we do not see any renormalization in the hybridisation and the only flow is towards a local moment fixed point with large impurity onsite energy  $U$ . In the presence of those additional exchange scattering terms, the corresponding couplings  $J$ (spin exchange) and  $K$ (isospin exchange) flow to large values for low values of  $\omega$ , signaling strong-coupling fixed points. At the spin-screened strong-coupling fixed point ( $J > K$ ), the ground state wavefunction is a superposition of a spin singlet and a charge-isospin triplet. The ground state for the isospin-dominated fixed point ( $K > J$ ) is an isospin singlet. Thermodynamic quantities are now calculated using zero-mode Hamiltonians of the low energy effective theories. The impurity susceptibility  $\chi_{\text{imp}}$  goes to the Curie-Weiss value of a four-fold degenerate system at large temperatures, and becomes constant (paramagnetic) at very low temperatures. With  $T_K$  defined suitably,  $\chi_{\text{imp}}$  takes the zero temperature value of  $(2\pi T_K)^{-1}$ . The impurity specific heat has also been calculated, and reveals a two-peak structure. The fixed-point Hamiltonian further allows us to calculate the impurity spectral function. For very small  $U$  we obtain a single-peak structure corresponding to a single spin-spin or isospin-isospin excitation at the Fermi surface, while two other side-peaks emerge at large  $U$  that correspond to excitations between the spin and charge sectors. By tweaking the values of the couplings in the fixed-point Hamiltonian, we can mimic the reverse RG flow and see how the impurity spectral function morphs along this journey. Both the single-peak and three-peak structures revert back to a two-peak spectral function corresponding to that of a local moment. We then extract the effective Hamiltonian for the Kondo cloud, up to two particle interactions, by tracing out the impurity from the coupled Hamiltonian. The Hamiltonian has both a Fermi liquid piece of the form  $\hat{n}_{k\sigma}\hat{n}_{q\sigma'}$  and a two-particle off-diagonal scattering piece of the form  $c_{k\uparrow}^\dagger c_{k'\downarrow}^\dagger c_{q\uparrow} c_{q'\downarrow}$ . It is the latter which is responsible for the screening mechanism. This conclusion is further strengthened by the studies of entanglement measures and correlations. The mutual information between the impurity and a cloud electron, as well as that between two cloud electrons increases as we go from the UV towards the IR fixed point. The off-diagonal correlation also increases from the UV towards the IR, which shows that the growth of the off-diagonal term is concomitant with the screening. We also obtain the Wilson ratio of the impurity by creating a local Fermi liquid from the fixed point Hamiltonian. Using the zero charge susceptibility at  $T = 0$  in the Kondo regime of the SIAM, we can show that the Wilson ratio goes to 2 at the fixed point. We also calculate the change in Luttinger's volume along the RG flow. At the free orbital or local moment fixed points, the Luttinger's volume is measured purely by the number of conduction electrons, but we see that at the strong-coupling fixed point, the correct Luttinger's volume is given by the total number of electrons in the conduction bath as well as the impurity. This is also connected to the increase in Wilson ratio from 1 to 2.

## Chapter 2

# Preliminaries and Existing Results

This chapter is devoted to an extensive literature survey of the Anderson impurity model (SIAM) (and the Kondo model to some extent, because it is closely related to the SIAM). It also includes discussions and derivations of some topics like the Friedel sum rule and some results from scattering theory, because these topics will often be invoked later.

### 2.1 $T$ – and $S$ –matrices, Greens function and scattering phase shifts

#### 2.1.1 $T$ –matrix and Greens function

We will first introduce the  $T$ –matrix and the Greens function operator, and derive a relation between them. It is assumed that we have an interacting system  $H = H_0 + V$ .  $H_0$  as the non-interacting part with the spectrum  $\{E_i, |\Phi_i\rangle\}$ .  $V$  represents the interaction between the states  $|\Phi_i\rangle$ . The  $T$ –matrix arises naturally when we write down the full Schrodinger equation of the problem:

$$(H_0 + V) |\Psi_i\rangle = E_i |\Psi_i\rangle \quad (2.1.1)$$

$|\Psi_i\rangle$  are the eigenstates of  $H$ . The eigenvalues are the same as  $H_0$  because we have assumed elastic scattering. The solutions  $|\Psi_i\rangle$  can be expressed as

$$|\Psi_i\rangle = \frac{1}{E_i - H_0} V |\Psi_i\rangle + |\Phi_i\rangle \quad (2.1.2)$$

The  $|\Phi_i\rangle$  was inserted to ensure that  $|\Psi_i\rangle \rightarrow |\Phi_i\rangle$  when  $V \rightarrow 0$ . That eq. 2.1.2 is equivalent to eq. 2.1.1 is easily verified by multiplying eq. 2.1.2 from the left with  $E_i - H_0$ . That will cancel the last term on the RHS because  $H_0 |\Phi_i\rangle = E_i |\Phi_i\rangle$ . Although we have presented eq. 2.1.2 as a solution for the Hamiltonian  $H$ , the problem is that the unknown  $|\Psi_i\rangle$  appears on the RHS. This is where the  $T$ –matrix comes in; we define  $T$  in order to write the RHS completely in terms of  $|\Phi_i\rangle$ :

$$V |\Psi_i\rangle = T |\Phi_i\rangle \quad (2.1.3)$$

With this, the solution becomes

$$|\Psi_i\rangle = \left(1 + \frac{1}{E_i - H_0} T\right) |\Phi_i\rangle \quad (2.1.4)$$

At this point, we can define the non-interacting Greens function operator  $G_0$ :

$$G_0(E) = \frac{1}{E - H_0} \quad (2.1.5)$$

Eq. 2.1.4 becomes

$$|\Psi_i\rangle = [1 + G_0(E_i)T] |\Phi_i\rangle \quad (2.1.6)$$

To obtain a relation between  $T$  and  $G_0$ , we substitute this equation back into the definition of  $T$  (eq. 2.1.3):

$$T |\Phi_i\rangle = V [1 + G_0(E_i)T] |\Phi_i\rangle \quad (2.1.7)$$

Since the  $|\Phi_i\rangle$  form a complete basis, we get the relation:

$$\begin{aligned} T(i) &= V [1 + G_0(E_i)T(i)] \\ T(i) &= \frac{1}{1 - VG_0(E_i)}V \end{aligned} \quad (2.1.8)$$

The last equation allows us to perturbatively expand the  $T$ -matrix, by substituting the RHS into the  $T$  on the RHS:

$$T(i) = V + VG_0(E_i)V + VG_0(E_i)VG_0(E_i)V + \dots \quad (2.1.9)$$

This is equivalent to a Dyson expansion in powers of  $V$ . More relations can be obtained by defining the full (interacting) counterpart of  $G_0$ :

$$G(E_i) = \frac{1}{E_i - H} = \frac{1}{E_i - H_0 - V} \quad (2.1.10)$$

That definition can be massaged into the following identity:

$$G^{-1} = G_0^{-1} - V \implies G_0 G^{-1} G = G_0 G_0^{-1} G - G_0 V G \implies G = G_0 + G_0 V G \quad (2.1.11)$$

By re-substituting  $G$  into the RHS, this can be made into a perturbative expansion:

$$\begin{aligned} G &= G_0 + G_0 V (G_0 + G_0 V G) = G_0 + G_0 V G_0 + G_0 V G_0 V G_0 + \dots \\ &= G_0 + G_0 (V + V G_0 V + \dots) G_0 \end{aligned} \quad (2.1.12)$$

By comparing with eq. 2.1.9, we can recognize the term inside the brackets as the  $T$ -matrix, and write

$$G(E_i) = G_0(E_i) + G_0(E_i)T(i)G_0(E_i) \quad (2.1.13)$$

### 2.1.2 $S$ -matrix

A plane wave can be represented as the sum of incoming waves  $\chi_{k,l}^-$  and outgoing spherical waves  $\chi_{k,l}^+$ . These incoming and outgoing waves are eigenstates of the total angular momentum squared  $L^2$  with eigenvalue  $l(l+1)$ .

$$|\Phi_k\rangle = \sum_l \left( |\chi_{k,l}^+\rangle + |\chi_{k,l}^-\rangle \right) \quad (2.1.14)$$

It is a standard result in scattering theory that the total scattered wavefunction can be written as the sum of the same incoming spherical wave and a modified outgoing spherical wave:

$$|\Psi_k\rangle = \sum_l \left[ (1 + 2ikf_l(k)) |\chi_{k,l}^+\rangle + |\chi_{k,l}^-\rangle \right] \quad (2.1.15)$$

where

$$kf_l(k) = -\pi\rho(E_k)T(k, l) = -\pi\rho(E_k) \langle l | T(k) | l \rangle \quad (2.1.16)$$

$\rho(E_k)$  is the density of states at energy  $E_k$ . Note that these are the non-interacting density of states: they count energy states that match with the kinetic energy  $E_k$  and do not take into account any self-energy term that may come from some interaction.

The  $S$ -matrix is defined to track the evolution of the outgoing spherical waves at very long time intervals:

$$S = \lim_{t \rightarrow \infty} U(-t, t) \quad (2.1.17)$$

Assuming momentum  $k$  is conserved in the scattering, we can relate the  $S$ -matrix to the  $T$ -matrix:

$$S(k) = \sum_l |\chi_{k,l}^+\rangle \langle \chi_{k,l}^+| \lim_{t \rightarrow \infty} \langle \chi_{k,l}^+ | U(-t, t) | \chi_{k,l}^+ \rangle = \sum_l |\chi_{k,l}^+\rangle \langle \chi_{k,l}^+| (1 + 2ikf_l(k)) = 1 - 2i\pi\rho(E_k)T(k) \quad (2.1.18)$$

The elements of  $S$ -matrix are called the partial wave  $S$ -matrix element:

$$S_l(k) = 1 - 2i\pi\rho(E_k)T_l(k) \quad (2.1.19)$$

By using the completeness and orthonormality of the kets  $|k\rangle$  and by assuming a uniform density of states  $\rho$ , we can write the entire  $S$ -matrix:

$$S = \sum_k |k\rangle \langle k| S(k) = 1 - 2\pi i \rho \sum_k |k\rangle \langle k| T(k) = 1 - 2\pi i \rho T \quad (2.1.20)$$

The  $S$ -matrix at a particular energy  $\omega$  then turns out to be

$$S(\omega) = \langle \omega | S | \omega \rangle = 1 - 2\pi i \rho T(\omega) \quad (2.1.21)$$

### 2.1.3 Scattering phase shifts and their relation to $T$ -matrix

$S(k)$  is unitary because  $U$  is. Expanding  $S(k)$  in its eigenbasis  $\{|i\rangle\}$  (not necessarily angular momentum) gives

$$S(k)^\dagger S(k) = \sum_i |i\rangle \langle i| |S_i(k)|^2 = 1 \implies |S_i(k)|^2 = 1 \implies S_i(k) = e^{2i\delta_i(k)} \quad (2.1.22)$$

The parameters  $\delta_i(k)$  are scattering phase shifts of the state  $|i\rangle$ . The total phase shift  $\delta(\omega) = \sum_i \delta_i(\omega)$  in the eigenbasis of  $S$  can be obtained by taking the trace and log of  $S$ :

$$\ln S = \ln \sum_i |i\rangle \langle i| e^{2i\delta_i} = 2i \sum_i |i\rangle \langle i| \delta_i \implies \frac{1}{2i} \text{Trace} [\ln S] = \delta(\omega) \quad (2.1.23)$$

These phase shifts can be expressed in terms of  $T$ . To prove this, first note that the determinant of the  $S$ -matrix is the exponential of the total phase shift:

$$\text{Det} [S(\omega)] = e^{2i \sum_i \delta_i(\omega)} = e^{2i\delta(\omega)}. \quad (2.1.24)$$

Taking the determinant of eq. 2.1.21 gives

$$e^{2i\delta(\omega)} = 1 - 2\pi i \text{Det} [T(\omega)] \implies \text{Det} [T(\omega)] = -\frac{\sin \delta(\omega)}{\pi \rho} e^{i\delta(\omega)} \quad (2.1.25)$$

If we define the argument of a complex number  $z(r, \phi) = re^{i\phi}$  as  $\arg(z) = \phi$ , then we can write

$$\arg [\text{Det} [T(\omega)]] = \delta(\omega) = \frac{1}{2i} \text{Trace} [\ln S] \quad (2.1.26)$$

## 2.2 The Friedel sum rule

The Friedel sum rule [5, 15, 16] is a very useful theorem that operates in the domain of impurity problems. In the presence of an impurity that interacts with the electrons of the system, the total number of particles in the ground state will generally be different from that in the absence of the impurity. This difference is given directly by the total scattering phase shift suffered by the conduction electrons at the Fermi surface as they scatter off the impurity. The more general version states that the difference in the number of particles is actually related to the scattering local  $S$ -matrix (against the impurity) of the conduction electrons at the Fermi surface. Here we will see a derivation of this theorem.

Consider a Hamiltonian

$$\mathcal{H} = H_0 + V \quad (2.2.1)$$

where  $H_0 = \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma}$ . We will define the number of states of the Hamiltonian by integrating over the density of states (dos), which is in turn defined using a retarded Green's function. The retarded Green's function for the full Hamiltonian is defined as

$$G(\omega) = \lim_{\eta \rightarrow 0} \frac{1}{\omega - \mathcal{H} + i\eta} = \frac{1}{\omega - \mathcal{H}} - i\pi \delta(\omega - \mathcal{H}) \quad (2.2.2)$$

The non-interacting Greens function is then

$$G_0(\omega) = \frac{1}{\omega - H_0} - i\pi \delta(\omega - H_0) \quad (2.2.3)$$

The dos  $\rho(\omega)$  and total number of states  $N$  are then defined as

$$\begin{aligned} \rho(\omega) &\equiv \sum_{\epsilon} \delta(\omega - \epsilon) = \text{Tr} [\delta(\omega - \mathcal{H})] = -\frac{1}{\pi} \text{ImTr} [G(\omega)], \quad \rho_0(\omega) = -\frac{1}{\pi} \text{ImTr} [G_0(\omega)] \\ N &= \int_{-\infty}^{\epsilon_F} \rho(\omega) d\omega = -\int_{-\infty}^{\epsilon_F} \frac{1}{\pi} \text{ImTr} [G(\omega)] d\omega, \quad N_0 = -\int_{-\infty}^{\epsilon_F} \frac{1}{\pi} \text{ImTr} [G_0(\omega)] d\omega \end{aligned} \quad (2.2.4)$$

The sum  $\sum_{\epsilon}$  is over all eigenstates of the system, including all degeneracies. The quantity  $N$  counts the total number of states in the system below the Fermi surface. The change in the density of states induced by the interaction term  $V$  is

$$\Delta \rho(\omega) = \rho(\omega) - \rho_0(\omega) = -\frac{1}{\pi} \text{ImTr} [G(\omega) - G_0(\omega)] \quad (2.2.5)$$



We can rewrite the trace of Green's function as

$$\begin{aligned}
\text{Tr} [G(\omega)] &= \sum_i \frac{1}{\omega - E_i} \\
&= \sum_i \frac{\partial}{\partial \omega} \ln (\omega - E_i) \\
&= \frac{\partial}{\partial \omega} \ln \prod_i (\omega - E_i) \\
&= -\frac{\partial}{\partial \omega} \ln \text{Det} [G(\omega)]
\end{aligned} \tag{2.2.6}$$

such that

$$\begin{aligned}
-\text{Tr} [G(\omega) - G_0(\omega)] &= \frac{\partial}{\partial \omega} \ln \left\{ \text{Det} [G] \left( \text{Det} [G_0] \right)^{-1} \right\} \\
&= \frac{\partial}{\partial \omega} \ln \text{Det} [G(\omega) G_0^{-1}(\omega)] \\
&= \frac{\partial}{\partial \omega} \ln \text{Det} [G_0^{-1}(\omega) G(\omega)]
\end{aligned} \tag{2.2.7}$$

which works because  $\text{Det} [AB] = \text{Det} [BA]$ . From eq. 2.1.13, we can write  $G_0^{-1}(\omega) G(\omega) = 1 + G_0 T$ , which means

$$\begin{aligned}
-\text{Tr} [G(\omega) - G_0(\omega)] &= \frac{\partial}{\partial \omega} \ln \text{Det} [1 + G_0 T] \\
&= \frac{\partial}{\partial \omega} \ln \text{Det} [V^{-1} T] \quad [\text{eq. 2.1.8}] \\
&= \frac{\partial}{\partial \omega} \ln \text{Det} [V^{-1}] \text{Det} [T] \\
&= \frac{\partial}{\partial \omega} \left( \ln \text{Det} [V^{-1}] + \ln \text{Det} [T] \right)
\end{aligned} \tag{2.2.8}$$

Since  $V$  is independent of  $\omega$ , the first term will vanish under the derivative.

$$-\text{Tr} [G(\omega) - G_0(\omega)] = \frac{\partial}{\partial \omega} \ln \text{Det} [T] \tag{2.2.9}$$

The change in the dos becomes

$$\begin{aligned}
\Delta \rho(\omega) &= \frac{1}{\pi} \text{Im} \left( \frac{\partial}{\partial \omega} \ln \text{Det} [T] \right) \\
&= \frac{1}{\pi} \frac{\partial}{\partial \omega} \text{Im} \left( \ln \text{Det} [T] \right) \\
&= \frac{1}{\pi} \frac{\partial}{\partial \omega} \arg [\text{Det} (T)]
\end{aligned} \tag{2.2.10}$$

At the last line, we used the relation  $\text{Im} \ln(z) = \arg(z)$ . From eq. 2.1.26, we get

$$\Delta \rho(\omega) = \frac{1}{2i\pi} \frac{\partial}{\partial \omega} \text{Trace} [\ln S(\omega)] \tag{2.2.11}$$

The change in the total number of states is obtained simply by integrating the dos from  $-\infty$  to the chemical potential  $\epsilon_F$ :

$$\Delta N = \int_{-\infty}^{\epsilon_F} d\omega \frac{1}{2i\pi} \frac{\partial}{\partial \omega} \text{Trace} [\ln S(\omega)] = \frac{1}{2\pi i} \text{Trace} \ln \frac{S(\epsilon_F)}{S(-\infty)} \tag{2.2.12}$$

For  $\omega \rightarrow -\infty$ , we can write  $\omega - \mathcal{H} \rightarrow \omega - H_0$  such that  $G(\omega) \rightarrow G_0(\omega)$  and hence  $S(-\infty) \rightarrow 1$ . On making this substitution, we derive the generalised Friedel sum rule [15]

$$\Delta N = \frac{1}{2\pi i} \text{Trace} [\ln S(\epsilon_F)] \tag{2.2.13}$$

## 2.3 The single-impurity Anderson model (SIAM)

The SIAM consists of a single localized impurity site talking to a conduction bath. The impurity site has an energy  $\epsilon_d$  which is typically below the Fermi surface and hence favours a bound state but can in general be positive as well. We will assume the impurities are from a d or f-electron such that the orbitals are localized and there is a local repulsion  $U$  produced by the localized orbitals. The conduction bath dispersion is  $\epsilon_k$ .

$$H = \epsilon_d \sum_{\sigma} c_{d\sigma}^{\dagger} c_{d\sigma} + \sum_{k\sigma} \epsilon_k c_{k\sigma}^{\dagger} c_{k\sigma} + \sum_{k\sigma} t \left( c_{k\sigma}^{\dagger} c_{d\sigma} + c_{d\sigma}^{\dagger} c_{k\sigma} \right) + U c_{d\uparrow}^{\dagger} c_{d\uparrow} c_{d\downarrow}^{\dagger} c_{d\downarrow} \quad (2.3.1)$$

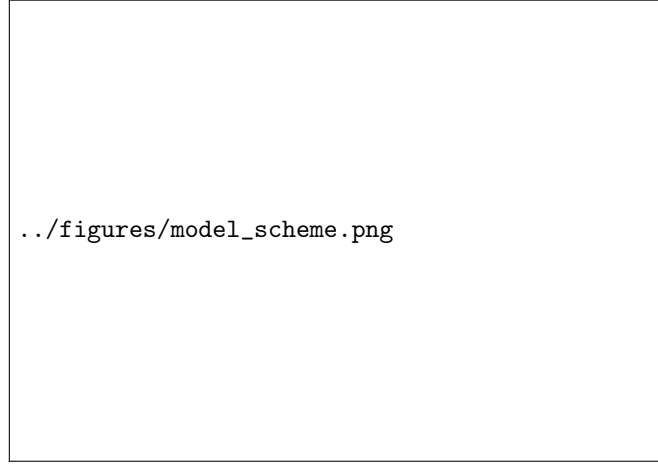


Figure 2.1: The single-impurity Anderson model Hamiltonian

The SIAM involves the following energy scales:

- the onsite energy:  $\epsilon_d$
- the onsite repulsion:  $U$
- the energy scale generated by the hybridisation:  $\Delta = \pi t^2 \sum_k \rho(\epsilon_k)$ . The rate of hybridisation is  $\frac{2\Delta}{\hbar}$ .

Let us discuss what might happen in various regimes of relative strengths of the energy scales:

$U \gg |\epsilon_d| \gg \Delta$  : Because of the very large on-site repulsion, the doublon configuration of the impurity is effectively at infinite energy. Since the onsite energy is sufficiently larger than the hybridisation, the eigenstates of the  $\Delta = 0$  model will be quite good approximations of the full problem. These eigenstates are, of course, the spin states and the holon state. If  $\epsilon_d < 0$ , then the spin states are below the Fermi energy and those will be the ground states, which means the impurity will be magnetic. If, however,  $\epsilon_d > 0$ , then the empty impurity is the ground state. Finally, if  $\epsilon_d = 0$ , all three configurations are degenerate, and this can lead to fractional occupation of the impurity (mixed-valence physics).

$U \gg \Delta \gg |\epsilon_d|$  : Double occupation of the impurity is still not possible. The impurity eigenstates are now, however, not good eigenstates of the interacting problem, because of the large  $\Delta$ . This large hybridisation will mix the spin states of the impurity, leading to a singlet ground state which is again non-magnetic. For  $\epsilon_d \geq 0$ , the holon state will again come into play, destroying the singlet and replacing it with a more complicated state.

$\Delta \gg U \gg \epsilon_d$  : This will be similar to the previous case, but now the hybridisation can mix the doublon with the spin and holon states. This can lead to a state consisting of spin singlet and charge triplet.

To get a feel for the model, we can consider the very simple atomic limit ( $V = 0$ ). The total Hamiltonian becomes a sum of the impurity part and the conduction bath part with no coupling between them, allowing us to solve one independent of the other. The impurity part of the Hamiltonian is

$$H_{\text{atomic}} = E_d + U n_{d\uparrow} n_{d\downarrow} \quad (2.3.2)$$

There are four states, two spin states ( $|\uparrow\rangle, |\downarrow\rangle$ ) and two charge states ( $|0\rangle, |2\rangle$ ).

$$E_\sigma = \epsilon_d, E_0 = 0, E_2 = 2\epsilon_d + U \quad (2.3.3)$$

For magnetic solutions, we need the energy  $E_\uparrow, E_\downarrow$  of the spin states to be lower than the energy  $E_0, E_2$  of the charge states:

$$-U < \epsilon_d < 0 \quad (2.3.4)$$

../figures//atomic.pdf

### 2.3.1 The non-interacting limit

The non-interacting limit consists of a non-interacting impurity site ( $U = 0$ ). This is often referred to as the resonant-level model.

$$H_{\text{non-int}} = \epsilon_d n_d + \sum_k \epsilon_k n_k + \sum_{k\sigma} t \left( c_{k\sigma}^\dagger c_{d\sigma} + c_{d\sigma}^\dagger c_{k\sigma} \right) \quad (2.3.5)$$

This is a single-electron problem and it can be exactly solved. The impurity and conduction electron Greens function can be obtained completely. The calculation of the conduction electron phase shifts also provides a demonstration of the Friedel sum rule.

#### Impurity Green's function

We want to write down diagonal the *Green's function*  $G_{d\sigma}$  for the excitation  $|d\sigma\rangle$ ; it is a single-particle state having an electron of spin  $\sigma$  on the impurity site. In the absence of the hybridisation, this Greens function is

$$G_0^{d\sigma}(\omega) = \langle d\sigma | \frac{1}{\omega - H_d} | d\sigma \rangle = \frac{1}{\omega - \epsilon_d} \quad (2.3.6)$$

$H_d = \sum_\sigma \epsilon_d \hat{n}_{d\sigma} + \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma}$  is the Hamiltonian in the absence of hybridisation. In the presence of the coupling with the conduction band, there are several ways of creating an excitation at the impurity site, with an energy  $\omega$ . The simplest is by putting an electron directly at the impurity site; this is just the bare Greens function  $G^0$ . But the electron can also tunnel into the conduction bath, spend time there and finally return to the impurity site. Such terms are captured by the Dyson expansion of the Greens function:

$$G = G_0 + G_0 V G_0 + G_0 V G_0 V G_0 + \dots \quad (2.3.7)$$

Using  $V = -t \sum_{k\sigma} c_{d\sigma}^\dagger c_{k\sigma} + \text{h.c.}$  and by taking the matrix element between  $|d\sigma\rangle$ , we get

$$G^{d\sigma} = \langle d\sigma | (G_0 + G_0 V G_0 + G_0 V G_0 V G_0 + \dots) | d\sigma \rangle \quad (2.3.8)$$

Note that only even powers of  $V$  will survive; with odd number of hopping, the electron cannot return to the impurity site:  $\langle d\sigma | V^3 | d\sigma \rangle = -t^3 \langle d\sigma | k\sigma \rangle = 0$ . A typical term with even number of hopping typical evaluates as:

$$\begin{aligned} \langle d\sigma | G_0 V G_0 V G_0 | d\sigma \rangle &= t^2 \sum_k \langle d\sigma | \frac{1}{\omega - H_d} c_{d\sigma}^\dagger c_{k\sigma} \frac{1}{\omega - H_d} c_{k\sigma}^\dagger c_{d\sigma} \frac{1}{\omega - H_d} | d\sigma \rangle \\ &= t^2 \sum_k G_0^{d\sigma} \langle d\sigma | c_{d\sigma}^\dagger c_{k\sigma} \frac{1}{\omega - H_d} c_{k\sigma}^\dagger c_{d\sigma} | d\sigma \rangle G_0^{d\sigma} \\ &= t^2 \sum_k G_0^{d\sigma} \langle k\sigma | \frac{1}{\omega - H_d} | k\sigma \rangle G_0^{d\sigma} \\ &= \left( G_0^{d\sigma} \right)^2 \sum_k \frac{t^2}{\omega - \epsilon_k} \end{aligned} \quad (2.3.9)$$

We can define the self-energy  $\Sigma(\omega) = \sum_k \frac{t^2}{\omega - \epsilon_k}$  which allows us to write the total Greens function as

$$G^{d\sigma} = G_0^{d\sigma} + \left( G_0^{d\sigma} \right)^2 \Sigma + \left( G_0^{d\sigma} \right)^3 \Sigma^2 + \dots = G_0^{d\sigma} \frac{1}{1 - G_0^{d\sigma} \Sigma} = \frac{1}{\left( G_0^{d\sigma} \right)^{-1} - \Sigma} = \frac{1}{\omega - \epsilon_d - \Sigma(\omega)} \quad (2.3.10)$$

The self-energy acts a single term that incorporates all single-particle scatterings in the form of a renormalization of the impurity energy  $\epsilon_d$ .

The self-energy can be simplified with some assumptions.

$$\frac{1}{t^2}\Sigma(\omega) = \sum_k \frac{1}{\omega - \epsilon_k} = \lim_{\eta \rightarrow 0} \int_{-W}^W d\epsilon \rho(\epsilon) \frac{1}{\omega - \epsilon + i\eta} \quad (2.3.11)$$

$$\Rightarrow \frac{1}{t^2}\text{Re}[\Sigma(\omega)] = \int_{-W}^W d\epsilon \rho(\epsilon) \frac{1}{\omega - \epsilon}, \text{ and } \frac{1}{t^2}\text{Im}[\Sigma(\omega)] = \int_{-W}^W d\epsilon \rho(\epsilon) (-i\pi) \delta(\omega - \epsilon) \quad (2.3.12)$$

Assuming  $\rho(\omega)$  varies sufficiently slowly, we can neglect the real part,

$$\Sigma(\omega) = \text{Im}[\Sigma(\omega)] = -i\pi t^2 \rho(\omega) = -i\Delta \quad (2.3.13)$$

Therefore,

$$G^{d\sigma}(\omega) = \frac{1}{\omega - \epsilon_d + i\Delta} \quad (2.3.14)$$

The difference from  $G_0^{d\sigma}$  can be seen by computing the density of states for both the bare and the interacting ones:

$$\rho_d^0(E) = -\frac{1}{\pi} \text{Im}[G_0^{d\sigma}] = -\frac{1}{\pi} \lim_{\eta \rightarrow 0} \frac{1}{E - \epsilon_d + i\eta} = \delta(E - \epsilon_d) \quad (2.3.15)$$

$$\rho_d(E) = -\frac{1}{\pi} \text{Im}[G^{d\sigma}] = -\frac{1}{\pi} \lim_{\eta \rightarrow 0} \frac{1}{E - \epsilon_d + i(\eta + \Delta)} = \frac{1}{\pi} \frac{\Delta}{(E - \epsilon_d)^2 + \Delta^2} \quad (2.3.16)$$

The first density of states is delta function, because  $\epsilon_d$  is an eigenstate in that case, and the poles of the corresponding Green's function are real poles. But the presence of the hybridisation means that is no longer the case in the second density of states, so the delta function fades into a Lorentzian in that case, and the poles of the Greens function move off the real axis. The total number of d-electrons can be calculated as:

$$\langle n_d \rangle = 2 \int d\epsilon \rho_d(\epsilon) = \frac{2\Delta}{\pi} \int \frac{d\epsilon}{(\epsilon - \epsilon_d)^2 + \Delta^2} = \frac{2}{\pi} \cot^{-1} \left( \frac{\epsilon_d}{\Delta} \right) \quad (2.3.17)$$

### Conduction bath Greens function and scattering phase shift

As mentioned before, the  $T$ -matrix satisfies the equation

$$T = V + VGT \quad (2.3.18)$$

We also have

$$\begin{aligned} G &= G_0 + G_0VG = G_0 + G_0T \frac{1}{1 + GT} G \\ &= G_0 + G_0T(1 - GT + \dots)(G_0 + G_0VG_0 + \dots) \\ &= G_0 + G_0TG_0 \end{aligned} \quad (2.3.19)$$

The conduction electron Green's function can be calculated as

$$\begin{aligned} G_c(k, k', E) &= \delta_{k,k'} G_c^0(k, E) + G_c^0(k) t G_0^{d\sigma} t G_c^0(k') + \\ &G_c^0(k) t G_0^{d\sigma} t \sum_q G_c^0(q) t G_0^{d\sigma} t G_c^0(k') + \dots \end{aligned} \quad (2.3.20)$$

Noting that

$$t \sum_q G_c^0(q) t = \Sigma_c, \quad (2.3.21)$$

we have

$$G_c(k, k', E) = \delta_{k,k'} G_c^0(k, E) + G_c^0(k) t^2 G^{d\sigma}(E) G_c^0(k') \quad (2.3.22)$$

Comparing with the final form of  $G$  in eq. 2.3.19, we can write

$$T(k, k', E) = t^2 G^{d\sigma}(E) = \frac{t^2}{E - \epsilon_d + i\Delta} = -\frac{t^2}{\Delta} \frac{1}{\frac{\epsilon_d - E}{\Delta} - i} \quad (2.3.23)$$

As an aside, this form of the transition matrix allows us to make a connection:

$$\text{Im}[T] = -\frac{t^2 \Delta}{(E - \epsilon_d)^2 + \Delta^2} = -\pi t^2 \rho_d \quad (2.3.24)$$

The density of states of the impurity site is proportional to the imaginary part of the transition matrix element. This is a general relation, because

$$\rho_d = -\frac{1}{\pi} \text{Im} [G_d] = -\frac{1}{\pi t^2} \text{Im} [t^2 G_d] = -\frac{1}{\pi t^2} \text{Im} [T] \quad (2.3.25)$$

This relation will hold as long as the  $T$ -matrix is of the form  $t^2 G_d$ .

If the phase shift of the conduction electrons due to scattering off the impurity is  $\delta$ , we have

$$T = e^{2i\delta} - 1 = e^{i\delta} (e^{i\delta} - e^{-i\delta}) \sim \frac{1}{\cot \delta - i} \quad (2.3.26)$$

Comparing with eq. 2.3.23, we can write

$$\delta(E) = \cot^{-1} \left( \frac{\epsilon_d - E}{\Delta} \right) \quad (2.3.27)$$

When  $E = \epsilon_d$ , the phase shift is  $\pi$ , and the scattering is head on (the conduction electron is reflected back). Comparing with eq. 2.3.17,

$$\frac{2}{\pi} \delta(0) = \langle n_d \rangle \quad (2.3.28)$$

This is an example of the Friedel sum rule which states that the total number of electrons bound inside a resonance is  $\frac{1}{\pi}$  times the total scattering phase shift at the Fermi surface. In other words, the impurity will be singly occupied when  $\delta(0) = \frac{\pi}{2}$ .

### 2.3.2 Total Hamiltonian: Mean field treatment

$$n_{d\uparrow} n_{d\downarrow} \approx n_{d\uparrow} \langle n_{d\downarrow} \rangle + n_{d\downarrow} \langle n_{d\uparrow} \rangle + \text{constant} \quad (2.3.29)$$

$$H \approx \sum_k \epsilon_k n_k + \sum_{\sigma} [\epsilon_d + U \langle n_{d\bar{\sigma}} \rangle] n_{d\sigma} + t \sum_{k\sigma} (c_{k\sigma}^\dagger c_{d\sigma} + c_{d\sigma}^\dagger c_{k\sigma}) \quad (2.3.30)$$

The only change is  $\epsilon_d \rightarrow \epsilon_{d\sigma} = \epsilon_d + U \langle n_{d\bar{\sigma}} \rangle$ . This allows us to write

$$\rho_{d\sigma} = \frac{1}{\pi} \frac{\Delta}{(E - \epsilon_{d\sigma})^2 + \Delta^2} \implies \langle n_{d\sigma} \rangle = \int \rho_{d\sigma} = \frac{1}{\pi} \cot^{-1} \left( \frac{\epsilon_{d\sigma}}{\Delta} \right) \quad (2.3.31)$$

An alternative way of writing that is

$$\frac{\epsilon_{d\sigma}}{\Delta} = \frac{\epsilon_d + U \langle n_{d\bar{\sigma}} \rangle}{\Delta} = \cot(\pi \langle n_{d\sigma} \rangle) \implies \langle n_{d\sigma} \rangle = \frac{\Delta}{U} \left[ \cot(\pi \langle n_{d\bar{\sigma}} \rangle) - \frac{\epsilon_d}{\Delta} \right] \quad (2.3.32)$$

Introducing  $n_d = \langle n_{d\uparrow} \rangle + \langle n_{d\downarrow} \rangle$  and  $m = \langle n_{d\uparrow} \rangle - \langle n_{d\downarrow} \rangle$ , we can write

$$\begin{aligned} \langle n_{d\uparrow} - n_{d\downarrow} \rangle \equiv m &= \frac{\Delta}{U} \left[ \cot(\pi \langle n_{d\downarrow} \rangle) - \cot(\pi \langle n_{d\uparrow} \rangle) \right] \\ &= \frac{\Delta}{U} \left[ \cot \frac{\pi}{2} (n_d - m) - \cot \frac{\pi}{2} (n_d + m) \right] \end{aligned} \quad (2.3.33)$$

We want to find the critical condition for the onset of magnetism. This occurs when  $m \rightarrow 0^+$ . This means we can expand the cot around  $m = 0$ . Since

$$\cot(a + x) \approx \cot a - x (\sin a)^{-2} \implies \cot(a - x) - \cot(a + x) \approx 2x (\sin a)^{-2} \quad (2.3.34)$$

we get

$$m = \frac{\Delta}{U} \left[ -\pi \frac{m}{\sin^2 \frac{\pi}{2} n_d} \right] \implies 1 = \lim_{m \rightarrow 0} \frac{U}{\pi \Delta} \frac{1}{1 + \cot^2 \frac{\pi n_d}{2}} \quad (2.3.35)$$

At  $m = 0$ ,  $\langle n_{d\uparrow} \rangle = \langle n_{d\downarrow} \rangle$ , therefore  $\cot \frac{\pi n_d}{2} = \frac{U n_d}{2\Delta} + \frac{\epsilon_d}{\Delta}$ . Substituting in eq. 2.3.35,

$$1 = \frac{U_c}{\pi} \frac{\Delta}{\Delta^2 + \left( \frac{U_c n_d}{2} + \epsilon_d \right)^2} \quad (2.3.36)$$

Magnetism will prevail for  $U \geq U_c$ . Comparing with eq. 2.3.32,

$$1 = U_c \rho_d(E = 0) \quad (2.3.37)$$

At half-filling,  $n_d = 1$  and  $\epsilon_d = -\frac{U}{2}$ , which gives

$$U_c = \pi \Delta \quad (2.3.38)$$

For higher values of  $U$ , we get a value of  $m$  far from 0. This provides two peaks in the density of states.

$$\langle n_{d\uparrow} \rangle = \frac{1+m}{2} \quad (2.3.39)$$

$$\langle n_{d\downarrow} \rangle = \frac{1-m}{2} \quad (2.3.40)$$

$$\epsilon_{d\sigma} = \epsilon_d + U \langle n_{d\bar{\sigma}} \rangle = \epsilon_d + \frac{U}{2} \pm \frac{U}{2} m = \pm \frac{U}{2} m \quad (2.3.41)$$

$$\rho_d = \rho_{d\uparrow} + \rho_{d\downarrow} = \frac{\Delta}{\pi} \left[ \frac{1}{\Delta^2 + \left( E - \frac{U m}{2} \right)^2} + \frac{1}{\Delta^2 + \left( E + \frac{U m}{2} \right)^2} \right] \quad (2.3.42)$$

We get two Lorentzian peaks at  $E = \pm \frac{U m}{2}$ , depending on whichever polarization the impurity local moment is in.

### 2.3.3 Discussions

The resonant-level model can be exactly solved, and The mean-field self-consistent hence predicts a magnetic ground state of the impurity for  $U$  larger than a critical value.

- At low temperatures, the resistivity is found to reach a minimum and then vary as  $\ln T$ . This behavior stops at some very low temperature  $T_K$ . The temperature  $T_K$  is also that at which the magnetization vanishes, and the susceptibility becomes constant, suggesting that the impurity spin has condensed into a singlet.
- Since the disappearance of the  $\ln T$  behavior is coincident with the condensation of the spin degree of freedom, it is natural to hope that the resistivity minimum is a result of the interaction between the impurity and the conduction spins.
- To describe such an interaction, the way to proceed is to strip the model of the charge excitations (via a *Schrieffer-Wolff transformation*). The resultant Hamiltonian consists of an anti-ferromagnetic interaction between the itinerant spins and the impurity spin, and is called the Kondo model.
- Calculating the scattering rate up to second order using the Kondo model produces a logarithmic term, which explains the log-dependence. Since this perturbative treatment will fail at small temperatures (where the log term diverges), we need some other technique to find out the fate of the model at low temperatures.
- Anderson's poor man's scaling wraps the effects of high energy scatterings into the low energy model, showing that the anti-ferromagnetic coupling diverges at low temperatures, producing a singlet.
- There are two routes that one can follow to note the changes in the system; one is by reducing the temperature which is equivalent to folding in the high energy fluctuations, aka scaling. The other is to reduce the onsite interaction  $U$  and note the changes in state.

- Reducing the temperature or performing the RG takes the model from the Anderson model ( $T > 0$ ) to the Fermi liquid state ( $T \sim T_K$ ). This Fermi liquid may have interactions, depending on the value of  $U$  we are working in.
- Coming down to  $T < T_K$ , we can now modify the  $U$  from  $\infty$  to 0. Large  $U$  means the Fermi liquid has large interactions. Reducing  $U$  means coming down to a Fermi gas. For  $T \neq 0$ , reducing  $U$  means going from local moment regime to non-magnetic regime. For  $T = 0$ , local moments persist for all  $U > 0$ .
- It will be seen that in the large  $U$  regime, the singlet channel scattering phase shift (phase shift incurred when one singlet state scatters into another singlet state) at the Fermi energy is  $\propto \tan^{-1} J_{\text{eff}}$ . This effective coupling  $J_{\text{eff}}$  flows to  $\infty$  under poor man's scaling as  $T \rightarrow 0$ . Thus, the singlet phase shift at  $\epsilon_F$  approaches  $\frac{\pi}{2}$  as  $T \rightarrow 0$ .

## 2.4 The Kondo model

To study the interactions of the spin degrees of freedom, it becomes necessary to integrate out the charge degrees of freedom from the general scattering term  $V c_k^\dagger c_d + \text{h.c.}$ . Doing so produces a simpler Hamiltonian that has the charge fluctuations projected out and only spin fluctuations remaining.

$$H_{\text{Kondo}} = \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{i=x,y,z} J_i S_d^i s^i \quad (2.4.1)$$

$S_i = \sum_{\alpha\beta} c_{d\alpha}^\dagger \sigma_{\alpha\beta}^i c_{d\beta}$ .  $s_i = \sum_{kk'\alpha\beta} c_{k\alpha}^\dagger \sigma_{\alpha\beta}^i c_{k'\beta}$ . Note that the impurity onsite energy has also been dropped because we are in the subspace of constant  $\hat{n}_d (= 1)$ .

### 2.4.1 Derivation of the Kondo Hamiltonian

Deriving the Kondo Hamiltonian involves separating the impurity spinon subspace ( $\hat{n}_{d\uparrow} \neq \hat{n}_{d\downarrow}$ ) from the doublon and holon subspaces ( $\hat{n}_{d\uparrow} = \hat{n}_{d\downarrow}$ ). The canonical (pun intended) way of doing this is via a Schrieffer-Wolff transformation [17]. It involves applying a unitary transformation on the original Hamiltonian such that the terms that scatter between the two subspaces disappear, up to leading order. We are then left with a higher order intra-subspace scattering. It is often referred to as a one-shot renormalization group method, because it kills all the off-diagonal terms in one iteration. The approach here follows that in [18]. An alternate derivation via a projector operator method due to [19] is shown in 4.4. The space of the impurity electron can be divided into low energy and high energy subspaces:

$$\begin{aligned} \text{low energy (L)} &\rightarrow \begin{cases} |\uparrow\rangle \\ |\downarrow\rangle \end{cases} \\ \text{high energy (H)} &\rightarrow \begin{cases} | \rangle \\ |\uparrow\downarrow\rangle \end{cases} \end{aligned} \quad (2.4.2)$$

$$H = H_0 + V = \begin{array}{cc} & \begin{matrix} \text{low} & \text{high} \end{matrix} \\ \begin{matrix} \text{low} \\ \text{high} \end{matrix} & \begin{pmatrix} H^L & v^\dagger \\ v & H^H \end{pmatrix} \end{array} \quad (2.4.3)$$

$$H_0 = \sum_k \epsilon_k n_k + \epsilon_d n_d + U n_{d\uparrow} n_{d\downarrow}, V = \sum_{k\sigma} \left( V_k c_{k\sigma}^\dagger c_{d\sigma} + V_k^* c_{d\sigma}^\dagger c_{k\sigma} \right) \quad (2.4.4)$$

Let  $S$  be some anti-Hermitian operator, of the order of  $V$ . Expanding in powers of  $V$ ,

$$\bar{H} = e^{-S} H e^S = H_0 + \left( V + [H_0, S] \right) + \frac{1}{2} \left( [V, S] + [[H_0, S], S] \right) \quad (2.4.5)$$

Defining  $S$  such that the first order term vanishes,

$$V = [S, H_0] \quad (2.4.6)$$

$$\bar{H} = H_0 + \frac{1}{2} [V, S] \quad (2.4.7)$$

Take  $S = \begin{pmatrix} 0 & -s^\dagger \\ s & 0 \end{pmatrix}$ . From eq. 2.4.6,

$$\begin{aligned} V &= \begin{pmatrix} 0 & -s^\dagger \\ s & 0 \end{pmatrix} \begin{pmatrix} H^L & 0 \\ 0 & H^H \end{pmatrix} - \begin{pmatrix} H^L & 0 \\ 0 & H^H \end{pmatrix} \begin{pmatrix} 0 & -s^\dagger \\ s & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & -s^\dagger H^H + H^L s^\dagger \\ s H^L - H^H s & 0 \end{pmatrix} \end{aligned} \quad (2.4.8)$$

Comparing with the definition of  $V$ , we can write

$$v_{ij}^\dagger = s_{ij}^\dagger (E_i^L - E_j^H), v_{ij} = s_{ij} (E_j^L - E_i^H) \quad (2.4.9)$$

$$\implies s_{ij}^\dagger = \frac{v_{ij}^\dagger}{E_i^L - E_j^H}, s_{ij} = \frac{v_{ij}}{E_j^L - E_i^H} \quad (2.4.10)$$

From the structure of  $S$ , it is clear that  $i \in H, j \in L$ .

$$[V, S] = \begin{pmatrix} 0 & v^\dagger \\ v & 0 \end{pmatrix} \begin{pmatrix} 0 & -s^\dagger \\ s & 0 \end{pmatrix} - \begin{pmatrix} 0 & -s^\dagger \\ s & 0 \end{pmatrix} \begin{pmatrix} 0 & v^\dagger \\ v & 0 \end{pmatrix} = \begin{pmatrix} v^\dagger s + s^\dagger v & 0 \\ 0 & -v s^\dagger - s v^\dagger \end{pmatrix} \quad (2.4.11)$$

Hence,

$$\bar{H} = H_0 + \frac{[V, S]}{2} = \begin{pmatrix} H^L + \frac{1}{2} (v^\dagger s + s^\dagger v) & 0 \\ 0 & H^H - v s^\dagger - s v^\dagger \end{pmatrix} \quad (2.4.12)$$

Since we want the low energy excitations, the effective low-energy Hamiltonian is

$$\mathcal{H} = \langle L | \bar{H} | L \rangle = H^L + \frac{1}{2} (v^\dagger s + s^\dagger v) \quad (2.4.13)$$

where  $H^L = \sum_\sigma \langle \sigma_d | H_0 | \sigma_d \rangle = \epsilon_d n_d + \sum_k n_k$ . Now,

$$\begin{aligned} \Delta H &= \frac{1}{2} (v^\dagger s + s^\dagger v) = \frac{1}{2} \left( v^\dagger \sum_{HL} s_{HL} |H\rangle \langle L| + \text{h.c.} \right) \\ &= \frac{1}{2} \sum_{HL} \left[ v^\dagger |H\rangle \langle L| \frac{v_{HL}}{E_L - E_H} + |L\rangle \langle H| \frac{v_{LH}^\dagger}{E_L - E_H} v \right] \end{aligned} \quad (2.4.14)$$

Taking a matrix element between two low energy states  $l, l'$ , we get

$$\Delta H_{ll'} = \langle l | \Delta H | l' \rangle = \frac{1}{2} \sum_H v_{lH}^\dagger v_{Hl'} \left( \frac{1}{E_{l'} - E_H} + \frac{1}{E_l - E_H} \right) \quad (2.4.15)$$

This can also be written as

$$\Delta H_{ll'} = \frac{1}{2} [T_{ll'}(E_l) + T_{ll'}(E_{l'})] \quad (2.4.16)$$



where

$$T_{ll'}(E) = \sum_H \frac{v_{lH}^\dagger v_{Hl'}}{E - E_H} = \sum_H \frac{V_{lH}^\dagger V_{Hl'}}{E - E_H} \quad (2.4.17)$$

$T(E)$ , here, is the second order contribution of the  $T$ -matrix due to scattering off the interaction  $V$ . The  $|H\rangle$  act as the intermediate states during the second order scatterings. This is a slight generalization from second order perturbation theory. In second order perturbation, we only consider the scattering amplitude between the same states, but here we consider the scattering between two potentially different states  $|l\rangle, |l'\rangle$ . The total amplitude is an average of these two amplitudes. If we assume the high energy subspace is very far away from the low energy one ( $E_H \gg E_L$ ), we can assume  $E_l \approx E_{l'} = E_L$ , we can write

$$\begin{aligned} \Delta H_{ll'} &= \sum_H v_{lH}^\dagger v_{Hl'} \frac{1}{E_L - E_H} \\ \Rightarrow \Delta H &= V \left( \sum_H \frac{1}{\Delta_{LH}} |H\rangle \langle H| \right) V \end{aligned} \quad (2.4.18)$$

where  $\Delta_{LH} = E_L - E_H$  is the energy difference between the low energy subspace and the high energy state  $|H\rangle$ . For our Hamiltonian,  $|H_1\rangle = |0\rangle, |H_2\rangle = |\uparrow\downarrow\rangle$ . Therefore,

$$\Delta_{LH_1} = \epsilon_d - 0 = \epsilon_d, \Delta_{LH_2} = \epsilon_d - (2\epsilon_d + U) = -\epsilon_d - U \quad (2.4.19)$$

Also,  $V = \sum_{k\sigma} [V(k)c_{k\sigma}^\dagger c_{d\sigma} + V^*(k)c_{d\sigma}^\dagger c_{k\sigma}]$ . Hence,

$$\begin{aligned} \Delta H &= V \frac{|0\rangle \langle 0|}{\epsilon_d} V - V \frac{|\uparrow\downarrow\rangle \langle \uparrow\downarrow|}{\epsilon_d + U} V \\ &= \sum_{k_1, k_2, \sigma_1, \sigma_2} V(k_1) V^*(k_2) \left[ \frac{c_{d\sigma_2}^\dagger c_{k_2\sigma_2} |0\rangle \langle 0| c_{k_1\sigma_1}^\dagger c_{d\sigma_1}}{\epsilon_d} - \frac{c_{k_1\sigma_1}^\dagger c_{d\sigma_1} |\uparrow\downarrow\rangle \langle \uparrow\downarrow| c_{d\sigma_2}^\dagger c_{k_2\sigma_2}}{\epsilon_d + U} \right] \\ &= \sum_{k_1, k_2, \sigma_1, \sigma_2} V(k_1) V^*(k_2) \frac{c_{d\sigma_2}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_1} |d\sigma_1, h_{k_1\sigma_1}\rangle \langle d\sigma_1, h_{k_1\sigma_1}|}{\epsilon_d} \\ &\quad - \sum_{k_1, k_2, \sigma_1, \sigma_2} V(k_1) V^*(k_2) \frac{c_{k_1\sigma_1}^\dagger c_{d\sigma_1} c_{d\sigma_2}^\dagger c_{k_2\sigma_2} |d\bar{\sigma}_2, e_{k_2\sigma_2}\rangle \langle d\bar{\sigma}_2, e_{k_2\sigma_2}|}{\epsilon_d + U} \\ &= \sum_{k_1, k_2, \sigma_1, \sigma_2} V(k_1) V^*(k_2) \left[ \frac{c_{d\sigma_2}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_1}}{\epsilon_d} - \frac{c_{k_1\sigma_1}^\dagger c_{d\sigma_1} c_{d\sigma_2}^\dagger c_{k_2\sigma_2}}{\epsilon_d + U} \right] P_{n_d=1} \end{aligned} \quad (2.4.20)$$

Using the Fierz identity  $\delta_{\sigma_1\sigma_3} \delta_{\sigma_4\sigma_2} = \frac{1}{2} \delta_{\sigma_1\sigma_2} \delta_{\sigma_3\sigma_4} + \frac{1}{2} \vec{\sigma}_{\sigma_1\sigma_2} \cdot \vec{\sigma}_{\sigma_3\sigma_4}$ , we can write

$$\begin{aligned} c_{d\sigma_2}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_1} &= \sum_{\sigma_3, \sigma_4} c_{d\sigma_3}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_4} \delta_{\sigma_1\sigma_3} \delta_{\sigma_4\sigma_2} \\ &= \frac{1}{2} \sum_{\sigma_3, \sigma_4} c_{d\sigma_3}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_4} (\delta_{\sigma_1\sigma_2} \delta_{\sigma_3\sigma_4} + \vec{\sigma}_{\sigma_1\sigma_2} \cdot \vec{\sigma}_{\sigma_3\sigma_4}) \\ &= \frac{1}{2} c_{k_2\sigma_1} c_{k_1\sigma_1}^\dagger n_d + c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} \cdot \sum_{\sigma_3, \sigma_4} c_{d\sigma_3}^\dagger \frac{\vec{\sigma}_{\sigma_3\sigma_4}}{2} c_{d\sigma_4} \end{aligned} \quad (2.4.21)$$

Now,  $c_{k_2\sigma_1} c_{k_1\sigma_1}^\dagger = \delta_{k_1, k_2} - c_{k_1\sigma_1}^\dagger c_{k_2\sigma_1}$ , and  $c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger = \delta_{\sigma_1, \sigma_2} \delta_{k_1, k_2} - c_{k_1\sigma_1}^\dagger c_{k_2\sigma_1}$ . The  $\delta$  will result in terms that have no interaction, so we drop these terms. Also, the  $P_{n_d=1}$  ensures we can substitute  $n_d = 1$ .

$$c_{d\sigma_2}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_1} = -\frac{1}{2} c_{k_1\sigma_1}^\dagger c_{k_2\sigma_1} - c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2} \cdot \sum_{\sigma_3, \sigma_4} c_{d\sigma_3}^\dagger \frac{\vec{\sigma}_{\sigma_3\sigma_4}}{2} c_{d\sigma_4} \quad (2.4.22)$$

Since the first term does not have any spin-spin interaction, we drop that term.

Defining  $\vec{\sigma}_d = \sum_{\sigma_3, \sigma_4} c_{d\sigma_3}^\dagger \vec{\sigma}_{\sigma_3\sigma_4} c_{d\sigma_4}$ , we have

$$c_{d\sigma_2}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_1} = -\frac{1}{2} c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2} \cdot \vec{\sigma}_d \quad (2.4.23)$$

Similarly,

$$c_{k_1\sigma_1}^\dagger c_{d\sigma_1} c_{d\sigma_2}^\dagger c_{k_2\sigma_2} = -\frac{1}{2} c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2} \cdot \vec{\sigma}_d \quad (2.4.24)$$

Finally, putting all this together,

$$\begin{aligned} \Delta H &= \frac{1}{2} \sum_{k_1, k_2, \sigma_1, \sigma_2} V(k_1) V^*(k_2) \left[ \frac{1}{\epsilon_d + U} - \frac{1}{\epsilon_d} \right] c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2} \cdot \vec{\sigma}_d \\ &= \frac{1}{2} \sum_{k_1, k_2, \sigma_1, \sigma_2} J(k_1, k_2) c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2} \cdot \vec{\sigma}_d \end{aligned} \quad (2.4.25)$$

where

$$J(k_1, k_2) = V(k_1) V^*(k_2) \left[ \frac{1}{\epsilon_d + U} - \frac{1}{\epsilon_d} \right] \quad (2.4.26)$$

Assuming  $V(k) \equiv t$ ,

$$H_K = \sum_k \epsilon_k n_k + \frac{J}{2} \vec{\sigma}_e \cdot \vec{\sigma}_d \quad (2.4.27)$$

where

$$\vec{\sigma}_e = \sum_{k_1, k_2, \sigma_1, \sigma_2} c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2} = \sum_{\sigma_1, \sigma_2} c_{\sigma_1}^\dagger (\vec{r}=0) \vec{\sigma}_{\sigma_1\sigma_2} c_{\sigma_2} (\vec{r}=0) \quad (2.4.28)$$

$\vec{\sigma}_e$  is thus the spin density at the origin.

### 2.4.2 Obtaining the resistivity minimum and log-dependence

The next few sections follow the approach in [20]. The model we are working with is

$$H_K = H_0 + V = \sum_k \epsilon_k n_k + \frac{J}{2} \sum_{k_1, k_2, \sigma_1, \sigma_2} c_{k_1\sigma_1}^\dagger \vec{\sigma}_d \cdot \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2} \quad (2.4.29)$$

$$\begin{aligned} \sum_{\sigma_1, \sigma_2} c_{k_1\sigma_1}^\dagger \vec{\sigma}_d \cdot \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2} &= \sigma_d^z \left( c_{k_1\uparrow}^\dagger c_{k_2\uparrow} - c_{k_1\downarrow}^\dagger c_{k_2\downarrow} \right) + \sigma_d^x \left( c_{k_1\downarrow}^\dagger c_{k_2\uparrow} + c_{k_1\uparrow}^\dagger c_{k_2\downarrow} \right) \\ &\quad - i\sigma_d^y \left( c_{k_1\uparrow}^\dagger c_{k_2\downarrow} - c_{k_1\downarrow}^\dagger c_{k_2\uparrow} \right) \end{aligned} \quad (2.4.30)$$

$$= \sigma_d^z \left( c_{k_1\uparrow}^\dagger c_{k_2\uparrow} - c_{k_1\downarrow}^\dagger c_{k_2\downarrow} \right) + c_{k_1\downarrow}^\dagger c_{k_2\uparrow} \sigma_d^+ + c_{k_1\uparrow}^\dagger c_{k_2\downarrow} \sigma_d^- \quad (2.4.31)$$

where  $\sigma^\pm = \sigma^x \pm i\sigma^y$ . Therefore,

$$\begin{aligned} H_K &= \sum_k \epsilon_k n_k + \frac{J}{2} \sum_{k_1, k_2} \left[ \sigma_d^z \left( c_{k_1\uparrow}^\dagger c_{k_2\uparrow} - c_{k_1\downarrow}^\dagger c_{k_2\downarrow} \right) + \sigma_d^+ c_{k_1\downarrow}^\dagger c_{k_2\uparrow} + \sigma_d^- c_{k_1\uparrow}^\dagger c_{k_2\downarrow} \right] \\ &= \sum_k \epsilon_k n_k + J \sum_{k_1, k_2} \left[ S_d^z \left( c_{k_1\uparrow}^\dagger c_{k_2\uparrow} - c_{k_1\downarrow}^\dagger c_{k_2\downarrow} \right) + S_d^+ c_{k_1\downarrow}^\dagger c_{k_2\uparrow} + S_d^- c_{k_1\uparrow}^\dagger c_{k_2\downarrow} \right] \end{aligned} \quad (2.4.32)$$

To see the log-dependence, we need to calculate the transition matrix up to second order:

$$T = V + V G_0 V \quad (2.4.33)$$

We wish to calculate the scattering probability of a conduction electron  $|k \uparrow\rangle$ .

**First order scattering**

$$\left. \begin{aligned} &|k \uparrow, d_\sigma\rangle \rightarrow |q \uparrow, d_\sigma\rangle \\ &|k \uparrow, d_\downarrow\rangle \rightarrow |q \downarrow, d_\uparrow\rangle \end{aligned} \right\} \begin{array}{l} \text{non-spin-flip} \\ \text{pro-spin-flip} \end{array}$$

For non-flip, the matrix elements for the  $T$ -matrix is

$$T_{\text{non-flip}}^{(1)} = T_{k_\uparrow, d_\sigma \rightarrow q_\uparrow, d_\sigma} = \langle q_\uparrow, d_\sigma | V | k_\uparrow, d_\sigma \rangle = m_d J \quad (2.4.34)$$

where  $m_d \in \{-s_d, s_d\}$  is the spin of the impurity electron. The probability for this scattering is

$$\mathcal{P}_{k_\sigma, d_{\sigma'} \rightarrow q_\sigma, d_{\sigma'}} = 2\pi \sum_{\epsilon} \rho(\epsilon) T_{k_\uparrow, d_\sigma \rightarrow q_\uparrow, d_\sigma}^2 = 2\pi \rho(0) J^2 m_d^2 \quad (2.4.35)$$

Since we are considering scattering close to the Fermi surface, we replaced the sum with  $\rho(0)$ .

$$\mathcal{P}_1 = 2\pi \rho(0) J^2 m_d^2 \quad (2.4.36)$$

For spin-flip, the matrix element is

$$T_{\text{flip}}^{(1)} = T_{k_\uparrow, d_\downarrow \rightarrow q_\downarrow, d_\uparrow} = \langle q_\downarrow, d_\uparrow | V | k_\uparrow, d_\downarrow \rangle = \lambda_+ J \quad (2.4.37)$$

where  $\lambda_\pm = \langle m_d \pm 1 | S_d^\pm | m_d \rangle = \sqrt{s_d(s_d + 1) - m_d(m_d \pm 1)}$ . The probability for this scattering is hence

$$\mathcal{P}_2 = \mathcal{P}_{k_\uparrow, d_\downarrow \rightarrow q_\downarrow, d_\uparrow} = 2\pi \rho(0) J^2 [s_d(s_d + 1) - m_d(m_d + 1)] \quad (2.4.38)$$

The total first order scattering probability is (averaged over all configurations of the impurity)

$$\begin{aligned} \mathcal{P}^{(1)} &= \frac{1}{2s_d + 1} \sum_{m_d = -s_d}^{s_d} (\mathcal{P}_1 + \mathcal{P}_2) = \frac{2\pi \rho(0) J^2}{(2s_d + 1)} \sum_{m_d = -s_d}^{s_d} (s_d(s_d + 1) - m_d) \\ &= 2\pi \rho(0) J^2 s_d(s_d + 1) \end{aligned} \quad (2.4.39)$$

**Second order scattering**

$$\left. \begin{aligned} &\text{no-impurity-flip} \left\{ \begin{array}{l} |k \uparrow, d_\sigma\rangle \rightarrow |q \uparrow, d_\sigma\rangle \rightarrow |k' \uparrow, d_\sigma\rangle \\ |k \uparrow, q \uparrow, d_\sigma\rangle \rightarrow |k \uparrow, k' \uparrow, d_\sigma\rangle \rightarrow |k' \uparrow, q \uparrow, d_\sigma\rangle \end{array} \right\} \\ &\text{pro-impurity-flip} \left\{ \begin{array}{l} |k \uparrow, d_\downarrow\rangle \rightarrow |q \downarrow, d_\uparrow\rangle \rightarrow |k' \uparrow, d_\downarrow\rangle \\ |k \uparrow, q \downarrow, d_\uparrow\rangle \rightarrow |k \uparrow, k' \uparrow, d_\downarrow\rangle \rightarrow |k' \uparrow, q \downarrow, d_\uparrow\rangle \end{array} \right\} \end{aligned} \right\} \text{no-cond-flip}$$

$$\left. \begin{aligned} &\text{flip-first} \left\{ \begin{array}{l} |k \uparrow, d_\downarrow\rangle \rightarrow |q \downarrow, d_\uparrow\rangle \rightarrow |k' \downarrow, d_\uparrow\rangle \\ |k \uparrow, q \uparrow, d_\downarrow\rangle \rightarrow |k \uparrow, k' \downarrow, d_\uparrow\rangle \rightarrow |k' \downarrow, q \uparrow, d_\downarrow\rangle \end{array} \right\} \\ &\text{flip-later} \left\{ \begin{array}{l} |k \uparrow, d_\downarrow\rangle \rightarrow |q \uparrow, d_\downarrow\rangle \rightarrow |k' \downarrow, d_\uparrow\rangle \\ |k \uparrow, q \downarrow, d_\downarrow\rangle \rightarrow |k \uparrow, k' \downarrow, d_\downarrow\rangle \rightarrow |k' \downarrow, q \downarrow, d_\uparrow\rangle \end{array} \right\} \end{aligned} \right\} \text{pro-cond-flip}$$

The second order transition matrix contribution is of the form

$$T_{i \rightarrow j}^{(2)} = \langle j | V G_0 V | i \rangle = \sum_l \frac{\langle j | V | l \rangle \langle l | V | i \rangle}{E_i - E_l} \quad (2.4.40)$$

The sum is over all the intermediate states in going from  $|i\rangle$  to  $|k\rangle$ . For no flipping of the conduction electron, there are four possible processes. The first process has the following  $T$ -matrix:

$$\begin{aligned} T_{11}^{(2)} &= \sum_q \frac{\langle k'_\uparrow d_\sigma | V | q_\uparrow d_\sigma \rangle \langle q_\uparrow d_\sigma | V | k_\uparrow d_\sigma \rangle}{\epsilon_k - \epsilon_q} \\ &= (Jm_d)^2 \sum_q \frac{1 - P(q)}{\epsilon_k - \epsilon_q} = J^2 m_d^2 \sum_q \frac{1 - P(q)}{\epsilon_k - \epsilon_q} \end{aligned} \quad (2.4.41)$$

where  $m_d = \langle d_\sigma | S_d^z | d_\sigma \rangle$  and  $1 - P(q)$  is the probability that the state  $q \uparrow$  is empty. For the second process,

$$T_{12}^{(2)} = \sum_q \frac{\langle q_\uparrow k'_\uparrow d_\sigma | V | k'_\uparrow k_\uparrow d_\sigma \rangle \langle k'_\uparrow k_\uparrow d_\sigma | V | q_\uparrow k_\uparrow d_\sigma \rangle}{\epsilon_q - \epsilon_{k'}} P(q) \quad (2.4.42)$$

Note that if  $\langle k'k | V | qk \rangle \sim \langle k'k | c_{k'}^\dagger c_q | qk \rangle = 1$ , then  $\langle qk' | V | k'k \rangle \sim \langle qk' | c_q^\dagger c_{k'} | k'k \rangle = -\langle qk' | c_q^\dagger c_{k'} | k'k' \rangle = -1$ . Assuming the scattering conserves energy ( $\epsilon_k = \epsilon_{k'}$ ), we get

$$T_{12}^{(2)} = -J^2 m_d^2 \sum_q \frac{P(q)}{\epsilon_q - \epsilon_k} = J^2 m_d^2 \sum_q \frac{P(q)}{\epsilon_k - \epsilon_q} \quad (2.4.43)$$

For the third process,

$$T_{13}^{(2)} = \sum_q \frac{\langle k'_\uparrow d_\downarrow | V | q_\downarrow d_\uparrow \rangle \langle q_\downarrow d_\uparrow | V | k_\uparrow d_\downarrow \rangle}{\epsilon_k - \epsilon_q} \quad (2.4.44)$$

Using  $\langle m_d \pm 1 | S_d^\pm | m_d \rangle = \sqrt{s_d(s_d + 1) - m_d(m_d \pm 1)} = \lambda_\pm$ , we get

$$T_{13}^{(2)} = \lambda_+^2 J^2 \sum_q \frac{1 - P(q)}{\epsilon_k - \epsilon_q} \quad (2.4.45)$$

For the fourth process,

$$\begin{aligned} T_{14}^{(2)} &= \sum_q \frac{\langle q_\downarrow k'_\uparrow d_\uparrow | V | k'_\uparrow k_\uparrow d_\downarrow \rangle \langle k'_\uparrow k_\uparrow d_\downarrow | V | q_\downarrow k_\uparrow d_\uparrow \rangle}{\epsilon_q - \epsilon'_k} \\ &= -\lambda_-^2 J^2 \sum_q \frac{P(q)}{\epsilon_q - \epsilon_k} \\ &= \lambda_-^2 J^2 \sum_q \frac{P(q)}{\epsilon_k - \epsilon_q} \end{aligned} \quad (2.4.46)$$

The sum of all the elements gives the transition matrix element for the scattering  $k \uparrow \rightarrow k' \uparrow$ :

$$\begin{aligned} T_{\text{nonflip}}^{(2)} &= \sum_{i=1}^4 T_{1i}^{(2)} = J^2 \sum_q \frac{m_d^2 + \lambda_+^2 - P(q) (\lambda_+^2 - \lambda_-^2)}{\epsilon_k - \epsilon_q} \\ &= J^2 \sum_q \frac{s(s+1) - m_d + 2m_d P(q)}{\epsilon_k - \epsilon_q} \\ &= J^2 [s(s+1) - m_d] (\alpha + \gamma) + 2J^2 m_d \gamma \end{aligned} \quad (2.4.47)$$

where  $\gamma = \sum_q \frac{P(q)}{\epsilon_k - \epsilon_q}$ ,  $\alpha = \sum_q \frac{1 - P(q)}{\epsilon_k - \epsilon_q}$ . The second term has the Fermi-Dirac distribution and hence is the only temperature dependent term. Accordingly, we drop the first term.

$$\begin{aligned} T_{\text{nonflip}}^{(2)} &= 2J^2 m_d \gamma \\ &= 2J^2 m_d \int d\epsilon N(\epsilon) \frac{P(\epsilon)}{\epsilon_k - \epsilon} = \frac{\sqrt{2} J^2 m_d m^{\frac{3}{2}}}{\pi^2 \hbar^3} \int d\epsilon \frac{\sqrt{\epsilon} P(\epsilon)}{\epsilon_k - \epsilon} \end{aligned} \quad (2.4.48)$$

Assuming  $T = 0$ ,  $P(\epsilon) = \theta(\epsilon_F - \epsilon)$ . Then

$$\begin{aligned} T_{\text{nonflip}}^{(2)} &= \frac{\sqrt{2}J^2m_d m^{\frac{3}{2}}}{\pi^2\hbar^3} \sqrt{\epsilon_k} \ln \left| \frac{\sqrt{\epsilon_k} + \sqrt{\epsilon_F}}{\sqrt{\epsilon_k} - \sqrt{\epsilon_F}} \right| \\ &= \frac{\sqrt{2}J^2m_d m^{\frac{3}{2}}}{\pi^2\hbar^3} \sqrt{\epsilon_k} \ln \left| \frac{\epsilon_k + \epsilon_F + 2\sqrt{\epsilon_k\epsilon_F}}{\epsilon_k - \epsilon_F} \right| \end{aligned} \quad (2.4.49)$$

For  $T > 0$  but  $\ll T_F$ , the excitation energy of the electrons is very small and of the order of  $k_B T$ . Hence, we can replace  $\epsilon_k - \epsilon_F = k_B T$  and everywhere else replace  $\epsilon_k = \epsilon_F$ .

$$T_{\text{nonflip}}^{(2)} = \frac{\sqrt{2}J^2m_d m^{\frac{3}{2}}}{\pi^2\hbar^3} \sqrt{\epsilon_F} \ln \left| \frac{4T_F}{T} \right| \quad (2.4.50)$$

Dropping the temperature-independent  $\log 4$  term and recognizing  $N(\epsilon_F)$  in the pre-factor,

$$T_{\text{nonflip}}^{(2)} = 2J^2m_d N(\epsilon_F) \ln \left| \frac{T_F}{T} \right| \quad (2.4.51)$$

Adding the first order non-flip contribution ( $T_{\text{nonflip}}^{(1)}$ ) to the  $T$ -matrix, we get

$$T_{\text{nonflip}} = Jm_d \left[ 1 + 2N(\epsilon_F)J \ln \frac{T_F}{T} \right] \quad (2.4.52)$$

The upshot is that the additional contribution in second order is obtained by replacing  $J \rightarrow 2JN(\epsilon_F) \ln \frac{T_F}{T}$ . For the spin-flip scatterings (processes 5<sup>th</sup> to 8<sup>th</sup>),

$$\begin{aligned} T_{21}^{(2)} &= -J^2(m_d + 1)\lambda_+ \sum_q \frac{1 - P_q}{\epsilon_k - \epsilon_q} \\ T_{23}^{(2)} &= J^2m_d\lambda_+ \sum_q \frac{1 - P_q}{\epsilon_k - \epsilon_q} \\ T_{22}^{(2)} &= J^2(m_d + 1)\lambda_+ \sum_q \frac{P(q)}{\epsilon_k - \epsilon_q} \\ T_{24}^{(2)} &= -\lambda_+m_dJ^2 \sum_q \frac{P(q)}{\epsilon_k - \epsilon_q} \end{aligned} \quad (2.4.53)$$

$$T_{\text{flip}}^{(2)} = -J^2\lambda_+ (\alpha - \gamma) \quad (2.4.54)$$

The total spin-flip matrix element (temperature-dependent part) is

$$\begin{aligned} T_{\text{flip}}^{(2)} &= 2J^2\lambda_+ \sum_q \frac{P(q)}{\epsilon_k - \epsilon_q} \\ &= 2J^2\lambda_+ N(\epsilon_F) \ln \left| \frac{T_F}{T} \right| \end{aligned} \quad (2.4.55)$$

Adding the first order contribution,

$$T_{\text{flip}} = \lambda_+ J \left[ 1 + 2N(\epsilon_F)J \ln \frac{T_F}{T} \right] \quad (2.4.56)$$

Here again, the second order contribution is obtained by replacing  $J \rightarrow 2JN(\epsilon_F) \ln \frac{T_F}{T}$ . Both the solutions together imply that the next order probability for scattering of  $k \uparrow$  is obtained by replacing the additional  $J$  with  $2JN(\epsilon_F) \ln \frac{T_F}{T}$ .

$$\mathcal{P} = \mathcal{P}^{(2)} \left[ 1 + 2JN(\epsilon_F) \ln \frac{T_F}{T} \right] \quad (2.4.57)$$

### 2.4.3 The Kondo resonance

Since  $V$  conserves total angular momentum,  $\langle s | V | s' \rangle \sim \delta_{ss'}$ . Hence

$$T_{a \rightarrow b} = \sum_{s, m_s} |\langle s, m_s | a \rangle|^2 T_s \quad (2.4.58)$$

Now,  $|k \uparrow, d_\uparrow\rangle = |s = 1\rangle$ , so

$$T_{|k \uparrow, d_\uparrow\rangle \rightarrow |k' \uparrow d_\uparrow\rangle} = T_1 \quad (2.4.59)$$

But, since  $|k \uparrow, d_\downarrow\rangle = \frac{|s=1\rangle + |s=0\rangle}{\sqrt{2}}$ ,

$$T_{|k \uparrow, d_\downarrow\rangle \rightarrow |k' \uparrow d_\downarrow\rangle} = \frac{T_1 + T_0}{2} \quad (2.4.60)$$

and  $|k \downarrow, d_\uparrow\rangle = \frac{|s=1\rangle - |s=0\rangle}{\sqrt{2}}$ ,

$$T_{|k \uparrow, d_\downarrow\rangle \rightarrow |k' \downarrow d_\uparrow\rangle} = \frac{T_1 - T_0}{2} \quad (2.4.61)$$

Therefore,

$$\begin{aligned} T_1 &= T_{|k \uparrow, d_\downarrow\rangle \rightarrow |k' \uparrow d_\downarrow\rangle} + T_{|k \uparrow, d_\downarrow\rangle \rightarrow |k' \downarrow d_\uparrow\rangle} = T_{\text{nonflip}} + T_{\text{flip}} \\ T_0 &= T_{|k \uparrow, d_\downarrow\rangle \rightarrow |k' \uparrow d_\downarrow\rangle} - T_{|k \uparrow, d_\downarrow\rangle \rightarrow |k' \downarrow d_\uparrow\rangle} = T_{\text{nonflip}} - T_{\text{flip}} \end{aligned} \quad (2.4.62)$$

Assuming spin-half impurity, ( $s = \frac{1}{2}$ )

$$T_{\text{nonflip}} = J \left[ m_d + \frac{J}{4} \{ 3(\alpha + \gamma) + 4m_d(\gamma - \alpha) \} \right] \quad (2.4.63)$$

$$T_{\text{flip}} = J \left[ 1 + J(\gamma - \alpha) \right] \quad (2.4.64)$$

Setting  $m_d = -\frac{1}{2}$ ,

$$\begin{aligned} T_1 &= \frac{J}{2} \left[ 1 + \frac{J}{2} (\alpha + 5\gamma) \right] \\ T_0 &= -\frac{3J}{2} \left[ 1 - \frac{3J}{2} \left( \alpha - \frac{\gamma}{3} \right) \right] \end{aligned} \quad (2.4.65)$$

The value of the prefactors can be understood as follows: The interaction term is

$$J \vec{S}_d \cdot \vec{\sigma}_e = 2J \vec{S}_d \cdot \vec{S}_e = J \left( S^2 - S_d^2 - S_e^2 \right) = J \left( s(s+1) - \frac{3}{2} \right) = \begin{cases} -\frac{3J}{2} & (\text{singlet}) \\ \frac{J}{2} & (\text{triplet}) \end{cases} \quad (2.4.66)$$

Hence, the pre-factors are just the bare values of the interaction Hamiltonian,  $V$ . Hence, the equations 2.4.65 can be written as

$$T = V(1 + TG) \quad (2.4.67)$$

For the singlet and triplet  $T$ -matrices, it becomes

$$\begin{aligned} T_1 &= \frac{J}{2} \left[ 1 + T_1 (\alpha + 5\gamma) \right] \implies T_1 = \frac{J/2}{1 - \frac{J}{2}(\alpha + 5\gamma)} \\ T_0 &= -\frac{3J}{2} \left[ 1 + T_0 \left( \alpha - \frac{\gamma}{3} \right) \right] \implies T_0 = \frac{-3J/2}{1 + \frac{3J}{2}(\alpha - \gamma/3)} \end{aligned} \quad (2.4.68)$$

We want to find the maximum value of  $|T_s|$ . To this end, rewrite

$$T_1 = \frac{1}{2/J - 5\gamma - \alpha} \quad (2.4.69)$$

$$T_0 = \frac{1}{-2/3J + \gamma/2 - \alpha} \quad (2.4.70)$$

For excitations ( $k$ ) just above the Fermi surface,  $\alpha$  will encounter a zero in its denominator, because the integral in  $\alpha$  is outside the Fermi surface. On the other hand, the integral in  $\gamma$  is inside the Fermi surface, so the denominator in  $\gamma$  will never become zero for  $k$  just outside the Fermi surface. Hence,  $\alpha = \text{real part} - i\pi N(0)$ ,  $\gamma = \text{real part}$ . Accordingly, the expressions for  $T_s$  can be written as

$$T_s = \frac{1}{\text{real part} + i\pi N(0)} \quad (2.4.71)$$

The maximum value of  $|T_s|$  will occur when the denominator is minimum, that is, when real part = 0. Hence,

$$|T_s| \leq \frac{1}{\pi N_0} \quad (2.4.72)$$

From eq. 2.1.25, we can write

$$T_s = -\frac{e^{i\delta_s} \sin \delta_s}{\pi N(0)} \quad (2.4.73)$$

Eq. 2.3.24 allows us to write

$$\rho_{d\sigma}(0) = -\frac{\text{Im}[T]}{t^2\pi} = \frac{\sin^2 \delta_s}{t^2\pi^2 N(0)} = \frac{\sin^2 \delta_s}{\pi\Delta} = \frac{1}{\pi\Delta} \sin^2 \left( \frac{\pi n_c}{2} \right) \quad (2.4.74)$$

where  $n_c = \langle n_{d\uparrow} + n_{d\downarrow} \rangle$ . This is in contrast to the value obtained from the mean field analysis of the Anderson model, eq. 2.3.31,

$$\rho_{d\sigma}(0) = \frac{1}{\pi\Delta} \left[ 1 + \left( \frac{\epsilon_d + U n_c}{\Delta} \right)^2 \right]^{-1} \quad (2.4.75)$$

For  $n_c = 1$  (half-filling), the mean field value is less than the one obtained from the spin-spin scattering. This is because the mean-field analysis does not take these scatterings into account. The large density of states at the Fermi level means that the spectral function has three peaks in general, two of which are revealed in the mean field analysis, but a third one exists, which is of a width of the order of a very low temperature  $T_K$ , and hence is not noticed at higher temperatures. Eq. 2.4.68 can be written as

$$T_1 = \frac{J/2}{1 - 2J\gamma - \frac{J}{2}(\alpha + \gamma)} \quad (2.4.76)$$

$$T_0 = \frac{-3J/2}{1 - 2J\gamma + \frac{3J}{2}(\alpha + \gamma)} \quad (2.4.77)$$

Defining  $J_{\text{eff}} = \frac{J}{1-2J\gamma}$ , the scattering amplitudes  $T_1$  and  $T_0$  can be written as

$$\begin{aligned} T_1 &= \frac{1}{\frac{2}{J_{\text{eff}}} - (\alpha + \gamma)} \\ T_0 &= \frac{-1}{\frac{2}{3J_{\text{eff}}} + \alpha + \gamma} \end{aligned} \quad (2.4.78)$$

$\alpha + \gamma$  can be calculated as

$$\begin{aligned} \alpha + \gamma &= \lim_{\eta \rightarrow 0} \int_0^\infty d\epsilon \frac{N(\epsilon)}{\epsilon_k - \epsilon + i\eta} \\ &\sim \lim_{\epsilon_{\text{up}} \rightarrow \infty} \ln \left| \frac{\sqrt{\epsilon_k} - \sqrt{\epsilon_{\text{up}}}}{\sqrt{\epsilon_k} + \sqrt{\epsilon_{\text{up}}}} \right| - i\pi N(0) \end{aligned} \quad (2.4.79)$$

In the limit of  $\epsilon_{\text{up}} \rightarrow \infty$ , the argument of the log becomes

$$\left| \frac{\sqrt{\epsilon_k} - \sqrt{\epsilon_{\text{up}}}}{\sqrt{\epsilon_k} + \sqrt{\epsilon_{\text{up}}}} \right| \approx \left| \frac{-\sqrt{\epsilon_{\text{up}}}}{\sqrt{\epsilon_{\text{up}}}} \right| = 1 \quad (2.4.80)$$

Hence, the real part vanishes, and the expression for  $T_1$  becomes

$$T_1 = \frac{1}{2J_{\text{eff}}^{-1} + i\pi N(0)} \sim \frac{1}{\frac{2}{\pi N(0)J_{\text{eff}}} + i} \quad (2.4.81)$$

Since

$$T_s \sim e^{i\delta_s} \sin \delta_s = \frac{1}{\cot \delta_s - i} \quad (2.4.82)$$

we can write

$$\cot \delta_1 = -\frac{2}{\pi N(0)J_{\text{eff}}} \implies \tan \delta_1 = -\frac{\pi}{2} N(0)J_{\text{eff}} \quad (2.4.83)$$

Similarly,

$$T_0 = \frac{-1}{\frac{2}{3J_{\text{eff}}} - i\pi N(0)} \sim \frac{-1}{\frac{2}{3J_{\text{eff}}\pi N(0)} - i} \quad (2.4.84)$$

giving

$$\cot \delta_0 = \frac{2}{3J_{\text{eff}}\pi N(0)} \implies \tan \delta_0 = \frac{3\pi}{2} J_{\text{eff}} N(0) \quad (2.4.85)$$

Since  $J_{\text{eff}} > 0$ ,  $\delta_1 < 0$  and  $\delta_0 > 0$ . The significance of this can be seen as follows. For scattering at the Fermi surface, the scattered wavefunction can be written as

$$\psi \sim \psi_{\text{in}} - e^{2i\delta_d} \psi_{\text{out}} \quad (2.4.86)$$

where  $\psi_{\text{in}} = \frac{e^{ik_F r}}{r}$  is the incoming wave and  $\psi_{\text{out}} = \frac{e^{-ik_F r}}{r}$  is the outgoing one. Hence,

$$\psi = \frac{e^{i\delta}}{r} \left( e^{-i(k_F r + \delta_d)} - e^{i(k_F r + \delta_d)} \right) \sim \frac{e^{i\delta}}{r} \sin [k_F (r + \Delta r)] \quad (2.4.87)$$

This scattered wave is thus another radial wave but its phase is shifted by an amount  $\Delta r = \frac{\delta_d}{k_F}$ . For a positive  $\Delta r$  (and hence a positive  $\delta_d$ ), the wave will be drawn inward. Hence, the singlet channel having a positive  $\delta$  will lead to formation of bound states. On the other hand, the triplet channel has a negative phase shift, meaning it is repulsive.

#### 2.4.4 Adiabatic route to the Kondo resonance

Assuming  $T = 0$ , the interactions due to a single impurity are unlikely to break adiabaticity. Hence, we replace the effect of the  $U$  on the impurity by adding a self energy  $\Sigma(\omega)$  to the bare energy  $\epsilon_d$ . This self energy can be Taylor-expanded about  $E = 0$ :

$$\Sigma(E) = \Sigma(0) + E \left. \frac{d\Sigma}{dE} \right|_{E=0} + O(E^2) \quad (2.4.88)$$

Defining

$$Z^{-1} \equiv 1 - \left. \frac{d\Sigma}{dE} \right|_{E=0} \quad (2.4.89)$$

we can write

$$\Sigma(E) = \Sigma(0) + (1 - Z^{-1}) E \quad (2.4.90)$$

The interacting Green's function for the impurity becomes

$$G_d(E) = \frac{1}{E - \epsilon_d - \Sigma - i\Delta} \quad (2.4.91)$$

where  $\Delta$  is the result of the hybridisation. Substituting eq. 2.4.90 and gathering the terms gives

$$G_d(E) = \frac{Z}{E - Z(\epsilon_d + \Sigma(0)) - iZ\Delta} \quad (2.4.92)$$



Defining the renormalised parameters

$$\epsilon_d^* = Z(\epsilon_d + \Sigma(0)) \quad (2.4.93)$$

$$\Delta^* = Z\Delta \quad (2.4.94)$$

we have

$$G_d(E) = \frac{Z}{E - \epsilon_d^* - i\Delta^*} \quad (2.4.95)$$

What this means is that as we adiabatically vary the interaction  $U$ , the parameters  $\epsilon_d^*$  and  $\Delta^*$  also morph, keeping the form of the Greens's function constant. In the non-interacting limit ( $U = 0$ ), we have

$$Z = 1, \Sigma = 0 \implies \epsilon_d^* = \epsilon_d, \Delta^* = \Delta \quad (2.4.96)$$

We then recover the atomic form of the Green's function.  $Z$  varies from 0 to 1.  $Z = 1$  is the non-interacting limit,  $Z = 0$  is the limit of  $U = \infty$ . The phase shift due to scattering can be calculated by looking at eq.2.3.27, and replacing the bare quantities with the renormalised versions:

$$\delta_d(0) = \cot^{-1} \frac{\epsilon_d^*}{\Delta^*} \quad (2.4.97)$$

Similarly, the renormalised version of eq. 2.3.16 is

$$\rho_d(0) = \frac{1}{\pi} \frac{\Delta^*}{\epsilon_d^{*2} + \Delta^{*2}} \quad (2.4.98)$$

Using eq. 2.4.97 gives

$$\rho_d(0) = \frac{1}{\pi} \frac{\Delta^*}{\Delta^{*2} \cot^2 \delta_d + \Delta^{*2}} = \frac{\sin^2 \delta_d}{\pi \Delta} \quad (2.4.99)$$

### 2.4.5 The Kondo temperature

We consider a simplified model where a single conduction electron forms a singlet with the d-electron, and the rest of the conduction electrons simply fill the Fermi sea. For the singlet state,  $\vec{S}_e \cdot \vec{S}_d = -\frac{3}{2}$ . So,

$$H_K = \sum_{k > k_F} \epsilon_k n_k - \frac{3J}{2} \sum_{k, k' > k_F} c_{k'\sigma}^\dagger c_{k\sigma} \quad (2.4.100)$$

The operator to create the singlet state  $|S_k\rangle = \frac{1}{\sqrt{2}} (|k \uparrow, d \downarrow\rangle - |k \downarrow, d \uparrow\rangle)$  off the Fermi sea ( $|\Phi\rangle$ ) is

$$b_k^\dagger = \frac{1}{\sqrt{2}} (c_{k\uparrow}^\dagger c_{d\downarrow}^\dagger - c_{k\downarrow}^\dagger c_{d\uparrow}^\dagger) \quad (2.4.101)$$

Hence the total wavefunction of singlet+Fermi-sea is

$$|\Psi\rangle = \sum_{k > k_F} a_k b_k^\dagger |\Phi\rangle = |\Phi\rangle \otimes \sum_{k > k_F} a_k |S_k\rangle \quad (2.4.102)$$

$a_k$  is the probability amplitude for the conduction electron in the single to have momentum  $k$ .

$$a_q = \langle \Phi | \langle S_q | \sum_k a_k |S_k\rangle |\Phi\rangle = \langle \Phi | b_q |\Psi\rangle \quad (2.4.103)$$

The Schrödinger equation for  $|\Psi\rangle$  is

$$\begin{aligned} E |\Psi\rangle &= H_K |\Psi\rangle = |\Phi\rangle \otimes H_K \sum_{k > k_F} a_k |S_k\rangle \\ &= |\Phi\rangle \otimes \sum_{k > k_F} a_k \left( \epsilon_k |S_k\rangle - \frac{3J}{2} \sum_{k' > k_F} |S_{k'}\rangle \right) \\ &= \sum_{k > k_F} a_k \left( \epsilon_k b_k^\dagger - \frac{3J}{2} \sum_{k' > k_F} b_{k'}^\dagger \right) |\Phi\rangle \end{aligned} \quad (2.4.104)$$

Multiplying  $b_q$  from left gives

$$Eb_q |\Psi\rangle = \epsilon_q a_q |\Phi\rangle - \frac{3J}{2} \sum_{k>k_F} a_k |\Phi\rangle \quad (2.4.105)$$

Multiplying  $\langle\Phi|$  from left and looking at eq. 2.4.103 gives

$$\begin{aligned} E \langle\Phi| b_q |\Psi\rangle &= E a_q = a_q \epsilon_q - \frac{3J}{2} \sum_k a_k \\ \implies a_q &= \frac{3J/2}{\epsilon_q - E} \sum_k a_k \\ \implies \sum_q a_q &= \sum_q \frac{3J/2}{\epsilon_q - E} \sum_k a_k \end{aligned} \quad (2.4.106)$$

Since  $\sum_q a_q = \sum_k a_k$ , we get an equation for  $E$

$$1 = \frac{3J}{2} \sum_{q>k_F} \frac{1}{\epsilon_q - E} \quad (2.4.107)$$

Converting to integral,

$$1 = \frac{3J}{2} \int_{\epsilon_F}^D d\epsilon \frac{N(\epsilon)}{\epsilon - E} \quad (2.4.108)$$

$D$  is the upper limit of the conduction band. Assuming  $N(\epsilon)$  is constant ( $N(0)$ ) in this range, we get

$$\begin{aligned} \frac{2}{3JN(0)} &= \ln \left| \frac{D - E}{\epsilon_F - E} \right| \approx \ln \left| \frac{D}{\epsilon_F - E} \right| \\ \implies E &= \epsilon_F - D e^{-\frac{2}{3N(0)J}} \end{aligned} \quad (2.4.109)$$

Thus, the energy of the ground state is lowered from the Fermi energy by an amount

$$E_b = D e^{-\frac{2}{3N(0)J}} \quad (2.4.110)$$

The temperature below which this will be stable,  $T_K$ , is given by the relation

$$k_B T_K \sim E_b \implies T_K = \frac{D}{k_B} e^{-\frac{2}{3N(0)J}} \quad (2.4.111)$$

## 2.4.6 Poor man's scaling

The idea is to reduce the bandwidth from  $D$  to  $D - \delta D$ , by considering all possible excitations in that range, up to second order. The transition matrix second order contributions in that range

$$T^{(2)} = V G_0 V \quad (2.4.112)$$

can be clubbed into a term  $\Delta V$ . This term is a representative of the scatterings from that range. After reducing the bandwidth to  $D - \delta D$ , the effect of the excluded region can be incorporated by changing the interaction term  $V \rightarrow V' = V + \Delta V$ . The interaction part is

$$H' = J_z \sum_{k_1, k_2} S_d^z \left( c_{k_1\uparrow}^\dagger c_{k_2\uparrow} - c_{k_1\downarrow}^\dagger c_{k_2\downarrow} \right) + J_T \sum_{k_1, k_2} \left( S_d^+ c_{k_1\downarrow}^\dagger c_{k_2\uparrow} + S_d^- c_{k_1\uparrow}^\dagger c_{k_2\downarrow} \right) \quad (2.4.113)$$

Incorporating  $\Delta V$  will involve changing the coupling constants  $J_z$  and  $J_T$ . There are three types of scattering processes at second order:

1. No spin-flip of impurity - involving  $(S_d^z)^2$
2. one spin-flip of impurity - involving  $S_d^z S_d^\pm$  or  $S_d^\pm S_d^z$
3. two spin-flips of impurity - involving  $S_d^\pm S_d^\mp$

The first kind does not involve any spin impurity operator ( $S_z^2 = \frac{1}{4}$ ), so it will be ignored. The second kind will leave the impurity spin flipped at the end, and will hence result in a renormalization of  $J_T$ . The third kind will leave the impurity spin unchanged (two flips), and hence will involve a renormalization of  $J_z$ .

**Renormalization of  $J_z$** 

First consider the process

$$k \uparrow, d \downarrow \rightarrow q \downarrow d \uparrow \rightarrow k' \uparrow d \downarrow \quad (2.4.114)$$

The  $T$ -matrix term is

$$T_1 = J_T^2 \sum_q S_d^- c_{k'\uparrow}^\dagger c_{q\downarrow} \frac{1}{E - H_0} S_d^+ c_{q\downarrow}^\dagger c_{k\uparrow} \quad (2.4.115)$$

If, for some operator  $A$ , we have  $[H, A] = \lambda A$ , where  $\lambda$  is some scalar, then we can write

$$HA = A(\lambda + H) \quad (2.4.116)$$

A consequence of this is, for another scalar  $E$ , we can write

$$(E - H)A = AE - A(\lambda + H) = A(E - \lambda - H) \quad (2.4.117)$$

$$\implies A(E - \lambda - H)^{-1} = (E - H)^{-1}A \quad (2.4.118)$$

$$(E - H_0)^{-1} c_{q\downarrow}^\dagger c_{k\uparrow} = c_{q\downarrow}^\dagger c_{k\uparrow} (E - \lambda - H_0)^{-1} \quad (2.4.119)$$

where  $\lambda$  is given by  $[H_0, c_{q\downarrow}^\dagger c_{k\uparrow}] = (\epsilon_q - \epsilon_k) c_{q\downarrow}^\dagger c_{k\uparrow} \implies \lambda = \epsilon_q - \epsilon_k$ . Hence,

$$T_1 = J_T^2 S_d^- S_d^+ \sum_q c_{k'\uparrow}^\dagger c_{q\downarrow} c_{q\downarrow}^\dagger c_{k\uparrow} (E - \epsilon_q + \epsilon_k - H_0)^{-1} \quad (2.4.120)$$

Since the upper momenta states are unoccupied,  $c_{q\downarrow} c_{q\downarrow}^\dagger = 1 - n_q = 1$ .

$$T_1 = J_T^2 S_d^- S_d^+ c_{k'\uparrow}^\dagger c_{k\uparrow} \sum_q (E - \epsilon_q + \epsilon_k - H_0)^{-1} \quad (2.4.121)$$

If we set the Fermi level to 0,  $H_0 = 0$ . Since the summation is over the narrow band  $\{D - \delta D, D\}$ , we can approximate the result of the summation as

$$\sum_q (E - \epsilon_q + \epsilon_k - H_0)^{-1} = N |\delta D| \frac{1}{E - D + \epsilon_k} \quad (2.4.122)$$

$N$  is the density of states. Also,

$$S^- S^+ = (S^x - iS^y) (S^x + iS^y) = \frac{1}{2} + i[S^x, S^y] = \frac{1}{2} - S^z \quad (2.4.123)$$

Putting it all together,

$$T_1 = J_T^2 \left( \frac{1}{2} - S_d^z \right) N |\delta D| c_{k'\uparrow}^\dagger c_{k\uparrow} \frac{1}{E - D + \epsilon_k} \quad (2.4.124)$$

For the second possible scattering,

$$q \downarrow k \uparrow d \uparrow \rightarrow k' \uparrow k \uparrow d \downarrow \rightarrow k' \uparrow q \downarrow d \uparrow \quad (2.4.125)$$

we get

$$T_2 = J_T^2 \sum_q S_d^+ S_d^- c_{q\downarrow}^\dagger c_{k\uparrow} \frac{1}{E - H_0} c_{k'\uparrow}^\dagger c_{q\downarrow} \quad (2.4.126)$$

Using  $[H_0, c_{k'\uparrow}^\dagger c_{q\downarrow}] = (\epsilon_{k'} - \epsilon_q) c_{k'\uparrow}^\dagger c_{q\downarrow} = (\epsilon_{k'} + D) c_{k'\uparrow}^\dagger c_{q\downarrow}$ , and  $S_d^+ S_d^- = \frac{1}{2} + S_d^z$ , we get

$$\begin{aligned} T_2 &= J_T^2 \left( \frac{1}{2} + S_d^z \right) N |\delta D| c_{k\uparrow} c_{k'\uparrow}^\dagger \frac{1}{E - D - \epsilon_{k'}} \\ &= -J_T^2 \left( \frac{1}{2} + S_d^z \right) N |\delta D| c_{k'\uparrow}^\dagger c_{k\uparrow} \frac{1}{E - D - \epsilon_{k'}} \end{aligned} \quad (2.4.127)$$

The constant term resulting from the commutator at the last line was dropped. For each of these two processes, there are identical processes that start with the conduction electron in  $\downarrow$ :

$$k \downarrow, d \uparrow \rightarrow q \uparrow d \downarrow \rightarrow k' \downarrow d \uparrow \quad (2.4.128)$$

$$q \uparrow k \downarrow d \downarrow \rightarrow k' \downarrow k \downarrow d \uparrow \rightarrow k' \downarrow q \uparrow d \downarrow \quad (2.4.129)$$

The only difference from the previous processes is that  $S^+$  is replaced by  $S^-$  and vice versa. Hence, these processes give

$$T_3 = J_T^2 \left( \frac{1}{2} + S_d^z \right) N |\delta D| c_{k'\downarrow}^\dagger c_{k\downarrow} \frac{1}{E - D + \epsilon_k} \quad (2.4.130)$$

$$T_4 = -J_T^2 \left( \frac{1}{2} - S_d^z \right) N |\delta D| c_{k'\downarrow}^\dagger c_{k\downarrow} \frac{1}{E - D - \epsilon_{k'}} \quad (2.4.131)$$

The total second order contribution is

$$T^{(2)} = -J_T^2 S_d^z N |\delta D| \left( \frac{1}{E - D + \epsilon_k} + \frac{1}{E - D - \epsilon_{k'}} \right) (c_{k'\uparrow}^\dagger c_{k\uparrow} - c_{k'\downarrow}^\dagger c_{k\downarrow}) \quad (2.4.132)$$

Comparing this with the  $S_d^z$  term in the Hamiltonian

$$J_z S_d^z (c_{k'\uparrow}^\dagger c_{k\uparrow} - c_{k'\downarrow}^\dagger c_{k\downarrow}) \quad (2.4.133)$$

we can easily write down the change in the coupling  $J_d^z$ ,

$$\delta J_d^z = -J_T^2 N |\delta D| \left( \frac{1}{E - D + \epsilon_k} + \frac{1}{E - D - \epsilon_{k'}} \right) \quad (2.4.134)$$

For low energy excitations, we can neglect  $E, \epsilon_k, \epsilon_{k'}$  with respect to  $D$ . Noting that the bandwidth is decreasing and hence  $\delta D < 0$ ,

$$\frac{dJ_d^z}{dD} = -J_T^2 N \frac{2}{D} \quad (2.4.135)$$

This is the scaling equation for the coupling  $J_d^z$ .

### Renormalization of $J_T$

Consider the scattering

$$k \uparrow d \downarrow \rightarrow q \downarrow d \uparrow \rightarrow k' \downarrow d \uparrow \quad (2.4.136)$$

$$T_1 = -J_T J_z S_d^+ S_d^+ N |\delta D| c_{k'\downarrow}^\dagger c_{k\uparrow} \frac{1}{E - D + \epsilon_k} \quad (2.4.137)$$

The minus sign at the front comes from the term

$$-S_d^z c_{k'\downarrow}^\dagger c_{q\downarrow} \quad (2.4.138)$$

in the Hamiltonian. Using  $S_d^z S_d^+ = \frac{S_d^+}{2}$ ,

$$T_1 = -J_T J_z \frac{S_d^+}{2} N |\delta D| c_{k'\downarrow}^\dagger c_{k\uparrow} \frac{1}{E - D + \epsilon_k} \quad (2.4.139)$$

The second process is

$$q \uparrow k \uparrow d \downarrow \rightarrow k' \downarrow k \uparrow d \uparrow \rightarrow q \uparrow k' \downarrow d \uparrow \quad (2.4.140)$$

$$T_2 = -J_T J_z \frac{S_d^+}{2} N |\delta D| c_{k'\downarrow}^\dagger c_{k\uparrow} \frac{1}{E - D - \epsilon_{k'}} \quad (2.4.141)$$

Two more processes can be constructed from the above two processes, by switching the  $S_d^+$  and  $S_d^z$  operations. The change in the first process is that the  $S_d^z$  term will now become

$$+S_d^z c_{k'\uparrow}^\dagger c_{q\uparrow} \quad (2.4.142)$$

so that will invert the sign. The change in the second process is that now the  $q$ -electron has to start off as  $\downarrow$ , which means that the  $S_d^z$  term for this process becomes

$$-S_d^z c_{k'\downarrow}^\dagger c_{q\downarrow} \quad (2.4.143)$$

So the sign of the second process will also invert. The change common to both the process is that  $S_d^z S_d^+$  becomes  $S_d^+ S_d^z$ . Since  $S_d^+ S_d^z = -\frac{S_d^+}{2}$ , this will involve a second change in sign for both processes. Thus, overall there is no change for either process.

$$T_3 = T_1 \quad (2.4.144)$$

$$T_4 = T_2 \quad (2.4.145)$$

The total contribution is

$$T^{(2)} = -J_T J_z S_d^+ N |\delta D| c_{k'\downarrow}^\dagger c_{k\uparrow} \left( \frac{1}{E - D - \epsilon_{k'}} + \frac{1}{E - D + \epsilon_k} \right) \quad (2.4.146)$$

Comparing with the  $S_d^+$  term in the Hamiltonian

$$J_T S_d^+ c_{k'\downarrow}^\dagger c_{k\uparrow} \quad (2.4.147)$$

we can write

$$\delta J_T = -J_T J_z N |\delta D| \left( \frac{1}{E - D - \epsilon_{k'}} + \frac{1}{E - D + \epsilon_k} \right) \quad (2.4.148)$$

Again neglecting the terms in the denominator, we get

$$\frac{dJ_T}{dD} = -J_T J_z N \frac{2}{D} \quad (2.4.149)$$

This is the scaling equation for  $J_T$ .

### Flow of the couplings

Switching to the dimensionless couplings

$$g_1 = N J_z, g_2 = N J_T \quad (2.4.150)$$

the equations become

$$\frac{dg_1}{dD} = -\frac{2g_2^2}{D} \quad (2.4.151)$$

$$\frac{dg_2}{dD} = -\frac{2g_1 g_2}{D} \quad (2.4.152)$$

The first equation says that as the cutoff decreases,  $g_1$  will always increase. For  $g < 0$  (ferromagnetic coupling), the coupling will go to zero. That is, at sufficiently low temperatures, the impurity electron becomes effectively decoupled from the conduction band. The phenomenon is called asymptotic freedom. For the antiferromagnetic case, the coupling should go to infinity. This means that at sufficiently low temperatures, the coupling will necessarily become appreciable large so as to render perturbation theory inapplicable. Dividing the two coupling equations gives

$$\frac{dg_1}{dg_2} = \frac{g_2}{g_1} \implies g_1^2 - g_2^2 = \text{constant} \quad (2.4.153)$$

Taking  $g_1$  as the x-axis and  $g_2$  as the y-axis, depending on the sign of the constant, the solution is a vertical hyperbola or horizontal hyperbola. Since the coupling equations are unchanged under the transformation  $g_2 \rightarrow -g_2$ , analyzing the upper half ( $g_2 > 0$ ) suffices. The antiferromagnetic case is easy.  $g_1 > 0$  means  $g_1$  will always increase the RG flow. The only solution is that both  $g_1$  and  $g_2$  flow to infinity. For the ferromagnetic case, if  $|g_1| > g_2$ ,  $g_1$  will increase and the representative point will reach the x-axis ( $g_2 = 0$ ). At this point, both the couplings will stop changing because both the derivatives involve  $g_2$ . So the fixed point in this case is  $g_2 = 0$  and  $g_1$  is some negative value. However, if  $|g_1| < g_2$ , the representative point will reach the positive y-axis. Since  $g_2 \neq 0$  here,  $g_1$  will

continue to grow and become positive at some point. From there, it becomes the antiferromagnetic case. Setting  $g_1 = g_2 = g > 0$  and integrating either of the scaling equations gives

$$\begin{aligned} g(D') &= \frac{g_0}{1 - 2g_0 \ln \frac{D}{D'}} \\ \implies 2g(D') &= \frac{1}{\ln \frac{D'}{T_K}} \end{aligned} \quad (2.4.154)$$

where  $T_K = \frac{D}{k_B} \exp \left\{ -\frac{1}{2g_0} \right\}$ .  $D'$  is the running bandwidth and  $D$  is the original bandwidth. This is almost the same as the one obtained in eq. 2.4.111, because  $g = NJ$ . The expression for  $g_{D'}$  shows that perturbation theory will work only for  $T \gg T_K$ , because close to  $T_K$ , the expression becomes non-analytic. The ferromagnetic case ( $g < 0$ ), on the other hand, remains perturbative.

$$g(D') = \frac{g_0}{1 - 2g_0 \ln \frac{D}{D'}} = -\frac{|g_0|}{1 + 2|g_0| \ln \frac{D}{D'}} \quad (2.4.155)$$

At all points, the expression remains analytic, and gradually goes to zero at  $D' = 0$ .

### Alternate way of obtaining the scaling equations

From eq. 2.4.16, the interaction part can be written as

$$\Delta H_{ll'} = \frac{1}{2} [T_{ll'}(E_l) + T_{ll'}(E_{l'})] \quad (2.4.156)$$

where the transition matrix  $T$  is

$$T_{ll'}(E) = \sum_H \frac{V_{lH} V_{Hl'}}{E - E_H} \quad (2.4.157)$$

Here,  $\{H\} = \{D - \delta D, D\}$  and

$$V = J \vec{S}_d \cdot \sum_{k, k', \alpha, \alpha'} c_{k\alpha}^\dagger \vec{\sigma}_{\alpha\alpha'} c_{k'\alpha'} \quad (2.4.158)$$

The first process is

$$k\alpha \xrightarrow{\sigma^b} q\lambda \xrightarrow{\sigma^a} k'\beta \quad (2.4.159)$$

$$d\sigma \xrightarrow{S_d^b} d\sigma'' \xrightarrow{S_d^a} d\sigma' \quad (2.4.160)$$

The transition matrix element is

$$\begin{aligned} T_1 &= \sum_{q \in \{D - \delta D\}, \lambda, \sigma''} \langle k'\beta, \sigma' | V | q\lambda, \sigma'' \rangle \langle q\lambda, \sigma'' | V | k\alpha, \sigma \rangle \frac{1}{E - E_q} \\ &= J^2 \sum_{\sigma''} (S_d^a)_{\sigma'\sigma''} (S_d^b)_{\sigma''\sigma} \sum_{\lambda} (\sigma^a)_{\beta\lambda} (\sigma^b)_{\lambda\alpha} \sum_{q \in \{D - \delta D\}} \frac{1}{E - E_q} \\ &\approx J^2 (S_d^a S_d^b)_{\sigma'\sigma} (\sigma^a \sigma^b)_{\beta\alpha} \frac{N|\delta D|}{E - D} \end{aligned} \quad (2.4.161)$$

The second process is

$$k\alpha \longrightarrow k\alpha \xrightarrow{\sigma^a} q\lambda \quad (2.4.162)$$

$$q\lambda \xrightarrow{\sigma^b} k'\beta \longrightarrow k'\beta \quad (2.4.163)$$

$$d\sigma \xrightarrow{S_d^b} d\sigma'' \xrightarrow{S_d^a} d\sigma' \quad (2.4.164)$$

Here the intermediate state consists of two electrons with energy  $E_k, E_{k'}$  and a hole with energy  $-E_q$ . The transition matrix element is

$$T_2 = \sum_{q \in \{D - |\delta D|\}, \lambda, \sigma''} \langle q\lambda, k'\beta, \sigma' | V | k'\beta, k\alpha, \sigma'' \rangle \langle k'\beta, k\alpha, \sigma'' | V | q\lambda, k\alpha, \sigma \rangle \frac{1}{E - (E_k + E_{k'} - E_q)} \quad (2.4.165)$$

$$\approx -J^2 \left( S_d^a S_d^b \right)_{\sigma'\sigma} \left( \sigma^b \sigma^a \right)_{\beta\alpha} \frac{N|\delta D|}{E - D}$$

Neglecting  $E$  with respect to  $D$  and adding the contributions, we get

$$T = \frac{J^2 N |\delta D|}{D} \left( S_d^a S_d^b \right)_{\sigma'\sigma} \left[ \sigma^b, \sigma^a \right]_{\beta\alpha} \quad (2.4.166)$$

$$= \frac{J^2 N |\delta D|}{2D} \left[ S_d^a, S_d^b \right]_{\sigma'\sigma} \left[ \sigma^b, \sigma^a \right]_{\beta\alpha}$$

In the last step, I used  $\{S^a, S^b\} = 0$ . Now,

$$\begin{aligned} \left[ S_d^a, S_d^b \right]_{\sigma'\sigma} \left[ \sigma^b, \sigma^a \right]_{\beta\alpha} &= - \left[ S_d^a, S_d^b \right]_{\sigma'\sigma} \left[ \sigma^a, \sigma^b \right]_{\beta\alpha} \\ &= -i\epsilon_{abc} S_{\sigma\sigma'}^c 2i\epsilon_{abd} \sigma_{\beta\alpha}^d \\ &= 4\delta_{cd} S_{\sigma\sigma'}^c \sigma_{\beta\alpha}^d \\ &= 4\vec{S}_{\sigma\sigma'} \cdot \vec{\sigma}_{\beta\alpha} \end{aligned} \quad (2.4.167)$$

Therefore,

$$T = \frac{2J^2 N |\delta D|}{D} \vec{S}_{\sigma\sigma'} \cdot \vec{\sigma}_{\beta\alpha} \quad (2.4.168)$$

The correction to the coupling  $J$  can be read off:

$$J(D - \delta D) = J(D) - \frac{2J^2 N \delta D}{D} \quad (2.4.169)$$

This gives the same scaling equations we found earlier.

### 2.4.7 Universality

Adding a higher order correction to the Poor Man's scaling gives

$$\frac{\partial g}{\partial \ln D} = -2g^2 + 2g^3 \quad (2.4.170)$$

It can be integrated from  $g^0(D)$  to  $g(D')$ :

$$\ln \frac{D'}{D} = - \int_{g_0}^g \frac{dg}{2g^2 - 2g^3} = - \int_{g_0}^g \frac{dg}{2g^2} (1 + g) \quad (2.4.171)$$

Defining  $D' = k_B T_K$  to be the temperature where  $g \sim 1$ , we can write

$$\begin{aligned} \ln \frac{k_B T_K}{D} &= - \int_{g_0}^1 \frac{dg}{2g^2} (1 + g) = - \frac{1}{2g_0} + \frac{1}{2} \ln g_0 + O(1) \\ &= - \frac{1}{2g_0} + \frac{1}{2} \ln 2g_0 + O(1) \end{aligned} \quad (2.4.172)$$

This gives a better estimate of the Kondo temperature

$$T_K = \frac{D}{k_B} \sqrt{2g_0} \exp \left\{ - \frac{1}{2g_0} \right\} \quad (2.4.173)$$

$T_K$  can also be determined by appealing to dimensional arguments and ideas of universality. Since the energy scale in question is  $D$ , we can write

$$k_B T_K = Dy(g) \quad (2.4.174)$$

where  $y$  is some dimensionless quantity. Since  $T_K$  is a physical quantity, it cannot change with our choice of the bandwidth  $D$ :

$$\frac{dT_K}{dD} = 0 \quad (2.4.175)$$

Substituting the form of  $T_K$ , eq. 2.4.174, in this equation gives

$$\begin{aligned} y(g) + D \frac{dy(g)}{dD} &= 0 \\ \implies y + D \frac{dy}{dg} \frac{dg}{dD} &= 0 \\ \implies y - 2g^2 \frac{dy}{dg} &= 0 \\ \implies y &= e^{-\frac{1}{2g}} \end{aligned} \quad (2.4.176)$$

This gives almost the same solution as eq. 2.4.173:

$$T_K = \frac{D}{k_B} e^{-\frac{1}{2g}} \quad (2.4.177)$$

The difference in the pre-factor arises from the extra contribution incorporated in that solution.

The fact that the scaling equations are universal can be seen by noting that from eq. 2.4.154, up to second order, we can write

$$g(D') = g_0 \left( 1 + 2g_0^2 \ln \frac{D}{D'} \right) \quad (2.4.178)$$

As we lower the temperature, the quantum processes are able to be coherent and lower energies. At temperature  $T$ , the order of energies that is explored by the processes is  $k_B T$ . Hence we can set  $\frac{D}{D'} = \frac{T}{T_F}$ . This says that the variation of the coupling from  $g_0$  to  $g$  is

$$g_0 \rightarrow g = g_0 \left( 1 + 2g_0 \ln \frac{T_F}{T} \right) \quad (2.4.179)$$

Since  $g \equiv NJ$ , we have recovered eq. 2.4.57. Since eq. 2.4.57 was obtained as a perturbation calculation, it should have been valid only at  $T \gg T_K$ , but the scaling relation holds at all temperatures.

### 2.4.8 Nozières' local Fermi liquid theory

Wilson's numerical renormalization group calculation showed that the low temperature specific heat contribution from the singlet is linear in temperature

$$C_V = \gamma T \quad (2.4.180)$$

This suggests that the strong-coupling limit of the Kondo model is a Fermi liquid.

The singlet state ( $s = 0$ ) has an energy

$$E_g = J \left[ 2\vec{S}_e \cdot \vec{S}_d \right] = J \left[ S^2 - S_d^2 - S_e^2 \right] = J \left[ s(s+1) - \frac{3}{2} \right] = -\frac{3J}{2} \quad (2.4.181)$$

Since the interaction term is spherically symmetric, it suffices to consider a one dimensional chain of conduction electrons with the impurity site coupling to the conduction electron at the origin. This electron forms a singlet with the impurity electron,

$$\frac{|0_\uparrow, d \downarrow\rangle - |0_\downarrow, d \uparrow\rangle}{\sqrt{2}} \quad (2.4.182)$$



Considering a tight-binding model, the only electron that can hop to the zeroth site is the one on the first site. The hopping of this electron on to the zeroth site would lead to an energy of

$$E_1 = -\frac{3}{2}J + \frac{3}{2}J = 0 \quad (2.4.183)$$

because the new electron would have the spin opposite to the other electron on the 0<sup>th</sup> site. This means that breaking the singlet raises the energy by  $\frac{3}{2}J$ . At low temperatures and very large  $J$ , this is not possible. That being said, there can always be virtual fluctuations into excited states. For example, the impurity electron can tunnel into the conduction band ( $n_d = 0$ ) or another conduction electron may scatter into the impurity site ( $n_d = 2$ ). Both these states have zero energy. With further virtual excitations, it is also possible to go into the triplet state with energy  $\frac{J}{2}$ . What this means is that although the singlet is stable with respect to energy-conserving transitions, the singlet is virtually polarizable, with the help of the site 1 electron. This induces an interaction on the site 1. Since the interaction on the site 1 is just a manifestation of the polarizability of the singlet, we can either take the singlet with its polarizability and assume the conduction band to be non-interacting, or we can assume the singlet to be static and take the Fermi sea to have a localised interaction at the site 1. In the latter picture, we have a frozen singlet (which can be ignored) and an interacting Fermi sea.

The goal [21] is to calculate the change in phase shift suffered by the conduction electrons in the presence of interactions. In the absence of interactions, the scattered wavefunction is

$$\psi \sim \frac{\sin [kr + \delta(E_k)]}{r} \quad (2.4.184)$$

That is, the phase shift is only a function of the energy. At the Fermi surface, this value  $\delta(0)$  is  $\frac{\pi}{2}$ , as known from the Friedel sum rule.

$$n = \sum_{\sigma} \frac{\delta}{\pi} \implies 1 = \frac{2\delta}{\pi} \implies \delta = \frac{\pi}{2} \quad (2.4.185)$$

$n$  is the number of conduction electrons bound in the resonance and the sum is over the possible quantum numbers (spin in this case).  $\delta(0)$  can also be obtained directly from eq. 2.4.184, by substituting  $k = k_F$  and noting that the isolation of the 0<sup>th</sup> site means all wavefunctions should shift by  $\Delta r = a$ :

$$k_F a = \delta(0) \implies \delta(0) = \frac{\pi}{2a} 2 = \frac{\pi}{2} \quad (2.4.186)$$

where the formula for  $k_F$  was used.

In a Fermi gas, the energy levels are separated by

$$\Delta\epsilon = \frac{\partial\epsilon}{\partial k} \Delta k \quad (2.4.187)$$

With the condition that the wavefunction should vanish at the boundary, we have  $\Delta k = k_n - k_{n-1} = \frac{\pi}{L}$ . Hence,

$$\Delta\epsilon = \frac{\partial\epsilon}{\partial k} \frac{\pi}{L} \quad (2.4.188)$$

However, this changes in the presence of the impurity. Because of eq. 2.4.184, the boundary condition becomes

$$k_n L + \delta(\epsilon_k) = n\pi \implies k_n = \frac{n\pi}{L} - \frac{\delta}{L} = k_n^0 - \frac{\delta(\epsilon_k)}{L} \quad (2.4.189)$$

The energy becomes

$$\begin{aligned} \epsilon(k) &= \epsilon(k^0) + \frac{\partial\epsilon}{\partial k} (k - k_0) \\ &= \epsilon_k - \frac{\partial\epsilon}{\partial k} \frac{\delta(\epsilon_k)}{L} \end{aligned} \quad (2.4.190)$$

In the Landau formulation of an interacting Fermi liquid, the phase shifts will depend on the quasiparticle occupation probabilities  $n_{k\sigma}$ . Hence,

$$\tilde{\epsilon}_{\sigma}(k) = \epsilon_k - \frac{\partial\epsilon}{\partial k} \frac{\delta_{\sigma}(\epsilon_k, \{n_{q,\sigma}\})}{L} \quad (2.4.191)$$

In bulk Fermi liquid, we expand the quasiparticle energy in the deviation of the quasiparticle distribution  $n_k$  from the ideal Fermi-Dirac distribution  $n_k^0$ ,

$$\begin{aligned} \tilde{\epsilon}_p = & \underbrace{\epsilon_F}_{\text{Fermi gas}} + \underbrace{\frac{p_F^*}{m} (p - p_F)}_{\text{linear contribution for } p \text{ close to } p_F} \\ & + \underbrace{\sum_{q\sigma} f(p, q) (n_q - n_q^0)}_{\text{interacting between two quasiparticles at momenta } p \text{ and } q} \end{aligned} \quad (2.4.192)$$

Similarly, for this local Fermi liquid, the phase shift depends on the energy of the quasiparticle  $\tilde{\epsilon}$  and the quasiparticle occupation  $n_{q\sigma}$ . Accordingly,

$$\delta_\sigma(\tilde{\epsilon}, \{n_{q,\sigma}\}) = \delta_\sigma(\tilde{\epsilon} = \epsilon_F, n_k = n_k^0) + \alpha (\tilde{\epsilon} - \epsilon_F) + \Phi \sum_{q\sigma'} (n_{q\sigma'} - n_{q\sigma'}^0) \quad (2.4.193)$$

This is just a Taylor expansion of  $\delta_\sigma$  around  $\tilde{\epsilon} = \epsilon_F$  and  $n_q = n_q^0$ .  $\Phi$  and  $\alpha$  play the same role as  $f$  and  $\frac{p_F^*}{m}$  in eq. 2.4.192. Specifically,  $\Phi$  represents the onsite interaction between quasiparticles of opposite spin and

$$\alpha = \frac{d\delta_\sigma}{dE} \quad (2.4.194)$$

Since  $\Phi$  acts only between quasiparticles of opposite spin, the last term can be simplified by requiring  $\sigma' = -\sigma$ ,

$$\delta_\sigma(\tilde{\epsilon}, \{n_{q,\sigma}\}) = \delta_\sigma(\tilde{\epsilon} = \epsilon_F, n_k = n_k^0) + \alpha (\tilde{\epsilon} - \epsilon_F) + \Phi \sum_q \delta n_{q,-\sigma} \quad (2.4.195)$$

Since the singlet is isolated from the Fermi liquid, any change in the chemical potential will not affect the average occupation of the impurity site  $\langle n_d \rangle$ , and since we know that  $\langle n_d \rangle = \frac{2\delta(0)}{\pi}$ , this means that  $\delta(0)$ , the phase shift at the Fermi surface, is invariant under a change of the chemical potential. This in turn means that the resonance scattering ( $\delta = \frac{\pi}{2}$ ) will always be pinned to the Fermi surface. With this knowledge, let us explicitly try to calculate the change in the phase shift at Fermi surface when we change the chemical potential by  $\Delta\mu$ . Before the change in chemical potential,

$$\delta_\uparrow^0 = \frac{\pi}{2} + \Phi \sum_q \delta n_{q\downarrow}^0 \quad (2.4.196)$$

Since  $\delta n^0 = n^0 - n^0 = 0$ ,

$$\delta_\uparrow^0 = \frac{\pi}{2} \quad (2.4.197)$$

After the change in chemical potential,  $\epsilon'_F = \epsilon_F + \Delta\mu$  and

$$N(\mu = 0) = N^0 \quad (2.4.198)$$

$$N(E' = E + \mu) = N(E' = E) + \frac{dN}{dE'} (E' - E) = N^0 + \rho \Delta\mu \quad (2.4.199)$$

$$\implies \sum_q \delta n_q = N - N^0 = \rho \Delta\mu \quad (2.4.200)$$

Hence, from eq. 2.4.195,

$$\begin{aligned} \delta_\uparrow &= \frac{\pi}{2} + \alpha (\epsilon'_F - \epsilon_F) + \Phi \sum_q \delta n_{q\downarrow} \\ &= \delta_\uparrow^0 + \alpha \Delta\mu + \Phi \rho \Delta\mu \end{aligned} \quad (2.4.201)$$

Hence the change in the phase is

$$0 = \Delta\delta_\uparrow = \Delta\mu (\alpha + \Phi\rho) \implies \alpha = -\Phi\rho \quad (2.4.202)$$

This shows that the interaction term  $\Phi$  is responsible for pinning the resonance at the Fermi level; without that term in the formalism, the occupancy of the impurity site will change. This is similar to the fact that the interaction term  $f(k, k')$  in the bulk Fermi liquid is responsible for making the Landau theory invariant under Galilean transformations.

Now we can calculate the density of states. From the boundary condition, we have

$$n_\sigma = \frac{kL}{\pi} + \frac{\delta_\sigma(E)}{\pi} = n^0 + \frac{\delta_\sigma(E)}{\pi} \quad (2.4.203)$$

Hence,

$$\begin{aligned} \rho &= \frac{dn_\sigma}{dE} = \rho^0 + \frac{1}{\pi} \frac{d\delta_\sigma}{dE} \\ \implies \rho &= \rho^0 + \frac{1}{\pi} \alpha \end{aligned} \quad (2.4.204)$$

$\rho^0$  is the density of states in absence of the impurity. The low temperature specific heat of an ideal Fermi liquid can be shown to be

$$C_v^0 = \gamma T = \frac{\pi^2 k_B^2}{3} \mathcal{N}(0) T \quad (2.4.205)$$

The interacting Fermi liquid is just a renormalised version of the Fermi gas, with a modified density of states  $\frac{1}{\pi} \alpha$ . Hence, the impurity contribution to the specific heat is

$$\begin{aligned} C_v &= \frac{\pi^2 k_B^2}{3} (\rho_\uparrow + \rho_\downarrow) T \\ &= \frac{2\alpha}{\pi} \frac{\pi^2 k_B^2}{3} T \end{aligned} \quad (2.4.206)$$

In presence of a magnetic field  $B$ , the magnetization is

$$m = \delta n \times \mu \quad (2.4.207)$$

where  $\mu$  is the magnetic moment

$$\mu = -\frac{g}{2} \mu_B \quad (2.4.208)$$

and  $\delta n$  is the difference in number between up and down electrons

$$\delta n = \langle n_\uparrow \rangle - \langle n_\downarrow \rangle = \frac{1}{\pi} (\delta_\uparrow - \delta_\downarrow) \quad (2.4.209)$$

In the presence of the magnetic field, all energies get modified,

$$E_\sigma^B = E - \sigma \frac{g\mu_B}{2} B \quad (2.4.210)$$

Hence,

$$\sum_k \delta n_{k\sigma} = N_\sigma(E_\sigma^B) - N(E) = \frac{dN}{dE^B} (E^B - E) = -\rho \frac{g\mu_B}{2} \sigma B \quad (2.4.211)$$

This modifies the phase shift at the Fermi surface,

$$\begin{aligned} \delta_\sigma(\epsilon_F) &= \frac{\pi}{2} + \alpha \left( \epsilon_F - \frac{g\mu_B}{2} \sigma B - \epsilon_F \right) + \Phi \sum_q \delta n_{q,-\sigma} \\ &= \frac{\pi}{2} - \sigma \frac{g\mu_B}{2} \alpha B + \Phi \rho \frac{g\mu_B}{2} \sigma B \\ &= \frac{\pi}{2} - 2\alpha \frac{g\mu_B}{2} \sigma B \end{aligned} \quad (2.4.212)$$

Hence,

$$\delta n = \frac{1}{\pi} (\delta_\uparrow - \delta_\downarrow) = -\frac{4\alpha B}{\pi} \frac{g\mu_B}{2} \quad (2.4.213)$$

The susceptibility is

$$\chi = \frac{\partial m}{\partial B} = \frac{\partial}{\partial B} \mu \delta n = \frac{4\alpha}{\pi} \left( \frac{g\mu_B}{2} \right)^2 \quad (2.4.214)$$

The susceptibility for an ideal Fermi gas can be calculated similarly. The additional energy of an electron with spin  $\sigma$  in a magnetic field  $B$  is  $-\sigma \frac{g}{2} \mu_B B$ . The magnetization induced at the Fermi surface is  $\delta n \times \mu$ , where  $\mu$  is the magnetic moment

$$\mu = -\frac{g}{2} \mu_B \quad (2.4.215)$$

and  $\delta n$  is the difference in number between up and down electrons

$$\delta n = n_{\uparrow}(0) - n_{\downarrow}(0) = n_{\uparrow}(\epsilon_F - \frac{g}{2} \mu_B B) - n_{\downarrow}(\epsilon_F + \frac{g}{2} \mu_B B) = -\frac{1}{2} \mathcal{N}(0) g B \mu_B \quad (2.4.216)$$

$\mathcal{N}(0) = \left. \frac{\partial n}{\partial E} \right|_{\epsilon_F}$  is the density of states at the Fermi energy and the  $\frac{1}{2}$  is because we are counting electrons of a particular spin only. Therefore,

$$m = \delta n \times \mu = \mathcal{N}(0) \left( \frac{g}{2} \mu_B \right)^2 B \quad (2.4.217)$$

The magnetic susceptibility comes out to be

$$\chi^0 = \left. \frac{\partial m}{\partial B} \right|_{B \rightarrow 0} = \mathcal{N}(0) \left( \frac{g}{2} \mu_B \right)^2 \quad (2.4.218)$$

The Wilson ratio  $R$  can now be computed,

$$R = \frac{\chi/\chi_0}{C_v/C_v^0} = \frac{4\alpha/\pi \mathcal{N}(0)}{2\alpha/\pi \mathcal{N}(0)} = 2 \quad (2.4.219)$$

## 2.5 Numerical renormalization group calculation

Wilson's idea [22] was to remove the limitations of the perturbative nature of Anderson's scaling method. To that end, we transformed the Hamiltonian into a one-dimensional chain, and then iteratively diagonalised chains of increasing length. The Hamiltonian we are working with is

$$H = \sum_k \epsilon_k n_k + J \vec{S}_d \cdot \vec{\sigma}_e \quad (2.5.1)$$

where  $\vec{\sigma}_e = \sum_{k_1, k_2, \alpha, \beta} c_{k_1 \alpha}^\dagger \vec{\sigma}_{\alpha \beta} c_{k_2 \beta}$  is the conduction electron spin at the origin. This assumes that the exchange interaction  $J(k, k')$  is independent of spin. To form the linear chain, we construct a new basis in which to express the conduction electron part  $H_c$ , out of the states  $|0\rangle, H_c|0\rangle, H_c^2|0\rangle, \dots$ .  $|0\rangle$  is the origin site, where the impurity resides. The first member of the new basis is  $|0\rangle$ . The next member is taken to be some state in the subspace of  $|0\rangle$  and  $H_c|0\rangle$ ,

$$|1\rangle = (\lambda_1 H_c |0\rangle + \lambda_2 |0\rangle) \quad (2.5.2)$$

This is a general form for any ket in the subspace spanned by  $|0\rangle$  and  $H_c|0\rangle$ . Since we want the state to be normalised, we can shift one of the parameters to the denominator:

$$|1\rangle = \frac{1}{\gamma_0} (H_c |0\rangle + \lambda |0\rangle) \quad (2.5.3)$$

where  $\gamma_0$  sets  $\langle 1|1\rangle = 1$ . The remaining parameter is set by requiring  $\langle 1|0\rangle = 0$ . That gives

$$\lambda = -\langle 0|H_c|0\rangle \quad (2.5.4)$$

Therefore,

$$|1\rangle = \frac{1}{\gamma_0} (H_c |0\rangle - \langle 0|H_c|0\rangle |0\rangle) \quad (2.5.5)$$

The general state can be shown to be

$$|n+1\rangle = \frac{1}{\gamma_n} (H_c |n\rangle - |n\rangle \langle n| H_c |n-1\rangle - |n-1\rangle \langle n-1| H_c |n\rangle) \quad (2.5.6)$$

From eq. 2.5.6, by multiplying  $\langle n'|$  from left, we get

$$\delta_{n',n+1} = \frac{1}{\gamma_n} \left[ (H_c)_{n',n} + (H_c)_{n,n-1} \delta_{n',n} + (H_c)_{n-1,n} \delta_{n',n-1} \right] \quad (2.5.7)$$

Clearly, for  $n' < n-1$  or  $n' > n+1$ , we get

$$(H_c)_{n',n} = 0 \quad (2.5.8)$$

so the only non-zero terms are for  $n' = n-1, n, n+1$ . For  $n' = n+1$  gives

$$(H_c)_{n+1,n} = \gamma_n \quad (2.5.9)$$

Taking the complex conjugate of this gives

$$\gamma_n^* = (H_c^\dagger)_{n,n+1} = (H_c)_{n,n+1} \quad (2.5.10)$$

Defining

$$(H_c)_{n,n} = \epsilon_n \quad (2.5.11)$$

we can write

$$\begin{aligned} H_c &= \sum_{n_1, n_2} |n_1\rangle \langle n_1| H_c |n_2\rangle \langle n_2| \\ &= \sum_n \epsilon_n |n\rangle \langle n| + \sum_n (\gamma_n |n\rangle \langle n+1| + \gamma_n^* |n+1\rangle \langle n|) \\ &= \sum_n \epsilon_n \hat{n}_n + \sum_n (\gamma_n c_n^\dagger c_{n+1} + \gamma_n^* c_{n+1}^\dagger c_n) \end{aligned} \quad (2.5.12)$$

The diagonalization of these chains become impossible for  $n > 8$ . To remedy this problem, Wilson, after diagonalization a chain of a particular length, retained only the lowest parts of the spectrum, and the Hamiltonian for the next stage was formed out of these low-lying states. This keeps the size of the Hilber space (and hence the matrices) manageable. Another problem is that as one goes on adding sites to the chain, the couplings need to die off, otherwise this process will never converge.

### Logarithmic discretization

First, note that up to first order

$$\epsilon_k = \epsilon_F + (k - k_F) \frac{\partial \epsilon_k}{\partial k} \quad (2.5.13)$$

By choosing  $k_F = \epsilon_F = 0$ , we get  $\epsilon_k = k$ .

Wilson divided the conduction band into patches,  $[\Lambda^{-(n+1)}, \Lambda^{-n}]$ , for  $n = 1, 2, 3, \dots$ . The width of each interval is

$$d_n = \Lambda^{-n} (1 - \Lambda^{-1}) \quad (2.5.14)$$

We can now define orthogonal functions in this  $n^{\text{th}}$  interval  $k \in [\Lambda^{-(n+1)}, \Lambda^{-n}]$ ,

$$\psi_{m,n}(k) = \frac{1}{\sqrt{d_n}} \exp \left\{ \frac{2\pi i m}{d_n} k \right\} \quad (2.5.15)$$

They allows us to define a new set of creation operators,

$$a_{m,n}^\dagger = \sum_k \psi_m(k) c_k^\dagger \quad (2.5.16)$$

Similarly functions can be defined in the negative interval  $-k \in [\Lambda^{-(n+1)}, \Lambda^{-n}]$ .

$$\phi_{m,n}(k) = \frac{1}{\sqrt{d_n}} \exp \left\{ -\frac{2\pi i m}{d_n} k \right\} \quad (2.5.17)$$

$$b_{m,n}^\dagger = \sum_k \phi_m(k) c_k^\dagger \quad (2.5.18)$$

Then,

$$a_{m,n}^\dagger + b_{m,n}^\dagger = \frac{2}{\sqrt{d_n}} \sum_{\pm k \in []} \cos \left( \frac{2\pi m k}{d_n} \right) c_k^\dagger \quad (2.5.19)$$

Summing over  $n$  involves summing over all momenta.

$$\begin{aligned} \sum_n (a_{m,n}^\dagger + b_{m,n}^\dagger) &= \frac{2}{\sqrt{d_n}} \sum_k \cos \left( \frac{2\pi m k}{d_n} \right) c_k^\dagger \\ \Rightarrow \sum_n (a_{0,n}^\dagger + b_{0,n}^\dagger) &= \frac{2}{\sqrt{d_n}} \sum_k c_k^\dagger \end{aligned} \quad (2.5.20)$$

For the momentum-independent  $J(k, k')$ , the coupling term involves.

$$\sum_{k,q} c_k^\dagger c_q = \sum_k c_k^\dagger \sum_q c_q \quad (2.5.21)$$

Looking at eq. 2.5.20, we see that the impurity spin is coupled only to the  $m = 0$  operators. This is where the approximation comes in, in Wilson's scheme. All the  $m$  values other than  $m = 0$  are ignored.

Wilson chose

$$\epsilon_n = 0, \gamma = D' \Lambda^{-\frac{n}{2}} \quad (2.5.22)$$

with  $\Lambda > 1$ . The Hamiltonian for  $N$  sites then turns out to be

$$H_N = D' \sum_{n=0}^{N-1} \Lambda^{-\frac{n}{2}} \left( c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n \right) + 2J \vec{S}_d \cdot \vec{S}_e \quad (2.5.23)$$

The next step involves adding another site to the chain. The next Hamiltonian is hence

$$H_{N+1} = H_N + D' \Lambda^{-\frac{N}{2}} \left( c_N^\dagger c_{N+1} + c_{N+1}^\dagger c_N \right) \quad (2.5.24)$$

To compare the couplings, and hence the Hamiltonians, at each value of  $N$ , we need to rescale the Hamiltonians  $H_N$  so that the lowest energy scale is independent of the running index  $N$ . Looking at eq. 2.5.23, the lowest energy scale is  $\Gamma_N = D' \Lambda^{-\frac{N-1}{2}}$ . Hence, the rescaled Hamiltonian is

$$\bar{H}_N = \frac{H_N}{\Gamma_N} = \frac{\Lambda^{\frac{N-1}{2}}}{D'} H_N \quad (2.5.25)$$

The utility can be seen by noting the relation between  $\bar{H}_{N+1}$  and  $\bar{H}_N$ ,

$$\begin{aligned} \bar{H}_{N+1} &= \frac{\Lambda^{\frac{N}{2}}}{D'} \left[ H_N + \Lambda^{-\frac{N}{2}} D' \left( c_N^\dagger c_{N+1} + c_{N+1}^\dagger c_N \right) \right] \\ \Rightarrow \bar{H}_{N+1} &= \Lambda^{\frac{1}{2}} \bar{H}_N + \left( c_N^\dagger c_{N+1} + c_{N+1}^\dagger c_N \right) \end{aligned} \quad (2.5.26)$$

In the series of Hamiltonians  $\{H_N\}$ , the couplings to the extra site are all same, so the lowest energy scales are all of the same order. This allows us to construct a flow of the Hamiltonians. The real Hamiltonian is the unscaled one, so it is given by

$$H = \lim_{N \rightarrow \infty} H_N = \lim_{N \rightarrow \infty} D' \Lambda^{\frac{1-N}{2}} \bar{H}_N \quad (2.5.27)$$

Since  $\bar{H}_N$  is exactly diagonalised with a spectrum  $\{E_m, |m\rangle\}$ , it can be written down as

$$\bar{H}_N = \sum_m E_m |m\rangle \langle m| \quad (2.5.28)$$

The next Hamiltonian is then

$$\bar{H}_{N+1} = \Lambda^{\frac{1}{2}} \sum_m E_m |m\rangle \langle m| + \sum_{m,m'} \left( C(m, m') |m\rangle \langle m'| + \text{h.c.} \right) \quad (2.5.29)$$

This is the same equation as eq. 2.5.26, with  $\bar{H}_N$  expressed in its eigenbasis and the creation and annihilation operators also expressed in that basis; the  $C(m, m')$  are just the matrix elements of  $c$  and  $c^\dagger$  in that basis.

To check whether the guesses about the fixed points are true, Wilson did the following. He set  $J = 0.009$  and then then calculated the lowest excitations of the Hamiltonians obtained from the NRG in the limit of large  $N$ . They indeed correspond to the excitations of the Kondo hamiltonian at  $J = \infty$ , meaning that under the application of the NRG, the  $J = 0.009$  Hamiltonian flowed to the fixed-point Hamiltonian  $J = \infty$ .

## 2.6 Correspondence between the Kondo model fixed-point and a local Fermi liquid

### Local Fermi liquid

The fixed-point Hamiltonians [23] are found to represent interacting Fermi liquids. The effective Hamiltonian can be shown to resemble the Anderson model, but with modified parameters,

$$H_{\text{eff}} = \sum_k \epsilon_k n_k + \sum_k V_k c_d^\dagger c_k + \text{h.c.} + U n_{d\uparrow} n_{d\downarrow} \quad (2.6.1)$$

The parameters  $\epsilon_k, V_k, U$  are not the same as the Anderson model we start with, but I am using the same symbols for convenience. The interaction term  $U$  is the leading irrelevant operator near the low-energy fixed point. For  $T \rightarrow 0$ , assuming only single excitations, the interacting term will not get invoked.

Under mean-field,

$$\begin{aligned} n_{d\uparrow} n_{d\downarrow} &\approx \langle n_{d\uparrow} \rangle n_{d\downarrow} + \langle n_{d\downarrow} \rangle n_{d\uparrow} - \langle n_{d\uparrow} \rangle \langle n_{d\downarrow} \rangle \\ \implies \langle n_{d\uparrow} n_{d\downarrow} \rangle &= \langle n_{d\uparrow} \rangle \langle n_{d\downarrow} \rangle \\ &= \sum_{k,q} \langle n_{k\sigma} \rangle \langle n_{q,-\sigma} \rangle \end{aligned} \quad (2.6.2)$$

where  $N$  is the number of sites. Note that the number of excitations,  $\langle n_q \rangle$  has to be defined differently for the states above and below the Fermi surface. For excited states above  $\epsilon_F$ , the number of excitations is given usually:

$$\langle n_q^> \rangle = \langle \psi^> | c_k^\dagger c_k | \psi^> \rangle = n_k^p \quad (2.6.3)$$

where  $n_k^p$  stands for the number of particles. For states below  $\epsilon_F$ , however, we need to count the number of holes:

$$\langle n_q^< \rangle = \langle \psi^< | c_k^\dagger c_k | \psi^< \rangle = - \langle \psi^< | c_k c_k^\dagger | \psi^< \rangle = -n_k^h \quad (2.6.4)$$

where  $n_k^h$  stands for the number of holes. We can thus define a generalized excitation:

$$\langle \delta n_{k,\sigma} \rangle = \begin{cases} n_k^p, & \epsilon_k > \epsilon_F \\ -n_k^h, & \epsilon_k < \epsilon_F \end{cases} \quad (2.6.5)$$

Replacing the quasiparticle excitations with their expectation values, the effective one-particle energy becomes

$$\epsilon_{k\sigma} = \epsilon_k + U \sum_q \langle \delta n_{q,-\sigma} \rangle \equiv \epsilon_k + U \langle \delta n_{-\sigma} \rangle \quad (2.6.6)$$

This is analogous to the Landau quasiparticle energy functional,  $U$  acting as the interaction between the quasiparticles.  $\delta n > 0$  acts as the excitations from the ground state.

The interacting density of states is

$$\rho_{d\sigma}(\omega) = \frac{\Delta}{\pi} \frac{1}{\left(\omega - \epsilon_d^*\right)^2 + \Delta^2} \quad (2.6.7)$$

where  $\epsilon_d^* = \epsilon_d + U\langle\delta n_{-\sigma}\rangle$ .

### Calculation of $C_v$

To calculate the specific heat,  $C_v = \frac{d\langle E \rangle}{dT}$ , note that a change in temperature would modify the quasiparticle distribution  $\delta n_{k\sigma}$  and hence the quasiparticle energies  $\epsilon_{k\sigma}$ . This leads to a complicated feedback effect. However, at low temperatures, higher order excitations will be very low and we can approximate by considering only the variation in the distribution:

$$\frac{d\langle E \rangle}{dT} = \sum_{k,\sigma} \epsilon_{k\sigma} \frac{d\langle \delta n_{k\sigma} \rangle}{dT} \quad (2.6.8)$$

Since the quasiparticle excitations are adiabatically connected to the free electron excitations,  $\langle \delta n_{k\sigma} \rangle$  will follow a Fermi-Dirac distribution:

$$\begin{aligned} \langle \delta n_{k\sigma} \rangle(T) &= \frac{1}{e^{\beta \epsilon_{k\sigma}} + 1} \\ \Rightarrow \frac{d\langle \delta n_{k\sigma} \rangle}{dT} &= \frac{e^{\beta \epsilon_{k\sigma}}}{\left(e^{\beta \epsilon_{k\sigma}} + 1\right)^2} \left[ \frac{1}{k_B T^2} \epsilon_{k\sigma} - \frac{1}{k_B T} (2\epsilon_{k\sigma} - \epsilon_k) \frac{d\langle \delta n_{k\sigma} \rangle}{dT} \right] \end{aligned} \quad (2.6.9)$$

At sufficiently low temperatures, the first term will dominate over the others ( $T^{-2} \gg T^{-1}$ ). Hence the low temperature specific heat can be written as

$$\begin{aligned} \frac{d\langle E \rangle}{dT} &= \sum_{k,\sigma} \epsilon_{k\sigma} \frac{e^{\beta \epsilon_{k\sigma}}}{\left(e^{\beta \epsilon_{k\sigma}} + 1\right)^2} \frac{1}{k_B T^2} \epsilon_{k\sigma} \\ &= \frac{1}{k_B T^2} \sum_{k,\sigma} \epsilon_{k\sigma}^2 \frac{e^{\beta \epsilon_{k\sigma}}}{\left(e^{\beta \epsilon_{k\sigma}} + 1\right)^2} \\ &= \frac{1}{k_B T^2} \sum_{\sigma} \int d\epsilon_{\sigma} \rho(\epsilon_{\sigma}) \epsilon_{\sigma}^2 \frac{e^{\beta \epsilon_{k\sigma}}}{\left(e^{\beta \epsilon_{k\sigma}} + 1\right)^2} \end{aligned} \quad (2.6.10)$$

The function  $\frac{e^{\beta \epsilon_{k\sigma}}}{\left(e^{\beta \epsilon_{k\sigma}} + 1\right)^2}$  is very sharply peaked at the Fermi surface  $\epsilon_{\sigma} = 0$ . Therefore we can replace the density of states by its value at the Fermi surface.

$$\begin{aligned} \frac{d\langle E \rangle}{dT} &= \frac{1}{k_B T^2} \sum_{\sigma} \rho_{\sigma}(0) \int_{-\infty}^{\infty} d\epsilon_{\sigma} \epsilon_{\sigma}^2 \frac{e^{\beta \epsilon_{k\sigma}}}{\left(e^{\beta \epsilon_{k\sigma}} + 1\right)^2} \\ &= -\frac{1}{T} \sum_{\sigma} \rho_{\sigma}(0) \int_{-\infty}^{\infty} d\epsilon_{\sigma} \epsilon_{\sigma}^2 f'(\epsilon_{\sigma}) \\ &= -\frac{1}{T} \sum_{\sigma} \rho_{\sigma}(0) \int_1^0 df \epsilon_{\sigma}^2 \end{aligned} \quad (2.6.11)$$

$f(\epsilon_{\sigma})$  is the Fermi-Dirac distribution. Note that

$$\epsilon = k_B T \ln \left( f^{-1} - 1 \right) \Rightarrow \epsilon^2 = k_B^2 T^2 \left[ \ln \left( f^{-1} - 1 \right) \right]^2 \quad (2.6.12)$$



Therefore,

$$\frac{d\langle E \rangle}{dT} = -k_B^2 T \sum_{\sigma} \rho_{\sigma}(0) \int_1^0 df \left[ \ln(f^{-1} - 1) \right]^2 \quad (2.6.13)$$

The remaining integral gives  $-\frac{\pi^2}{3}$ . For  $T \rightarrow 0$ , quasiparticle excitations will be absent and we can write  $\rho_{\uparrow} = \rho_{\downarrow} = \rho_d$ :

$$\begin{aligned} \frac{d\langle E \rangle}{dT} &= k_B^2 T \sum_{\sigma} \rho_d(0) \frac{\pi^2}{3} \\ &= 2k_B^2 T \rho_d(0) \frac{\pi^2}{3} \\ &= \gamma_{\text{imp}} T \end{aligned} \quad (2.6.14)$$

where

$$\gamma_{\text{imp}} \equiv \frac{C_v}{T} = \frac{2\pi^2}{3} k_B^2 \rho_d(0) \quad (2.6.15)$$

This is identical in structure to the Fermi gas result  $C_v^{(0)} \equiv \gamma^{(0)} T = \frac{2\pi^2}{3} k_B^2 \rho_d^{(0)}(0) T$ :

$$\frac{\gamma_{\text{imp}}}{\gamma^{(0)}} = \frac{\rho_d(0)}{\rho_d^{(0)}(0)} \quad (2.6.16)$$

### Calculation of $\chi$

Under a magnetic field  $B$ ,  $\epsilon_{k\sigma} \rightarrow \epsilon_{k\sigma} + \sigma h$ , where  $h = \frac{1}{2} g B \mu_B$ . The magnetisation is

$$\begin{aligned} m &= \frac{g\mu_B}{2} (\delta n_{\uparrow} - \delta n_{\downarrow}) \\ &= \frac{g\mu_B}{2} \sum_{\sigma} \sigma \delta n_{\sigma} \\ &= \frac{g\mu_B}{2} \sum_{k\sigma} \sigma \frac{\partial n_{\sigma}}{\partial \epsilon_{k\sigma}} \delta \epsilon_{k\sigma} \\ &= \frac{g\mu_B}{2} \sum_{k\sigma} \sigma \rho_{k\sigma} (\sigma h + U \delta n_{-\sigma}) \\ &= \frac{g\mu_B}{2} \sum_{\sigma} \sigma \rho_{\sigma} (\sigma h + U \delta n_{-\sigma}) \end{aligned} \quad (2.6.17)$$

On applying the magnetic field, the Fermi energy of spin  $-\sigma$  decreases as  $\epsilon_F - \sigma h$ . Hence, more number of spin  $-\sigma$  electrons will get excited, the number of such excitations being

$$\delta n_{-\sigma} = \sum_q \delta n_{q,-\sigma} = \sum_q \Delta \epsilon_F \rho_{q-\sigma} = \sigma h \rho_{-\sigma}(0) \quad (2.6.18)$$

In the last step, I used the fact that the density of states is non-zero only very close to the Fermi surface. Substituting this in the magnetization gives

$$\begin{aligned} m &= \frac{g\mu_B}{2} h \sum_{\sigma} \sigma^2 \rho_{\sigma}(0) (1 + U \rho_{-\sigma}(0)) \\ &= \left( \frac{g\mu_B}{2} \right)^2 B \sum_{\sigma} \rho_{\sigma}(0) [1 + U \rho_{-\sigma}(0)] \end{aligned} \quad (2.6.19)$$

The susceptibility is

$$\begin{aligned} \chi_{\text{imp}} &= \lim_{h \rightarrow 0} \frac{\partial m}{\partial B} \\ &= \left( \frac{g\mu_B}{2} \right)^2 \rho_d(0) [1 + U \rho_d(0)] \sum_{\sigma} \\ &= \frac{(g\mu_B)^2}{2} \rho_d(0) [1 + U \rho_d(0)] \\ &= \chi^{(0)} \frac{\rho_d(0)}{\rho_d^{(0)}(0)} [1 + U \rho_d(0)] \end{aligned} \quad (2.6.20)$$

There I used the fact that in the absence of any field and  $T \rightarrow 0$ ,  $\rho_{\uparrow} = \rho_{\downarrow} = \rho_d$ .

The Wilson ratio is

$$R \equiv \frac{\chi_{\text{imp}}}{\chi^{(0)}} \frac{\gamma^{(0)}}{\gamma_{\text{imp}}} = 1 + U\rho_d(0) \quad (2.6.21)$$

### Relation between the density of states and scattering phase shift

The Green's function is of the general form

$$G_d(\omega) = \frac{1}{\omega - \epsilon_d - i\Delta - \Sigma(\omega)} \quad (2.6.22)$$

Close to the Fermi surface, the imaginary part of the self energy goes as  $\omega^2$ . Therefore, up to first order in  $\omega$ , the self energy is completely real close to the Fermi surface:

$$\begin{aligned} \Sigma(\omega) &= \Sigma(0, 0) + \omega\Sigma'(0) + O(i\omega^2) \\ &\equiv \Sigma(0) + (1 - Z^{-1})\omega \end{aligned} \quad (2.6.23)$$

where  $Z = (1 - \Sigma')^{-1}$ . Substituting this in  $G_d(\omega)$  gives

$$\begin{aligned} G_d(\omega) &= \frac{1}{\omega - \epsilon_d - i\Delta - \Sigma(0) - (1 - Z^{-1})\omega} \\ &= \frac{Z}{Z\omega - Z\epsilon_d - iZ\Delta - Z\Sigma(0) - Z\omega + \omega} \\ &= \frac{Z}{\omega - Z(\epsilon_d + \Sigma(0)) - iZ\Delta} \\ &\equiv \frac{Z}{\omega - \epsilon_d^* - i\Delta^*} \end{aligned} \quad (2.6.24)$$

The density of states at the Fermi surface is given by

$$\begin{aligned} \rho_d(0) &= \frac{1}{\pi} \text{Im } G_d(\omega) \Big|_{\omega=0} \\ &= \frac{1}{\pi} \frac{Z\Delta^*}{(\omega - \epsilon_d^*)^2 + \Delta^{*2}} \Big|_{\omega=0} \\ &= \frac{1}{\pi} \frac{Z\Delta^*}{\epsilon_d^{*2} + \Delta^{*2}} \end{aligned} \quad (2.6.25)$$

The total Green's function for the conduction electrons can be expressed in powers of the scattering potential  $V$ :

$$\begin{aligned} G &= G^{(0)} + G^{(0)}VG_d^{(0)}VG^{(0)} + G^{(0)}VG_d^{(0)}VG^{(0)}VG_d^{(0)}VG^{(0)} + \dots \\ &= G^{(0)} + G^{(0)}V \left[ G_d^{(0)} + G_d^{(0)}VG^{(0)}VG_d^{(0)} \right] VG^{(0)} \\ &= G^{(0)} + G^{(0)}V^2G_dG^{(0)} \end{aligned} \quad (2.6.26)$$

Here,  $G^{(0)}$  are the bare Green functions of the conduction and impurity electron and  $G_d$  is the interaction impurity Green's function. Comparing with

$$G = G_0 + G_0TG_0 \quad (2.6.27)$$

we can write

$$T = V^2G_d \quad (2.6.28)$$

where  $T$  is the  $T$ -matrix for scattering of conduction electrons off the impurity. From the optical theorem, we know that the  $S$ -matrix ( $S(\omega) \equiv e^{2i\delta(\omega)}$ ) is related to the  $T$ -matrix as

$$\begin{aligned} e^{2i\delta(\omega)} &= 1 - 2\pi i \rho T(\omega) \\ \implies T &= V^2 G_d = \frac{1}{2\pi i \rho} \left( 1 - e^{2i\delta(\omega)} \right) = \frac{e^{i\delta(\omega)}}{2\pi i \rho} (-2i \sin \delta) \\ \implies G_d &= -\frac{e^{i\delta(\omega)}}{V^2 \pi \rho} \sin \delta \end{aligned} \quad (2.6.29)$$

Since  $-\frac{1}{V^2 \pi \rho} \sin \delta$  is real, we can write

$$G_d = |G_d| e^{i\delta(\omega)} \quad (2.6.30)$$

From the expression for  $G_d$  in eq. 2.6.24, we can find the phase of  $G_d$ :

$$\begin{aligned} \delta(\omega) &= \tan^{-1} \frac{\Delta^*}{\omega - \epsilon_d^*} \\ \implies \epsilon_d^* &= -\Delta^* \cot \delta(0) \end{aligned} \quad (2.6.31)$$

Substituting this in the density of states expression gives

$$\rho_d(0) = \frac{Z \sin^2 \delta(0)}{\pi \Delta^*} \quad (2.6.32)$$

Substituting this expression for the density of states in the expression for the Wilson ratio gives

$$R = 1 + \frac{U Z \sin^2 \delta(0)}{\pi \Delta^*} \quad (2.6.33)$$

From the definition  $\Delta^* \equiv Z \Delta$ , we get

$$R = 1 + \frac{U}{\pi \Delta} \sin^2 \delta(0) \quad (2.6.34)$$

### The case of $\langle n_d \rangle = 1$

Exactly at the strong-coupling fixed point, for particle-hole symmetry, we expect the occupancy of the impurity to be  $\langle n_d \rangle = 1$ , because the singly-occupied state is below the Fermi level while the doubly occupied state is above. If we now lower the Fermi level by  $\Delta\mu$  while keeping the particle-hole symmetry intact (by suitably shifting the impurity levels), the resonance in the spectral function at the Fermi surface will persist, because the electrons at the Fermi surface will always form a singlet with the impurity and go into a bound state.

Since the energies are measured relative to the Fermi level, all quasiparticle energies will increase by  $\Delta\epsilon_{k\sigma} = \Delta\mu$ . However, some of the quasiparticles closer to the Fermi surface will now come below it, so that the number of quasiparticles will decrease by  $\Delta n = -\Delta\mu \rho_d(0)$ . The net change in  $n_\uparrow$  is thus

$$\begin{aligned} \Delta n_\uparrow &= \delta n_\uparrow(\epsilon_{k\uparrow} + \mu) - \delta n_\uparrow(\epsilon_{k\uparrow}) \\ &= \rho_d(0) \left( \Delta\mu + U \Delta n_\downarrow \right) \\ &= \rho_d(0) \left( \Delta\mu - U \rho_d(0) \Delta\mu \right) \\ &= \rho_d(0) \Delta\mu \left( 1 - U \rho_d(0) \right) \end{aligned} \quad (2.6.35)$$

At the Kondo limit, the impurity occupation is fixed at 1 because the resonance in the spectral function of the conduction electrons is pinned at the Fermi energy. This means that even if we shift the Fermi energy, the resonance moves with it, and there should be no change  $\Delta n_\uparrow$ . Hence,

$$1 - U \rho_d(0) = 0 \implies U \rho_d(0) = 1 \quad (2.6.36)$$

Substituting  $\langle n_{d\sigma} \rangle = \frac{1}{2}$  and  $\epsilon_d = -\frac{U}{2}$  in the density of states eq. 2.6.7 gives  $\rho_d(0) = \frac{1}{\pi \Delta} = \frac{1}{U}$ . This can be substituted in the Wilson ratio to give

$$R = 1 + \sin^2 \delta(0) \quad (2.6.37)$$

## 2.7 Topological interpretation of Wilson ratio

From the Friedel sum rule[15], we can relate the phase shift  $\delta(0)$  due to scattering (at the Fermi surface) off a local impurity to the number of electrons bound in the potential well produced by that impurity:

$$\tilde{N} = \frac{1}{2\pi i} \text{Tr} \ln S(0) = \int_{\Gamma} dz \partial_z \frac{1}{2\pi i} \text{Tr} \ln S(0) \quad (2.7.1)$$

From the optical theorem, we can write

$$S = 1 + TG_0 = \frac{G}{G_0} \quad [\text{eq. 2.6.27}] \quad (2.7.2)$$

This allows us to write [1]

$$\tilde{N} = \int_{\Gamma} dz \partial_z \frac{1}{2\pi i} \text{Tr} \ln \frac{G}{G_0} \quad (2.7.3)$$

Since  $\text{Tr} \ln \hat{O} = \sum_{\lambda} \ln O_{\lambda} = \ln \prod_{\lambda} O_{\lambda} = \ln \text{Det} \hat{O}$ , we get

$$\begin{aligned} \tilde{N} &= \int_{\Gamma} dz \partial_z \frac{1}{2\pi i} \ln \text{Det} \frac{G}{G_0} \\ &= - \int_{\Gamma} dz \partial_z \frac{1}{2\pi i} \ln \frac{\text{Det } G_0}{\text{Det } G} \\ &\equiv - \int_{\Gamma} dz \partial_z \frac{1}{2\pi i} \ln D \\ &= - \int_{\Gamma(D)} \frac{dD}{D} \end{aligned} \quad (2.7.4)$$

From the work of Seki and Yunoki [24], we know that this quantity is essentially the winding number of the curve  $\Gamma(D)$  in the complex plane spanned by the real and imaginary parts of  $D$ , and is equal to the change in Luttinger's volume  $V_L$  at  $T = 0$ .

$$\tilde{N} = - \int_{\Gamma(D)} \frac{dD}{D} = -\Delta V_L \quad (2.7.5)$$

The incoming electrons can have  $\sigma = \uparrow, \downarrow$ . Since the impurity singlet ground state is rotationally invariant, we have  $\delta_{\uparrow} = \delta_{\downarrow} = \delta(0)$ .

$$\begin{aligned} \tilde{N} &= \frac{1}{\pi} \sum_{\sigma} \delta_{\sigma}(0) \\ \implies \delta(0) &= \frac{\pi}{2} \tilde{N} = -\frac{\pi}{2} \Delta V_L \end{aligned} \quad (2.7.6)$$

$$\begin{aligned} R &= 1 + \sin^2 \left( \frac{\pi}{2} \tilde{N} \right) \\ &= 1 + \sin^2 \left( \frac{\pi}{2} \Delta V_L \right) \end{aligned} \quad (2.7.7)$$

We note that this connection between  $R$  and  $\Delta V_L$  has not been obtained in the existing literature thus far. In the unitary limit,  $\delta(0) = \frac{\pi}{2}$ , giving  $\Delta V_L = -1 = -\tilde{N}$  [25] (i.e., one electronic state from the impurity has been absorbed into the Luttinger volume of the conduction bath), such that  $R = 2$  in this limit. In this way, we see that a change in the topological quantum number  $\tilde{N}$  causes the well known renormalisation of the Wilson ratio  $R$  from its non-interacting value (1) to the value (2) obtained for the local Fermi liquid [12].

## 2.8 Renormalized perturbation theory

This is a perturbative expansion of the Hamiltonian in terms of the renormalized interaction  $\tilde{U}$ , and the second order results obtained from this approach coincide with the phenomenological results at  $T, h \rightarrow 0$ . This approach is obviously more general as all terms in the original Hamiltonian are retained. This is an alternative to the full microscopic approach. In the microscopic approach, we take the exact microscopic Hamiltonian and calculate

observables from it. In the renormalized perturbation, we separate the Hamiltonian into a non-interacting quasiparticle Hamiltonian which is like the low-energy free Hamiltonian, and an interacting part, and also a counter-term to prevent divergences. The original parameters of the model get replaced by renormalized parameters, and we can analyze the model perturbatively in powers of the renormalized interaction.

To do a perturbative expansion of the Hamiltonian in terms of the interaction  $U$ , it is useful to introduce the self energy  $\Sigma(E) = \Sigma(0) + E\Sigma' + \Sigma^{\text{rem}}(E)$ . In the absence of interaction, the impurity Green's function is

$$G_d^0 = \frac{1}{E - \epsilon_d + i\Delta} \quad (2.8.1)$$

Including the self energy gives

$$G_d = \frac{1}{E - \epsilon_d + i\Delta - \Sigma(E)} \quad (2.8.2)$$

As shown previously in section 2.4.4, the impurity Green's function can be shown to take the form

$$G_d = \frac{Z}{E - \tilde{\epsilon}_d + i\tilde{\Delta} - \tilde{\Sigma}(E)} \quad (2.8.3)$$

where the  $\tilde{\phantom{x}}$  represents the renormalised quantities

$$\begin{aligned} \tilde{\epsilon}_d &= Z(\epsilon_d + \Sigma(0)) \\ \tilde{\Delta} &= Z\Delta \\ \tilde{\Sigma} &= Z\Sigma^{\text{rem}}(E) \\ Z^{-1} &= 1 - \Sigma(0)' \\ \tilde{\Gamma}_{\sigma\sigma'}(E, E') &= z^2\Gamma_{\sigma\sigma'}(E, E') \\ \tilde{U} &= z^2\Gamma_{\uparrow\downarrow}(0, 0) \end{aligned} \quad (2.8.4)$$

The perturbative expansion is about the bare Hamiltonian, that is, the one with  $\tilde{\Sigma} = 0$ . The corresponding Greens function (non-interacting quasiparticle Green's function) is

$$\tilde{G}_d = \frac{1}{E - \tilde{\epsilon}_d + i\tilde{\Delta}} \quad (2.8.5)$$

The Anderson hamiltonian

$$H = \epsilon_d n_d + U n_{d\uparrow} n_{d\downarrow} + \sum_k \epsilon_k n_k + \sum_k \left( V_k c_{d\sigma}^\dagger c_{k\sigma} + V_k^* c_{k\sigma}^\dagger c_{d\sigma} \right) \quad (2.8.6)$$

can be written in the form

$$H = \tilde{H}_{qp} - \tilde{H}_c \quad (2.8.7)$$

$\tilde{H}_{qp} = \tilde{H}_{qp}^0 + \tilde{H}_{qp}^I$  is the total quasiparticle Hamiltonian, consisting of a non-interacting part  $\tilde{H}_{qp}^0$  and an interaction  $\tilde{H}_{qp}^I$ .

$$\tilde{H}_{qp}^0 = \tilde{\epsilon}_d \tilde{n}_d + \sum_k \epsilon_k n_k + \sum_k \left( \tilde{V}_k \tilde{c}_{d\sigma}^\dagger c_{k\sigma} + \tilde{V}_k^* c_{k\sigma}^\dagger \tilde{c}_{d\sigma} \right) \quad (2.8.8)$$

$$\tilde{H}_{qp}^I = \tilde{U} \tilde{n}_{d\uparrow} \tilde{n}_{d\downarrow} \quad (2.8.9)$$

The renormalised parameters are defined in eq. 2.8.4. The renormalised operators are

$$\tilde{c}_d^\dagger = \sqrt{z} c_d^\dagger \quad (2.8.10)$$

$$\tilde{c}_d = \sqrt{z} c_d \quad (2.8.11)$$

The  $\tilde{H}_c$  that satisfies eq. 2.8.7 is

$$\tilde{H}_c = \lambda_1 \tilde{n}_d + \lambda_2 \tilde{n}_{d\uparrow} \tilde{n}_{d\downarrow} \quad (2.8.12)$$

where

$$\lambda_1 = z\Sigma(0, 0) \quad (2.8.13)$$

$$\lambda_2 = z^2 \left[ \Gamma_{\uparrow\downarrow}(0, 0) - U \right] \quad (2.8.14)$$

$\tilde{H}_{qp}$  is the effective Hamiltonian close to the strong-coupling fixed point.  $\tilde{H}_c$  is the counter-term. It is introduced to cancel divergences. Close to the Fermi surface, we want the renormalised self-energy  $\tilde{\Sigma}(E)$  to vary as  $E^2$ . That gives two constraints

$$\begin{aligned} \tilde{\Sigma}(0) &= 0 \\ \tilde{\Sigma}'(0) &= 0 \end{aligned} \quad (2.8.15)$$

Close to the Fermi surface, we also have

$$\tilde{\Gamma}_{\uparrow\downarrow}(0) = \tilde{U} \quad (2.8.16)$$

$$\tilde{\Gamma}_{\sigma\sigma}(0) = 0 \quad (2.8.17)$$

$$\implies \Gamma_{\sigma\sigma'}(0) = \tilde{U}(1 - \delta_{\sigma\sigma'}) \quad (2.8.18)$$

This is the third constraint. The perturbation expansion is in powers of the renormalised interaction  $\tilde{U}$ . The parameters that are determined by the expansion are  $\lambda_1, \lambda_2, z$ . Hence, they should be expanded in powers of  $\tilde{U}$ .

$$\lambda_i = \sum_n \lambda_i^{(n)} \tilde{U}^n \quad (2.8.19)$$

$$z = \sum_n z^{(n)} \tilde{U}^n \quad (2.8.20)$$

$$(2.8.21)$$

The expansion is about the non-interacting quasiparticle Hamiltonian. The corresponding Green's function is

$$G^0 = \frac{1}{E - \tilde{\epsilon}_d + i\tilde{\Delta}} \quad (2.8.22)$$

From the Friedel sum rule in the next section, we get

$$\langle n_{d\sigma} \rangle = \frac{1}{2} - \frac{1}{\pi} \tan^{-1} \frac{\epsilon_d + \Sigma(0, h)}{\Delta} \quad (2.8.23)$$

Multiplying the numerator and denominator by  $z$ , we get the same occupancy in terms of the renormalised parameters.

$$\langle n_{d\sigma} \rangle = \frac{1}{2} - \frac{1}{\pi} \tan^{-1} \frac{\tilde{\epsilon}_d + \tilde{\Sigma}(0, h)}{\tilde{\Delta}} \quad (2.8.24)$$

For  $T, h \rightarrow 0$ , the counter-term cancels appropriate terms from the quasiparticle Hamiltonian leading to the vanishing of the effects of the self-energy, eq. 2.8.15. In that case,  $\langle n_{d\sigma} \rangle = \langle n_{d\sigma}^0 \rangle$ , that is, the quasiparticle distribution becomes the same as the free fermionic distribution.

The first order Feynman diagram for the self-energy is of the Hartree type. They give a contribution

$$\tilde{\Sigma}(\omega, H, T) = \tilde{U} \left( n_{d\sigma}^{(0)}(0, H, T) - n_{d\sigma}^{(0)}(0, 0, 0) \right) \quad (2.8.25)$$

This satisfies the constraint eq. 2.8.15. That is,  $\Sigma^{(1)}(0, 0) = 0$ . With the expression for self-energy, we can write down the impurity magnetic susceptibility,  $\chi_d = \frac{\partial m}{\partial B}$ , where

$$m = \frac{g\mu_B}{2} \langle n_{d\uparrow} - n_{d\downarrow} \rangle \quad (2.8.26)$$

We can substitute the expression for the self-energy into eq. 2.8.24. That gives

$$\chi_d = \frac{1}{2} (g\mu_B)^2 \frac{\partial \langle n_{d\uparrow} - n_{d\downarrow} \rangle}{\partial h} = \frac{1}{2\pi} (g\mu_B)^2 \frac{\partial}{\partial h} \left( \tan^{-1} \frac{\tilde{\epsilon}_{d\downarrow}}{\tilde{\Delta}} - \tan^{-1} \frac{\tilde{\epsilon}_{d\uparrow}}{\tilde{\Delta}} \right) \quad (2.8.27)$$

where  $h = g\mu_B B$  and  $\tilde{\epsilon}_{d\sigma} = \tilde{\epsilon}_d + \tilde{U}n_{d\sigma}^{(0)}$ . Performing the derivative and taking the limits of  $T \rightarrow 0$  and  $B \rightarrow 0$  gives

$$\chi_d = \frac{1}{2\pi} (g\mu_B)^2 \frac{1}{1 + \left(\frac{\tilde{\epsilon}_d}{\tilde{\Delta}}\right)^2} \frac{1}{\tilde{\Delta}} \frac{\partial}{\partial h} [\tilde{\epsilon}_{d\downarrow} - \tilde{\epsilon}_{d\uparrow}] \quad (2.8.28)$$

We can recognize that

$$\frac{1}{1 + \left(\frac{\tilde{\epsilon}_d}{\tilde{\Delta}}\right)^2} \frac{1}{\pi \tilde{\Delta}} = \frac{1}{\pi} \frac{\tilde{\Delta}}{\tilde{\Delta}^2 + \tilde{\epsilon}_d^2} = \rho_d(0) \quad (2.8.29)$$

Therefore,

$$\chi_d = \frac{1}{2} (g\mu_B)^2 \rho_d(0) \frac{\partial}{\partial h} [\tilde{\epsilon}_{d\downarrow} - \tilde{\epsilon}_{d\uparrow}] \quad (2.8.30)$$

Up to first order, we can write

$$\tilde{\epsilon}_{d\downarrow} - \tilde{\epsilon}_{d\uparrow} = \epsilon_{d\downarrow} - \epsilon_{d\uparrow} + \tilde{U} (n_{d\downarrow}^{(0)} - n_{d\uparrow}^{(0)}) = 2\epsilon_d + h + \tilde{U} (n_{d\downarrow}^{(0)} - n_{d\uparrow}^{(0)}) \quad (2.8.31)$$

where I used  $\epsilon_{d\sigma}(h) = \epsilon_d - \frac{h}{2}\sigma$ . Substituting this in the expression for  $\chi_d$  gives

$$\frac{\partial}{\partial h} [\tilde{\epsilon}_{d\downarrow} - \tilde{\epsilon}_{d\uparrow}] = 1 + \tilde{U} \left( \frac{\partial n_{d\downarrow}^{(0)}}{\partial \epsilon_{d\downarrow}} \frac{\partial \epsilon_{d\downarrow}}{\partial h} - \frac{\partial n_{d\uparrow}^{(0)}}{\partial \epsilon_{d\uparrow}} \frac{\partial \epsilon_{d\uparrow}}{\partial h} \right) \quad (2.8.32)$$

Up to first order, we can approximate  $\frac{\partial \epsilon_{d\sigma}}{\partial h} = \frac{\sigma}{2}$ , therefore,

$$\frac{\partial}{\partial h} [\tilde{\epsilon}_{d\downarrow} - \tilde{\epsilon}_{d\uparrow}] = 1 + \tilde{U} \rho_d(0) \quad (2.8.33)$$

Substituting in to the parent equation, we get

$$\chi_d = \frac{1}{2} (g\mu_B)^2 \rho_d(0) (1 + \tilde{U} \rho_d(0)) \quad (2.8.34)$$

which is same as the one obtained from mean-field.

It is possible to take higher order contributions into account, but there are identities which show that these results are exact.

$$\left( \frac{\partial}{\partial E} + \frac{\partial}{\partial \mu} \right) \Sigma(E) \Big|_{E=0} = -\rho_{d\sigma}(0) \Gamma_{\uparrow\downarrow}(0,0) \quad (2.8.35)$$

$$\left( \frac{\partial}{\partial h} - \frac{\partial}{\partial E} \right) \Sigma(E) \Big|_{E=0} = -\rho_{d\sigma}(0) \Gamma_{\uparrow\downarrow}(0,0) \quad (2.8.36)$$

Multiplying both equations throughout by  $Z$ , we get

$$\left( \frac{\partial}{\partial E} + \frac{\partial}{\partial \mu} \right) \tilde{\Sigma}(E) \Big|_{E=0} = -Z \rho_{d\sigma}(0) \Gamma_{\uparrow\downarrow}(0,0) = -\frac{1}{Z} \rho_{d\sigma}(0) \tilde{U} \quad (2.8.37)$$

$$\left( \frac{\partial}{\partial h} - \frac{\partial}{\partial E} \right) \tilde{\Sigma}(E) \Big|_{E=0} = -Z \rho_{d\sigma}(0) \Gamma_{\uparrow\downarrow}(0,0) = -\frac{1}{Z} \rho_{d\sigma}(0) \tilde{U} \quad (2.8.38)$$

where I used  $Z^2 \Gamma = \tilde{U}$ . We also have the relation  $\tilde{\rho}_d = \frac{1}{Z} \rho_d$ , because

$$\tilde{\rho}(0) \sim \frac{\tilde{\Delta}}{\tilde{\epsilon}_d^2 + \tilde{\Delta}^2} = \frac{1}{Z} \frac{\Delta}{\epsilon_d^2 + \Delta^2} = \frac{1}{Z} \rho_d(0) \quad (2.8.39)$$

Noting that the derivative of the renormalised self energy goes to zero at the Fermi surface, we get

$$\left. \frac{\partial \tilde{\Sigma}(E)}{\partial \mu} \right|_{E=0} = \left. \frac{\partial \tilde{\Sigma}(E)}{\partial h} \right|_{E=0} = -\tilde{\rho}_{d\sigma}(0) \tilde{U} \quad (2.8.40)$$

These can be used to prove the mean-field results regarding specific heat and the susceptibilities. Similar to the mean field treatment, close to  $T = 0$ , the effects of the self energy vanish, and the specific heat linear term,  $\gamma$ , involves only the non-interacting density of states.

$$\tilde{\gamma} \sim \tilde{\rho}_d(0) \quad (2.8.41)$$

The susceptibilities are given by

$$\chi_m = - \left( \frac{g\mu_B}{2} \right)^2 \tilde{\rho}_d \sum_{\sigma} \frac{\partial (\epsilon_k - h\sigma + \tilde{\Sigma})}{\partial h} = \frac{g^2 \mu_B^2}{2} \tilde{\rho}_d \left( 1 - \frac{\partial \tilde{\Sigma}}{\partial h} \right) \quad (2.8.42)$$

Substituting from eq. 2.8.40,

$$\chi_m = \frac{g^2 \mu_B^2}{2} \tilde{\rho}_d \left( 1 + \tilde{U} \tilde{\rho}_d(0) \right) \quad (2.8.43)$$

Similarly,

$$\chi_c = \frac{dn}{d\mu} = \tilde{\rho}_d(0) \sum_{\sigma} \frac{d(\epsilon_F + \tilde{\Sigma})}{d\mu} = 2\tilde{\rho}_d(0) \left( 1 + \frac{\partial \tilde{\Sigma}}{\partial \mu} \right) = 2\tilde{\rho}_d(0) \left( 1 - \tilde{U} \tilde{\rho}_d(0) \right) \quad (2.8.44)$$

### Friedel sum rule

Looking at eq. 2.8.2, we can write down the density of states and hence the average occupancy of the impurity site

$$\rho_{d\sigma} = \frac{-1}{\pi} \text{Im} [G_d] \quad (2.8.45)$$

$$\langle n_{d\sigma} \rangle = \int_{-\infty}^0 dE \rho_{d\sigma} = -\frac{1}{\pi} \text{Im} \int_{-\infty}^0 dE G_d(E) \quad (2.8.46)$$

Luttinger proved that

$$\int_{-\infty}^0 \Sigma' G dE = 0 \quad (2.8.47)$$

In order to use this, note that

$$\begin{aligned} \ln G_d^{-1} &= \ln (E - \epsilon_d + i\Delta - \Sigma) \\ \implies \frac{d \ln G_d^{-1}}{dE} &= \frac{1}{E - \epsilon_d + i\Delta - \Sigma} (1 - \Sigma') = G_d - \Sigma' G_d \\ \implies G_d &= \Sigma' G_d - \frac{d \ln G_d}{dE} \end{aligned} \quad (2.8.48)$$

Substituting this expression for  $G_d$  in eq. 2.8.46,

$$\langle n_{d\sigma} \rangle = -\frac{1}{\pi} \text{Im} \int_{-\infty}^0 \Sigma' G dE + \frac{1}{\pi} \text{Im} \int_{-\infty}^0 \frac{d \ln G_d}{dE} dE \quad (2.8.49)$$



The first integral is zero, courtesy Luttinger. We get

$$\begin{aligned}
\langle n_{d\sigma} \rangle &= \frac{1}{\pi} \text{Im} \left[ \ln \frac{1}{E - \epsilon_d + i\Delta - \Sigma} \right]_{-\infty}^0 \\
&= -\frac{1}{\pi} \text{Im} \left[ \ln (E - \epsilon_d + i\Delta - \Sigma) \right]_{-\infty}^0 \\
&= -\frac{1}{\pi} \text{Im} \left[ \ln e^{i\theta} \right]_{-\infty}^0 \quad \left[ \tan \theta = \frac{\Delta}{E - \epsilon_d - \Sigma} \right] \\
&= -\frac{1}{\pi} [\theta(0) - \theta(-\infty)] \\
&= \frac{1}{\pi} \tan^{-1} \frac{\Delta}{\epsilon_d + \Sigma(0, h)} \\
&= \frac{1}{2} - \frac{1}{\pi} \tan^{-1} \frac{\epsilon_d + \Sigma(0, h)}{\Delta}
\end{aligned} \tag{2.8.50}$$

We can now relate the average occupancy with the density of states. From eq. 2.8.45,

$$\begin{aligned}
\rho_{d\sigma} &= \frac{1}{\pi} \frac{\Delta}{(\epsilon_d + \Sigma(0))^2 + \Delta^2} \\
&= \frac{1}{\pi\Delta} \left[ 1 + \left( \frac{\epsilon_d + \Sigma(0)}{\Delta} \right)^2 \right]^{-1} \\
&= \frac{1}{\pi\Delta} \left[ 1 + \cot^2 \pi \langle n_{d\sigma} \rangle \right]^{-1} \\
&= \frac{\sin^2 \pi \langle n_{d\sigma} \rangle}{\pi\Delta}
\end{aligned} \tag{2.8.51}$$

## 2.9 Poor Man's scaling of the SIAM

First consider the case in which  $\epsilon_d \ll -D, U + \epsilon_d \gg D$ . The situation is such that both the impurity levels are far outside the bandwidth, as shown in the left of fig. 2.2. The maximum energy scale at which scattering with conduction electrons can take place is of the order of the bandwidth  $D$ . Since the impurity energies are much higher than the bandwidth, no charge fluctuation can take place. The impurity state will be fixed at  $\epsilon_d$ . The only remaining degree of freedom will be the spin fluctuations, and we can then do the S-W transformation.

On the other hand, if we take the situation in the right of fig. 2.2 where both the impurity levels are far inside the bandwidth, then both the impurity levels will be on energy scales completely different from the bandwidth. So there won't be any renormalization of the impurity levels. From another perspective, it can be said that there won't be any renormalization because both the impurity levels  $|0\rangle, |1\rangle$  will be able to hybridize with two states each:  $|0\rangle$  can hybridize with  $|k \uparrow\rangle, |k \downarrow\rangle$  and  $|1\rangle$  can hybridize with  $|0\rangle, |2\rangle$ .

The limit where there will be some renormalization is the following. We are working with the asymmetric Anderson model, that is,  
 $U + \epsilon_d \gg D \gg |\epsilon_d|, \Delta$ . The total Hamiltonian is

$$H = \sum_{k\sigma} \epsilon_{k\sigma} n_{k\sigma} + \epsilon_d \sum_{\sigma} n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow} + \sum_{k\sigma} \left( V_{kd} c_{k\sigma}^\dagger c_{d\sigma} + V_{kd}^* c_{d\sigma}^\dagger c_{k\sigma} \right) \tag{2.9.1}$$

This means that the doubly-occupied state is decoupled from the conduction band; it cannot hybridize through the  $V_{kd}$  because the virtual transition will involve a huge amount of energy and so it is practically impossible.

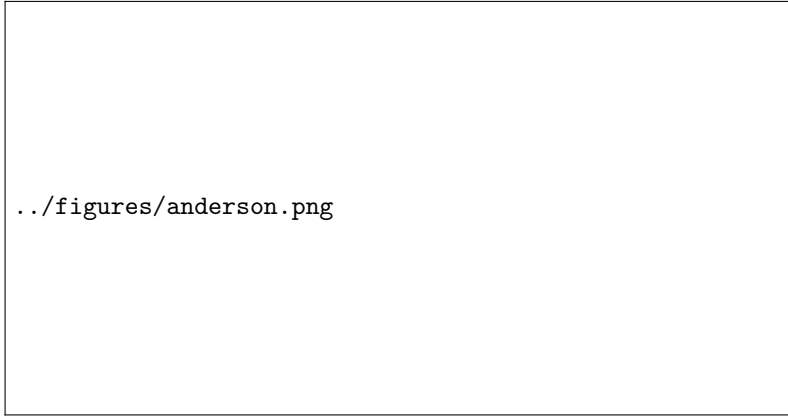


Figure 2.2: *Left*: Both impurity levels far outside the bandwidth. *Right*: Both impurity levels comfortably inside the bandwidth.

At the first iteration, we will reduce the cut-off from  $D$  to  $D - \delta D$ . The zeroth approximation to this Hamiltonian is

$$H^{(0)} = \sum_{k < D - \delta D, \sigma} \epsilon_{k\sigma} n_{k\sigma} + \epsilon_d \sum_{\sigma} n_{d\sigma} + \sum_{k < D - \delta D, \sigma} \left( V_{kd} c_{k\sigma}^{\dagger} c_{d\sigma} + V_{kd}^* c_{d\sigma}^{\dagger} c_{k\sigma} \right) \quad (2.9.2)$$

As is apparent, the zeroth approximation involves completely ignoring the region to be integrated out. All kinetic energies and actual scatterings are strictly within the smaller region  $[-D + \delta D, D - \delta D]$ . The higher approximations allow these states to make virtual transitions to the band edge states and then come back. The Hamiltonian term for the virtual excitation in to the upper band edge (with a particle in the intermediate state) is

$$H_{\sigma}^{(1,p)} = \sum_{k \in k^+} \alpha_{k\sigma} c_{d\sigma}^{\dagger} c_{k\sigma} c_{k\sigma}^{\dagger} c_{d\sigma} \quad (2.9.3)$$

There are two things to note here. Firstly,  $\alpha_{k\sigma}$  is the probability of such a virtual transition and is found from perturbation theory. Secondly, the summation  $k^+$  is over the states in  $[D - \delta D, D]$ . To calculate  $\alpha_{k\sigma}$ , note that such a virtual excitation can take place only from the state  $1_{d\sigma}$ . Therefore, we look at the first order correction to this state under the perturbation  $V_{kd}$ .

$$\alpha_{k\sigma} = \frac{\langle 1_{d\sigma} | V_{kd}^* c_{d\sigma}^{\dagger} c_{k\sigma} | k\sigma \rangle \langle k\sigma | V_{kd} c_{k\sigma}^{\dagger} c_{d\sigma} | 1_{d\sigma} \rangle}{E_{1_{d\sigma}} - E_{k\sigma}} = \frac{|V_{kd}|^2}{\epsilon_d - \epsilon_k} \quad (2.9.4)$$

The analogous term in the same order for the virtual transition to the lower edge consists of a hole in the intermediate state, because the lower edge states are already filled. This term is of the form

$$H^{(1,h)} = \sum_{k \in k^-, \sigma} \beta_{k\sigma} c_{k\sigma}^{\dagger} c_{d\sigma} c_{k\sigma} c_{d\sigma}^{\dagger} \quad (2.9.5)$$

$\beta_{k\sigma}$  is calculated similarly, using perturbation theory.

$$\beta_{k\sigma} = \frac{\langle 0 | V_{kd}^* c_{d\sigma} c_{k\sigma}^{\dagger} | k\sigma \rangle \langle k\sigma | V_{kd} c_{k\sigma} c_{d\sigma}^{\dagger} | 0 \rangle}{E_0 - E_{k\sigma}} = \frac{|V_{kd}|^2}{\epsilon_k - \epsilon_d} \quad (2.9.6)$$

The total first order correction to the Hamiltonian is of the form

$$H^{(1)} = \sum_{k^+, \sigma} \alpha_{k\sigma} T_{k\sigma}^+ + \sum_{k^-, \sigma} \beta_{k\sigma} T_{k\sigma}^- \quad (2.9.7)$$

$T^{+,-}$  represent virtual transitions to the upper and lower edges. Since these terms do not cause any real fluctuations in the impurity sites, they renormalize only the impurity energy  $\epsilon_d$ , and not the hybridisation coupling  $V_{kd}$ . To find the renormalization in the site energies  $\epsilon_0$  and  $\epsilon_1$  (and hence in  $\epsilon_d \equiv \epsilon_1 - \epsilon_0$ ), note that the term  $T^+$  virtually excites the state  $n_{d\sigma} = 1$ , and hence the change in  $\epsilon_1$  is

$$\delta\epsilon_1 = \alpha_{k\sigma} = \sum_{k^+} \frac{|V_{kd}|^2}{\epsilon_d - \epsilon_k} \quad (2.9.8)$$

We can write this summation in terms of  $\Delta(E) = \pi N(E)V^2(E)$ , under the assumption  $\Delta(E) \approx \Delta$  for  $E \in \{-D, D\}$ .

$$\delta\epsilon_1 = \sum_{k^+} \frac{|V_{kd}|^2}{\epsilon_d - \epsilon_k} = \int_{D-\delta D}^D dE N(E) \frac{|V(E)|^2}{\epsilon_d - E} \approx \frac{\Delta}{\pi} \frac{|\delta D|}{\epsilon_d - D} \quad (2.9.9)$$

The change in  $\epsilon_0$  is

$$\delta\epsilon_0 = \sum_{\sigma} \beta_{k\sigma} \approx -2 \frac{\Delta}{\pi} \frac{|\delta D|}{\epsilon_d + D} \quad (2.9.10)$$

The change in the denominator occurs because in the lower edge,  $\epsilon_k = -D$ . The change in  $\epsilon_d$  is

$$\delta\epsilon_d = \delta\epsilon_1 - \delta\epsilon_0 = \frac{\Delta|\delta D|}{\pi} \left[ \frac{1}{\epsilon_d - D} + \frac{2}{\epsilon_d + D} \right] = \frac{\Delta}{\pi} \frac{|\delta D|}{D} = -\frac{\Delta}{\pi} \delta \ln D \quad (2.9.11)$$

We assumed  $D \gg \epsilon_d$ . In the limit of infinitesimal change, we get the equation

$$\frac{d\epsilon_d}{d \ln D} = -\frac{\Delta}{\pi} \quad (2.9.12)$$

If we had allowed the  $|1_{d\sigma}\rangle$  to hybridize with the state  $|2_d\rangle$  (that is, if we had assumed both  $U$  and  $\epsilon_d$  to be  $\ll D$ ), then  $\alpha_{k\sigma}$  would have had another term added to it:

$$\frac{|V_{kd}|^2}{\epsilon_k - U - \epsilon_d} \approx \frac{|V|^2}{-D - U - \epsilon_d} \quad (2.9.13)$$

$-(U + \epsilon_d)$  is the change in energy from  $|1_d\rangle$  to  $|2_d\rangle$  and  $-D$  is the energy of the hole created in the process. The renormalization in  $\epsilon_d$  would then have been

$$\delta\epsilon_d = \frac{\Delta|\delta D|}{\pi} \left( \frac{1}{\epsilon_d - D} - \frac{1}{D + U + \epsilon_d} + \frac{2}{\epsilon_d + D} \right) \quad (2.9.14)$$

which is zero in the limit of  $U, |\epsilon_d| \ll D$ . This is the equal renormalization in  $\epsilon_0$  and  $\epsilon_1$  discussed earlier.

We do not yet know whether  $\Delta$  is a function of the cutoff  $D$ . To find the renormalization of  $\Delta$ , we need to find the renormalization of  $V_{kd}$ . Note that the lowest order virtual transitions do not cause any actual charge fluctuation, and hence they do not renormalize  $V_{kd}$ . To see the renormalization of  $V_{kd}$ , we need to consider one order higher. These higher order terms involve transitions within the lower subspace along with virtual transitions into the higher subspaces.

$$H^{(2)} = \sum_{k^+, q, \sigma} \alpha_{k\sigma} T_{k\sigma}^+ \gamma_{q, k, \sigma} c_{d\sigma}^\dagger c_{q\sigma} + \sum_{k^-, q, \sigma} \beta_{k\sigma} T_{k\sigma}^- \gamma_{q, k, \sigma} c_{d\sigma} c_{q\sigma}^\dagger \quad (2.9.15)$$

The  $\gamma_{k\sigma}$  can be calculated as

$$\begin{aligned} \alpha_{k\sigma} \gamma_{q, k, \sigma} &= \frac{\langle 1_{d\sigma} | V_{kd}^* c_{d\sigma}^\dagger c_{k\sigma} | k\sigma \rangle \langle k\sigma | V_{kd} c_{k\sigma}^\dagger c_{d\sigma} | 1_{d\sigma} \rangle \langle 1_{d\sigma} | V_{kd} c_{q\sigma} c_{d\sigma}^\dagger | q\sigma \rangle}{(E_{1_{d\sigma}} - E_{k\sigma})(E_q - E_k)} \\ &= \alpha_{k\sigma} \frac{V_{kd}}{\epsilon_q - \epsilon_k} \end{aligned} \quad (2.9.16)$$

The renormalization in  $V_{kd}$  is therefore

$$\delta V_{kd} = \frac{\Delta}{\pi} \frac{|\delta D|}{\epsilon_d - D} \frac{V_{kd}}{\epsilon_q - \epsilon_k} \quad (2.9.17)$$

Close to the band edge, we get

$$\delta V = \frac{\Delta}{\pi} \frac{|\delta D|}{\epsilon_d - D} \frac{V}{D} \approx \frac{\Delta}{\pi} \frac{|\delta D|}{D^2} V \quad (2.9.18)$$

Therefore,

$$\delta\Delta \sim V\delta V = \frac{\Delta V^2}{\pi D^2} |\delta D| \implies \frac{d\Delta}{dD} \sim \left( \frac{\Delta}{D} \right)^2 \quad (2.9.19)$$

For  $D \gg \Delta$ , this will vanish very quickly. Hence, in this regime, there is no renormalization of  $\Delta$ , and we can take it to be a constant in the renormalization flow. Integrating eq. 2.9.12 gives

$$\epsilon_d = -\frac{\Delta}{\pi} \ln D + \text{constant} \quad (2.9.20)$$

Defining the constant as

$$\text{constant} = \epsilon_d^* + \frac{\Delta}{\pi} \ln \Delta \quad (2.9.21)$$

we get

$$\epsilon_d = -\frac{\Delta}{\pi} \ln D + \epsilon_d^* + \frac{\Delta}{\pi} \ln \Delta \quad (2.9.22)$$

$$\implies \epsilon_d = \epsilon_d^* - \frac{\Delta}{\pi} \ln \frac{D}{\Delta} \quad (2.9.23)$$

This result is in the regime  $U + \epsilon_d \gg D \gg |\epsilon_d|$ . Even if  $U \ll D$  initially, scaling will begin once  $D \sim U$ . Until then, as mentioned previously, both  $\epsilon_1$  and  $\epsilon_0$  will change equally and there won't be any scaling in  $\epsilon_d$ . If we start with  $U \ll D$ , under scaling, as  $D$  will decrease, there won't be any renormalization until we reach the point  $D \sim U$ .

Say, as a result of scaling, the bandwidth decreases and  $\epsilon_d$  increases (which it will, as is apparent from the eq. 2.9.23). At some point,  $-D \lesssim \epsilon_d$ . At this point, perturbation theory breaks down and we resort to SWT. We denote this point of the scaling by  $D = -a\tilde{\epsilon}_d, a > 1$ . We can then express the SWT coupling constant  $\tilde{J}$  by replacing  $\epsilon_d$  with  $\tilde{\epsilon}_d$  in eq. 2.4.26. For simplicity set  $U = \infty$ . Then,

$$\tilde{J} = -\frac{|V|^2}{\tilde{\epsilon}_d} = \frac{a|V|^2}{D} \quad (2.9.24)$$

We can then do the poor man's scaling with this coupling. From eq. 2.4.173,

$$\begin{aligned} T_K &\sim D \sqrt{\tilde{J}N(0)^2} \exp \left\{ -\frac{1}{2\tilde{J}N(0)^2} \right\} = \sqrt{\Delta D} \exp \left\{ -\frac{D}{2\Delta} \right\} \\ &\sim D \sqrt{\frac{\Delta}{D}} \exp \left\{ \frac{\epsilon_d}{2\Delta} \right\} \end{aligned} \quad (2.9.25)$$

A different result is obtained if one is in the regime of  $\epsilon_d < -D$ . This is the situation mentioned at the very beginning of the discussion, left of fig. 2.2. Assuming  $U \rightarrow \infty$  and  $\epsilon_d$  outside the conduction band, we can do a SWT and the  $T_K$  obtained is q. 2.4.173,

$$J = -\frac{V^2}{\epsilon_d} \quad (2.9.26)$$

$$g = J\rho = -\frac{\Delta}{\epsilon_d} \quad (2.9.27)$$

$$\implies T_K = D \sqrt{\frac{\Delta}{\epsilon_d}} \exp \left\{ \frac{\epsilon_d}{2\Delta} \right\} \quad (2.9.28)$$

The two forms of the Kondo temperature show that the prefactor is not a universal function; it depends on the starting conditions (the microscopic Hamiltonian from which we start the scaling). But the universal fact is that in the local moment regime ( $U \rightarrow \infty$ ), all physical quantities will involve only one energy scale,  $T_K$ . This  $T_K$  itself might be different based on the starting Hamiltonian.

For  $\epsilon_d^* \gg \Delta$ , the renormalization will stop at  $D \sim \epsilon_d$ . Note that we had assumed  $D \gg \epsilon_d$ . That was the starting condition, that is,  $\epsilon_d$  deep inside the Fermi surface. During the renormalization,  $D$  will keep on decreasing and  $\epsilon_d$  will continuously increase. At some value of  $D$ , they will become equal and the impurity level will go outside the Fermi surface. At this point, none of the impurity levels can renormalize any more, because the relevant energy scales are greater than the cutoff. Hence the renormalization stops at this point. This point is given by  $\bar{D} = a\epsilon_d(\bar{D}) \equiv \bar{\epsilon}_d$  where  $a$  is a constant of order unity. It satisfies the equation

$$\bar{\epsilon}_d = \epsilon_d^* - \frac{\Delta}{\pi} \ln \frac{a\bar{\epsilon}_d}{\Delta} \quad (2.9.29)$$

Figure 2.3: Renormalization in the energy levels when  $\epsilon_d^* \gg \Delta$ 

which is just eq. 2.9.23 with the substitution  $D = a\bar{\epsilon}_d$ . In this regime, because  $\epsilon_d \gg \Delta$ , we can do a perturbative expansion of the bare Hamiltonian in terms of  $\frac{\Delta}{\epsilon_d}$ . The susceptibility is

$$\chi_d = \frac{\Delta}{2\pi} \left( \frac{g\mu_B}{\epsilon_d} \right)^2 \left[ 1 + \frac{2\Delta}{\pi\epsilon_d} \ln \frac{\epsilon_d}{D} + \dots \right] \quad (2.9.30)$$

From the scaling, we know that  $D$  can be decreased to  $\bar{D}$ . We can hence substitute  $D = a\bar{\epsilon}_d$ ,  $\epsilon_d = \bar{\epsilon}_d$ . With this in mind, the susceptibility becomes

$$\begin{aligned} \chi_d &= \frac{\Delta}{2\pi} \left( \frac{g\mu_B}{\bar{\epsilon}_d} \right)^2 \left[ 1 + \frac{2\Delta}{\pi\bar{\epsilon}_d} \ln a + \dots \right] \\ &= \frac{\Delta}{2\pi} \left( \frac{g\mu_B}{\bar{\epsilon}_d} \right)^2 \left[ 1 + \mathcal{O} \left( \frac{2\Delta}{\pi\bar{\epsilon}_d} \right) \right] \end{aligned} \quad (2.9.31)$$

where I used the fact that  $\ln a$  will be of order 1. As we go on decreasing the cutoff, the impurity level will go on moving farther away from the Fermi level, and impurity site will become null occupied:  $\langle n_d \rangle \approx 0$ . The critical cutoff  $\bar{D}$  can be associated with a temperature scale  $k_b \bar{T} = \bar{D}$ . At temperatures sufficiently below this temperature ( $T \ll \bar{T}$ ), the susceptibility becomes (again from perturbation theory)

$$\chi_d(T) = \frac{\Delta}{2\pi} \left( \frac{g\mu_B}{\bar{\epsilon}_d} \right)^2 + \frac{1}{4T} \left[ 1 + \frac{1}{2} \exp \left\{ \frac{T^*}{T} \right\} \right]^{-1} \quad (2.9.32)$$

For temperatures sufficiently low, which we demarcate by a temperature  $T_{FL}$ , the denominator in the second term will be sufficiently large so that we can ignore that term with respect to the first term:

$$T \gg T_{FL} \implies e^{\frac{T^*}{T}} \gg 1 \implies \left[ 1 + \frac{1}{2} \exp \left\{ \frac{T^*}{T} \right\} \right]^{-1} \approx 0 \quad (2.9.33)$$

The susceptibility in this low temperature range can thus be written as

$$\chi_d = \frac{\Delta}{2\pi} \left( \frac{g\mu_B}{\bar{\epsilon}_d} \right)^2 \quad (2.9.34)$$

This is analogous to the result obtained in eq. 2.6.20, from the mean field version of the Fermi liquid theory, and also obtained from a renormalized perturbation theory of Anderson model. To see how, note that since we are in

the limit  $\langle n_d \rangle = 0$ , the onsite repulsion term  $U$  can be dropped because there is no probability of double occupation. Eq. 2.6.20 then becomes

$$\chi_d = \frac{g^2 \mu_B^2}{2} \rho_d(0) = \frac{g^2 \mu_B^2}{2} \frac{\Delta}{\pi} \frac{1}{\bar{\epsilon}_d^2 + \Delta^2} \quad (2.9.35)$$

Next note that we had assumed at the beginning that  $\epsilon_d^* \gg \Delta$ . We need to find the relative order difference between  $\bar{\epsilon}_d$  and  $\Delta$ . From eq. 2.9.29, we can drop the  $\pi$  and  $a$  because they are of order 1.

$$\bar{\epsilon}_d = \epsilon_d^* - \Delta \ln \frac{\bar{\epsilon}_d}{\Delta} \quad (2.9.36)$$

Dividing through by  $\Delta$  and defining  $x_1 = \frac{\bar{\epsilon}_d}{\Delta}, x_2 = \frac{\epsilon_d^*}{\Delta}$ , we get

$$x_1 + \ln x_1 = x_2 \quad (2.9.37)$$

Since  $O(\ln x_1) \leq O(x_1)$ , we can write

$$O(x_1) = O(x_2) \quad (2.9.38)$$

$$\implies O\left(\frac{\bar{\epsilon}_d}{\Delta}\right) = O\left(\frac{\epsilon_d^*}{\Delta}\right) \quad (2.9.39)$$

$$\implies O(\bar{\epsilon}_d) = O(\epsilon_d^*) \quad (2.9.40)$$

$$(2.9.41)$$

Since  $\bar{\epsilon}_d$  and  $\epsilon_d^*$  are of the same order, we can say:

$$\epsilon_d^* \gg \Delta \implies \bar{\epsilon}_d \gg \Delta \quad (2.9.42)$$

Applying this to eq. 2.9.35 means

$$\chi_d \approx \frac{g^2 \mu_B^2}{2} \frac{\Delta}{\pi} \frac{1}{\bar{\epsilon}_d^2} \quad (2.9.43)$$

which is the same as eq. 2.9.34. This tells us that scaling all the way down to very low temperatures in regime  $\epsilon_d^* \gg \Delta$  brings us into a Fermi liquid state, characterized by a temperature-independent susceptibility (as is standard in a Fermi liquid). The crossovers can be seen by looking at the variation of the Curie constant  $\chi T$ .

Since the susceptibility is proportional to the magnetic moment, presence of degeneracy will reduce this moment because the probability of occupying the states will decrease. As a result, the Curie constant is also a measure of the effective degeneracy of the impurity orbital. At very high temperatures  $T \gg U, \epsilon_d$ , all the impurity levels  $0, \epsilon_d$  and  $2\epsilon_d + U$  will become degenerate on energy scales of the order of  $k_B T$ . As a result, the Curie constant is approximately  $\frac{1}{8}$  in this range. The impurity occupancy is  $n_d = 1$ , because there are 4 degenerate states and the average number of electrons on them is 1. At lower temperatures  $U \gg T \gg T^*$ , the degeneracy gets lowered; now, only the vacant and single-occupied states are degenerate. Here the Curie constant is  $\frac{1}{6}$ . In this case, the average occupancy is  $n_d = \frac{0+1+1}{3} = \frac{2}{3}$ . At still lower temperatures, we saw that the impurity becomes vacant and  $n_d = 0$ . The Curie constant becomes linear in temperature, going down to 0. More formally,

$$m = \frac{1}{\beta} \frac{\partial \ln Z}{\partial B} \implies \chi = \lim_{B \rightarrow 0} \frac{\partial m}{\partial B} = \lim_{B \rightarrow 0} \frac{1}{Z^2 \beta} \left[ Z \frac{\partial^2 Z}{\partial B^2} - \left( \frac{\partial Z}{\partial B} \right)^2 \right] \quad (2.9.44)$$

For the case of four-fold degeneracy, all the states can be assumed to be at zero energy. Then, under a magnetic field  $B$  ( $h = \frac{g\mu_B}{2} B$ ), the partition function is

$$Z = 1 + \exp\{\beta h\} + \exp\{-\beta h\} + 1 = 2(1 + \cosh \beta h) \quad (2.9.45)$$

$$\implies \frac{\partial Z}{\partial B} = g\mu_B \beta \sinh \beta h \quad (2.9.46)$$

$$\implies \frac{\partial^2 Z}{\partial B^2} = \frac{1}{2} (g\mu_B)^2 \beta^2 \cosh \beta h \quad (2.9.47)$$

Since  $\lim_{h \rightarrow 0} \sinh \beta h = 0$  and  $\lim_{h \rightarrow 0} \cosh \beta h = 1$ , we get

$$\chi = \frac{\beta g^2 \mu_B^2}{2Z(h=0)} \quad (2.9.48)$$

Setting  $g\mu_B = k_B = 1$ , we get

$$\chi T = \frac{1}{2\mathcal{D}} \quad (2.9.49)$$

where  $Z(h=0) = 2 + 2 = 4 = \mathcal{D}$  is the degeneracy.

Similarly, for the triplet case ( $\epsilon_d$  and 0 are degenerate while  $U \gg T$ ), the doubly occupied case is essentially cut off from the available states, so  $Z = 1 + 2 \cosh \beta h$ . The proof again goes through similarly. But this time, we have  $Z(h=0) = 1 + 2 = 3 = \mathcal{D}$ .

For  $\epsilon_d = k_B T^* > k_B T$  such that  $k_B T^* \gg \Delta$ , we can find the magnetic moment in a perturbative fashion. At the zeroth order, we can neglect the hybridisation  $\Delta$ . Then,

$$m^{(0)} = \frac{1}{\beta} \frac{\partial \ln Z(h)}{\partial B} \quad (2.9.50)$$

where

$$Z(h) = 1 + e^{-\beta(k_B T^* - h)} + e^{-\beta(k_B T^* + h)} = 1 + e^{-\frac{\beta}{\beta^*}} 2 \cosh \beta h \quad (2.9.51)$$

Therefore,

$$\chi^{(0)} = \lim_{h \rightarrow 0} \frac{1}{\beta Z} \frac{\partial^2 Z}{\partial B^2} = \lim_{h \rightarrow 0} \frac{g^2 \mu_B^2}{4\beta Z} \frac{\partial^2 Z}{\partial h^2} = \frac{g^2 \mu_B^2}{4} \beta \frac{2e^{-\frac{\beta}{\beta^*}}}{1 + 2e^{-\frac{\beta}{\beta^*}}} \quad (2.9.52)$$

Again setting  $g\mu_B = k_B = 1$ , we get,

$$\chi^{(0)} = \frac{1}{4T} \frac{2e^{-\frac{\beta}{\beta^*}}}{1 + 2e^{-\frac{\beta}{\beta^*}}} = \frac{1}{4T} \frac{2}{e^{\frac{\beta}{\beta^*}} + 2} \quad (2.9.53)$$

As a first approximation, we can include the hybridisation by using the expression for the average number of spin up or spin down impurity as obtained from the non-interacting treatment, eq. 2.3.17

$$m^{(1)} = \frac{g\mu_B}{2} (n_\uparrow - n_\downarrow) = \frac{g\mu_B}{2\pi} \left[ \tan^{-1} \frac{\Delta}{k_B T^* - h} - \tan^{-1} \frac{\Delta}{k_B T^* + h} \right] \quad (2.9.54)$$

Since  $\Delta \ll T^*$ , we can expand the arctan in a Taylor series. Up to first order, we get

$$m^{(1)} = \frac{g\mu_B}{2\pi} \left[ \frac{\Delta}{k_B T^* - h} - \frac{\Delta}{k_B T^* + h} \right] = \frac{g\mu_B \Delta}{\pi} \frac{h}{k_B (T^*)^2 - h^2} \quad (2.9.55)$$

Differentiating with  $B$  gives

$$\chi^{(1)} = \lim_{h \rightarrow 0} \frac{\partial m^{(1)}}{\partial B} = \frac{g^2 \mu_B^2}{2} \frac{\Delta}{\pi} \frac{1}{k_B^2 T^{*2}} = \frac{\Delta}{2\pi T^{*2}} \quad (2.9.56)$$

Combining the zeroth and first order terms, the susceptibility in the regime  $T \lesssim T^*$  is

$$\chi = \frac{1}{4T} \frac{2}{e^{\frac{\beta}{\beta^*}} + 2} + \frac{\Delta}{2\pi T^{*2}} \quad (2.9.57)$$

Below some temperature  $T_{FL} \ll T^*$ , the susceptibility reduces to

$$\chi \approx \frac{1}{4T} \frac{2}{e^{\frac{\beta}{\beta^*}}} + \frac{\Delta}{2\pi T^{*2}} \approx \frac{\Delta}{2\pi T^{*2}} \quad (2.9.58)$$

$$\implies \chi T \propto T \quad (2.9.59)$$

Figure 2.4: Renormalization in energy levels when  $|\epsilon_d^*| \lesssim \Delta$ 

We can now visualize the various phases as the temperature is changed. For  $T \gg U, \epsilon_d$ , all the four states  $|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |2\rangle$  are degenerate ( $\mathcal{D} = 4$ ), the average occupancy is  $\langle n_d \rangle = \frac{0+1+1+2}{4} = 1$  and the effective Curie constant is  $\frac{1}{2\mathcal{D}} = \frac{1}{8}$ . At lower temperatures  $U \gg T \gg T^*$ , the level  $|2\rangle$  is disconnected from the conduction band and the three remaining states are now degenerate ( $\mathcal{D} = 3$ ). The average occupancy becomes  $\frac{0+1+1}{3} = \frac{2}{3}$  and the effective Curie constant is now  $\frac{1}{2 \times 3} = \frac{1}{6}$ . At still lower temperatures  $T^* \gg T$ , the singly-occupied levels become disconnected and the impurity occupancy becomes 0. The effective Curie constant in this regime is linear in  $T$ .

$$\begin{array}{ccc} n_d = 1 & & n_d = \frac{2}{3} & & n_d = 0 \\ \chi T \sim \frac{1}{8} & \implies & \chi T \sim \frac{1}{6} & \implies & \chi T \sim T \\ T \gg U & & T \gg T^* & & T \ll T^* \end{array}$$

Next we consider the mixed valence regime, described by  $|\epsilon_d^*| < \Delta$ . It is clear that since the impurity level is within an interval of the hybridisation from the Fermi surface, the charge fluctuations can cause transitions between the various states of the impurity. This means that the occupation number of the impurity site is not a good quantum number in this regime, and the average number of impurity electrons will be fractional. This definition is a bit arbitrary because any observed sample will display an eigenstate in which the impurity states have contributions from both  $\langle n_d \rangle = 0$  and  $\langle n_d \rangle = 1$ , so any sample will be mixed in that sense. However, if we are not in the mixed valence regime ( $|\epsilon_d| \gg \Delta$ ), then the contribution from any one state will far outweigh the other. If  $\epsilon_d > 0$ , then the impurity level is far above the Fermi level and it will most probably not be occupied and the majority of the contribution will come from  $\langle n_d \rangle = 0$ . Similarly, if  $\epsilon_d < 0$ , then the impurity level is far below the Fermi level and the average occupation will be close to 1. The regime of mixed valence is one in which these two contributions are comparable.

Since we have  $|\epsilon_d^*| \lesssim \Delta$ , as we renormalize, the decreasing cutoff will first match  $\Delta$  or  $k_B T$ , whichever is greater. From eq. 2.9.19, we know that if  $D$  comes close to  $\Delta$ , our analysis will break down because we can no longer ignore that term. Since that term represents the broadening of the impurity level, this same broadening can also be brought about by the thermal fluctuations which are of the scale  $k_B T$ . This means that real valence fluctuations will now renormalize the potential  $V_{kd}$ . Hence, our analysis will stop at  $D = \max\{\Delta, k_B T\}$ . For the simpler situation in which  $T = 0$ , the renormalization will stop at  $D = \Delta$ . From eq. 2.9.23, putting  $D = \Delta$ , we get

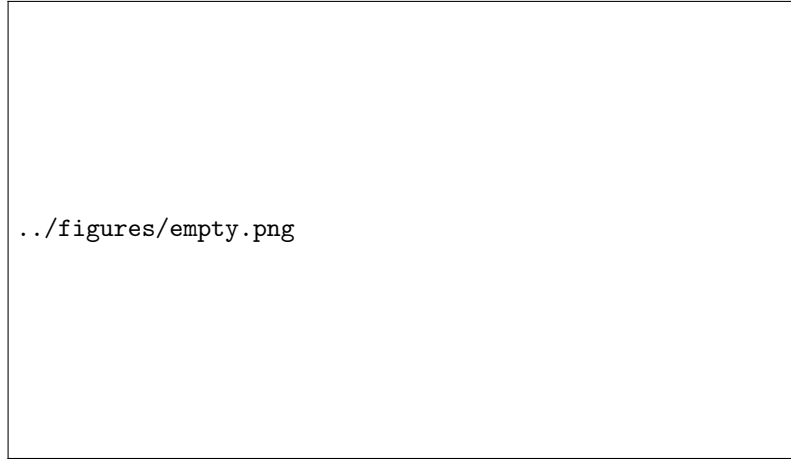
$$(\epsilon_d)_{\text{MV}} = \epsilon_d^* \quad (2.9.60)$$

This is the renormalized impurity level in the mixed valence regime. A characteristic feature of this regime is that the charge fluctuations can be thermally excited. This can be seen as follows. The probability of a transition from, say,  $|n_d = 0\rangle$  to  $|n_d = 1\rangle$  is

$$\sim \frac{k_B T}{\epsilon_d} \quad (2.9.61)$$

Assuming the thermal fluctuations are more or less of the order  $\Delta$ , for  $\epsilon_d \gg \Delta$ , this transition will not be possible. However, in the mixed valence regime, because  $\epsilon_d \sim \Delta$ , these excitations do occur. These fluctuations, as well as



Figure 2.5: Renormalization in energy levels when  $\epsilon_d^* \ll -\Delta$ 

the ones from the hybridisation with the conduction band, are responsible for the mixing of the singly-occupied and null-occupied states.

The crossovers in the mixed valence regime are as follows. Similar to the previous case, at high and intermediate temperatures, we have  $n_d = 1$  and  $n_d = \frac{2}{3}$  respectively. However, while the triplet degeneracy lasted upto  $T \sim T^*$  in the previous case, here it continues up to  $T \sim \Delta$  because that is where the scaling breaks down. That is,  $T = \Delta$  is the point where we can no longer ignore the renormalization in  $V$  and it begins to increase with scaling. Beyond this point, the impurity occupation remains fractional and not much else can be said.

$$\begin{array}{ccccc} n_d = 1 & & n_d = \frac{2}{3} & & n_d = \text{fractional} \\ \chi T = \frac{1}{8} & \implies & \chi T = \frac{1}{6} & \implies & \chi T \propto T \\ T \gg U & & T \gg \Delta & & T \ll \Delta \end{array}$$

For  $\epsilon_d^* \ll -\Delta$ , the scaling will stop when the impurity level again goes out of the Fermi surface. But this time, it goes out from below. This again decouples the singly-occupied state from the conduction band and the scaling stops. This happens at say  $\tilde{D} = -\tilde{\epsilon}_d = \tilde{T}$ . Since the singly-occupied impurity level is now well below  $-D$ , we have  $\langle n_d \rangle = 1$  and we are comfortably in the Kondo limit and the SWT and a consequent poor man's scaling can be performed, which will give eqs. 2.9.24 through 2.9.28. The result of the Schrieffer-Wolff transformation is a Hamiltonian that couples the impurity to the conduction electrons only through their spins; there is no charge fluctuation. At high temperatures  $T \gg T_K$ , the impurity is essentially decoupled and we get a susceptibility of the form eq. 2.9.49, but with a degeneracy of 2. To go to lower temperatures, we can do a Poor Man's scaling which suggests that the Hamiltonian at  $T \ll T_K$  is one with a large coupling between the impurity and the conduction electrons.

$$\begin{array}{ccccccc} n_d = 1 & & n_d = \frac{2}{3} & & n_d = 1 & & n_d = 1 \\ \chi T = \frac{1}{8} & = & \chi T = \frac{1}{6} & \implies & \chi T = \frac{1}{4} & \implies & \chi T \propto T \\ \frac{1}{8}T \gg U & \implies & T \gg \tilde{T} & & T \ll \tilde{T} & & T \ll \tilde{T}_K \end{array}$$

## Chapter 3

# 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.

### 3.1 Formalism

#### 3.1.1 Description of the problem

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

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

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

$$\mathcal{H} = \begin{pmatrix} |1\rangle & |0\rangle \\ H_1 & T \\ T^\dagger & H_0 \end{pmatrix} \quad (3.1.2)$$

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.

$$\tilde{\mathcal{H}} \equiv U\mathcal{H}U^\dagger = \begin{pmatrix} |1\rangle & |0\rangle \\ \tilde{H}_1 & 0 \\ 0 & \tilde{H}_0 \end{pmatrix} \quad (3.1.3)$$

$U_q$  is defined by

$$\tilde{\mathcal{H}} = U_q \mathcal{H} U_q^\dagger \text{ such that } [\tilde{\mathcal{H}}, n_q] = 0 \quad (3.1.4)$$

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

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

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

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

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

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

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

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

This gives

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

### 3.1.2 Obtaining the decoupling transformation

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

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

From the definition of  $\hat{\omega}_i$ , we can see that it is Hermitian and has no term that scatters in the subspace of  $q\beta$ , so it is diagonal in  $q\beta$  and we can expand it as  $\hat{\omega}_i = \hat{\omega}_i^1 \hat{n}_{q\beta} + \hat{\omega}_i^0 \left( 1 - \hat{n}_{q\beta} \right)$ . Using the expansion 3.1.6, we can write

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

Since the only requirement on  $|\psi_i\rangle$  is that it diagonalize the Hamiltonian in the subspace of  $q\beta$ , there is freedom in the choice of this state. We can exploit this freedom and choose the  $|\phi_0^i\rangle$  to be an eigenstates of  $\hat{\omega}_i^{1,0}$  corresponding to real eigenvalues  $\omega_i^{1,0}$ :

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

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

$$c_{q\beta}^\dagger T |0\rangle |\phi_0^i\rangle = \left( \omega_i^1 - \mathcal{H}^d \right) |1\rangle |\phi_1^i\rangle \quad (3.1.12)$$

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

$$T^\dagger c_{q\beta} |1\rangle |\phi_1^i\rangle = \left( \omega_i^0 - \mathcal{H}^d \right) |0\rangle |\phi_0^i\rangle \quad (3.1.13)$$

We now define two many-particle transition operators:

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

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

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

where  $\hat{\omega}_i = \omega_i^0 \left( 1 - \hat{n}_{q\beta} \right) + \omega_i^1 \hat{n}_{q\beta} = \begin{pmatrix} \omega_i^1 & \\ & \omega_i^0 \end{pmatrix}$  is a 2x2 matrix and  $\mathcal{H}^d = \mathcal{H}_0^d \left( 1 - \hat{n}_{q\beta} \right) + \mathcal{H}_1^d \hat{n}_{q\beta}$  and  $G = \left( \hat{\omega} - \mathcal{H}^d \right)^{-1}$ . It is easy to check that this reproduces the previous forms of  $\eta_0$  and  $\eta_1^\dagger$ . 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:

$$\eta^\dagger(\omega_i^0) = \eta^\dagger(\omega_i^1) \implies \frac{1}{\omega_i^1 - \mathcal{H}^d} c_{q\beta}^\dagger T = c_{q\beta}^\dagger T \frac{1}{\omega_i^0 - \mathcal{H}^d} \quad (3.1.16)$$

Henceforth we will assume that this constraint has been imposed.

In terms of these operators, eq. 3.1.13 becomes

$$\begin{aligned} |1\rangle |\phi_1^i\rangle &= \eta^\dagger |0\rangle |\phi_0^i\rangle \\ |0\rangle |\phi_0^i\rangle &= \eta |1\rangle |\phi_1^i\rangle \end{aligned} \quad (3.1.17)$$

These allow us to write

$$\begin{aligned} |\psi_1\rangle &= |1\rangle |\phi_1^i\rangle + |0\rangle |\phi_0^i\rangle = (1 + \eta) |1\rangle |\phi_1^i\rangle \\ |\psi_0\rangle &= (1 + \eta^\dagger) |0\rangle |\phi_0^i\rangle \end{aligned} \quad (3.1.18)$$

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

$$U_1 = 1 + \eta \quad (3.1.19)$$

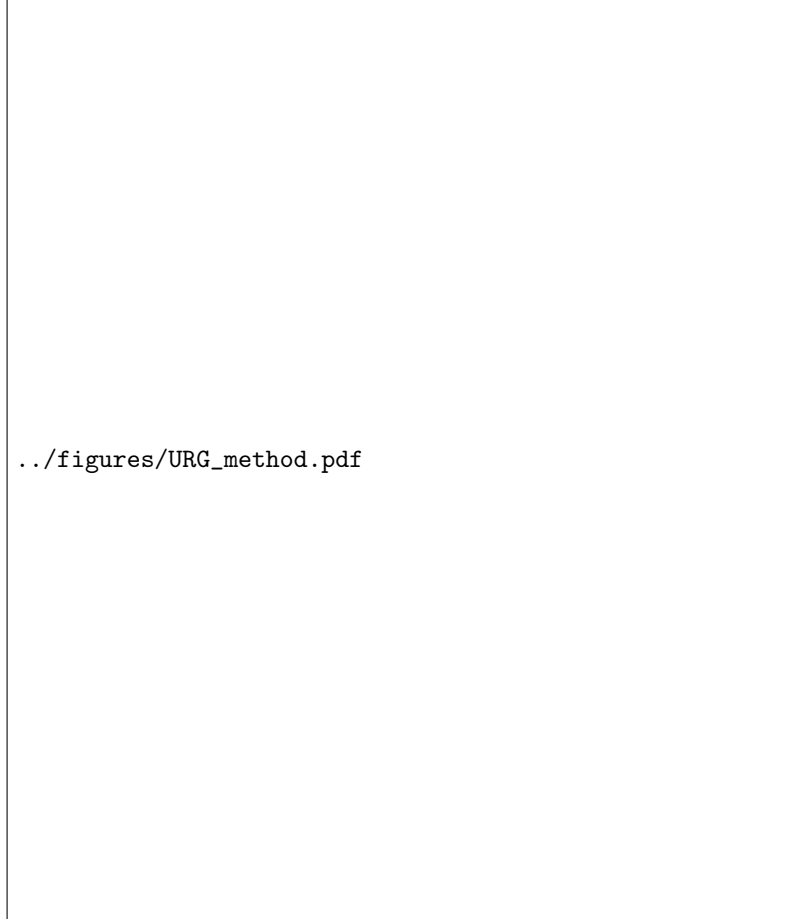


Figure 3.1: Three steps of the URG: Decompose the Hamiltonian in a  $2 \times 2$  matrix, apply the unitary operator to rotate it, then repeat these steps with one of the rotated blocks.

### 3.1.3 Properties of the many-body transition operators

The operators  $\eta$  have some important properties. First is the Fermionic nature:

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

Second is:

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

and hence the anticommutator

$$\implies \{\eta, \eta^\dagger\} = 1 \quad (3.1.22)$$

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

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

### 3.1.4 Form of the unitary operators

Although we have found the correct similarity transformations  $U_i$  (eqs. 3.1.19), we need to convert them into a unitary transformation. Say we are trying to rotate the eigenstate  $|\psi_1\rangle$  into the state  $|1\rangle$ . We can then work with the transformation

$$U_1 = 1 + \eta \quad (3.1.23)$$

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

$$U_1 = e^\eta \quad (3.1.24)$$

using the fact that  $\eta^2 = 0$ . It is shown in ref. [26] that corresponding to a similarity transformation  $e^\omega$ , there exists a unitary transformation  $e^G$  where

$$G = \tanh^{-1}(\omega - \omega^\dagger) \quad (3.1.25)$$

Applying that to the problem at hand gives

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

Let  $x = \tanh y$ . Then,

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

Therefore,

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

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

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

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

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

There we used

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

and hence

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

and so on.

### 3.1.5 Effective Hamiltonian

We can now compute the form of the effective Hamiltonian that comes about when we apply  $U_1$  - that is - when we rotate one exact eigenstate  $|\psi_1\rangle$  into the occupied Fock space basis  $|1\rangle$ . From eq. 3.1.29,

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

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

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

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

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

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

and

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

Group 2 becomes

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

To simplify this, we use the relation

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

which gives

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

Taking the Hermitian conjugate of eq. 3.1.39 gives

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

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

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

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

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

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

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

It can also be shown that

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

Putting it all together,

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

The renormalizing in the Hamiltonian is

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

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

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

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

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

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

### 3.1.6 Fixed point condition

Within the URG, it is a prescription that the fixed point is reached when the denominator of the RG equation vanishes. This is equivalent to either  $\omega_i^1 = \mathcal{H}_1^d$  or  $\omega_i^0 = \mathcal{H}_0^d$ . This shows that at the fixed point, one of the eigenvalues of  $\hat{\omega}_i$  matches the corresponding eigenvalue of the diagonal blocks. This also leads to the vanishing of the off-diagonal block, because eqs. 3.1.12 and 3.1.13 gives

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

### 3.1.7 Multiple off-diagonal terms

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

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

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

$$\omega^0 - E_1^0 = \omega^1 - E_1^1, \quad \omega^0 - E_2^0 = \omega^1 - E_2^1 \quad (3.1.51)$$

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

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

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

$$\omega_i^0 - \omega_i^1 = E_i^0 - E_i^1 \quad (3.1.53)$$

and so

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

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

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



### 3.1.8 Equivalence of the two unitaries and preservation of partial trace

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

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

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

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

This  $\eta$  will however be different from the  $\eta$  in eq. 3.1.29. The reason is, in order to get  $U_1$ , we must start from the eigenvalue equation  $\mathcal{H} |\psi_1\rangle = \tilde{H}_1 |\psi_1\rangle$ . This means that the corresponding  $\hat{\omega}$  will be defined as  $\hat{\omega}_1 = \tilde{H}_1 - \mathcal{H}^i$ . On the other hand, in order to get  $U_0$  we must start with  $\mathcal{H} |\psi_0\rangle = \tilde{H}_0 |\psi_0\rangle$ , and hence this  $\hat{\omega}$  will be  $\hat{\omega}_0 = \tilde{H}_0 - \mathcal{H}^i$ . This difference in the  $\hat{\omega}$  will define two different sets of  $\eta$ :

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

The  $\omega_j^i$  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  $\omega_j$ . The two unitaries are

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

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

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

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

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

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

$$\tilde{H} = \begin{pmatrix} E_1 & 0 \\ 0 & E_0 \end{pmatrix} \quad (3.1.61)$$

Therefore, the trace of the rotated Hamiltonian is  $t_{\text{new}} = E_1 + E_0$ . The trace of the LHS in the final equation of 3.1.60 is  $\text{tr}(\tilde{H}_1 + \tilde{H}_0) = \text{tr}(E_1 \otimes I + E_0 \otimes I) = 2(E_1 + E_0) = 2t_{\text{new}}$ . The trace of the RHS in final equation of 3.1.60 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  $t_{\text{new}} = t_{\text{old}}$ .

### 3.1.9 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  $U(t)$ :

$$O_j = U_j O(0) U_j^\dagger, \quad j = 1, 2, \dots \quad (3.1.62)$$

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

$$\Delta O_j \equiv O_{j+1} - O_j = [O_j, S_j] \quad (3.1.63)$$

where

$$S_j = U_j \Delta U_j^\dagger. \quad (3.1.64)$$

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. 3.1.62 is indeed the solution of eq. 3.1.63, we differentiate eq. 3.1.62:

$$O_{j+1} - O_j = \Delta U_j O(0) U_j^\dagger + U_j O(0) \Delta U_j^\dagger = \Delta U_j U_j^\dagger O_j + O_j U_j \Delta U_j^\dagger = [O_j, S_j] \quad (3.1.65)$$

This shows that given a family of operators eq. 3.1.62 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:

$$U_j = \frac{1}{\sqrt{2}} (1 + \eta_j^\dagger - \eta_j) \quad (3.1.66)$$

From the definition of the generator  $S_j$ , we then get

$$S_j = \frac{1}{2} (1 + \eta_j^\dagger - \eta_j) (\eta_{j+1} - \eta_{j+1}^\dagger - \eta_j + \eta_j^\dagger) \quad (3.1.67)$$

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

$$\eta_j |1\rangle |\phi_1\rangle = |0\rangle |\phi_0\rangle, \quad \eta_j |0\rangle |\phi_0\rangle = 0, \quad \eta_j^\dagger |0\rangle |\phi_0\rangle = |1\rangle |\phi_1\rangle, \quad \eta_j^\dagger |1\rangle |\phi_1\rangle = 0, \quad (3.1.68)$$

$$(3.1.69)$$

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

$$\begin{aligned} S^x &= \frac{1}{2} (S^+ + S^-) = \frac{1}{2} (\eta_j^\dagger + \eta_j) \\ S^y &= \frac{1}{2i} (S^+ - S^-) = \frac{1}{2i} (\eta_j^\dagger - \eta_j) \\ S^z &= \hat{n} - \frac{1}{2} \end{aligned} \quad (3.1.70)$$

The commutation relations give

$$\begin{aligned} [S^x, S^y] &= \frac{1}{4i} [\eta_j^\dagger + \eta_j, \eta_j^\dagger - \eta_j] = \frac{1}{2i} [\eta_j, \eta_j^\dagger] = \frac{1}{2i} (1 - \hat{n} - \hat{n}) = \frac{-1}{i} \left( \hat{n} - \frac{1}{2} \right) = iS^z \\ [S^y, S^z] &= \frac{1}{2i} \left[ \eta_j^\dagger - \eta_j, \hat{n} - \frac{1}{2} \right] = \frac{1}{2i} [-\eta_j \hat{n} - \hat{n} \eta_j^\dagger] = \frac{1}{2i} (-\eta_j - \eta_j^\dagger) = \frac{i}{2} (\eta_j^\dagger + \eta_j) = iS^x \\ [S^z, S^x] &= \frac{1}{2} \left[ \hat{n} - \frac{1}{2}, \eta_j^\dagger + \eta_j \right] = \frac{1}{2} [\hat{n} \eta_j^\dagger - \eta_j \hat{n}] = \frac{1}{2} (\eta_j^\dagger - \eta_j) = i \frac{1}{2i} (\eta_j^\dagger - \eta_j) = iS^y \end{aligned} \quad (3.1.71)$$

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

### 3.1.10 A note on the various quantum fluctuation scales $\omega_i^j$

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

$$\begin{aligned}\omega_1^0 - \omega_1^1 &= \mathcal{H}_d^0 - \mathcal{H}_d^1 \\ \omega_0^0 - \omega_0^1 &= \mathcal{H}_d^0 - \mathcal{H}_d^1 \\ \omega_1^0 + \omega_0^0 &= 2\mathcal{H}_d^0\end{aligned}\tag{3.1.72}$$

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  $\omega_1^0$  and  $\omega_0^1$  can be derived from these. This means that we have four  $\omega$  and three constraints, such that each step of the URG is characterized by just a single independent quantum fluctuation scale.

## 3.2 Prescription

Given a Hamiltonian

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

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

From eq. 3.1.45, the first two terms in the rotated Hamiltonian are just the diagonal parts of the bare Hamiltonian; they are unchanged in that part. The renormalization comes from the third term. For one electron  $q\beta$  on the shell, the renormalization is

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

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

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

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

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

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

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

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

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

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

$$\Delta\mathcal{H} = c_{q\beta}^\dagger \text{Tr}(\mathcal{H}c_{q\beta}) \eta_1 + \text{Tr}(c_{q\beta}^\dagger \mathcal{H}) c_{q\beta} \eta_0^\dagger \quad (3.2.7)$$

This form of the total renormalization is identical to the one we use in the "Poor Man's scaling"-type of renormalization that was used to get the scaling equations in the Kondo and Anderson models [27, 28]. Writing down the forms of  $\eta$  and  $\eta^\dagger$  explicitly, we get

$$\Delta\mathcal{H} = c_{q\beta}^\dagger \text{Tr}(\mathcal{H}c_{q\beta}) \frac{1}{\omega_1^0 - \mathcal{H}_0^d} \text{Tr}(c_{q\beta}^\dagger \mathcal{H}) c_{q\beta} + \text{Tr}(c_{q\beta}^\dagger \mathcal{H}) c_{q\beta} \frac{1}{\omega_0^1 - \mathcal{H}_1^d} c_{q\beta}^\dagger \text{Tr}(\mathcal{H}c_{q\beta}) \quad (3.2.8)$$

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

$$\Delta\mathcal{H} = \sum_{q\beta} \left[ c_{q\beta}^\dagger \text{Tr}(\mathcal{H}c_{q\beta}) \frac{1}{\omega_1^0 - \mathcal{H}_0^d} \text{Tr}(c_{q\beta}^\dagger \mathcal{H}) c_{q\beta} + \text{Tr}(c_{q\beta}^\dagger \mathcal{H}) c_{q\beta} \frac{1}{\omega_0^1 - \mathcal{H}_1^d} c_{q\beta}^\dagger \text{Tr}(\mathcal{H}c_{q\beta}) \right] \quad (3.2.9)$$

These equations will now need to be simplified. For example, in the particle sector, we can set  $\hat{n}_{q\beta} = 0$  in the numerator, because there is no such excitation in the initial state. Similarly, in the hole sector, we can set  $\hat{n}_{q\beta} = 1$  because that state was occupied in the initial state. Another simplification we typically employ is that  $\mathcal{H}_{0,1}^d$  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;  $\text{Tr}(c_{q\beta}^\dagger \mathcal{H}) c_{q\beta}$  is the off-diagonal term that has  $c_{q\beta}$  in it, and  $c_{q\beta}^\dagger \text{Tr}(\mathcal{H}c_{q\beta})$  is the off-diagonal term that has  $c_{q\beta}^\dagger$  in it.  $\mathcal{H}^D$  is just the diagonal part of the Hamiltonian.

### 3.3 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. [29]. 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  $\epsilon_i$ . 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,  $\epsilon_1$  is the infrared limit and  $\epsilon_N$  is the ultraviolet limit.

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

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

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

#### 3.3.1 Calculation of Renormalization

The RG involves decoupling the nodes  $N$  through 1, and looking at the resultant renormalization in  $\epsilon_i$  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

$$\mathcal{H}^D = \epsilon_0 S_0^z + \epsilon_N S_N^z + J_N S_0^z S_N^z \quad (3.3.3)$$

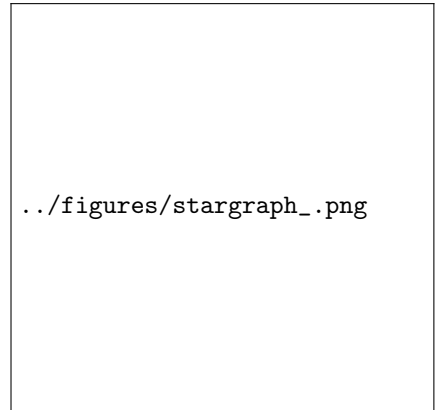


Figure 3.2: Star Graph model

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

$$\mathcal{H}_X = S_N^+ T + T^\dagger S_N^- = \frac{1}{2} J_N (S_N^+ S_0^- + S_N^- S_0^+) \quad (3.3.4)$$

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

$$\begin{aligned} \Delta\mathcal{H} &= S_N^+ T \frac{1}{\omega_0^1 - \mathcal{H}^D} T^\dagger S_N^- + T^\dagger S_N^- \frac{1}{\omega_1^0 - \mathcal{H}^D} S_N^+ T \\ &= \frac{J_N^2}{4} S_N^+ S_0^- \frac{1}{\omega_0^1 - \epsilon_0 S_0^z - \epsilon_N S_N^z - J_N S_0^z S_N^z} S_0^+ S_N^- + \frac{J_N^2}{4} S_0^+ S_N^- \frac{1}{\omega_1^0 - \epsilon_0 S_0^z - \epsilon_N S_N^z - J_N S_0^z S_N^z} S_N^+ S_0^- \end{aligned} \quad (3.3.5)$$

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.

$$\Delta\mathcal{H} = \frac{J_N^2}{4} S_N^+ S_0^- \frac{1}{\omega_1^0 - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} S_0^+ S_N^- + \frac{J_N^2}{4} S_0^+ S_N^- \frac{1}{\omega_0^1 + \frac{1}{2}\epsilon_0 - \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} S_N^+ S_0^- \quad (3.3.6)$$

To relate  $\omega_1^0$  and  $\omega_0^1$ , we use eq. 3.1.72:

$$\omega_1^0 + \omega_0^1 = \mathcal{H}_0^D + \mathcal{H}_1^D = -\frac{1}{2} J_N \implies \omega_1^0 \equiv \omega, \quad \omega_0^1 \equiv \omega' = -\frac{1}{2} J_N - \omega \quad (3.3.7)$$

So, the renormalization becomes

$$\Delta\mathcal{H} = \frac{J_N^2}{4} \frac{1}{\omega - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} (S_N^+ S_0^- S_0^+ S_N^- - S_0^+ S_N^- S_N^+ S_0^-) = \frac{J_N^2}{4} \frac{1}{\omega - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} (S_N^z - S_0^z) \quad (3.3.8)$$

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  $\epsilon_N$  and  $\epsilon_0$ .

$$\begin{aligned} \Delta\epsilon_N &= \frac{1}{4} J_N^2 \frac{1}{\omega - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \\ \Delta\epsilon_0 &= -\frac{1}{4} J_N^2 \frac{1}{\omega - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \end{aligned} \quad (3.3.9)$$

### 3.3.2 Nature of flows

We are interested in looking at the renormalization of the central node energy  $\epsilon_0$ , 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  $i \in \{1, N\}$ .

$$\Delta\epsilon_0 = -\frac{1}{4} J^2 \frac{1}{\omega - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon + \frac{1}{4}J} \quad (3.3.10)$$

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

$$\Delta\epsilon_0 = -\frac{1}{4} J^2 \frac{1}{\tilde{\omega} - \frac{1}{2}\epsilon_0} \quad (3.3.11)$$

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  $\epsilon_0$  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  $\epsilon_0$  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  $\epsilon_0$  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  $\epsilon_0$  will keep on increasing, and the denominator will keep on becoming more and more negative, meaning there cannot be a fixed point in this situation either. These situations are depicted in figure 3.3.

Since we cannot find a fixed point, we will use a different  $\omega$ . Instead of  $\omega_1^0$ , we will use  $\omega_1^1$ . From eq. 3.1.72, we have

$$\omega_1^0 - \omega_1^1 = \mathcal{H}_0^D - \mathcal{H}_1^D = \epsilon_0 - \epsilon_N = \epsilon_0 - \epsilon \quad (3.3.12)$$

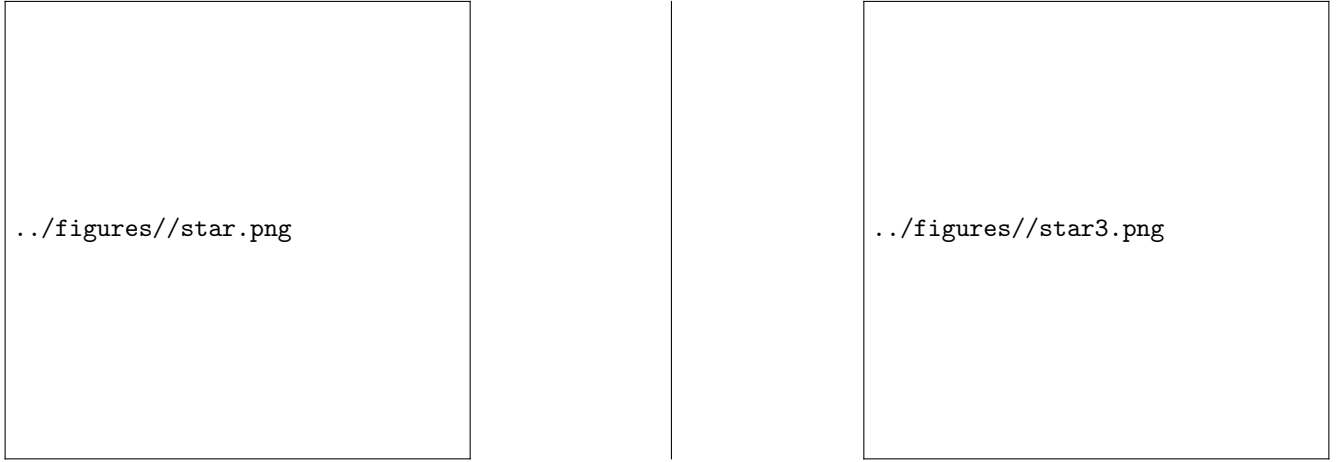


Figure 3.3: Left: RG flow for the two cases. The green line is the distance between the bare values of the two couplings, and hence also the magnitude of the denominator. The red arrow denotes the direction in which  $\epsilon_0$  will flow. Upward flow is increase. In both cases, the flow is such that 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.

Defining  $\omega_1^1 = \omega'$  and substituting this in eq. 3.3.10 gives

$$\Delta\epsilon_0 = -\frac{1}{4}J^2 \frac{1}{\omega' - \frac{1}{2}\epsilon + \frac{1}{2}\epsilon_0 + \frac{1}{4}J} \quad (3.3.13)$$

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

$$\Delta\epsilon_0 = \frac{1}{4}J^2 \frac{1}{\tilde{\omega} - \frac{1}{2}\epsilon_0} \quad (3.3.14)$$

We now repeat the exercise of determining the relevance of the flows under various regime. If we start with a bare  $\epsilon_0$  such that  $\tilde{\omega} + \frac{1}{2}\epsilon_0 > 0$ , then the denominator is positive so the renormalization will be irrelevant.  $\epsilon_0$  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  $\epsilon_0$  such that  $\tilde{\omega} + \frac{1}{2}\epsilon_0 < 0$ , then the denominator is negative so the renormalization will be relevant.  $\epsilon_0$  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 3.3.

### 3.3.3 Effective Hamiltonians

If  $\tilde{\omega}$  and  $\epsilon_0$  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

$$\mathcal{H}^* = 2\tilde{\omega}S_0^z + \epsilon \sum_i S_i^z + J \sum_i \vec{S}_i \cdot \vec{S}_0, \quad \text{if } \tilde{\omega}\epsilon_0 > 0 \quad (3.3.15)$$

If, at the bare level,  $\epsilon_0$  and  $\tilde{\omega}$  are of opposite signs, then  $\epsilon_0$  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.

$$\mathcal{H}^* = \epsilon \sum_i S_i^z + J \sum_i \vec{S}_i \cdot \vec{S}_0, \quad \text{if } \tilde{\omega}\epsilon_0 < 0 \quad (3.3.16)$$

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

$$\begin{aligned} \mathcal{H}^* &= 2\tilde{\omega}S_0^z + J \sum_i \vec{S}_i \cdot \vec{S}_0, & \text{if } \tilde{\omega}\epsilon_0 > 0 \\ \mathcal{H}^* &= J \sum_i \vec{S}_i \cdot \vec{S}_0, & \text{if } \tilde{\omega}\epsilon_0 < 0 \end{aligned} \quad (3.3.17)$$

### 3.3.4 Fixed points

The fixed points are obtained numerically by solving the RG equation. As mentioned before, there are two types of solutions: The first kind is those in which  $\epsilon_0$  and  $\tilde{\omega}$  are of the same sign, and the former flows to the latter without crossing the 0 axis. These flows are shown (obtained numerically) in fig. 3.4. The second kind are those where the two couplings have different signs, and so  $\epsilon_0$  flows to 0. These are shown in fig. 3.5.



Figure 3.4: Flows where  $\epsilon_0$  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  $\epsilon_0$ , the other less than that. The fixed point value is  $2\tilde{\omega}$ .



Figure 3.5: Flows where  $\epsilon_0$  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  $\epsilon_0$ , the other less than that. The fixed point value is 0.

## 3.4 URG analysis of the single-channel Kondo model

The Kondo model URG analysis was originally carried out in ref. [1]. A specific version of the model is described by the Hamiltonian

$$\mathcal{H} = \sum_{k\sigma} \epsilon_k \tau_{k\sigma} + \sum_{k,l} J^z S_d^z s_{kl}^z + \frac{1}{2} \sum_{k,l} J^t \left( S_d^+ s_{kl}^- + S_d^- s_{kl}^+ \right) \quad (3.4.1)$$

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  $s_{kl}^+ = s_{lk}^-$ . 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  $\beta$  the spin. The diagonal part of the Hamiltonian under this scheme is

$$H_{q\beta}^D = \epsilon_q \tau_{q\beta} + J^z S_d^z s_{qq}^z \quad (3.4.2)$$

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

$$\begin{aligned} H_1^I &= \sum_{|k| < \Lambda, q} J^z S_d^z s_{kq}^z + \frac{1}{2} \sum_{|k| < \Lambda, q} J^t \left( S_d^+ s_{kq}^- + S_d^- s_{kq}^+ \right) \\ H_0^I &= \sum_{|k| < \Lambda, q} J^z S_d^z s_{qk}^z + \frac{1}{2} \sum_{|k| < \Lambda, q} J^t \left( S_d^+ s_{qk}^- + S_d^- s_{qk}^+ \right) \end{aligned} \quad (3.4.3)$$

$H_1^I$  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.

### 3.4.1 Particle sector

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

$$H_0^I \frac{1}{\omega - H_{q\beta}^D} H_1^I \quad (3.4.4)$$

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

$$\begin{aligned} \frac{1}{\omega - D/2 + J/4} \sum_{|k, k'| < \Lambda, q} & \left[ \frac{1}{2} J^z J^t \left( S_d^z S_d^+ s_{qk'}^z s_{kq}^- + S_d^z S_d^- s_{qk'}^z s_{kq}^+ \right) + \frac{1}{2} J^t J^z \left( S_d^+ S_d^z s_{qk'}^- s_{kq}^z + S_d^- S_d^z s_{qk'}^+ s_{kq}^z \right) \right. \\ & \left. + \frac{1}{4} J^{t2} \left( S_d^- S_d^+ s_{qk'}^+ s_{kq}^- + S_d^+ S_d^- s_{qk'}^- s_{kq}^+ \right) \right] \end{aligned} \quad (3.4.5)$$

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

$$\frac{1}{\omega - D/2 + J/4} \sum_{|k, k'| < \Lambda, q} \left[ \frac{1}{4} J^z J^t \left( -\frac{1}{2} S_d^+ \hat{n}_q s_{kk'}^- - \frac{1}{4} S_d^- \hat{n}_q s_{kk'}^z \right) - \frac{1}{4} J^{t2} S_d^z \left( -\hat{n}_{q\uparrow} c_{k\downarrow}^\dagger c_{k'\downarrow} + \hat{n}_{q\downarrow} c_{k\uparrow}^\dagger c_{k'\uparrow} \right) \right] \quad (3.4.6)$$

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

$$\Delta H_1 = -\frac{1}{2} \frac{n(D)}{\omega - D/2 + J/4} \sum_{|k, k'| < \Lambda} \left[ J^z J^t \frac{1}{2} \left( S_d^+ s_{kk'}^- + S_d^- s_{kk'}^z \right) + J^{t2} S_d^z s_{kk'}^z \right] \quad (3.4.7)$$

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

$$\Delta J^z = -\frac{1}{2} \frac{J^{t2} n(D)}{\omega - D/2 + J/4}, \quad \Delta J^t = -\frac{1}{2} \frac{J^z J^t n(D)}{\omega - D/2 + J/4} \quad (3.4.8)$$



### 3.4.2 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

$$H_1^I \frac{1}{\omega - H_{q\beta}^D} H_0^I \quad (3.4.9)$$

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  $\Delta H_0 = \Delta H_1^\dagger = \Delta H_1$ .

### 3.4.3 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. 3.4.8):

$$\Delta J^z = -\frac{J^{t^2} n(D)}{\omega - D/2 + J/4}, \quad \Delta J^t = -\frac{J^z J^t n(D)}{\omega - D/2 + J/4} \quad (3.4.10)$$

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

$$\Delta J = -\frac{J^2 n(D)}{\omega - D/2 + \frac{1}{4}J} \quad (3.4.11)$$

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

$$\Delta J \approx \frac{J^2 n(D)}{D} \quad (3.4.12)$$

### 3.4.4 Numerical Solutions

The symmetric scaling equation 3.4.11 was solved numerically with the choice  $\omega = -\frac{\epsilon_q}{2}$ , for both positive and negative bare values of  $J$ . For sufficiently low values of  $\omega$ , 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. 3.7



Figure 3.6: 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).

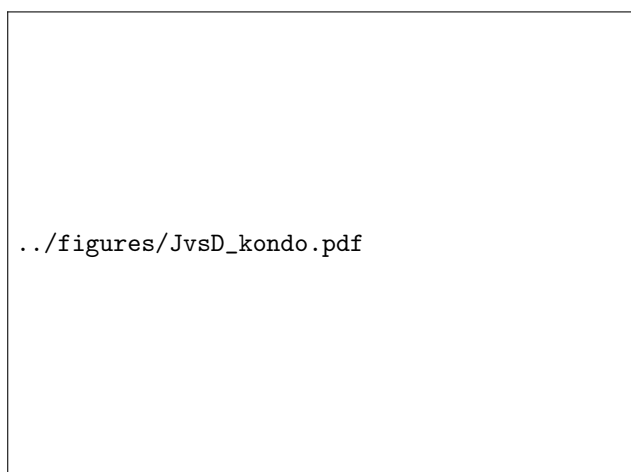


Figure 3.7: Variation of the fixed point value  $J^*$  against the bare bandwidth, in log scale.

## Chapter 4

# Connection between URG and Other Canonical Transformations

### 4.1 Poor man's scaling (PMS)

#### 4.1.1 Formalism

We first describe the formalism of the poor man's scaling (PMS) method, first formulated by Anderson [6]. The problem is defined as

$$\mathcal{H}|\Psi\rangle = E|\Psi\rangle \quad (4.1.1)$$

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

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

$$|\Psi\rangle = \sum_i |\phi_0^i\rangle + \sum_i |\phi_1^i\rangle \quad (4.1.2)$$

The Hamiltonian can also be split as

$$\mathcal{H} = H_0 + V_+ + V_- \quad (4.1.3)$$

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

$$\begin{aligned} V_+ \{|0\rangle\} &\mapsto \{|1\rangle\}, & V_+ |1\rangle &\rightarrow 0 \\ V_- \{|1\rangle\} &\mapsto \{|0\rangle\}, & V_- |0\rangle &\rightarrow 0 \end{aligned} \quad (4.1.4)$$

The Schrodinger equation can thus be split into

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

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

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

The effective Hamiltonian in this subspace is therefore

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

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

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

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

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

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

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

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

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

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

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

The second term similarly gives

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

The total renormalization becomes

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

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

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

However, closer inspection reveals that this choice makes the renormalization non-Hermitian. So the correct choice

is to keep both the initial and final energies.

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

Therefore,

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

In summary, the prescription of replacing all  $\omega$  with the initial state energy will be correct only if the initial and final states are the same. This happens when we are decoupling a single-electron state - then the total renormalization is of the form  $c^\dagger T^\dagger c$  such that we start from an initial state, scatter to an intermediate state and then go back to the initial state so that the final state is the same as the initial state. However, if we are using PMS to decouple states in one-shot, each subspace will have multiple states and there might be terms where we do not end up at the initial state we started with. Then the correct prescription would be to use the mean of the initial and final state denominators.

One might wonder how we can generate higher order terms in this method. Eq. 4.1.17, as it stands, has only  $\mathcal{O}(V^2)$  terms. The higher order terms were actually dropped when we replaced  $H_0$  with its diagonal part in eq. 4.1.12. To see the higher order term, we do not drop the off-diagonal part in the denominator, but split the total  $H_0$  into a diagonal and an off-diagonal part:  $H_0 = H_d + X$ . Note that  $X$  is off-diagonal in the subspace of the states that have not been decoupled yet but will be decoupled later. They represent scattering between the lower energy states.  $X$  is still diagonal with respect to the states that we are decoupling presently. The total effective Hamiltonian becomes

$$\tilde{\mathcal{H}}(E) = H_0 + V \frac{1}{G_0(E)^{-1} - X} V^\dagger + V^\dagger \frac{1}{G_0(E)^{-1} - X} V \tag{4.1.18}$$

where  $G_0(E)^{-1} = E - H_d$  is the inverse of the non-interacting Greens function. To allow computation, we can expand the denominator in powers of  $XG_0(E)^{-1}$ :

$$\begin{aligned}
\Delta H \equiv \tilde{\mathcal{H}}(E) - H_0 &= V G_0(E) [1 + X G_0(E) + X G_0(E) X G_0(E) + \dots] V^\dagger + V^\dagger \frac{1}{G_0(E)^{-1} - X} V \\
&= \underbrace{V G_0(E) V^\dagger + V^\dagger G_0(E) V}_{\text{two vertex or one loop correction}} + \underbrace{V G_0(E) X G_0(E) V^\dagger + V^\dagger G_0(E) X G_0(E) V}_{\text{three vertex or two loop correction}} \\
&\quad + \text{higher loop corrections}
\end{aligned} \tag{4.1.19}$$

### 4.1.2 PMS third order equations for symmetric multi-channel Kondo model

To get a clear idea of what the various terms in eq. 4.1.19 mean, we will calculate the multi-channel Kondo model RG equations up to third order. The model is

$$H = \sum_{k\sigma,\gamma} \epsilon_{k\sigma}^{(\gamma)} c_{k\sigma}^\dagger c_{k\sigma}^{(\gamma)} + \sum_{k\alpha,k'\alpha',\gamma,a} J^a S_d^a \sigma_{\alpha\alpha'}^a c_{k\alpha}^{(\gamma)\dagger} c_{k'\alpha'}^{(\gamma)} \tag{4.1.20}$$

$a$  goes over  $x, y, z$  and represents the directions.  $S_d^a$  therefore represents the spin operators for the impurity along the  $x, y$  and  $z$  directions. The labels  $k\alpha$  and  $k'\alpha'$  sum over the conduction electrons, while the index  $\gamma$  represents

the channel. We will first calculate the second order terms. The virtual particle term is

$$VG_0(E)V^\dagger = \sum_{k,k',\alpha,\alpha',q,\beta,\gamma,a,b} c_{q\beta}^{(\gamma)\dagger} c_{k\alpha}^{(\gamma)} S_d^a \sigma_{\beta\alpha}^a \frac{J^a J^b}{E - H_d} c_{k'\alpha'}^{(\gamma)\dagger} c_{q\beta}^{(\gamma)} S_d^b \sigma_{\alpha'\beta}^b \quad (4.1.21)$$

The label  $q$  sums over the momentum states being decoupled ( $|\epsilon_q| \in [D - |\delta D|, D]$ ). The labels  $k, k'$ , on the other hand, sum over the momentum states that are not being decoupled, so they lie in the complimentary range. The denominator of the Greens function is the excitation energy  $\epsilon_q - \epsilon_{k'}$ . We will now simplify the term.

$$\begin{aligned} VG_0(E)V^\dagger &= \sum_{k,k',\alpha,\alpha',q,\beta,\gamma,a,b} \frac{J^a J^b}{\epsilon_q - \epsilon_{k'}} S_d^a \sigma_{\beta\alpha}^a S_d^b \sigma_{\alpha'\beta}^b c_{q\beta}^{(\gamma)\dagger} c_{k\alpha}^{(\gamma)} c_{k'\alpha'}^{(\gamma)\dagger} c_{q\beta}^{(\gamma)} \\ &= \sum_{k,k',\alpha,\alpha',\beta,\gamma,a,b} \frac{J^a J^b}{\epsilon_q - \epsilon_{k'}} S_d^a \sigma_{\beta\alpha}^a S_d^b \sigma_{\alpha'\beta}^b c_{k\alpha}^{(\gamma)} c_{k'\alpha'}^{(\gamma)\dagger} \sum_q \hat{n}_{q\beta}^{(\gamma)} \\ &= \sum_{k,k',\alpha,\alpha',\beta,\gamma,a,b} S_d^a \sigma_{\beta\alpha}^a S_d^b \sigma_{\alpha'\beta}^b c_{k\alpha}^{(\gamma)} c_{k'\alpha'}^{(\gamma)\dagger} \int_{-D}^{-D+|\delta D|} d\epsilon \rho(\epsilon) \frac{J^a J^b \hat{n}^{(\gamma)}(\epsilon)_\beta}{\epsilon_q - \epsilon_{k'}} \\ &= \sum_{k,k',\alpha,\alpha',\beta,\gamma,a,b} S_d^a \sigma_{\beta\alpha}^a S_d^b \sigma_{\alpha'\beta}^b c_{k\alpha}^{(\gamma)} c_{k'\alpha'}^{(\gamma)\dagger} \frac{J^a J^b \rho(0)|\delta D|}{-D} [\hat{n}(\epsilon) = \theta(-\epsilon), |\epsilon_{k'}| \ll D] \\ &= \sum_{\alpha,\alpha',a,b} S_d^a S_d^b (\sigma^b \sigma^a)_{\alpha',\alpha} \sum_{k,k',\gamma} c_{k\alpha}^{(\gamma)} c_{k'\alpha'}^{(\gamma)\dagger} \frac{J^a J^b \rho(0)|\delta D|}{-D} \\ &= \sum_{\alpha,\alpha',a,b} \left( \frac{1}{4} \delta_{ab} + \frac{i}{2} \sum_c \epsilon^{abc} S_d^c \right) \left( \delta_{ab} + i \sum_c \epsilon^{bac} \sigma^c \right) \sum_{\alpha',\alpha} c_{k\alpha}^{(\gamma)} c_{k'\alpha'}^{(\gamma)\dagger} \frac{J^a J^b \rho(0)|\delta D|}{-D} \end{aligned} \quad (4.1.22)$$

The spin part can now be simplified:

$$\begin{aligned} \sum_{a,b} J^a J^b \left( \frac{1}{4} \delta_{ab} + \frac{i}{2} \sum_c \epsilon^{abc} S_d^c \right) \left( \delta_{ab} + i \sum_c \epsilon^{bac} \sigma^c \right)_{\alpha',\alpha} &= \frac{\sum_a J^{a2}}{4} \delta_{\alpha,\alpha'} + \frac{1}{2} \sum_{a,b,c,c'} J^a J^b \epsilon^{abc} \epsilon^{abc'} S_d^c (\sigma^c)_{\alpha'\alpha} \\ &= \frac{\sum_a J^{a2}}{4} \delta_{\alpha,\alpha'} + \frac{1}{2} \sum_c S_d^c \sigma_{\alpha'\alpha}^c \left( \sum_{\substack{a,b \\ a \neq b}} J^a J^b - 2J^c \sum_{\substack{a \\ a \neq c}} J^a \right) \end{aligned} \quad (4.1.23)$$

The constant part renormalizes a potential scattering, so we drop that part. The renormalization from the other part is

$$\begin{aligned} \sum_{\alpha,\alpha',c} S_d^c \sigma_{\alpha'\alpha}^c \sum_{k,k',\gamma} c_{k\alpha}^{(\gamma)} c_{k'\alpha'}^{(\gamma)\dagger} \frac{\frac{1}{2} \left( \sum_{\substack{a,b \\ a \neq b}} J^a J^b - 2J^c \sum_{\substack{a \\ a \neq c}} J^a \right) \rho(0)|\delta D|}{-D} \\ = \sum_{\alpha,\alpha',c} S_d^c \sigma_{\alpha'\alpha}^c \sum_{k,k',\gamma} c_{k'\alpha'}^{(\gamma)\dagger} c_{k\alpha}^{(\gamma)} \frac{\frac{1}{2} \left( \sum_{\substack{a,b \\ a \neq b}} J^a J^b - 2J^c \sum_{\substack{a \\ a \neq c}} J^a \right) \rho(0)|\delta D|}{D} \end{aligned} \quad (4.1.24)$$

The virtual hole term  $V^\dagger G_0(E)V$  gives the same contribution. The total renormalization at second order is therefore

$$\delta J^c = \frac{\left( \sum_{\substack{a,b \\ a \neq b}} J^a J^b - 2J^c \sum_{\substack{a \\ a \neq c}} J^a \right) \rho(0)|\delta D|}{D} = \frac{2J^{c+1} J^{c-1} \rho(0)|\delta D|}{D} \quad (4.1.25)$$

where  $\{c-1, c, c+1\}$  is a cyclic permutation of  $\{x, y, z\}$ . This reveals that the anisotropic Kondo coupling RG equations have a cyclic form:

$$\delta J^x = \frac{2J^y J^z \rho(0)|\delta D|}{D} \quad (4.1.26)$$

Cyclic permutations of the labels  $x, y, z$  produce the other equations. From here on, we will assume  $J^a = J$  for simplicity. This gives, at second order,

$$\delta J = \frac{2J^2 \rho(0) |\delta D|}{D} \quad (4.1.27)$$

We now consider the third order term. The virtual hole three vertex term,  $V^\dagger G_0(E) X G_0(E) V$ , is of the form

$$J^3 \sum_{\substack{q, k_1, k_2, k, k', \\ \alpha, \alpha', \alpha_1, \alpha_2, \beta, \\ \gamma_1, \gamma_2}} c_{q\beta}^{(\gamma_1)\dagger} c_{k\alpha}^{(\gamma_1)} \vec{S}_d \cdot \vec{\sigma}_{\beta\alpha} \frac{1}{E - H_d} c_{k_1\alpha_1}^{(\gamma_2)\dagger} c_{k_2\alpha_2}^{(\gamma_2)} \vec{S}_d \cdot \vec{\sigma}_{\alpha_1\alpha_2} \frac{1}{E - H_d} c_{k'\alpha'}^{(\gamma_1)\dagger} c_{q\beta}^{(\gamma_1)} \vec{S}_d \cdot \vec{\sigma}_{\alpha'\beta} \quad (4.1.28)$$

The other term among the two third order terms is the virtual particle term. The labels  $q, k, k', k_1, k_2$  run over the momentum states,  $\alpha, \alpha', \alpha_1, \alpha_2, \beta$  run over the spin indices and  $\gamma_1, \gamma_2$  run over the channel indices.  $q, \beta$  are the labels of the momentum states that are being decoupled.  $|\epsilon_q|$  therefore lies in the range  $[D, D - \delta D]$ . The rest of the labels  $(k, \alpha), (k_1, \alpha_1), (k_2, \alpha_2)$  lie in the compliment range and represent electrons that are not being decoupled at this step.

The denominator of the right-most Greens function measures the energy difference between the initial state and the state reached after the first excitation. This difference is  $\epsilon_q - \epsilon_{k'}$ . Similarly, the second Greens function has the energy difference between the initial state and the one obtained after two subsequent excitations. This difference is  $\epsilon_q - \epsilon_{k'} + \epsilon_{k_2} - \epsilon_{k_1}$ . With this substitution, we get

$$V^\dagger G_0(E) X G_0(E) V = J^3 \sum_{\substack{q, k_1, k_2, k, k', \\ \alpha, \alpha', \alpha_1, \alpha_2, \beta, \\ \gamma_1, \gamma_2}} \frac{c_{q\beta}^{(\gamma_1)\dagger} c_{k\alpha}^{(\gamma_1)} \vec{S}_d \cdot \vec{\sigma}_{\beta\alpha} c_{k_1\alpha_1}^{(\gamma_2)\dagger} c_{k_2\alpha_2}^{(\gamma_2)} \vec{S}_d \cdot \vec{\sigma}_{\alpha_1\alpha_2} c_{k'\alpha'}^{(\gamma_1)\dagger} c_{q\beta}^{(\gamma_1)} \vec{S}_d \cdot \vec{\sigma}_{\alpha'\beta}}{(\epsilon_q - \epsilon_{k'} + \epsilon_{k_2} - \epsilon_{k_1})(\epsilon_q - \epsilon_{k'})} \quad (4.1.29)$$

The sum over  $q$  can be performed in the usual manner.

$$\begin{aligned} \sum_q \frac{c_{q\beta}^\dagger c_{q\beta}}{(\epsilon_q - \epsilon_{k'} + \epsilon_{k_2} - \epsilon_{k_1})(\epsilon_q - \epsilon_{k'})} &= \int_{-D}^{-D+|\delta D|} \frac{d\epsilon \rho(\epsilon) \hat{n}(\epsilon)}{(\epsilon - \epsilon_{k'} + \epsilon_{k_2} - \epsilon_{k_1})(\epsilon - \epsilon_{k'})} \\ &= \frac{\rho(0) |\delta D|}{(D + \epsilon_{k'} - \epsilon_{k_2} + \epsilon_{k_1})(D + \epsilon_{k'})} \end{aligned} \quad (4.1.30)$$

where we have taken  $\rho(\epsilon) = \rho(0)$ ,  $\hat{n}(\epsilon) = \theta(-\epsilon)$  and  $\epsilon_q \simeq -D$ .

For the next step, note that  $\vec{S}_d \cdot \vec{\sigma}_{x,y} = \sum_a S_d^a \sigma_{x,y}^a$ . Substituting this into  $V^\dagger G_0(E) X G_0(E) V$  gives

$$\sum_{\gamma_1, \gamma_2} \sum_{k_1, k_2, k, k', \alpha, \alpha', \alpha_1, \alpha_2, \beta} \sum_{a, b, c} \frac{J^3 \rho(0) |\delta D|}{(D + \epsilon_{k'} - \epsilon_{k_2} + \epsilon_{k_1})(D + \epsilon_{k'})} S_d^a \sigma_{\beta\alpha}^a S_d^b \sigma_{\alpha_1\alpha_2}^b S_d^c \sigma_{\alpha'\beta}^c c_{k_1\alpha_1}^{(\gamma_2)\dagger} c_{k_2\alpha_2}^{(\gamma_2)} c_{k\alpha}^{(\gamma_1)\dagger} c_{q\beta}^{(\gamma_1)} \quad (4.1.31)$$

Now, note that all not all combinations of the momenta will renormalize the  $\vec{S}_d \cdot \vec{s}$  term of the Hamiltonian. In order for such a term to come out, the four remaining momenta must be contracted to two. The first set of terms that satisfy this requirement is given by the condition  $k'\alpha' = k\alpha$ . The renormalization from this subset of terms is

$$\begin{aligned} &\sum_{\gamma_1, \gamma_2} \sum_{k_1, k_2, k} \sum_{\alpha, \alpha_1, \alpha_2, \beta} \sum_{a, b, c} \frac{J^3 \rho(0) |\delta D|}{(D + \epsilon_k - \epsilon_{k_2} + \epsilon_{k_1})(D + \epsilon_k)} S_d^a \sigma_{\beta\alpha}^a S_d^b \sigma_{\alpha_1\alpha_2}^b S_d^c \sigma_{\alpha\beta}^c c_{k_1\alpha_1}^{(\gamma_2)\dagger} c_{k_2\alpha_2}^{(\gamma_2)} c_{k\alpha}^{(\gamma_1)\dagger} c_{k\alpha}^{(\gamma_1)} \\ &= \sum_{\gamma_2} \sum_{k_1, k_2} \sum_{\alpha, \alpha_1, \alpha_2, \beta} \sum_{a, b, c} J^3 \rho(0) |\delta D| S_d^a \sigma_{\beta\alpha}^a S_d^b \sigma_{\alpha_1\alpha_2}^b S_d^c \sigma_{\alpha\beta}^c c_{k_1\alpha_1}^{(\gamma_2)\dagger} c_{k_2\alpha_2}^{(\gamma_2)} \sum_{\gamma_1} \int_0^{D-|\delta D|} \frac{d\epsilon \rho(\epsilon)}{(D + \epsilon - \epsilon_{k_2} + \epsilon_{k_1})(D + \epsilon)} \\ &\simeq \sum_{\gamma_2} \sum_{k_1, k_2} \sum_{\alpha, \alpha_1, \alpha_2, \beta} \sum_{a, b, c} J^3 \rho(0) |\delta D| S_d^a \sigma_{\beta\alpha}^a S_d^b \sigma_{\alpha_1\alpha_2}^b S_d^c \sigma_{\alpha\beta}^c c_{k_1\alpha_1}^{(\gamma_2)\dagger} c_{k_2\alpha_2}^{(\gamma_2)} \sum_{\gamma_1} \int_0^{D-|\delta D|} \frac{d\epsilon \rho(\epsilon)}{(D + \epsilon)^2} \\ &= \frac{K \rho^2(0) J^3 |\delta D|}{2D} \sum_{\alpha, \beta} \sum_{a, c, b} \sum_{\alpha_1, \alpha_2} S_d^a S_d^b S_d^c \sigma_{\beta\alpha}^a \sigma_{\alpha_1\alpha_2}^b \sigma_{\alpha\beta}^c \sum_{k_1, k_2, \gamma_2} c_{k_1\alpha_1}^{(\gamma_2)\dagger} c_{k_2\alpha_2}^{(\gamma_2)}. \end{aligned} \quad (4.1.32)$$

$K = \sum_{\gamma_1}$  is the total number of channels. The other set of terms is given by the condition  $k_1\alpha_1 = k_2\alpha_2$ . The renormalization from these terms can be calculated similarly:

$$\begin{aligned} & \sum_{\gamma_1, \gamma_2} \sum_{k_1, k, k'} \sum_{\alpha, \alpha', \alpha_1, \beta} \sum_{a, b, c} \frac{J^3 \rho(0) |\delta D|}{(D + \epsilon_{k'})^2} S_d^a \sigma_{\beta\alpha}^a S_d^b \sigma_{\alpha_1\alpha_1}^b S_d^c \sigma_{\alpha'\beta}^c c_{k\alpha}^{(\gamma_1)} c_{k_1\alpha_1}^{(\gamma_2)\dagger} c_{k_1\alpha_1}^{(\gamma_2)} c_{k'\alpha'}^{(\gamma_1)\dagger} \\ &= \sum_{\gamma_1} \sum_{k, k'} \sum_{\alpha, \alpha', \beta} \sum_{a, b, c} \frac{J^3 \rho(0) |\delta D|}{(D + \epsilon_{k'})^2} S_d^a \sigma_{\beta\alpha}^a S_d^b \text{Trace}(\sigma^b) S_d^c \sigma_{\alpha'\beta}^c c_{k\alpha}^{(\gamma_1)} \sum_{\gamma_2} \left[ \int_{-D+|\delta D|}^0 d\epsilon \rho(\epsilon) \right] c_{k'\alpha'}^{(\gamma_1)\dagger} \\ &= 0 \end{aligned} \quad (4.1.33)$$

The spin products can be simplified using the identity

$$\sum_{\alpha\beta} \sigma_{\beta\alpha}^a \sigma_{\alpha\beta}^c = \text{Trace}[\sigma^a \sigma^c] = 2\delta_{ac}. \quad (4.1.34)$$

Using this identity, we get

$$V^\dagger G_0(E) X G_0(E) V = \frac{K \rho^2(0) J^3 |\delta D|}{D} \sum_{a,b} \sum_{\alpha_1, \alpha_2} S_d^a S_d^b S_d^a \sigma_{\alpha_1\alpha_2}^b \sum_{k_1, k_2, \gamma_2} c_{k_1\alpha_1}^{(\gamma_2)\dagger} c_{k_2\alpha_2}^{(\gamma_2)} \quad (4.1.35)$$

The products of the impurity spin operators can now be simplified:

$$\sum_a S_d^a S_d^b S_d^a = \sum_a \left[ S_d^b S_d^a + i \sum_c \epsilon^{abc} S_d^c \right] S_d^a = \frac{3}{4} S_d^b + i \sum_{a,c} \epsilon^{abc} S_d^c S_d^a = \frac{3}{4} S_d^b + \frac{1}{2} i^2 \sum_{a,c,e} \epsilon^{abc} \epsilon^{aec} S_d^e = -\frac{1}{4} S_d^b \quad (4.1.36)$$

Substituting this result in the renormalization gives

$$\begin{aligned} V^\dagger G_0(E) X G_0(E) V &= -\frac{K \rho(0)^2 J^3 |\delta D|}{4D} \sum_{k_1, k_2, \alpha_1, \alpha_2, b, \gamma_2} S_d^b \sigma_{\alpha_1\alpha_2}^b c_{k_1\alpha_1}^{(\gamma_2)\dagger} c_{k_2\alpha_2}^{(\gamma_2)} \\ &= -\frac{K \rho(0)^2 J^3 |\delta D|}{4D} \sum_{k_1\alpha_1, k_2\alpha_2, \gamma_2} \vec{S}_d \cdot \vec{\sigma}_{\alpha_1\alpha_2} c_{k_1\alpha_1}^{(\gamma_2)\dagger} c_{k_2\alpha_2}^{(\gamma_2)} \end{aligned} \quad (4.1.37)$$

The other term (virtual particle term) gives an equal contribution. The total renormalization is

$$\delta J = \frac{2J^2 \rho(0) |\delta D|}{D} \left( 1 - \frac{K \rho(0) J}{4} \right) \quad (4.1.38)$$

### 4.1.3 PMS in the language of the URG - obtaining the $\eta$ operators

To make a better connection with URG, we next show how the PMS formalism works out for a single-electron decoupling. The corresponding problem can be phrased in the following manner. We want to decouple one electron at momentum  $q$  from the full Hamiltonian. We can split the exact wavefunction as

$$|\Psi\rangle = |\Psi_0\rangle + |\Psi_1\rangle \quad (4.1.39)$$

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

$$\mathcal{H} = \mathcal{H}^d + V_0 + V_+ + V_- \quad (4.1.40)$$

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



Substituting eqs. 4.1.40 and 4.1.39 in eq. 4.1.1 gives

$$\left(\mathcal{H}^d + V_0 + V_+ + V_-\right) (|\Psi_0\rangle + |\Psi_1\rangle) = E (|\Psi_0\rangle + |\Psi_1\rangle) \quad (4.1.41)$$

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

$$\begin{aligned} \left(\mathcal{H}_0^d + V_0\right) |\Psi_0\rangle + V_- |\Psi_1\rangle &= E |\Psi_0\rangle \\ \left(\mathcal{H}_1^d + V_0\right) |\Psi_1\rangle + V_+ |\Psi_0\rangle &= E |\Psi_1\rangle \end{aligned} \quad (4.1.42)$$

The second equation can be written as

$$|\Psi_1\rangle = \eta^\dagger |\Psi_0\rangle \quad (4.1.43)$$

where

$$\left(\eta^\dagger\right)_{\text{PMS}} = \frac{1}{E - \mathcal{H}_1^d - V_0} V_+ \quad (4.1.44)$$

Substituting this in the first equation gives

$$\left(\mathcal{H}_0^d + V_0 + V_- \eta^\dagger\right) |\Psi_0\rangle = E |\Psi_0\rangle \quad (4.1.45)$$

This new Hamiltonian,

$$\tilde{\mathcal{H}}_0 = \mathcal{H}_0^d + V_0 + V_- \eta^\dagger \quad (4.1.46)$$

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

$$\Delta V_0 = V_- \eta^\dagger \quad (4.1.47)$$

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

$$|\Psi_0\rangle = \eta |\Psi_1\rangle \quad (4.1.48)$$

where

$$(\eta)_{\text{PMS}} = \frac{1}{E - \mathcal{H}_0^d - V_0} V_- \quad (4.1.49)$$

,so

$$\left(\mathcal{H}_1^d + V_0 + V_+ \eta\right) |\Psi_1\rangle = E |\Psi_1\rangle \quad (4.1.50)$$

The renormalized Hamiltonian in the high energy subspace is thus

$$\tilde{\mathcal{H}}_1 = \mathcal{H}_1^d + V_0 + V_+ \eta \quad (4.1.51)$$

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

$$\begin{aligned} \tilde{\mathcal{H}} &= \tilde{\mathcal{H}}_1 \hat{n} + \tilde{\mathcal{H}}_0 (1 - \hat{n}) \\ &= \mathcal{H}_0^d + \mathcal{H}_1^d + V_0 + V_+ \eta + V_- \eta^\dagger \end{aligned} \quad (4.1.52)$$

The total renormalization is

$$(\Delta \mathcal{H})_{\text{PMS}} = V_+ (\eta)_{\text{PMS}} + V_- (\eta^\dagger)_{\text{PMS}} \quad (4.1.53)$$

It can be shown that if we define a unitary operator  $U = 1 - \eta + \eta^\dagger$ , the transformed Hamiltonian  $U \mathcal{H} U^\dagger$  is the same as eq. 4.1.52. This, along with the properties of  $\eta$ , have been shown in section 3. The important feature of eq. 4.1.52 is that there is no term in the transformed Hamiltonian which scatters between  $|\Psi_0\rangle$  and  $|\Psi_0\rangle$ - the two subspaces have been truly decoupled.

$$\left[U \mathcal{H} U^\dagger, n_q\right] = 0 \quad (4.1.54)$$

We can write down the renormalized Schrodinger equation in the low energy subspace, from eq. 4.1.45,

$$\tilde{\mathcal{H}}_0 |\Psi_0\rangle = E |\Psi_0\rangle \quad (4.1.55)$$

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

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

$$\mathcal{H} |\Phi\rangle = \mathcal{H}' |\Phi\rangle \quad (4.1.56)$$

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

The operators  $\eta$  and its conjugate change accordingly:

$$\begin{aligned} (\eta)_{\text{URG}} &= \frac{1}{\tilde{\mathcal{H}} - \mathcal{H}_0^d - V_0} V_- \\ &= \frac{1}{\hat{\omega} - \mathcal{H}_0^d} V_- \end{aligned} \quad (4.1.57)$$

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

$$(\eta^\dagger)_{\text{URG}} = \frac{1}{\hat{\omega} - \mathcal{H}_1^d} V_+ \quad (4.1.58)$$

The renormalization is again

$$(\Delta\mathcal{H})_{\text{URG}} = V_+ (\eta)_{\text{URG}} + V_- (\eta^\dagger)_{\text{URG}} \quad (4.1.59)$$

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

$$U = 1 - \eta + \eta^\dagger, \left[ \hat{n}_q, U\mathcal{H}U^\dagger \right] = 0 \quad (4.1.60)$$

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

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

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

$$(\hat{\omega} - \mathcal{H}_1^d) V_+ |\Psi_0\rangle \text{ or } (\hat{\omega} - \mathcal{H}_1^d) V_- |\Psi_1\rangle \quad (4.1.61)$$

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

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

#### 4.1.4 PMS for the single impurity Anderson model

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

$$\mathcal{H} = \sum_{k\sigma} \left( \epsilon_k \tau_{k\sigma} + V c_{k\sigma}^\dagger c_{d\sigma} + \text{h.c.} \right) \quad (4.1.62)$$

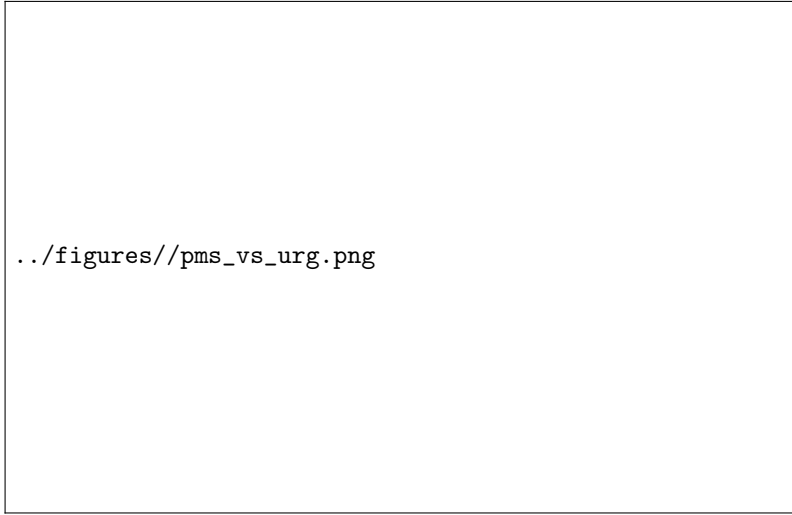


Figure 4.1: Flows of PMS(green) and URG(blue)

where  $\tau = \hat{n} - \frac{1}{2}$ . We want to decouple the state  $q\beta$  from the rest of the electrons. We have  $H_0 = \epsilon_d \hat{n}_d + U \hat{n}_{d\uparrow} n_{d\downarrow} + \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma}$ ,  $V_0 = \sum_{k<q,\sigma} c_{k\sigma}^\dagger c_{d\sigma} + \text{h.c.}$ ,  $V_+ = V c_{q\beta}^\dagger c_{d\beta}$  and  $V_- = V c_{d\beta}^\dagger c_{q\beta}$ . The renormalization in particle sector

$$\Delta V_0 = c_{d\beta}^\dagger c_{q\beta} \frac{1}{(E - V_0) - \hat{\mathcal{H}}_0^d} c_{q\beta}^\dagger c_{d\beta} \quad (4.1.63)$$

The intermediate energy (at the propagator) is

$$\hat{\mathcal{H}}_0^d = \sum_{k,\sigma} \epsilon_k \tau_{k\sigma} + \epsilon_d \hat{n}_{d\bar{\beta}} \quad (4.1.64)$$

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

$$\Delta V_0 = c_{d\beta}^\dagger c_{q\beta} \frac{1}{(E - V_0) - \sum_{k,\sigma} \epsilon_k \tau_{k\sigma} - \epsilon_d \hat{n}_{d\bar{\beta}}} c_{q\beta}^\dagger c_{d\beta} \quad (4.1.65)$$

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

$$E - V_0 = \sum_{k<q,\sigma} \epsilon_k \tau_{k\sigma} - \frac{1}{2} \epsilon_q + \epsilon_d + (\epsilon_d + U) \hat{n}_{d\bar{\beta}} \quad (4.1.66)$$

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

Substituting this in  $\Delta V_0$  gives

$$\begin{aligned} \Delta V_0 &= c_{d\beta}^\dagger c_{q\beta} \frac{1}{-\frac{1}{2} \epsilon_q - \epsilon_q \tau_{q\beta} + \epsilon_d + U \hat{n}_{d\bar{\beta}}} c_{q\beta}^\dagger c_{d\beta} \\ &= c_{d\beta}^\dagger c_{q\beta} \frac{1}{-\epsilon_q + \epsilon_d + U \hat{n}_{d\bar{\beta}}} c_{q\beta}^\dagger c_{d\beta} \\ &= c_{d\beta}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{d\beta} \frac{1}{-\epsilon_q + \epsilon_d + U \hat{n}_{d\bar{\beta}}} \\ &= -c_{d\beta}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{d\beta} \frac{1}{\epsilon_q - \epsilon_d - U \hat{n}_{d\bar{\beta}}} \\ &= (1 - \hat{n}_{q\beta}) \left( \frac{-\hat{n}_{d\beta} \hat{n}_{d\bar{\beta}}}{\epsilon_q - \epsilon_d - U} + \frac{-\hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}})}{\epsilon_q - \epsilon_d} \right) \end{aligned} \quad (4.1.67)$$

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

$$\begin{aligned}\Delta E_2 &= \frac{-1}{\epsilon_q - \epsilon_d - U} \\ \Delta E_1 &= \frac{-1}{\epsilon_q - \epsilon_d}\end{aligned}\tag{4.1.68}$$

The renormalization in the hole sector is

$$\begin{aligned}\Delta V_0 &= c_{q\beta}^\dagger c_{d\beta} \frac{1}{(E - V_0) - \hat{\mathcal{H}}_0^d} c_{d\beta}^\dagger c_{q\beta} \\ &= c_{q\beta}^\dagger c_{d\beta} \frac{1}{(E - V_0) - \sum_{k,\sigma} \epsilon_k \tau_{k\sigma} - \epsilon_d - (\epsilon_d + U) \hat{n}_{d\bar{\beta}}} c_{d\beta}^\dagger c_{q\beta}\end{aligned}\tag{4.1.69}$$

This time we substitute

$$\begin{aligned}E - V_0 &= \sum_{k < q, \sigma} \epsilon_k \tau_{k\sigma} + \tau_{q\beta} \epsilon_q^- + \epsilon_d \hat{n}_{d\bar{\beta}} \\ &= \sum_{k < q, \sigma} \epsilon_k \tau_{k\sigma} + \frac{1}{2} \epsilon_q^- + \epsilon_d \hat{n}_{d\bar{\beta}}\end{aligned}\tag{4.1.70}$$

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

$$\begin{aligned}\Delta V_0 &= c_{q\beta}^\dagger c_{d\beta} \frac{1}{-\frac{1}{2} \epsilon_q - \epsilon_q^- \tau_{q\beta} - \epsilon_d - U \hat{n}_{d\bar{\beta}}} c_{d\beta}^\dagger c_{q\beta} \\ &= c_{q\beta}^\dagger c_{d\beta} c_{d\beta}^\dagger c_{q\beta} \frac{1}{-\epsilon_q - \epsilon_d - U \hat{n}_{d\bar{\beta}}} \\ &= \hat{n}_{q\beta} \left( \frac{-\left(1 - \hat{n}_{d\beta}\right) \hat{n}_{d\bar{\beta}}}{\epsilon_q + \epsilon_d + U} + \frac{-\left(1 - \hat{n}_{d\beta}\right) \left(1 - \hat{n}_{d\bar{\beta}}\right)}{\epsilon_q + \epsilon_d} \right)\end{aligned}\tag{4.1.71}$$

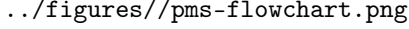
In the second line, we put  $\epsilon_q^- = -\epsilon_q$  and  $\tau_{q\beta} = -\frac{1}{2}$ . The first term renormalizes the singly-occupied state while the second term renormalizes the holon state. Combining with the particle sector results, the total renormalization in all the three impurity states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

$$\begin{aligned}\Delta E_0 &= -\frac{1}{\epsilon_q + \epsilon_d} \\ \Delta E_1 &= -\frac{1}{\epsilon_q + \epsilon_d + U} - \frac{1}{\epsilon_q - \epsilon_d} \\ \Delta E_2 &= -\frac{1}{\epsilon_q - \epsilon_d - U}\end{aligned}\tag{4.1.72}$$

These results are also obtained in ref. [30]. The complete process is depicted in fig. 4.2.

#### Some conclusions:

- The *only* difference in the formalism of PMS and URG is that while PMS uses the exact energy eigenvalue  $E$  to parameterise the flow, URG uses a general intermediate decoupled Hamiltonian to do the same. Since the  $E$  is also, technically, an intermediate decoupled Hamiltonian (it is the final Hamiltonian), PMS can be seen as an URG but with a specific choice for the paramter.
- In practise, PMS replaces  $E - V_0$  with the diagonal part of the initial state at the current step of the RG. We are talking about the energy of the initial state, not the intermediate state. This is because, from eq. 4.1.1,  $E$  is the energy of the initial state on which  $V_\pm$  act.



../figures//pms-flowchart.png

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

- The ideal solution would have been to substitute the exact energy and the total scattering term  $V$ , but since we do not know  $E$  and keeping the  $V$  would make the thing untractable, we use our current best guess (renormalised diagonal part). As the RG flows, both  $E_j$  and  $V$  flow, such that at the fixed point,  $V$  becomes zero (scattering terms get removed) and  $E_j$  morphs into the exact  $E$ .
- In practise, URG replaces the  $\hat{\omega}$  with a guess for the final energy  $E$ . This however ignores the renormalization of  $\hat{\omega}$ . A better approach would be to replace it with  $E_j$ , following PMS. That would act like the one-particle renormalization of  $\hat{\omega}$ .
- PMS usually drops any diagonal component of the scattering from the denominator. For example, in the PMS of the Kondo model by Anderson [6] or that of the anisotropic power law Kondo model by Chenge et.al [31], they do not keep the term  $J_z S_d^z s^z$  in the denominator although it is number (spin) conserving. Such terms are kept in the denominator of the URG though. It must be mentioned however that ref. [32] *does* bring a diagonal charge-charge interaction in the denominator in the PMS of the extended Anderson model.

## 4.2 Schrieffer-Wolff transformation (SWT)

### 4.2.1 Formalism

We have a general Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_X \quad (4.2.1)$$

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

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

where  $H_1$  is diagonal and  $H_2$  is off-diagonal.

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

The decoupling condition is  $H_2 = 0$ .

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

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

The second order decoupling condition is thus

$$[S, \mathcal{H}_0] = -\mathcal{H}_X \quad (4.2.5)$$

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

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

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

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

There we used

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

and hence

$$(\eta^\dagger - \eta)^3 = -1 (\eta^\dagger - \eta) \quad (4.2.9)$$

and so on. This simplification allows us to write

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

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

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

and

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

The off-diagonal part now becomes

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

The vanishing of this quantity is now the decoupling condition, and is also given in eq 16 of ref. [1].

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

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

That gives

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

The decoupling condition becomes

$$[S, \mathcal{H}_0] = -\frac{\pi}{4} \mathcal{H}_X + \frac{4}{\pi} S \mathcal{H}_X S \quad (4.2.15)$$

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

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

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

#### 4.2.2 Obtaining renormalization via Schrieffer-Wolff transformation - comparison with "poor man's scaling" and URG

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

$$S = \sum_{ij} [s |\phi_1^i\rangle \langle \phi_0^j| - s^\dagger |\phi_0^j\rangle \langle \phi_1^i|] \quad (4.2.17)$$

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

$$-\mathcal{H}_X = [S, H_0] = SH_0 - H_0S \quad (4.2.18)$$

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

$$-\langle \phi_0^a | V + V^\dagger | \phi_1^b \rangle = \langle \phi_0^a | SH_0 - H_0S | \phi_1^b \rangle \quad (4.2.19)$$

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

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

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

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

The renormalization is thus

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

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

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

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

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



where

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

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

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

### 4.3 A comparison of URG, SWT and PMS on the Anderson model

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

$$-\epsilon_q (A + B\hat{n}_{d\bar{\beta}}) + \epsilon_d (A + B\hat{n}_{d\bar{\beta}}) + U(A + B)\hat{n}_{d\bar{\beta}} = -V \tag{4.3.1}$$

which gives

$$S = V \left[ \frac{1 - \hat{n}_{d\bar{\beta}}}{\epsilon_q - \epsilon_d} + \frac{\hat{n}_{d\bar{\beta}}}{\epsilon_q - \epsilon_d - U} \right] (c_{q\beta}^\dagger c_{d\beta} - \text{h.c.}) \tag{4.3.2}$$

The remaining diagonal part constitutes the effective Hamiltonian.

$$\begin{aligned}
U\mathcal{H}U^\dagger &= H_1 = \mathcal{H}_0 + \frac{1}{2} \left\{ \mathcal{H}_0, S^2 \right\} - S\mathcal{H}_0S + [S, \mathcal{H}_X] \\
&= \mathcal{H}_0 + \frac{1}{2} \left[ [\mathcal{H}_0, S], S \right] + [S, \mathcal{H}_X] \\
&= \mathcal{H}_0 + \frac{1}{2} [\mathcal{H}_X, S] + [S, \mathcal{H}_X] \\
&= \mathcal{H}_0 + \frac{1}{2} [S, \mathcal{H}_X]
\end{aligned} \tag{4.3.3}$$

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

$$\begin{aligned}
\mathcal{H}_0 &= \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \epsilon_d \hat{n}_d + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \sum_{k\sigma \neq q\beta} \left( c_{k\sigma}^\dagger c_{d\sigma} + \text{h.c.} \right) \\
\mathcal{H}_X &= c_{q\beta}^\dagger c_{d\beta} + \text{h.c.}
\end{aligned} \tag{4.3.4}$$

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

$$\begin{aligned}
\frac{1}{2} [S, \mathcal{H}_X] \Big|_{\hat{n}_{q\beta}=0} &= |V|^2 \left[ \frac{1 - \hat{n}_{d\bar{\beta}}}{\epsilon_q - \epsilon_d} + \frac{\hat{n}_{d\bar{\beta}}}{\epsilon_q - \epsilon_d - U} \right] \left[ \hat{n}_{q\beta} (1 - \hat{n}_{d\beta}) - \hat{n}_{d\beta} (1 - \hat{n}_{q\beta}) \right] \Big|_{\hat{n}_{q\beta}=0} \\
&= -\hat{n}_{d\beta} |V|^2 \left[ \frac{1 - \hat{n}_{d\bar{\beta}}}{\epsilon_q - \epsilon_d} + \frac{\hat{n}_{d\bar{\beta}}}{\epsilon_q - \epsilon_d - U} \right]
\end{aligned} \tag{4.3.5}$$

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

$$\left. \frac{1}{2} [S, \mathcal{H}_X] \right|_{\hat{n}_{q\beta}=1} = - \left( 1 - \hat{n}_{d\beta} \right) |V|^2 \left[ \frac{1 - \hat{n}_{d\bar{\beta}}}{\epsilon_q + \epsilon_d} + \frac{\hat{n}_{d\bar{\beta}}}{\epsilon_q + \epsilon_d + U} \right] \quad (4.3.6)$$

These two results - the renormalization in the particle and hole sectors - is identical to the result (see [19]) obtained from PMS of the SIAM. The renormalizations in the various energy levels of the impurity can be read off now, after summing over all states in the interval we are decoupling.

$$\begin{aligned} \Delta E_2 &= -2 \sum_q \frac{|V_q|^2}{\epsilon_q - \epsilon_d - U} \\ \Delta E_1 &= - \sum_q \frac{|V_q|^2}{\epsilon_q - \epsilon_d} - \sum_q \frac{|V_q|^2}{\epsilon_q + \epsilon_d + U} \\ \Delta E_0 &= -2 \sum_q \frac{|V_q|^2}{\epsilon_q + \epsilon_d} \end{aligned} \quad (4.3.7)$$

This can be compared with the URG result, eq. 5.3.1,

$$\begin{aligned} \Delta E_2 &= 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d + U} \\ \Delta E_1 &= \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d - U} + \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d} \\ \Delta E_0 &= 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d} \end{aligned} \quad (4.3.8)$$

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

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

## 4.4 Deriving the Kondo model from the Anderson model via a one-shot URG

Here we will show how we can obtain the spin-spin interaction of the Kondo model by performing a one-shot URG on the SIAM. This should justify that the action of performing an SWT is analogous to decoupling the whole band via URG. There are three departures from the conventional way of doing URG (or PMS).

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

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

$$\mathcal{H}^I = \sum_{k\sigma} \left[ V_k c_{k\sigma}^\dagger c_{d\sigma} + \text{h.c.} \right] \quad (4.4.1)$$

The diagonal part is the rest of the Hamiltonian.

$$\begin{aligned} \mathcal{H}^d &= \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \epsilon_d \hat{n}_d + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \\ &= \sum_{k\sigma} \epsilon_k \tau_{k\sigma} + \epsilon_d \hat{n}_d + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \end{aligned} \quad (4.4.2)$$

Following eq. 3.1.47, the renormalization is

$$\Delta\mathcal{H} = \frac{1}{2} \left[ \eta^\dagger - \eta, \mathcal{H}_X \right] \quad (4.4.3)$$

The transition operator  $\eta$  is

$$\begin{aligned} \eta &= \frac{1}{\omega - \mathcal{H}^d} \sum_{k\sigma} V_k^* c_{d\sigma}^\dagger c_{k\sigma} \\ &= \sum_{k\sigma} \frac{1}{\omega + \frac{1}{2}\epsilon_k - \epsilon_d - (\epsilon_d + U) \hat{n}_{d\bar{\sigma}}} V_k^* c_{d\sigma}^\dagger c_{k\sigma} \\ &= \sum_{k\sigma} \left[ \frac{\hat{n}_{d\bar{\sigma}}}{\omega_1 + \frac{1}{2}\epsilon_k - 2\epsilon_d - U} + \frac{1 - \hat{n}_{d\bar{\sigma}}}{\omega_0 + \frac{1}{2}\epsilon_k - \epsilon_d} \right] V_k^* c_{d\sigma}^\dagger c_{k\sigma} \\ &= \sum_{k\sigma} \left[ \frac{\hat{n}_{d\bar{\sigma}}}{E_k^1} + \frac{1 - \hat{n}_{d\bar{\sigma}}}{E_k^0} \right] V_k^* c_{d\sigma}^\dagger c_{k\sigma} \end{aligned} \quad (4.4.4)$$

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

$$\eta^\dagger - \eta = \sum_{k\sigma} \left[ \frac{\hat{n}_{d\bar{\sigma}}}{E_k^1} + \frac{1 - \hat{n}_{d\bar{\sigma}}}{E_k^0} \right] \left( V_k c_{k\sigma}^\dagger c_{d\sigma} - V_k^* c_{d\sigma}^\dagger c_{k\sigma} \right) \quad (4.4.5)$$

The renormalization is

$$\Delta\mathcal{H}(\omega_1, \omega_0) = \frac{1}{2} \sum_{kq\sigma\alpha} \left[ \left( \frac{\hat{n}_{d\bar{\sigma}}}{E_k^1} + \frac{1 - \hat{n}_{d\bar{\sigma}}}{E_k^0} \right) \left( V_k c_{k\sigma}^\dagger c_{d\sigma} - V_k^* c_{d\sigma}^\dagger c_{k\sigma} \right), V_q c_{q\alpha}^\dagger c_{d\alpha} + V_q^* c_{d\alpha}^\dagger c_{q\alpha} \right] \quad (4.4.6)$$

The summation has two parts,  $\Delta_{1,2}$  - one where  $\sigma = \alpha$  and another where  $\sigma = \bar{\alpha}$ . The first part  $\Delta_1$  gives

$$\begin{aligned} \Delta_1 &= \frac{1}{2} \sum_{kq\sigma=\alpha} \left[ \left( \frac{\hat{n}_{d\bar{\sigma}}}{E_k^1} + \frac{1 - \hat{n}_{d\bar{\sigma}}}{E_k^0} \right) \left( V_k c_{k\sigma}^\dagger c_{d\sigma} - V_k^* c_{d\sigma}^\dagger c_{k\sigma} \right), V_q c_{q\sigma}^\dagger c_{d\sigma} + V_q^* c_{d\sigma}^\dagger c_{q\sigma} \right] \\ &= \frac{1}{2} \sum_{kq\sigma} \left( \frac{\hat{n}_{d\bar{\sigma}}}{E_k^1} + \frac{1 - \hat{n}_{d\bar{\sigma}}}{E_k^0} \right) \left[ V_k c_{k\sigma}^\dagger c_{d\sigma} - V_k^* c_{d\sigma}^\dagger c_{k\sigma}, V_q c_{q\sigma}^\dagger c_{d\sigma} + V_q^* c_{d\sigma}^\dagger c_{q\sigma} \right] \\ &= \frac{1}{2} \sum_{kq\sigma} \left( \frac{\hat{n}_{d\bar{\sigma}}}{E_k^1} + \frac{1 - \hat{n}_{d\bar{\sigma}}}{E_k^0} \right) \left\{ V_k V_q^* \left[ c_{k\sigma}^\dagger c_{d\sigma}, V_q c_{d\sigma}^\dagger c_{q\sigma} \right] - V_k^* V_q \left[ c_{d\sigma}^\dagger c_{k\sigma}, c_{q\sigma}^\dagger c_{d\sigma} \right] \right\} \\ &= \frac{1}{2} \sum_{kq\sigma} \left( \frac{\hat{n}_{d\bar{\sigma}}}{E_k^1} + \frac{1 - \hat{n}_{d\bar{\sigma}}}{E_k^0} \right) \left\{ V_k V_q^* \left[ c_{k\sigma}^\dagger c_{d\sigma}, V_q c_{d\sigma}^\dagger c_{q\sigma} \right] + V_k^* V_q \left[ c_{q\sigma}^\dagger c_{d\sigma}, c_{d\sigma}^\dagger c_{k\sigma} \right] \right\} \\ &= \frac{1}{2} \sum_{kq\sigma} \left[ \hat{n}_{d\bar{\sigma}} \left( \frac{1}{E_k^1} + \frac{1}{E_q^1} \right) + (1 - \hat{n}_{d\bar{\sigma}}) \left( \frac{1}{E_k^0} + \frac{1}{E_q^0} \right) \right] V_k V_q^* \left[ c_{k\sigma}^\dagger c_{d\sigma}, c_{d\sigma}^\dagger c_{q\sigma} \right] \\ &= \sum_{kq\sigma} \left[ \frac{1}{2} V_k V_q^* \left( \frac{1}{E_k^0} + \frac{1}{E_q^0} \right) + \hat{n}_{d\bar{\sigma}} \frac{1}{2} V_k V_q^* \left( \frac{1}{E_k^1} + \frac{1}{E_q^1} - \frac{1}{E_k^0} - \frac{1}{E_q^0} \right) \right] \left( c_{k\sigma}^\dagger c_{q\sigma} - c_{d\sigma}^\dagger c_{d\sigma} \delta_{kq} \right) \end{aligned} \quad (4.4.7)$$

We can now define two new energy scales:

$$W_{kq} = \frac{1}{2} V_k V_q^* \left( \frac{1}{E_k^0} + \frac{1}{E_q^0} \right), \quad J_{kq} = \frac{1}{2} V_k V_q^* \left( \frac{1}{E_k^1} + \frac{1}{E_q^1} - \frac{1}{E_k^0} - \frac{1}{E_q^0} \right) \quad (4.4.8)$$

The renormalization  $\Delta_1$  becomes

$$\begin{aligned} \Delta_1 &= \sum_{kq\sigma} \left[ W_{kq} + \hat{n}_{d\bar{\sigma}} J_{kq} \right] \left( c_{k\sigma}^\dagger c_{q\sigma} - c_{d\sigma}^\dagger c_{d\sigma} \delta_{kq} \right) \\ &= \sum_{kq\sigma} \left[ W_{kq} + \hat{n}_{d\bar{\sigma}} J_{kq} \right] c_{k\sigma}^\dagger c_{q\sigma} - \sum_{k\sigma} \left[ W_{kk} + \hat{n}_{d\bar{\sigma}} J_{kk} \right] \hat{n}_{d\sigma} \\ &= \sum_{kq\sigma} \left[ W_{kq} + \frac{1}{2} \hat{n}_d J_{kq} \right] c_{k\sigma}^\dagger c_{q\sigma} - \sum_{kq\sigma} \sigma J_{kq} S_d^z c_{k\sigma}^\dagger c_{q\sigma} - \sum_{k\sigma} \left[ W_{kk} + \hat{n}_{d\bar{\sigma}} J_{kk} \right] \hat{n}_{d\sigma} \end{aligned} \quad (4.4.9)$$

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

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

$$\begin{aligned} \Delta_2 &= \frac{1}{2} \sum_{kq\bar{\sigma}=\alpha} \left[ \left( \frac{\hat{n}_{d\bar{\sigma}}}{E_k^1} + \frac{1 - \hat{n}_{d\bar{\sigma}}}{E_k^0} \right) \left( V_k c_{k\sigma}^\dagger c_{d\sigma} - V_k^* c_{d\sigma}^\dagger c_{k\sigma} \right), V_q c_{q\bar{\sigma}}^\dagger c_{d\bar{\sigma}} + V_q^* c_{d\bar{\sigma}}^\dagger c_{q\bar{\sigma}} \right] \\ &= \frac{1}{2} \sum_{kq\sigma} \left( V_k c_{k\sigma}^\dagger c_{d\sigma} - V_k^* c_{d\sigma}^\dagger c_{k\sigma} \right) \left[ \frac{\hat{n}_{d\bar{\sigma}}}{E_k^1} + \frac{1 - \hat{n}_{d\bar{\sigma}}}{E_k^0}, V_q c_{q\bar{\sigma}}^\dagger c_{d\bar{\sigma}} + V_q^* c_{d\bar{\sigma}}^\dagger c_{q\bar{\sigma}} \right] \\ &= \frac{1}{2} \sum_{kq\sigma} \left( V_k c_{k\sigma}^\dagger c_{d\sigma} - V_k^* c_{d\sigma}^\dagger c_{k\sigma} \right) \left( V_q^* c_{d\bar{\sigma}}^\dagger c_{q\bar{\sigma}} - V_q c_{q\bar{\sigma}}^\dagger c_{d\bar{\sigma}} \right) \left( \frac{1}{E_k^1} - \frac{1}{E_k^0} \right) \\ &= \frac{1}{2} \sum_{kq\sigma} \left( V_k V_q^* c_{k\sigma}^\dagger c_{d\sigma} c_{d\bar{\sigma}}^\dagger c_{q\bar{\sigma}} - V_k V_q c_{k\sigma}^\dagger c_{d\sigma} c_{q\bar{\sigma}}^\dagger c_{d\bar{\sigma}} - V_k^* V_q^* c_{d\sigma}^\dagger c_{k\sigma} c_{d\bar{\sigma}}^\dagger c_{q\bar{\sigma}} + V_k^* V_q c_{d\sigma}^\dagger c_{k\sigma} c_{q\bar{\sigma}}^\dagger c_{d\bar{\sigma}} \right) \\ &\quad \times \left( \frac{1}{E_k^1} - \frac{1}{E_k^0} \right) \end{aligned} \quad (4.4.10)$$

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

$$\begin{aligned} &\frac{1}{2} \sum_{kq\sigma} \left( V_k V_q^* c_{k\sigma}^\dagger c_{d\sigma} c_{d\bar{\sigma}}^\dagger c_{q\bar{\sigma}} + V_k^* V_q c_{d\sigma}^\dagger c_{k\sigma} c_{q\bar{\sigma}}^\dagger c_{d\bar{\sigma}} \right) \times \left( \frac{1}{E_k^1} - \frac{1}{E_k^0} \right) \\ &= \frac{1}{2} \sum_{kq\sigma} V_k V_q^* c_{k\sigma}^\dagger c_{d\sigma} c_{d\bar{\sigma}}^\dagger c_{q\bar{\sigma}} \left( \frac{1}{E_k^1} - \frac{1}{E_k^0} \right) + \frac{1}{2} \sum_{kq\sigma} V_k^* V_q c_{d\sigma}^\dagger c_{k\sigma} c_{q\bar{\sigma}}^\dagger c_{d\bar{\sigma}} \left( \frac{1}{E_k^1} - \frac{1}{E_k^0} \right) \\ &= \frac{1}{2} \sum_{kq\sigma} V_k V_q^* c_{k\sigma}^\dagger c_{d\sigma} c_{d\bar{\sigma}}^\dagger c_{q\bar{\sigma}} \left( \frac{1}{E_k^1} - \frac{1}{E_k^0} \right) + \frac{1}{2} \sum_{qk\sigma} V_q^* V_k c_{d\bar{\sigma}}^\dagger c_{q\bar{\sigma}} c_{k\sigma}^\dagger c_{d\sigma} \left( \frac{1}{E_q^1} - \frac{1}{E_q^0} \right) \\ &= - \sum_{kq\sigma} J_{kq} c_{k\sigma}^\dagger c_{q\bar{\sigma}} c_{d\bar{\sigma}}^\dagger c_{d\sigma} \end{aligned} \quad (4.4.11)$$

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

Similarly, for the second term, we get

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

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

where  $K_{kq}$  is yet another energy scale.

$$K_{kq} = \frac{1}{2} V_k V_q \left( \frac{1}{E_k^1} - \frac{1}{E_k^0} + \frac{1}{E_q^1} - \frac{1}{E_q^0} \right) \quad (4.4.12)$$

The third term gives

$$\frac{1}{2} \sum_{kq\sigma} V_k^* V_q c_{d\sigma}^\dagger c_{k\sigma} c_{d\bar{\sigma}}^\dagger c_{q\bar{\sigma}} \left( \frac{1}{E_k^1} - \frac{1}{E_k^0} \right) = \sum_{kq\sigma} K_{kq} c_{d\sigma}^\dagger c_{k\sigma} c_{d\bar{\sigma}}^\dagger c_{q\bar{\sigma}} \quad (4.4.13)$$

The total renormalization can thus be written as

$$\begin{aligned}
\Delta \mathcal{H}(\omega_1, \omega_0) &= - \sum_{k\sigma} [W_{kk} + \hat{n}_{d\bar{\sigma}} J_{kk}] \hat{n}_{d\sigma} && [\text{renormalization in } \epsilon_d, U] \\
&+ \sum_{kq\sigma} \left[ W_{kq} + \frac{1}{2} \hat{n}_d J_{kq} \right] c_{k\sigma}^\dagger c_{q\sigma} && [\text{potential scattering}] \\
&- \sum_{kq\sigma} J_{kq} \left[ S_d^z c_{k\sigma}^\dagger c_{q\sigma} + \sum_{kq\sigma} J_{kq} c_{k\sigma}^\dagger c_{q\bar{\sigma}} c_{d\bar{\sigma}}^\dagger c_{d\sigma} \right] && [\text{spin Kondo}] \\
&+ \sum_{kq\sigma} K_{kq} c_{k\sigma}^\dagger c_{d\sigma} c_{q\bar{\sigma}}^\dagger c_{d\bar{\sigma}} + \text{h.c.} && [\text{charge Kondo}]
\end{aligned} \quad (4.4.14)$$

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

$$\begin{aligned}
W_{kq}^{SWT} &= \frac{1}{2} V_k V_q^* \left( \frac{1}{\epsilon_k - \epsilon_d} + \frac{1}{\epsilon_q - \epsilon_d} \right) \\
J_{kq}^{SWT} &= \frac{1}{2} V_k V_q^* \left( \frac{1}{\epsilon_k - \epsilon_d - U} + \frac{1}{\epsilon_q - \epsilon_d - U} - \frac{1}{\epsilon_k - \epsilon_d} - \frac{1}{\epsilon_q - \epsilon_d} \right) \\
W_{kq}^{URG}(\omega) &= \frac{1}{2} V_k V_q^* \left( \frac{1}{\omega_0 + \frac{1}{2}\epsilon_k - \epsilon_d} + \frac{1}{\omega_0 + \frac{1}{2}\epsilon_q - \epsilon_d} \right) \\
J_{kq}^{URG}(\omega) &= \frac{1}{2} V_k V_q^* \left( \frac{1}{\omega_1 + \epsilon_k - \epsilon_d - U} + \frac{1}{\omega_1 + \epsilon_q - \epsilon_d - U} - \frac{1}{\omega_0 + \epsilon_k - \epsilon_d} - \frac{1}{\omega_0 + \epsilon_q - \epsilon_d} \right)
\end{aligned} \quad (4.4.15)$$

To recover the SWT scales from the URG ones, we have to substitute each  $\omega_i$  by the energy of the initial state to which it corresponds. From eq. 4.4.4, we note that  $\omega_1$  refers to the initial state in which  $\hat{n}_{k\sigma} = \hat{n}_{d\bar{\sigma}} = 1 - \hat{n}_{d\sigma} = 1$ . Therefore,  $\omega_1 = \frac{1}{2}\epsilon_k + \epsilon_d$ . Similarly,  $\omega_0$  refers to the initial state in which  $\hat{n}_{k\sigma} = 1 - \hat{n}_{d\bar{\sigma}} = 1 - \hat{n}_{d\sigma} = 1$ . Therefore,  $\omega_0 = \frac{1}{2}\epsilon_k$ . Substituting these into the URG energy scales gives back the SWT scales.

## 4.5 Continuous unitary transformation RG

### 4.5.1 Formalism

The following equation generates a family of unitary Hamiltonians.

$$\frac{d\mathcal{H}(l)}{dl} = [\mathcal{H}, \eta(l)] \quad (4.5.1)$$

To prove the unitarity[33], we construct the unitary operator  $U(l)$  that connects the Hamiltonians  $\mathcal{H}(l)$  and  $\mathcal{H}(l=0)$ . Let  $\mathcal{H}(l) = U(l)\mathcal{H}(l=0)U^\dagger(l)$ , where  $U(l)$  is defined by

$$\eta(l) = \frac{dU}{dl}U^\dagger = -U\frac{dU^\dagger}{dl} \quad \left[ UU^\dagger = 1 \implies \frac{d(UU^\dagger)}{dl} = 0 \right] \quad (4.5.2)$$

This will give

$$\begin{aligned} \frac{d\mathcal{H}(l)}{dl} &= \frac{dU}{dl}\mathcal{H}(0)U^\dagger(l) + U\mathcal{H}(0)\frac{dU^\dagger}{dl} \\ &= \frac{dU}{dl}U^\dagger\mathcal{H}(l) + \mathcal{H}(l)U\frac{dU^\dagger}{dl} \\ &= \eta(l)\mathcal{H}(l) - \mathcal{H}(l)\eta(l) \\ &= [\eta(l), \mathcal{H}(l)] \end{aligned} \quad (4.5.3)$$

This proves that the family of Hamiltonians  $\mathcal{H}(l)$  satisfy the flow equation eq. 4.5.1.  $\eta(l)$  is referred to as the generator of the flow equation. It is chosen so as to reduce the off-diagonal part of the Hamiltonian, either progressively or in one shot. In Schrieffer-Wolff transformation, the transformation is one-shot, and the  $\eta$  there is the  $S$  that sits on top of the exponential in the unitary transformation. In URG, the generator to decouple one electron  $q\beta$  is  $\eta_{q\beta}^\dagger - \eta_{q\beta}$ .

In Continuous unitary transformation (CUT) RG [34], we progressively block-diagonalize the Hamiltonian by removing off-diagonal terms that are farthest from the diagonal, through infinitesimal unitary transformations. The change is described as a flow against the parameter  $l$ . The canonical choice of the generator is  $\eta(l) = [\mathcal{H}_d, \mathcal{H}_X]$ , where  $\mathcal{H}_d$  is the diagonal part of the Hamiltonian and  $\mathcal{H}_X = \mathcal{H} - \mathcal{H}_d$  is the off-diagonal part of the Hamiltonian. Therefore,

$$\frac{d\mathcal{H}}{dl} = [\mathcal{H}_d(l), \mathcal{H}_X(l)], \mathcal{H}(l) \quad (4.5.4)$$

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

$$\mathcal{H} = \sum_i \epsilon_i \hat{n}_i + \sum_{i \neq j} g_{ij} c_i^\dagger c_j \quad (4.5.5)$$

where  $g_{ij}^* = g_{ji}$ . The canonical generator then turns out to be

$$\eta = \left[ \sum_i \epsilon_i \hat{n}_i, \sum_{j \neq k} g_{jk} c_j^\dagger c_k \right] = \sum_{k \neq i} \epsilon_i \left[ g_{ik} c_i^\dagger c_k - g_{ki} c_k^\dagger c_i \right] = \sum_{k \neq i} g_{ik} c_i^\dagger c_k (\epsilon_i - \epsilon_k) \quad (4.5.6)$$

and the renormalization in the Hamiltonian is

$$\frac{d\mathcal{H}}{dl} = [\eta, \mathcal{H}] = \left[ \sum_{k \neq i} g_{ik} c_i^\dagger c_k (\epsilon_i - \epsilon_k), \sum_i \epsilon_i \hat{n}_i + \sum_{i \neq j} g_{ij} c_i^\dagger c_j \right] \quad (4.5.7)$$

The first commutator gives

$$- \sum_{i \neq k} g_{ik} (\epsilon_i - \epsilon_k)^2 c_i^\dagger c_k \quad (4.5.8)$$

The second commutator gives

$$\sum_{\substack{k \neq i \\ j}} \left[ g_{kj} g_{ik} (\epsilon_i - \epsilon_k) c_i^\dagger c_j + g_{ji} g_{ik} (\epsilon_k - \epsilon_i) c_j^\dagger c_k \right] = \sum_{\substack{k \neq i \\ j}} g_{ik} g_{kj} (\epsilon_i + \epsilon_j - 2\epsilon_k) c_i^\dagger c_j \quad (4.5.9)$$

The total renormalization is

$$\frac{d\mathcal{H}}{dl} = - \sum_{i \neq j} g_{ij} (\epsilon_i - \epsilon_j)^2 c_i^\dagger c_j + \sum_{\substack{k \neq i \\ j}} g_{ik} g_{kj} (\epsilon_i + \epsilon_j - 2\epsilon_k) c_i^\dagger c_j \quad (4.5.10)$$

The couplings renormalize as

$$\begin{aligned} \frac{d\epsilon_i}{dl} &= \sum_{k \neq i} 2|g_{ik}|^2 (\epsilon_i - \epsilon_k) \\ \frac{dg_{ij}}{dl} &= -g_{ij} (\epsilon_i - \epsilon_j)^2 + \sum_{k \neq i} g_{ik} g_{kj} (\epsilon_i + \epsilon_j - 2\epsilon_k) \end{aligned} \quad (4.5.11)$$

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

$$0 = \frac{d\text{Tr}(\mathcal{H})^2}{dl} = \frac{d\text{Tr}(\mathcal{H})^2}{dl} = \sum_i \frac{d\epsilon_i^2}{dl} + \sum_{i \neq j} \frac{d|g_{ij}|^2}{dl} \implies \sum_{i \neq j} \frac{d|g_{ij}|^2}{dl} = - \sum_i \frac{d\epsilon_i^2}{dl} \quad (4.5.12)$$

From the flow equation, we can see that

$$\sum_i \frac{d\epsilon_i^2}{dl} = 2 \sum_{i \neq k} \epsilon_i \frac{d\epsilon_i}{dl} = 2 \sum_i |g_{ik}|^2 (\epsilon_i - \epsilon_k)^2 \geq 0 \quad (4.5.13)$$

Therefore,

$$\sum_{i \neq j} \frac{d|g_{ij}|^2}{dl} \leq 0 \quad (4.5.14)$$

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

#### 4.5.2 CUT-RG for the Fröhlick Hamiltonian

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

$$\mathcal{H} = \mathcal{H}_d + \mathcal{H}_X \quad (4.5.15)$$

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

$$\sum_{kq} g_q b_{-q}^\dagger c_{k+q,\sigma}^\dagger c_{k\sigma} + \text{h.c.} \quad (4.5.16)$$

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

$$\eta(l) = [\mathcal{H}_d, \mathcal{H}] = [\mathcal{H}_d, \mathcal{H}_X] \quad (4.5.17)$$

It is easy to compute the commutators.

$$\begin{aligned} \left[ \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma}, \sum_{kq\sigma} b_{-q}^\dagger c_{k+q,\sigma}^\dagger c_{k\sigma} \right] &= \sum_{kq\sigma} g_q (\epsilon_{k+q} - \epsilon_k) g_q b_{-q}^\dagger c_{k+q,\sigma}^\dagger c_{k\sigma} \\ \left[ \sum_q \hbar\omega_q b_q^\dagger b_q, \sum_{kq} g_q b_{-q}^\dagger c_{k+q,\sigma}^\dagger c_{k\sigma} \right] &= \sum_{kq} g_q \hbar\omega_q b_{-q}^\dagger c_{k+q,\sigma}^\dagger c_{k\sigma} \end{aligned} \quad (4.5.18)$$

Therefore,

$$\eta = \sum_{kq\sigma} g_q (\epsilon_{k+q} - \epsilon_k + \hbar\omega_q) b_{-q}^\dagger c_{k+q,\sigma}^\dagger c_{k\sigma} - \text{h.c.} \quad (4.5.19)$$

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

$$\frac{d\mathcal{H}}{dl} = [\eta, \mathcal{H}] \quad (4.5.20)$$

The flow equation for the electron-phonon coupling is

$$\frac{dg_q}{dl} = -\xi^2 g_q \implies g_q(l) = g_q(0) \exp\{-\xi^2 l\} \quad (4.5.21)$$

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

$$V_{k,-k,q}(\infty) = V_{k,-k,-q}(0) - \frac{g_q^2 \omega_q}{\omega_q^2 + (\epsilon_{k+q} - \epsilon_k)^2} \quad (4.5.22)$$

Off-diagonal terms that connect larger energy differences  $\xi$  decay the fastest.

### 4.5.3 Deriving CUT RG from URG

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

$$\Delta\mathcal{H}^0 = \frac{1}{2} [\eta^\dagger - \eta, \mathcal{H}] \quad (4.5.23)$$

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

$$\begin{aligned} \eta^\dagger - \eta &= G_1 c^\dagger T - G_0 T^\dagger c \\ &= \frac{1}{\omega_1 - \omega_0} \left[ G_1 (\omega_1 - \omega_0) c^\dagger T - G_0 (\omega_1 - \omega_0) T^\dagger c \right] \\ &= \frac{1}{\omega_1 - \omega_0} \left[ G_1 \omega_1 c^\dagger T - c^\dagger T \omega_0 G_0 - T^\dagger c \omega_1 G_1 + G_0 \omega_0 T^\dagger c \right] \end{aligned} \quad (4.5.24)$$

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

$$\begin{aligned} \eta^\dagger - \eta &= \frac{1}{\omega_1 - \omega_0} \left[ G_1 (\omega_1 - G_1^{-1}) c^\dagger T + c^\dagger T - c^\dagger T (\omega_0 - G_0^{-1}) G_0 - c^\dagger T \right. \\ &\quad \left. - T^\dagger c (\omega_1 - G_1^{-1}) G_1 - T^\dagger c + G_0 (\omega_0 - G_0^{-1}) T^\dagger c + T^\dagger c \right] \\ &= \frac{1}{\omega_1 - \omega_0} \left[ G_1 (\omega_1 - G_1^{-1}) c^\dagger T - c^\dagger T (\omega_0 - G_0^{-1}) G_0 \right. \\ &\quad \left. - T^\dagger c (\omega_1 - G_1^{-1}) G_1 + G_0 (\omega_0 - G_0^{-1}) T^\dagger c \right] \end{aligned} \quad (4.5.25)$$

In the last step, the extra  $c^\dagger T$  and  $T^\dagger c$  terms canceled out. In the second and third terms, we can bring the Greens function closer to the operators  $c^\dagger T$  and  $T^\dagger c$  because  $(\omega_j - G_j^{-1}) G_j = G_j (\omega_j - G_j^{-1})$ :

$$\begin{aligned} \eta^\dagger - \eta &= \frac{1}{\omega_1 - \omega_0} \left[ G_1 (\omega_1 - G_1^{-1}) c^\dagger T - c^\dagger T G_0 (\omega_0 - G_0^{-1}) \right. \\ &\quad \left. - T^\dagger c G_1 (\omega_1 - G_1^{-1}) + G_0 (\omega_0 - G_0^{-1}) T^\dagger c \right] \\ &= \frac{1}{\omega_1 - \omega_0} \left[ G_1 (\omega_1 - G_1^{-1}) c^\dagger T - G_1 c^\dagger T (\omega_0 - G_0^{-1}) \right. \\ &\quad \left. - G_0 T^\dagger c (\omega_1 - G_1^{-1}) + G_0 (\omega_0 - G_0^{-1}) T^\dagger c \right] \end{aligned} \quad (4.5.26)$$



In the last step, we again used the constraint  $G_1 c^\dagger T = c^\dagger T G_0$  and its partner. From the definition of the Green's function  $G = (\omega - \mathcal{H}^d)^{-1}$ , we can write  $\omega_j - G_j^{-1} = \mathcal{H}_j^d$ . Therefore,

$$\begin{aligned} \eta^\dagger - \eta &= \frac{1}{\omega_1 - \omega_0} \left[ G_1 \mathcal{H}_1^d c^\dagger T - G_1 c^\dagger T \mathcal{H}_0^d - G_0 T^\dagger c \mathcal{H}_1^d + G_0 \mathcal{H}_0^d T^\dagger c \right] \\ &= \frac{1}{\omega_1 - \omega_0} \left[ G \mathcal{H}^d c^\dagger T - G c^\dagger T \mathcal{H}^d - G T^\dagger c \mathcal{H}^d + G \mathcal{H}^d T^\dagger c \right] \\ &= \frac{1}{\omega_1 - \omega_0} G \left[ \mathcal{H}^d, c^\dagger T + T^\dagger c \right] \end{aligned} \quad (4.5.27)$$

where  $\mathcal{H}^d = \mathcal{H}_1^d \hat{n} + \mathcal{H}_0^d (1 - \hat{n})$  and  $G = G_1 \hat{n} + G_0 (1 - \hat{n}) = (\hat{\omega} - \mathcal{H}^d)^{-1}$ . For URG, the relevant off-diagonal part of the Hamiltonian for the current node is  $\mathcal{H}^I = c^\dagger T + T^\dagger c$ . Therefore,

$$\eta^\dagger - \eta = \frac{1}{\omega_1 - \omega_0} G \left[ \mathcal{H}^d, \mathcal{H}^I \right] = \left[ \mathcal{H}^d, \frac{1}{\omega_1 - \omega_0} G \mathcal{H}^I \right] \quad (4.5.28)$$

The last equality comes about because both  $G$  and  $\mathcal{H}^d$  are completely diagonal and hence commute. The renormalization in the Hamiltonian under URG, which is a function of both the quantum fluctuation scale  $\omega$  and the running bandwidth  $D$ , can thus be written as

$$\Delta \mathcal{H}(\omega, D) = \left[ \left[ \mathcal{H}^d, \tilde{\mathcal{H}}^I \right], \mathcal{H} \right] - \mathcal{H}_X \quad (4.5.29)$$

The most obvious difference with the CUT version is the presence of the off-diagonal piece  $-\mathcal{H}_X$ . This is a result of the philosophical difference between URG and CUT-RG - while CUT-RG gradually suppresses the off-diagonal matrix elements, URG makes the off-diagonal components in each  $2 \times 2$  block vanish completely. We can instead look at the renormalization in the diagonal part of the Hamiltonian under URG:

$$\Delta \mathcal{H}^0(\omega, D) = \left[ \left[ \mathcal{H}^d, \tilde{\mathcal{H}}^I \right], \mathcal{H} \right] \quad (4.5.30)$$

where  $\tilde{\mathcal{H}}^I = \frac{1}{\omega_1 - \omega_0} G \mathcal{H}^I$ . This can be compared to the analogous equation for CUT (eq. 4.5.4),

$$\Delta \mathcal{H}(\lambda) = \Delta \lambda \left[ \left[ \mathcal{H}_d, \mathcal{H}_X \right], \mathcal{H} \right] \quad (4.5.31)$$

Leaving aside the obvious differences in the philosophies (the presence of  $\omega$  in URG or the fact that while URG decouples as a flow in the bandwidth, CUT uses a general parameter  $\lambda$  or the algorithmic difference that while URG decouples one specific node, CUT tries to make the Hamiltonian band-diagonal), the major physical difference is the presence of the total Green's function in the URG equation. It must be noted that while CUT employs the entire off-diagonal part in  $\mathcal{H}_X$ , the  $\mathcal{H}^I$  of URG contains only those parts that are off-diagonal with respect to the node being decoupled at this step.

To bring the URG form closer to CUT, we can make some approximations.

$$G = (\hat{\omega} - \mathcal{H}^d)^{-1} \approx -(\mathcal{H}^d)^{-1} \quad (4.5.32)$$

where we assumed that the quantum fluctuations are small and can be ignored w.r.t the diagonal contribution  $\mathcal{H}^d$ . This gives

$$\frac{\Delta \mathcal{H}^0(\omega, D)}{\left[ \mathcal{H}_1^d (\omega_0 - \omega_1) \right]^{-1}} = \left[ \left[ \mathcal{H}^d, \mathcal{H}^I \right], \mathcal{H} \right] \quad (4.5.33)$$

We can thus make the connection,

$$\Delta \lambda \sim \left[ \mathcal{H}_1^d (\omega_0 - \omega_1) \right]^{-1} \quad (4.5.34)$$

Note that in going from eq. 4.5.30 to the simplified form eq. 4.5.33, we had to drop all quantum fluctuations in the denominator and we lose the fixed point structure in the process. This results in the distinction that while URG can reach a fixed point theory in a finite number of steps, CUT cannot do so.

## 4.6 Comparison of the Canonical Transformations

We have considered three canonical transformations in this section: the Poor Man's scaling (PMS), the Schrieffer-Wolff transformation (SWT) and the continuous unitary transformation renormalization group (CUT-RG). PMS and SWT are more or less identical; they differ in the context in which they are used. PMS is used when there is an entire spectrum of energies in the model, ranging from a low energy limit to a high energy; it is then employed to decouple the highest energy modes in an iterative fashion. SWT is used when the Hamiltonian can be split into one high and one low energy part, and we need to decouple these two modes. It is clear when seen from this perspective that SWT is like a one-shot PMS; it decouples the UV from the IR in one step, compared to the iterative approach of PMS. However, as has been shown in the previous subsections, both PMS and SWT can be formalized in an identical fashion, so that one can be switched for the other in both contexts.

Now that we have established that PMS and SWT are formally identical, we can relate them to URG. URG is similar in philosophy to PMS in the fact that URG also successively decouples high energy modes from the low energy ones. The difference is that URG takes care of the quantum fluctuations, at least in principle, by introducing a new set of energy scales  $\omega$ . These  $\omega$  then parameterise the RG flows of URG, compared to the single RG flow of PMS. Since SWT is formally the same as PMS, there is also a comparison between SWT and URG. Both PMS and SWT trivialize the quantum fluctuation scales of URG by replacing it with the bare energy values.

CUT-RG is philosophically different from the other transformations. Its goal is to gradually reduce the contributions of the off-diagonal terms by making them decay along a certain scale  $l$ . Off-diagonal terms that connect states with large energy differences decay faster. In this sense, there is no sequential dropping out of off-diagonal terms; all off-diagonal terms disappear at  $l = \infty$ . In this sense, it is like a continuous version of SWT. While SWT strives to remove an entire off-diagonal term in one-shot, CUT RG does this gradually by introducing a scale  $l$ . This separation of scales is absent in SWT. It does exist in URG and PMS, albeit in a different fashion. There, the separation comes in when we decouple single electron states starting from the Brillouin zone boundary  $\Lambda_N$  and come down to the Fermi surface  $\Lambda_0$ . Each  $\Lambda$  provides a natural energy scale for separating the high and low energy physics.

If one integrates the continuum generator  $\eta$  over all the scales, one should recover something analogous to the SWT generator. This generator is however necessarily perturbative in the off-diagonal term, since by definition  $\eta$  will only be of first order in  $\mathcal{H}_X$ . This is in contrast to the non-perturbative generators in URG and, at least in principle, PMS. This non-perturbative form is encapsulated in the presence of a second completely different set of energy scales  $\omega$  (or  $E$  in PMS). This second energy scale is absent in CUT RG because it takes care of at most the second order term.

Another point to note is that since SWT keeps the entire off-diagonal piece in the generator, new terms will almost certainly be generated at every step, and they have to be truncated. This is not the case with URG or PMS, because in those methods, we decouple just a single-electron at each step, and so those electrons become integrals of motion at that step, leading to their removal from the off-diagonal piece, and very often the Hamiltonian retains the same form as the bare model. This makes the philosophy of URG and PMS easier to work with. Tied to this is the fact that CUT RG often takes a certain type of interaction in the generator part, and not the entire off-diagonal piece. Hence, at the limit of the flow parameter going to  $\infty$ , the chosen off-diagonal piece goes to zero but the remaining off-diagonal pieces still remain. As a result, the Hamiltonian is at most block diagonal at this stage. On the other hand, URG progressively decouples single electrons, meaning all scattering terms corresponding to that electron vanish at each step.

One last thing to note is that URG, being unitarily implemented with a well-defined generator, does not accommodate for spontaneous symmetry breaking (SSB). In order to see SSB, the symmetry-breaking term has to be added to the bare model explicitly; if this term grows under the RG, then the ground state will be symmetry-broken. CUT RG, however, does allow for SSB through the idea that the generator is not uniquely defined. If the generator commutes with a particular symmetry, then the family of Hamiltonians will also have the symmetry [33]. However, if the generator is replaced by something that is normal ordered w.r.t a particular expectation value, then the CUT RG flow will usually be towards either the symmetry-preserved state or the symmetry-broken state, depending on whichever is stable [35].



Figure 4.3: Comparison of the various unitary transformations and their relationships to each other.

## Chapter 5

# URG of generalised SIAM: RG flows and fixed point Hamiltonian

### 5.1 The single-impurity Anderson model

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

$$\mathcal{H} = \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{k\sigma} \left( V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right) + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \quad (5.1.1)$$

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.

$$\mathcal{H} = \sum_{k\sigma} \epsilon_k \tau_{k\sigma} + \sum_{k\sigma} \left( V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right) + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \quad (5.1.2)$$

### 5.2 Calculation of renormalisation

The renormalisation is

$$c_{q\beta}^\dagger T \frac{1}{\omega - H^D} T^\dagger c_{q\beta} + T^\dagger c_{q\beta} \frac{1}{\omega' - H^D} c_{q\beta}^\dagger T \quad (5.2.1)$$

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

$$H^D = \epsilon_q \tau_{q\beta} + \epsilon_d \hat{n}_{d\beta} + U \hat{n}_{d\beta} \hat{n}_{d\bar{\beta}} \quad (5.2.2)$$

The off-diagonal part is

$$c_{q\beta}^\dagger T = V_q c_{q\beta}^\dagger c_{d\beta} \quad (5.2.3)$$

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

$$\begin{aligned} \Delta H &= c_{q\beta}^\dagger c_{d\beta} \frac{1|V_q|^2}{\omega - H^D} c_{d\beta}^\dagger c_{q\beta} + c_{d\beta}^\dagger c_{q\beta} \frac{1|V_q|^2}{\omega' - H^D} c_{q\beta}^\dagger c_{d\beta} \\ &= c_{q\beta}^\dagger c_{d\beta} \frac{|V_q|^2}{\omega - D/2 - \epsilon_d - U \hat{n}_{d\bar{\beta}}} c_{d\beta}^\dagger c_{q\beta} + c_{d\beta}^\dagger c_{q\beta} \frac{|V_q|^2}{\omega' - D/2} c_{q\beta}^\dagger c_{d\beta} \\ &= \frac{\hat{n}_{q\beta} (1 - \hat{n}_{d\beta}) |V_q|^2}{\omega - D/2 - \epsilon_d - U \hat{n}_{d\bar{\beta}}} + \frac{\hat{n}_{d\beta} (1 - \hat{n}_{q\beta}) |V_q|^2}{\omega' - D/2} \end{aligned} \quad (5.2.4)$$

For comparing the two  $\omega$ s, we will use the relation eq. 3.1.72:  $\omega_0^1 + \omega_0^1 = H_0^D + H_1^D$  where  $\omega_0^1 = \omega'$ .  $\omega_0^1$  however is not  $\omega$ . This is because the relation assumes the  $\omega$ s to be calculated at the same energy - while  $\omega'$  is calculated at energy  $-D$ ,  $\omega$  is at energy  $D$ . The  $\omega_0^1$  should hence be the  $\omega$  at energy  $-D$ , which is  $-\omega$ . With this in mind, the relation says

$$\omega' - \omega = D/2 + \epsilon_d + U \hat{n}_{d\beta} - D/2 \quad (5.2.5)$$

This gives an expression of  $\omega'$  in terms of  $\omega$ . Substituting this into  $\Delta H$  gives

$$\Delta H = \frac{\hat{n}_{q\beta} (1 - \hat{n}_{d\beta}) |V_q|^2}{\omega - D/2 - \epsilon_d - U \hat{n}_{d\bar{\beta}}} + \frac{\hat{n}_{d\beta} (1 - \hat{n}_{q\beta}) |V_q|^2}{\omega - D/2 + \epsilon_d + U \hat{n}_{d\bar{\beta}}} \quad (5.2.6)$$

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

$$\begin{aligned} \Delta H &= \sum_{q\beta} |V_q|^2 \left[ \frac{\hat{n}_{q\beta} (1 - \hat{n}_{d\beta})}{\omega - D/2 - \epsilon_d - U \hat{n}_{d\bar{\beta}}} + \frac{\hat{n}_{d\beta} (1 - \hat{n}_{q\beta})}{\omega - D/2 + \epsilon_d + U \hat{n}_{d\bar{\beta}}} \right] \\ &= \sum_q |V_q|^2 \left[ \frac{(1 - \hat{n}_{d\beta}) \hat{n}_{d\bar{\beta}}}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d - U} + \frac{(1 - \hat{n}_{d\beta}) (1 - \hat{n}_{d\bar{\beta}})}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d} + \frac{\hat{n}_{d\beta} \hat{n}_{d\bar{\beta}}}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d + U} + \frac{\hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}})}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d} \right] \end{aligned} \quad (5.2.7)$$

### 5.3 Scaling equations for the SIAM

Once we have the renormalisation for decoupling one electronic or hole state, we can just sum over the spins and momenta to get the total renormalisation upon decoupling the entire shells  $\pm\epsilon_q$ . From the structure of  $\Delta\mathcal{H}$  in eq. 5.2.7, we can see that there are renormalisations 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  $(1 - \hat{n}_{d\beta})(1 - \hat{n}_{d\bar{\beta}}) + \hat{n}_{d\bar{\beta}}(1 - \hat{n}_{d\beta})$ .

$$\begin{aligned} \Delta E_2 &= +2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d + U} \\ \Delta E_1 &= + \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d} + \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d - U} \\ \Delta E_0 &= +2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d} \end{aligned} \quad (5.3.1)$$

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

$$\begin{aligned} \Delta\epsilon_d &= + \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d} + \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d - U} - 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d} \\ \Delta U &= \sum_q \frac{2|V_q|^2}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d + U} + \sum_q \frac{2|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d} - \sum_q \frac{2|V_q|^2}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d} - \sum_q \frac{2|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d - U} \end{aligned} \quad (5.3.2)$$

### 5.4 Connection to poor man's scaling

To obtain the results of Poor Man's scaling [28][36], we can look at various regimes. First we look at the case when both  $\epsilon_d$  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  $\epsilon_d$  and  $U$  in the denominator compared to the  $\epsilon_q$ .

$$\begin{aligned} \Delta\epsilon_d &= \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} + \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} - 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} \\ \Delta U &= 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} + 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} - 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} - 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} \end{aligned} \quad (5.4.1)$$

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

$$\begin{aligned}\Delta\epsilon_d &= \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} - 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} \\ \Delta U &= 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} - 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q}\end{aligned}\tag{5.4.2}$$

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

$$\begin{aligned}\Delta U &= 0 \\ \delta\epsilon_d &= -\frac{\Delta}{\pi} \frac{1}{\omega - \frac{1}{2}D}\end{aligned}\tag{5.4.3}$$

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

$$\delta\epsilon_d = \frac{\Delta}{\pi} \frac{\delta D}{D}\tag{5.4.4}$$

This is the one-loop scaling equation.

## 5.5 Preservation of particle-hole symmetry

The Anderson model Hamiltonian, eq. 5.1.1, 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

$$\epsilon_d \sum_\sigma \hat{n}_{d\sigma} \rightarrow 2\epsilon_d - \epsilon_d \sum_\sigma \hat{n}_{d\sigma}\tag{5.5.1}$$

$$U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \rightarrow U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} - U \sum_\sigma \hat{n}_{d\sigma} + U\tag{5.5.2}$$

$$\sum_{k\sigma} V(k) c_{k\sigma}^\dagger c_{d\sigma} + hc \rightarrow \sum_{k\sigma} -V(k) c_{k\sigma} c_{d\sigma}^\dagger + hc = \sum_{k\sigma} V^*(k) c_{k\sigma}^\dagger c_{d\sigma} + hc\tag{5.5.3}$$

The impurity-bath hopping term can be made symmetric by making  $V(k)$  real; we would then have, from eq. 5.5.3,

$$V(k) \left( c_{k\sigma}^\dagger c_{d\sigma} + c_{d\sigma}^\dagger c_{k\sigma} \right) \rightarrow V(k) \left( c_{d\sigma}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger c_{d\sigma} \right)\tag{5.5.4}$$

The impurity diagonal terms,  $\epsilon_d$  and  $U$ , require a specific condition. Combining eqs. 5.5.1 and 5.5.2,

$$\epsilon_d \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \rightarrow (-\epsilon_d - U) \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow}\tag{5.5.5}$$

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

$$\epsilon_d = -\epsilon_d - U \implies \epsilon_d + \frac{1}{2}U = 0\tag{5.5.6}$$

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. 5.5.6.

../figures//phsymm.pdf

Figure 5.1: 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

$$\Delta \left( \epsilon_d + \frac{1}{2}U \right) = 0 \quad (5.5.7)$$

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  $\epsilon_d$  and  $U$ , we can find the RG equation for the asymmetry parameter. The slightly easier way is to just note that the renormalisation in  $E_2$  should be equal to the renormalisation in  $E_0$ , in order for p-h symmetry to hold.

$$\Delta E_2 = 2 \frac{\Delta}{\pi} \frac{1}{\omega - D + \epsilon_d + U}, \Delta E_0 = 2 \frac{\Delta}{\pi} \frac{1}{\omega - D - \epsilon_d} \quad (5.5.8)$$

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.

## 5.6 Numerical analysis of the particle-hole symmetric RG equations

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  $\epsilon_d$ .

$$\Delta \epsilon_d = -4|V|^2 \frac{\epsilon_d}{\left(\omega - \frac{1}{2}D\right)^2 - \epsilon_d^2} \quad (5.6.1)$$


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

$$\Delta |\epsilon_d| = -4|V|^2 \frac{|\epsilon_d|}{\left(\omega - \frac{1}{2}D\right)^2 - \epsilon_d^2} \quad (5.6.2)$$

Depending on the signature of the denominator, the flows will be either relevant or irrelevant. For the flow to 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. 5.3.


## 5.7 Introduction of spin-exchange and charge isospin-exchange interactions into the SIAM: the generalised SIAM

We will now study the generalised SIAM obtained by introducing spin-exchange and charge isospin-exchange interactions between the impurity and the conduction bath. 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.



../figures/ed\_pure\_siam.pdf

Figure 5.2: Left: Irrelevant flow towards  $|\epsilon_d| = 0$ , at low  $\omega$ . Right: Relevant flow towards large  $|\epsilon_d|$ , at large  $\omega$ . 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  $\epsilon_d$ .



../figures/ed\_vs\_size.pdf

Figure 5.3: Change in fixed point value of  $|\epsilon_d|$  with system size.



The spin-exchange interaction has the form

$$J\vec{S}_d \cdot \vec{s} = J \left[ S_d^z s^z + \frac{1}{2} (S_d^+ s^- + S_d^- s^+) \right], \quad (5.7.1)$$

where  $\vec{S}_d = (S_d^x, S_d^y, S_d^z) = \sum_{\alpha\beta} \vec{\sigma}_{\alpha\beta} c_{d\alpha}^\dagger c_{d\beta}$  is the impurity spin operator,  $\vec{s} = \sum_{kk'\alpha\beta} \vec{\sigma}_{\alpha\beta} c_{k\alpha}^\dagger c_{k'\beta}$  is the spin operator for the conduction bath and  $J$  is the spin-exchange coupling. The bath spin operator actually acts locally, as can be seen by Fourier transforming to real space (using the definition  $f(k) = \frac{1}{\sqrt{N}} \sum_r g(r) \exp(ikr)$ ):

$$\vec{s} = \sum_{kk'rr'} \frac{1}{N} e^{ikr - ik'r'} \vec{\sigma}_{\alpha\beta} c_{r\alpha}^\dagger c_{r'\beta} = \sum_{rr'} \frac{1}{N} \vec{\sigma}_{\alpha\beta} c_{r\alpha}^\dagger c_{r'\beta} N \delta(r) \delta(r') = \vec{\sigma}_{\alpha\beta} c_{0\alpha}^\dagger c_{0\beta} \quad (5.7.2)$$

In order to introduce the charge isospin coupling, we define the Nambu spinor [37, 38]  $\psi^k = \begin{pmatrix} c_{k\uparrow} & c_{k\downarrow}^\dagger \end{pmatrix}$ , and the charge isospin [39] for the mobile conduction electrons

$$\vec{C} = \sum_{kk'} \psi^{k\dagger} \vec{S} \psi^{k'} = \frac{1}{2} \sum_{kk'\alpha\beta} \psi_\alpha^{k\dagger} \vec{\sigma}_{\alpha\beta} \psi_\beta^{k'} \quad (5.7.3)$$

The various components of the isospin are

$$\begin{aligned} C^z &= \sum_{kk'\sigma} \frac{1}{2} \psi_\sigma^{k\dagger} \sigma_{\sigma\sigma}^z \psi_\sigma^{k'} = \frac{1}{2} \sum_{kk'\sigma} \left( c_{k\sigma}^\dagger c_{k'\sigma} - \frac{1}{2} \delta_{kk'} \right) \\ C^x &= \sum_{kk'\sigma} \frac{1}{2} \psi_\sigma^{k\dagger} \sigma_{\sigma\bar{\sigma}}^x \psi_\sigma^{k'} = \sum_{kk'\sigma} \frac{\sigma}{4} \left( c_{k\sigma}^\dagger c_{k'\bar{\sigma}} + \text{h.c.} \right) \\ C^y &= \sum_{kk'\sigma} \frac{1}{2} \psi_\sigma^{k\dagger} \sigma_{\sigma\bar{\sigma}}^y \psi_\sigma^{k'} = \sum_{kk'\sigma} -\frac{i\sigma}{4} \left( c_{k\sigma}^\dagger c_{k'\bar{\sigma}} - \text{h.c.} \right) \end{aligned} \quad (5.7.4)$$

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

$$[A, B^\dagger] = \frac{1}{4} \sum_{kk', qq'} \left[ c_{k\uparrow}^\dagger c_{k'\downarrow}^\dagger, i c_{q'\downarrow} c_{q\uparrow} \right] = \frac{i}{4} \sum_{kq} \left( c_{k\uparrow}^\dagger c_{q\uparrow} - c_{k\downarrow} c_{q\downarrow}^\dagger \right) \quad (5.7.5)$$

and therefore

$$\Rightarrow [C^x, C^y] = \frac{i}{2} \sum_{kq} \left( c_{k\uparrow}^\dagger c_{q\uparrow} - c_{k\downarrow} c_{q\downarrow}^\dagger \right) = iC^z \quad (5.7.6)$$

There are similar operators for the impurity electron:

$$\psi_d = \begin{pmatrix} c_{d\uparrow} & c_{d\downarrow}^\dagger \end{pmatrix}, \quad \vec{C}_d = \frac{1}{2} \sum_\beta \psi_{d,\alpha}^\dagger \vec{\sigma}_{\alpha\beta} \psi_{d,\beta} \quad (5.7.7)$$

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

$$K\vec{C}_d \cdot \vec{C} = K \left[ C_d^z C^z + \frac{1}{2} (C_d^+ C^- + C_d^- C^+) \right] \quad (5.7.8)$$

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

$$C^+ = \sum_{kk'} c_{k\uparrow}^\dagger c_{k'\downarrow}^\dagger, \quad C^- = \sum_{kk'} c_{k'\downarrow} c_{k\uparrow} \quad (5.7.9)$$

The full generalised Anderson model Hamiltonian, at particle-hole symmetry, is

$$\mathcal{H} = \sum_{k\sigma} \epsilon_k \tau_{k\sigma} + \epsilon_d \left( \hat{n}_{d\uparrow} - \hat{n}_{d\downarrow} \right)^2 + \sum_{k\sigma} \left( V_k c_{k\sigma}^\dagger c_{d\sigma} + \text{h.c.} \right) + J\vec{S}_d \cdot \vec{s} + K\vec{C}_d \cdot \vec{C} \quad (5.7.10)$$

For the URG analysis, at each RG step, we decouple the electronic states  $q\beta$  on the  $k$ -space shell of radius  $\Lambda_j$ . For simplicity, we will only consider those diagonal terms in the denominator that either have both  $q\beta$  and  $q\bar{\beta}$  or both  $q\beta$  and  $d$  or both  $q\bar{\beta}$  and  $d$ . Terms that have purely  $q\bar{\beta}$  will not be considered. Also, the scattering between just  $d$  and  $q\bar{\beta}$  can be ignored since it is diagonal in  $q\beta$ . The diagonal (number-preserving) part is

$$H_D = \sum_{\beta} \epsilon_q \tau_{q\beta} + \epsilon_d \left( \hat{n}_{d\uparrow} - \hat{n}_{d\downarrow} \right)^2 + JS_d^z s_q^z + KC_d^z C_q^z \quad (5.7.11)$$

where  $s_q^z = \frac{1}{2} \left( \hat{n}_{q\uparrow} - \hat{n}_{q\downarrow} \right)$  and  $C_q^z = \frac{1}{2} \left( \hat{n}_{q\uparrow} + \hat{n}_{q\downarrow} - 1 \right)$ . The off-diagonal part is:

$$H_X = \sum_{\beta=\uparrow,\downarrow} \left[ V c_{d\beta}^\dagger c_{q\beta} + \frac{1}{2} J \sum_{k < \Lambda_N} \left\{ \left( \hat{n}_{d\beta} - \hat{n}_{d\bar{\beta}} \right) \frac{1}{2} c_{k\beta}^\dagger c_{q\beta} + c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \right\} + \frac{1}{2} K \sum_{k < \Lambda_N} \left\{ \left( \hat{n}_d - 1 \right) \frac{1}{2} c_{k\beta}^\dagger c_{q\beta} + c_{d\beta}^\dagger c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}} c_{q\beta} \right\} \right] + \text{h.c.} \quad (5.7.12)$$

## 5.8 Calculation of renormalisation

### 5.8.1 Renormalisation of the impurity energy $\epsilon_d$

The coupling  $\epsilon_d$  is renormalised by three kinds of vertices:  $V^2$ ,  $J^2$  and  $K^2$ . We will consider these processes one after another. We define  $n_j$  as the number of states being decoupled on each side of the Fermi surface, at the  $j^{\text{th}}$  RG step. In order to treat both spin and isospin exchanges democratically, we take  $|\Psi\rangle_i = \frac{1}{2} (|0\rangle + |q\uparrow\rangle + |q\downarrow\rangle + |q\uparrow, q\downarrow\rangle)$  as the *initial* state for the scattering processes. The intermediate states  $|\Psi\rangle_{\text{int}}$  in the particle sector ( $c_{q\beta} |\Psi\rangle_i$ ) and hole sector ( $c_{q\beta}^\dagger |\Psi\rangle_i$ ) will then have both spin and isospin excitations which can couple with the corresponding impurity degree of freedom. We will assume that states  $q > k_F$  ( $\epsilon_q > 0$ ) above the Fermi surface can have only particle excitations and states below the Fermi surface can only have hole excitations. The kinetic energy part  $\epsilon_q \tau_{q\beta}$  of  $H_D$  for  $|\Psi\rangle_i$  is then zero, whereas it is always  $D/2$  for  $|\Psi\rangle_{\text{int}}$ . To demonstrate this for a typical  $q < k_F$ , the hole excitation is  $c_{q\uparrow} |\Psi\rangle_i = \frac{1}{\sqrt{2}} (|0\rangle + |q\downarrow\rangle)$ . This has an isospin term in the form of the *holon* and a spin term in the form of the down state. Since  $\tau_{q\uparrow} = -\frac{1}{2}$  in the excited state, the kinetic energy for  $|\Psi\rangle_{\text{int}}$  is  $\epsilon_q \tau_{q\uparrow} = (-D) \times \left(-\frac{1}{2}\right) = D/2$ .

The renormalisation arising from the first kind of terms, in the particle sector, is

$$\sum_{q\beta} c_{q\beta}^\dagger c_{d\beta} \frac{V^2}{\omega - H_D} c_{d\beta}^\dagger c_{q\beta} = \sum_{q\beta} V^2 \hat{n}_{q\beta} \left( 1 - \hat{n}_{d\beta} \right) \left( \frac{1 - \hat{n}_{d\bar{\beta}}}{\omega - E_0} + \frac{\hat{n}_{d\bar{\beta}}}{\omega' - E_1} \right) = V^2 n_j \sum_{\beta} \left( 1 - \hat{n}_{d\beta} \right) \left( \frac{1 - \hat{n}_{d\bar{\beta}}}{\omega_0 - E_0} + \frac{\hat{n}_{d\bar{\beta}}}{\omega_1 - E_1} \right) \quad (5.8.1)$$

$q$  runs over the momentum states that are being decoupled at this RG step:  $|q| = \Lambda_j$ .  $E_{1,0}$  are the diagonal parts of the Hamiltonian at  $\hat{n}_{d\bar{\beta}} = 0, 1$  respectively. We have  $\hat{n}_{d\beta} = 1$  in the intermediate state because of the  $c_{d\beta}^\dagger$  in front of the Greens function. Applying  $c_{q\beta}$  on the initial state  $|\Psi\rangle_i$  leaves us with  $C_q^z = -\frac{1}{2}$  and  $s_q^z = \frac{1}{2}\bar{\beta}$ . We also know that

$$\hat{n}_{d\beta} = 1, \begin{cases} \hat{n}_{d\bar{\beta}} = 0 & \implies S_d^z = \frac{1}{2}\beta, C_d^z = 0, \epsilon_d \left( \hat{n}_{d\uparrow} - \hat{n}_{d\downarrow} \right)^2 = \epsilon_d \\ \hat{n}_{d\bar{\beta}} = 1 & \implies S_d^z = 0, C_d^z = \frac{1}{2}, \epsilon_d \left( \hat{n}_{d\uparrow} - \hat{n}_{d\downarrow} \right)^2 = 0 \end{cases} \quad (5.8.2)$$

Combining all this, we can write  $E_1 = \frac{D}{2} - \frac{K}{4}$  and  $E_0 = \frac{D}{2} + \epsilon_d - \frac{J}{4}$ . In order to relate  $\omega_0$  with  $\omega_1$  with the common fluctuation scale  $\omega$  for the conduction electrons, we will replace these quantum fluctuation scales by the current renormalised values of the single-particle self-energy for the initial state from which we started scattering. For  $\hat{n}_{d\bar{\beta}} = 0$ , there is no additional self-energy because the impurity does not have any spin:  $\omega_0 = \omega$ . For  $\hat{n}_{d\bar{\beta}} = 1$ , we have an additional self-energy of  $\epsilon_d$  arising from the correlation on the impurity:  $\omega_1 = \omega + \epsilon_d$ . Substituting the

values of  $E_{0,1}$  and  $\omega_{0,1}$ , we get

$$V^2 n_j \sum_{\beta} \left(1 - \hat{n}_{d\beta}\right) \left( \frac{1 - \hat{n}_{d\bar{\beta}}}{\omega - \frac{D}{2} - \epsilon_d + \frac{J}{4}} + \frac{\hat{n}_{d\bar{\beta}}}{\omega - \frac{D}{2} + \epsilon_d + \frac{K}{4}} \right) \quad (5.8.3)$$

Performing a similar calculation for the hole sector gives the contribution:

$$V^2 n_j \sum_{\beta} \hat{n}_{d\beta} \left( \frac{1 - \hat{n}_{d\bar{\beta}}}{\omega - \frac{D}{2} + \epsilon_d + \frac{K}{4}} + \frac{\hat{n}_{d\bar{\beta}}}{\omega - \frac{D}{2} - \epsilon_d + \frac{J}{4}} \right) \quad (5.8.4)$$

We now come to the second type of terms: spin-spin. We first look at the particle sector:

$$\frac{J^2}{4} \sum_{q\beta} c_{d\bar{\beta}}^{\dagger} c_{d\beta} c_{q\beta}^{\dagger} c_{-q\bar{\beta}} \frac{1}{\omega - H_D} c_{d\beta}^{\dagger} c_{d\bar{\beta}} c_{q\bar{\beta}}^{\dagger} c_{q\beta} = \frac{J^2}{4} n_j \frac{1}{\omega - \frac{D}{2} + \frac{J}{4}} \sum_{\beta} \hat{n}_{d\bar{\beta}} \left(1 - \hat{n}_{d\beta}\right) \quad (5.8.5)$$

The diagonal part in the denominator was simple to deduce in this case, because the nature of the scattering requires the spins  $S_d^z$  and  $\frac{\beta}{2} \left( \hat{n}_{q\beta} - \hat{n}_{q\bar{\beta}} \right)$  to be anti-parallel. This ensures that the intermediate state has an energy of  $E = \frac{D}{2} + \epsilon_d - \frac{J}{4}$ , and the quantum fluctuation scale is  $\omega' = \omega + \epsilon_d$ , such that  $\omega' - E = \omega - \frac{D}{2} + \frac{J}{4}$ . In the hole sector, we have

$$\frac{J^2}{4} n_j \frac{1}{\omega - \frac{D}{2} + \frac{J}{4}} \sum_{\beta} \hat{n}_{d\beta} \left(1 - \hat{n}_{d\bar{\beta}}\right) \quad (5.8.6)$$

The final kind of scattering is the  $K^2$  type. Similar to the  $J^2$  term, we get the following contribution:

$$\frac{K^2}{4} \sum_{q\beta} c_{q\beta}^{\dagger} c_{q\bar{\beta}}^{\dagger} c_{d\bar{\beta}} c_{d\beta} \frac{1}{\omega - H_D} c_{d\beta}^{\dagger} c_{d\bar{\beta}}^{\dagger} c_{q\bar{\beta}} c_{q\beta} = \frac{K^2}{2} n_j \frac{1}{\omega - \frac{D}{2} + \frac{K}{4}} \left(1 - \hat{n}_{d\uparrow}\right) \left(1 - \hat{n}_{d\downarrow}\right) \quad (5.8.7)$$

in the particle sector. This is again because  $E = \frac{D}{2} - \frac{K}{4}$  in the intermediate state and  $\omega' = \omega$ . In the hole sector, we get

$$\frac{K^2}{2} n_j \frac{1}{\omega - \frac{D}{2} + \frac{K}{4}} \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} . \quad (5.8.8)$$

We now have all possible renormalisation to the impurity energy  $\epsilon_d$ . To actually compute the renormalisation, we will first calculate the renormalisation in the energies  $\epsilon_0, \epsilon_1$  and  $\epsilon_2$  of the impurity states  $|\hat{n}_d = 0\rangle, |\hat{n}_d = 1\rangle, |\hat{n}_d = 2\rangle$  respectively. The renormalisation of these states are given by the following terms:

- $\Delta\epsilon_0$  is given by the renormalisation of the term  $\left(1 - \hat{n}_{d\uparrow}\right) \left(1 - \hat{n}_{d\downarrow}\right)$
- $\Delta\epsilon_1$  is given by the renormalisation of either  $\left(1 - \hat{n}_{d\uparrow}\right) \hat{n}_{d\downarrow}$  or  $\left(1 - \hat{n}_{d\downarrow}\right) \hat{n}_{d\uparrow}$
- $\Delta\epsilon_2$  is given by the renormalisation of  $\hat{n}_{d\uparrow} \hat{n}_{d\downarrow}$

From eqs. 5.8.3, 5.8.4, 5.8.5, 5.8.6, 5.8.7 and 5.8.8, we write

$$\Delta\epsilon_0 = \Delta\epsilon_2 = \frac{2V^2 n_j}{\omega - \frac{D}{2} - \epsilon_d + \frac{J}{4}} + \frac{K^2 n_j / 2}{\omega - \frac{D}{2} + \frac{K}{4}}, \quad \Delta\epsilon_1 = \frac{2V^2 n_j}{\omega - \frac{D}{2} + \epsilon_d + \frac{K}{4}} + \frac{J^2 n_j / 2}{\omega - \frac{D}{2} + \frac{J}{4}} \quad (5.8.9)$$

We had started with a particle-hole symmetric Hamiltonian ( $2\epsilon_d + U = 0$ ); the fact that  $\Delta\epsilon_0 = \Delta\epsilon_2$  means the RG transformation has preserved that symmetry. The renormalisation of  $\epsilon_d$  is simply the renormalisation in the energy difference between the singly-occupied and vacant impurity levels:  $\Delta\epsilon_d = \Delta\epsilon_1 - \Delta\epsilon_0$ . This gives our first RG equation:

$$\Delta\epsilon_d = 2V^2 n_j \left( \frac{1}{\omega - \frac{D}{2} + \epsilon_d + \frac{K}{4}} - \frac{1}{\omega - \frac{D}{2} - \epsilon_d + \frac{J}{4}} \right) + \frac{n_j}{2} \left( \frac{J^2}{\omega - \frac{D}{2} + \frac{J}{4}} - \frac{K^2}{\omega - \frac{D}{2} + \frac{K}{4}} \right) \quad (5.8.10)$$

### 5.8.2 Renormalisation of the hybridisation $V$

Renormalisation of  $V$  happens through two kinds of processes:  $VJ$  and  $VK$ . In order words, the two vertices involve one single-particle scattering and one spin or isospin exchange respectively. We first look at the vertices that involve a spin-exchange scattering.

Within spin-exchange, the scattering can be either via  $S_d^z$  or through  $S_d^\pm$ . For the first kind, we have the following contribution in the particle sector:

$$\sum_{q\beta} V c_{q\beta}^\dagger c_{d\beta} \frac{1}{\omega - H_D} \frac{1}{4} J \sum_k \left( \hat{n}_{d\beta} - \hat{n}_{d\bar{\beta}} \right) c_{k\beta}^\dagger c_{q\beta} = \frac{1}{4} V J n_j \frac{1}{2} \left( \frac{1}{\omega'_1 - E} + \frac{1}{\omega'_2 - E} \right) \sum_{k\beta} \left( 1 - \hat{n}_{d\bar{\beta}} \right) c_{d\beta} c_{k\beta}^\dagger \quad (5.8.11)$$

The transformation from  $\frac{1}{\omega - H_D}$  to  $\frac{1}{2} \left( \frac{1}{\omega'_1 - E} + \frac{1}{\omega'_2 - E} \right)$  is made so that we can account for both the initial state and the final state energies through the two fluctuation scales  $\omega'_1$  and  $\omega'_2$  respectively; we calculate the denominators for both the initial and final states, and then take the mean of the two (hence the factor of half in front). This was not required previously because in the earlier scattering processes, the impurity returned to its initial state at the end, at least in terms of  $\epsilon_d \left( \hat{n}_{d\uparrow} - \hat{n}_{d\downarrow} \right)^2$ , and so we had  $\omega'_1 = \omega'_2 = \omega'$ .

Note that the  $c_{d\beta}$  in front of the Greens function resulted in  $\left( \hat{n}_{d\beta} - \hat{n}_{d\bar{\beta}} \right) \rightarrow \left( 1 - \hat{n}_{d\bar{\beta}} \right)$ . The intermediate state is characterised by  $\hat{n}_{d\beta} = 1 - \hat{n}_{d\bar{\beta}} = 1$ , which means that  $E = \frac{D}{2} + \epsilon_d - \frac{J}{4}$ . Moreover, the initial state gives  $\omega'_1 = \omega + \epsilon_d$  while the final state gives  $\omega'_2 = \omega$ . Therefore, the renormalisation becomes

$$-\frac{n_j}{4} V J \frac{1}{2} \left( \frac{1}{\omega - \frac{D}{2} + \frac{J}{4}} + \frac{1}{\omega - \frac{D}{2} - \epsilon_d + \frac{J}{4}} \right) \sum_{k\beta} \left( 1 - \hat{n}_{d\bar{\beta}} \right) c_{k\beta}^\dagger c_{d\beta} \quad (5.8.12)$$

One can generate another such process by exchanging the single-particle process and the spin-exchange process:

$$\sum_{q\beta} \frac{1}{4} J \sum_k \left( \hat{n}_{d\beta} - \hat{n}_{d\bar{\beta}} \right) c_{q\beta}^\dagger c_{k\beta} \frac{1}{\omega - H_D} V c_{d\beta}^\dagger c_{q\beta} \quad (5.8.13)$$

This is simply the Hermitian conjugate of the previous contribution. Combining this with the previous then gives

$$-\frac{n_j}{8} V J \left( \frac{1}{\omega - \frac{D}{2} + \frac{J}{4}} + \frac{1}{\omega - \frac{D}{2} - \epsilon_d + \frac{J}{4}} \right) \sum_{k\beta} \left( 1 - \hat{n}_{d\bar{\beta}} \right) \left( c_{d\beta}^\dagger c_{k\beta} + \text{h.c.} \right) \quad (5.8.14)$$

We now consider the spin-exchange processes involving  $S_d^\pm$ :

$$\sum_{q\beta} V c_{q\beta}^\dagger c_{d\beta} \frac{1}{\omega - H_D} \frac{1}{2} J \sum_k c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} = \frac{1}{2} V J n_j \frac{1}{2} \left( \frac{1}{\omega'_1 - E} + \frac{1}{\omega'_2 - E} \right) \sum_{k\beta} \left( 1 - \hat{n}_{d\beta} \right) c_{d\bar{\beta}} c_{k\beta}^\dagger \quad (5.8.15)$$

We again have  $E = \frac{D}{2} + \epsilon_d - \frac{J}{4}$ ,  $\omega'_1 = \omega + \epsilon_d$  and  $\omega'_2 = \omega$ , which gives

$$-\frac{1}{2} V J n_j \frac{1}{\omega - \frac{D}{2} + \frac{J}{4}} \sum_{k\beta} \left( 1 - \hat{n}_{d\beta} \right) c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} \quad (5.8.16)$$

Combining this with the Hermitian conjugate obtained from exchanging the processes gives

$$-\frac{1}{4} V J n_j \left( \frac{1}{\omega - \frac{D}{2} + \frac{J}{4}} + \frac{1}{\omega - \frac{D}{2} - \epsilon_d + \frac{J}{4}} \right) \sum_{k\beta} \left( 1 - \hat{n}_{d\beta} \right) \left( c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} + \text{h.c.} \right) \quad (5.8.17)$$

The contributions from the hole sector are obtained making the transformation  $\hat{n}_{d\bar{\beta}} \rightarrow 1 - \hat{n}_{d\bar{\beta}}$  on the particle sector contributions. The total renormalisation to  $V$  from  $VJ$  processes are

$$-\frac{3n_j}{8} V J \left( \frac{1}{\omega - \frac{D}{2} + \frac{J}{4}} + \frac{1}{\omega - \frac{D}{2} - \epsilon_d + \frac{J}{4}} \right) \sum_{k\beta} \left( c_{d\beta}^\dagger c_{k\beta} + \text{h.c.} \right) \quad (5.8.18)$$

We now look at the  $VK$  processes. The first one is

$$\sum_{q\beta} V c_{q\beta}^\dagger c_{d\beta} \frac{1}{\omega - H_D} \frac{1}{4} K \sum_k (\hat{n}_d - 1) c_{k\beta}^\dagger c_{q\beta} = -\frac{1}{8} V K n_j \left( \frac{1}{\omega - \frac{D}{2} + \frac{K}{4}} + \frac{1}{\omega - \frac{D}{2} + \epsilon_d + \frac{K}{4}} \right) \sum_{k\beta} \hat{n}_{d\beta} c_{k\beta}^\dagger c_{d\beta} \quad (5.8.19)$$

The exchanged process again gives the Hermitian conjugate, so the combined contribution is

$$-\frac{1}{8} V K n_j \left( \frac{1}{\omega - \frac{D}{2} + \frac{K}{4}} + \frac{1}{\omega - \frac{D}{2} + \epsilon_d + \frac{K}{4}} \right) \sum_{k\beta} \hat{n}_{d\beta} (c_{k\beta}^\dagger c_{d\beta} + \text{h.c.}) \quad (5.8.20)$$

The isospin-flip vertex gives

$$\sum_{q\beta} V c_{q\beta}^\dagger c_{d\beta} \frac{1}{\omega - H_D} \frac{1}{2} K \sum_k c_{d\beta}^\dagger c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}} c_{q\beta} = \frac{1}{4} K V n_j \left( \frac{1}{\omega - \frac{D}{2} + \frac{K}{4}} + \frac{1}{\omega - \frac{D}{2} + \epsilon_d + \frac{K}{4}} \right) \sum_{k\beta} (1 - \hat{n}_{d\beta}) c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}}. \quad (5.8.21)$$

Combining with Hermitian conjugate gives

$$\frac{1}{4} K V n_j \left( \frac{1}{\omega - \frac{D}{2} + \frac{K}{4}} + \frac{1}{\omega - \frac{D}{2} + \epsilon_d + \frac{K}{4}} \right) \sum_{k\beta} (1 - \hat{n}_{d\beta}) (c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}} + \text{h.c.}) . \quad (5.8.22)$$

After obtaining the hole sector contributions, the total renormalisation from  $VK$  processes is

$$-\frac{3n_j}{4} V K \left( \frac{1}{\omega - \frac{D}{2} + \frac{K}{4}} + \frac{1}{\omega - \frac{D}{2} + \epsilon_d + \frac{K}{4}} \right) \sum_{k\beta} (c_{d\beta}^\dagger c_{k\beta} + \text{h.c.}) . \quad (5.8.23)$$

The RG equation for  $V$  is

$$\Delta V = -\frac{3n_j V}{8} \left[ J \left( \frac{1}{\omega - \frac{D}{2} + \frac{J}{4}} + \frac{1}{\omega - \frac{D}{2} - \epsilon_d + \frac{J}{4}} \right) + K \left( \frac{1}{\omega - \frac{D}{2} + \frac{K}{4}} + \frac{1}{\omega - \frac{D}{2} + \epsilon_d + \frac{K}{4}} \right) \right] \quad (5.8.24)$$

### 5.8.3 Renormalisation of the exchange couplings $J$ and $K$

We will just note the renormalisation in  $J^z$ , which will be equal to  $J^\pm$  due to spin-rotation symmetry. The terms that renormalise  $J^z$  are of the form  $S_d^\pm S_d^\mp$ . In the particle sector, we have

$$\sum_q \sum_{kk'} \frac{1}{4} J^2 S_d^\pm c_{q\mp}^\dagger c_{k'\pm} \frac{1}{\omega - H_D} S_d^\mp c_{k\pm}^\dagger c_{q\mp} = -n_j \frac{1}{4} J^2 \left( \frac{1}{2} \pm S_d^z \right) \sum_{kk'} c_{k\pm}^\dagger c_{k\pm} \frac{1}{\omega - \frac{D}{2} + \frac{J}{4}} . \quad (5.8.25)$$

The denominator is determined using  $E = \frac{D}{2} + \epsilon_d - \frac{J}{4}$  and  $\omega' = \omega + \epsilon_d$ . In the hole sector, we similarly have

$$\sum_q \sum_{kk'} \frac{1}{4} J^2 S_d^\mp c_{k\pm}^\dagger c_{q\mp} \frac{1}{\omega - H_D} S_d^\pm c_{q\mp}^\dagger c_{k'\pm} = n_j \frac{1}{4} J^2 \left( \frac{1}{2} \mp S_d^z \right) \sum_{kk'} c_{k\pm}^\dagger c_{k\pm} \frac{1}{\omega - \frac{D}{2} + \frac{J}{4}} . \quad (5.8.26)$$

Adding all four expressions and dropping the constant part, we get

$$-n_j \frac{1}{2} J^2 S_d^z \sum_{kk'} (c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow}) \frac{1}{\omega - \frac{D}{2} + \frac{J}{4}} . \quad (5.8.27)$$

We can now directly read off the RG equation for  $J$ :

$$\Delta J = -\frac{n_j J^2}{\omega - \frac{D}{2} + \frac{J}{4}} \quad (5.8.28)$$

Since the spin and charge degrees of freedom are treated on an equal footing in the model, we obtain the RG equation for  $K$  by simply changing  $J \rightarrow K$ :

$$\Delta K = -\frac{n_j K^2}{\omega - \frac{D}{2} + \frac{K}{4}} \quad (5.8.29)$$

## 5.9 RG equations for generalised SIAM

$$\begin{aligned}
\Delta\epsilon_d &= 2V^2 n_j \left( \frac{1}{\omega - \frac{D}{2} + \epsilon_d + \frac{K}{4}} - \frac{1}{\omega - \frac{D}{2} - \epsilon_d + \frac{J}{4}} \right) + \frac{n_j}{2} \left( \frac{J^2}{\omega - \frac{D}{2} + \frac{J}{4}} - \frac{K^2}{\omega - \frac{D}{2} + \frac{K}{4}} \right), \\
\Delta V &= -\frac{3n_j V}{8} \left[ J \left( \frac{1}{\omega - \frac{D}{2} + \frac{J}{4}} + \frac{1}{\omega - \frac{D}{2} - \epsilon_d + \frac{J}{4}} \right) + K \left( \frac{1}{\omega - \frac{D}{2} + \frac{K}{4}} + \frac{1}{\omega - \frac{D}{2} + \epsilon_d + \frac{K}{4}} \right) \right], \\
\Delta J &= -\frac{n_j J^2}{\omega - \frac{D}{2} + \frac{J}{4}}, \\
\Delta K &= -\frac{n_j K^2}{\omega - \frac{D}{2} + \frac{K}{4}}
\end{aligned} \tag{5.9.1}$$

In terms of  $U = -2\epsilon_d$ , the equations become

$$\Delta U = 4V^2 n_j \left( \frac{1}{d_0} - \frac{1}{d_1} \right) - n_j \left( \frac{J^2}{d_2} - \frac{K^2}{d_3} \right), \tag{5.9.2}$$

$$\Delta V = -\frac{3n_j V}{8} \left[ J \left( \frac{1}{d_2} + \frac{1}{d_1} \right) + K \left( \frac{1}{d_3} + \frac{1}{d_0} \right) \right], \tag{5.9.3}$$

$$\Delta J = -\frac{n_j J^2}{d_2}, \quad \Delta K = -\frac{n_j K^2}{d_3} \tag{5.9.4}$$

$d_i$  are the denominators:

$$d_0 = \omega - \frac{D}{2} - \frac{U}{2} + \frac{K}{4}, \quad d_1 = \omega - \frac{D}{2} + \frac{U}{2} + \frac{J}{4}, \quad d_2 = \omega - \frac{D}{2} + \frac{J}{4}, \quad d_3 = \omega - \frac{D}{2} + \frac{K}{4} \tag{5.9.5}$$

## 5.10 Nature of coupling RG flows

### 5.10.1 Repulsive interaction on impurity: $U > 0$

For the Hamiltonians with positive on-site correlation, we will assume that the spin-exchange coupling is positive and charge isospin-exchange coupling is negative:  $J > 0, K < 0$ . This choice is motivated by the signs of the corresponding terms when they are generated via a Schrieffer-Wolff transformation [17]. The impurity-bath hybridisation  $V$  is always positive. The sign of the couplings lead to inequalities among the denominators which we will utilise at various points. First of all, since  $U > 0$ , we have  $d_1 - d_2 = \frac{U}{2} > 0$ . Secondly, since  $K < 0$ , we have  $d_2 - d_3 = \frac{J-K}{4} > 0$ . And finally, we have  $d_3 - d_0 = \frac{U}{2} > 0$ . Combining these, we can write

$$d_1 > d_2 > d_3 > d_0 \tag{5.10.1}$$

The strong-coupling regime is defined as the range of values of  $\omega$  where the hybridisation is relevant. This is ensured by the assumption  $d_1 < 0$ . From eq. 5.10.1, we can then conclude that all denominators are negative:  $d_i = -|d_i|$ . The simplest consequence of this is the RG flow of  $K$ :

$$\Delta K = -\frac{n_j K^2}{d_3} = \frac{n_j K^2}{|d_3|} > 0 \implies K_{j+1} > K_j \implies K_0 = -|K_0|, K^* \rightarrow 0 \tag{5.10.2}$$

$K_j$  is the value of  $K$  after the  $j^{\text{th}}$  RG step,  $K_0$  representing the bare value. In other words, since  $d_3 < 0$ , the RG equation for  $K$  provides an algebraic increment, and the negative  $K$  increases and flows towards zero. The  $*$  indicates a fixed point value. The isospin coupling is irrelevant in this regime, and we will ignore it.

The coupling  $J$ , on the other hand, is relevant and flows from a small positive value towards a large value at strong-coupling.

$$\Delta J = -\frac{n_j J^2}{d_2} = \frac{n_j J^2}{|d_2|} > 0 \implies J_{j+1} > J_j \implies J_0 \rightarrow \text{large } J^* \text{ (strong-coupling)} \tag{5.10.3}$$

The value of  $J^*$  is obtained when the denominator  $d_2$  vanishes.

Because of the RG irrelevance of  $K$ , we can simplify the RG equation for  $V$ :

$$\Delta V = -\frac{3n_j V J}{8} \left( \frac{1}{d_2} + \frac{1}{d_1} \right) = \frac{3n_j V J}{8} \left( \frac{1}{|d_2|} + \frac{1}{|d_1|} \right) > 0 \quad (5.10.4)$$

Since both the denominators are positive,  $V$  is relevant. The fixed point value  $V^*$  is attained when the denominator  $d_1$  vanishes ( $d_1$  will vanish earlier than  $d_2$ ).

We can compare the rate of flows of  $V$  and  $J$ :

$$\frac{\Delta V}{\Delta J} = \frac{3V}{8J} \left( 1 + \frac{|d_2|}{|d_1|} \right) > \frac{3V}{4J} \quad (5.10.5)$$

There we used the fact that  $|d_2| > |d_1|$ . We finally come to the RG equation for  $U$ :

$$\Delta U = 4V^2 n_j \left( \frac{1}{d_1} - \frac{1}{d_0} \right) - n_j \frac{J^2}{d_2} = -4V^2 \left( U + \frac{J}{4} \right) \frac{n_j}{d_0 d_1} - \frac{n_j J^2}{d_2} \quad (5.10.6)$$

For  $V > J$ , we can expect  $U$  to be irrelevant. On the other hand,  $V < J$  makes  $U$  relevant.

In short, the  $U > 0$  regime is characterised by an irrelevant isospin-exchange coupling  $K$  and a relevant spin-exchange coupling  $J$ , and the following set of RG equations for the remaining couplings  $U$  and  $V$ :

$$\Delta U = 4V^2 n_j \left( \frac{1}{d_1} - \frac{1}{d_0} \right) - n_j \frac{J^2}{d_2}, \quad \Delta V = -\frac{3n_j V J}{8} \left( \frac{1}{d_2} + \frac{1}{d_1} \right) \quad (5.10.7)$$

../figures/U_irr,U>0,U.pdf	../figures/U_irr,U>0,V.pdf	../figures/U_irr,U>0,J.pdf
../figures/U_rel,U>0,U.pdf	../figures/U_rel,U>0,V.pdf	../figures/U_rel,U>0,J.pdf

### 5.10.2 Attractive interaction on impurity: $U < 0$

Here, we have  $J < 0$  and  $K > 0$ . The denominators satisfy the following inequality in this regime:

$$d_0 > d_3 > d_2 > d_1 \quad (5.10.8)$$

The strong-coupling regime here corresponds to  $d_0 < 0$ . This again means that all the denominators are negative. The spin-exchange coupling  $J$  is now irrelevant, because its bare value is negative while its RG equation

../figures/VvsJ\_relvsirr.pdf

../figures/UvsJ\_relvsirr.pdf

../figures/VcvsJ.pdf

../figures/UcvsJ.pdf



is positive:  $\Delta J > 0$ . Moreover, the isospin coupling  $K$  is now positive and so is its RG equation:  $\Delta K > 0$ , which means it flows to strong-coupling.  $V$  also flows to strong-coupling. The RG equation for  $U$  can be written as

$$\Delta U = 4V^2 \left( \frac{K}{4} - U \right) \frac{n_j}{d_0 d_1} + \frac{n_j K^2}{d_3} \quad (5.10.9)$$

The first term is necessarily positive, while the second term is negative. This means that for roughly  $V_0 > J_0$ , we will have  $\Delta U > 0$ , and since  $U_0 < 0$ , this amounts to an irrelevant flow of  $U$  towards zero. On the other hand, for  $J_0 > V_0$ , we will have  $\Delta U < 0$ , and this corresponds to a relevant flow of  $U$  towards large negative value.

In other words, the RG flows in this regime can be exactly mapped to those in the positive  $U$  regime. The general statement is: in the strong-coupling regime of positive(negative)  $U$ ,  $V$  is always relevant,  $J(K)$  is relevant,  $K(J)$  is irrelevant, and  $U$  is relevant when  $J(K) > V$ , otherwise  $U$  is irrelevant.

## 5.11 Effective Hamiltonian and ground state

The fixed point Hamiltonian can, in general, be written as

$$\mathcal{H}^* = \sum_{\sigma, k} \epsilon_k \tau_{k\sigma} - \frac{U^*}{2} (\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow})^2 + \sum_{\sigma, k < \Lambda^*} \left( V^* c_{k\sigma}^\dagger c_{d\sigma} + \text{h.c.} \right) + J^* \vec{S}_d \cdot \vec{s} + K^* \vec{C}_d \cdot \vec{C} \quad (5.11.1)$$

The first term is the kinetic energy of all the electrons. The next two terms are the impurity-diagonal pieces, featuring the renormalised interaction  $U^*$ . The next three terms are the residual interactions between the impurity and the metal, with the renormalised couplings  $V^*$ ,  $J^*$  and  $K^*$ . The summations in these terms extend from the fixed point momentum cutoff  $\Lambda^*$  to 0. This is the region of momentum space which the URG was unable to decouple. The operators  $\vec{s}$  and  $\vec{C}$  represent the macroscopic magnetic and charge spins formed by the remaining electrons that are lying inside the window  $[0, \Lambda^*]$ :

$$\vec{s} = \sum_{\substack{k, k' < \Lambda^* \\ \alpha, \beta}} c_{k\alpha}^\dagger \vec{\sigma}_{\alpha\beta} c_{k'\beta} \quad (5.11.2)$$

Our goal here is to write down the ground state wavefunction for this low-energy Hamiltonian.

To make progress, we will simplify the effective Hamiltonian by taking the zero bandwidth limit. This reduces it to a two-site problem. One site is of course the impurity site, and this site will be labeled as site 1. The other site will be formed by the center of mass degree of freedom of the conduction electrons, and will be labeled as site 2. The Hamiltonian for this two-site problem is

$$\mathcal{H}_{IR} = -\frac{U^*}{2} (\hat{n}_{1\uparrow} - \hat{n}_{1\downarrow})^2 + V^* \sum_{\sigma} \left( c_{1\sigma}^\dagger c_{2\sigma} + \text{h.c.} \right) + J^* \vec{S}_1 \cdot \vec{S}_2 + K^* \vec{C}_1 \cdot \vec{C}_2 \quad (5.11.3)$$

The subscripts on the operators designate the site on which they act;  $\hat{n}_1$  is the number operator for the first site.

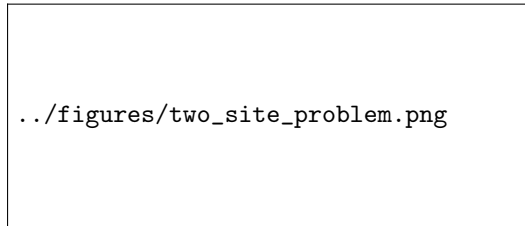


Figure 5.4: Two-site effective problem of fixed point Hamiltonian

We will adopt the following notation to represent the states in this Hilbert space. A general state will be represented in the Fock space basis as  $|n_{1\uparrow} n_{1\downarrow} n_{2\uparrow} n_{2\downarrow}\rangle$ . For example,

$$|1101\rangle = c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger c_{2\downarrow}^\dagger |-\rangle \quad (5.11.4)$$

$|-\rangle$  is the vacuum state.

For  $U > 0$ , the ground state is given by

$$|\Psi\rangle_1 = c_s \frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + c_c \frac{1}{\sqrt{2}} (|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle), \quad E_1 = -V^* \sqrt{\gamma^2 + 4} - \frac{1}{4}U^* - \frac{3}{8}J^* \quad (5.11.5)$$

where  $\gamma = \frac{1}{2V^*} \left[ \frac{1}{4} (3J^* + K^*) + \frac{1}{2}U^* \right]$ . The probabilities for the spin and charge sectors for the ground state are

$$(c_s)^2 = \frac{1}{2\sqrt{\gamma^2 + 4}} \left( \sqrt{\gamma^2 + 4} + \gamma \right), \quad (c_c)^2 = \frac{1}{2\sqrt{\gamma^2 + 4}} \left( \sqrt{\gamma^2 + 4} - \gamma \right). \quad (5.11.6)$$

For (roughly)  $J_0 > V_0$ , we get  $J^* \gg V^*$  and  $U^* \gg U_0$  so that  $\gamma \gg 1$ . This gives  $(c_s)^2 \sim 1$  and  $(c_c)^2 \sim 0$ . The entire contribution to the ground state then comes from the spin sectors of the two sites. This is calculated numerically in fig. 5.5.

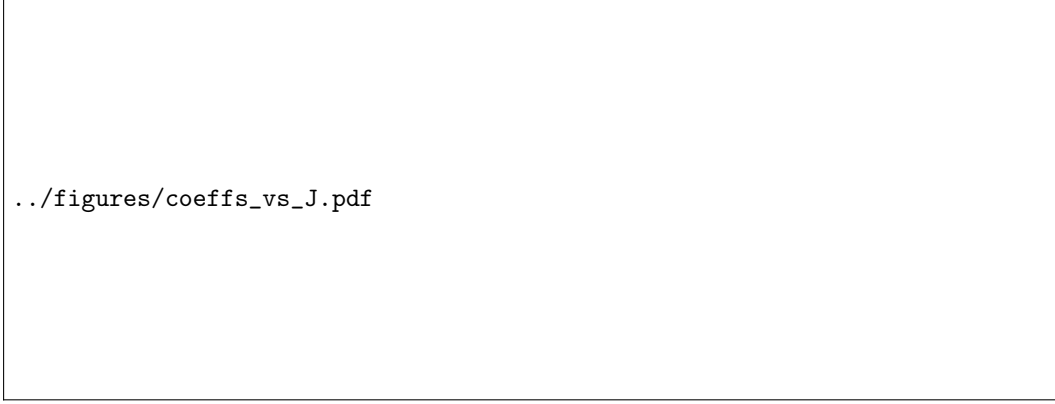


Figure 5.5: Variation of relative weights  $c_s$  and  $c_c$  with  $J_0$

In the other regime of  $U < 0$ , the two competing states are  $|\Psi\rangle_1$  defined above (with energy  $E_1$ ), and  $|\Psi_2\rangle$ , the charge singlet:  $|\Psi\rangle_2 = \frac{1}{\sqrt{2}} (|2, 0\rangle - |0, 2\rangle)$  having energy  $E_2$ .

$$E_2 = -\frac{3}{4}K^*, \quad E_1 - E_2 = -\frac{1}{4} \sqrt{\left( \frac{1}{2}K^* + U^* \right)^2 + (4V^*)^2} - \frac{1}{4}U^* + \frac{3}{4}K^* \quad (5.11.7)$$

For  $V_0 \gg K_0$ , the largest energy scale will be  $V^*$ , and we can then approximate this difference as

$$E_1 - E_2 \simeq -V^* < 0 \quad (5.11.8)$$

In such a case,  $|\Psi\rangle_1$  will therefore be the ground state. In the other regime  $V_0 \ll K_0$ , the largest energy scale will be  $K^*$ , and we can then write

$$E_1 - E_2 \simeq -\frac{1}{8}K^* + \frac{3}{4}K^* > 0 \quad (5.11.9)$$

In this case, the ground state will be  $|\Psi\rangle_2$ . There exists, therefore, a phase transition at a critical plane  $(U_c, K_c, V_c)$ , where the ground state changes between the charge singlet  $|\Psi\rangle_2$  and the spin singlet + charge triplet  $|\Psi\rangle_1$ .

## 5.12 Approach towards the thermodynamic limit

The URG method works strictly on finite systems and leads to finite values of fixed point couplings. The behaviour of the Hamiltonian in the thermodynamic limit can then be determined using finite-size scaling where we increase the bandwidth and decrease the width of each RG step. When applied to the fixed point value of the impurity-bath hybridisation parameter  $V$  (fig. 5.6), it can be seen that the fixed point value increases as the system size is increased, implying that the continuum limit of  $V^*$  is  $\infty$ . This holds for both  $V_0 > J_0$  and  $V_0 < J_0$ , as shown in the two panels of fig. 5.6.

In a similar manner, we checked the variation of the spin and charge probabilities,  $c_s$  and  $c_c$ , in the ground state, with increasing bandwidth. The result is shown in fig. 5.7. For both  $V_0 < J_0$  and  $V_0 > J_0$ , we see that



Figure 5.6: Variation of fixed point value  $V^*$  with increasing bandwidth  $D_0$ , for both  $V_0 > J_0$  and  $V_0 < J_0$ .

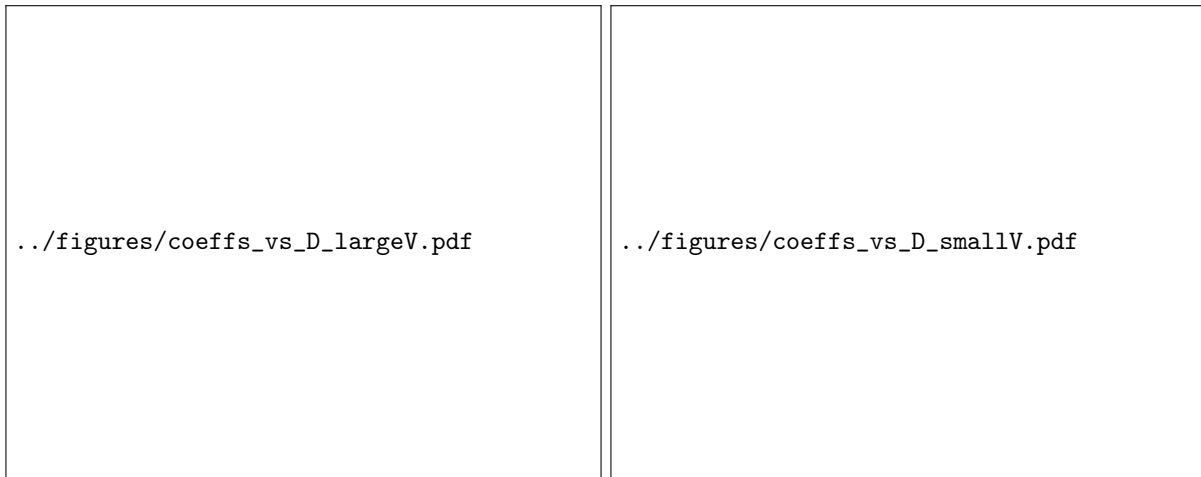


Figure 5.7: Variation of spin and charge fractions,  $c_s$  and  $c_c$ , of the ground state, as a function of bare bandwidth  $D_0$ . Left and right panels show the cases of  $J_0 < V_0$  and  $J_0 > V_0$  respectively.

the spin contribution increases towards unity while the charge contribution vanishes. This indicates that at large bandwidth, the ground state becomes purely a spin singlet, formed purely by singly-occupied impurity states.

$$\lim_{D_0 \rightarrow \infty} |\Psi\rangle_1 = \frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) \quad (5.12.1)$$

## Chapter 6

# Properties of the Low-Energy Theory: Thermodynamics and low-energy excitations

### 6.1 Effective temperature scale at the fixed point

We will first change the discrete RG equation to a continuum equation by interpreting  $\Delta J$  as  $\frac{\Delta J}{\Delta \ln D}$ , where the denominator is unity:  $\Delta \ln D = 1$ . Now, since the bandwidth is decreasing under the RG, we can write  $\Delta \ln D = -d \ln D$ . The continuum equation (for  $K = 0$ ) becomes

$$\frac{dJ}{d \ln D} = n(0)J^2 \frac{1}{\omega - \frac{D}{2} + \frac{J}{4}} \quad (6.1.1)$$

where we have replaced by the number of states at each shell with that at the Fermi surface (uniform DOS). We can define a dimensionless quantity  $g \equiv \frac{J}{\frac{D}{2}} - \omega$ . In terms of  $g$ , the continuum RG equation becomes

$$-\frac{dg}{d \ln D} + \frac{Dg}{2\omega - D} = \frac{n(0)g^2}{1 - \frac{g}{4}} \quad (6.1.2)$$

Now, for the specific case where  $D$  is small ( $D \rightarrow 0$ ), we can simplify and integrate this equation:

$$\begin{aligned} \frac{dg}{d \ln D} &= \frac{n(0)g^2}{\frac{g}{4} - 1} \\ \Rightarrow \left[ \frac{1}{g} + \frac{1}{4} \ln g \right]_{g_0}^{g^*} &= n(0) \ln D \Big|_{D_0}^{D^*} \end{aligned} \quad (6.1.3)$$

$g^*(0), D^*(0)$  are the fixed point (bare) values of  $g, D$ . From the denominator structure, the fixed-point value is  $g^* = 4$ . This gives an estimate of the bandwidth of the emergent window:

$$D^* = D_0 \left( \frac{4}{g_0} \right)^{\frac{1}{4n(0)}} \exp \left\{ -\frac{1}{n(0)} \left( \frac{1}{g_0} - \frac{1}{4} \right) \right\} \quad (6.1.4)$$

We can now define a temperature scale for the fixed-point theory:

$$T_K \equiv \frac{2N^*}{\pi} D^* = \frac{2N^*}{\pi} D_0 \left( \frac{4}{g_0} \right)^{\frac{1}{4n(0)}} \exp \left\{ -\frac{1}{n(0)} \left( \frac{1}{g_0} - \frac{1}{4} \right) \right\} \quad (6.1.5)$$

The factor of  $2N^*$  is inserted to make the Kondo temperature intensive (we will see below that the  $N^*$  allows it to be written in terms of parameters of the two-site Hamiltonian) -  $2N^*$  is the total number of momentum states in

the fixed point theory. The factor of  $\frac{1}{\pi}$  is for aesthetic reasons. Since we have and will primarily work with  $\omega = 0$ , the fixed point condition can be used to write  $D^* = \frac{J^* + K^*}{2}$ .

$$T_K = \frac{2N^*}{\pi} \frac{1}{2} (J^* + K^*) = \frac{1}{\pi} (j + k) \quad (6.1.6)$$

## 6.2 Impurity susceptibilities

### 6.2.1 Spin susceptibility

The spin susceptibility is defined as

$$\chi(\beta) = \beta \left( \left\langle (S_d^z)^2 \right\rangle - \langle S_d^z \rangle^2 \right) \quad (6.2.1)$$

There is an alternate way of calculating this. We insert a fictitious magnetic field that couples only to the impurity site. The Hamiltonian in the presence of this field is

$$\mathcal{H}'(B) = \mathcal{H} + BS_d^z \quad (6.2.2)$$

The susceptibility is then given by

$$\chi(\beta) = \lim_{B \rightarrow 0} \frac{1}{\beta} \left[ \frac{1}{Z(B)} \frac{\partial^2 Z(B)}{\partial B^2} - \frac{1}{Z(B)^2} \left( \frac{\partial Z(B)}{\partial B} \right)^2 \right] \quad (6.2.3)$$

where  $Z(B)$  is the partition function of the Hamiltonian  $\mathcal{H}'(B)$ . The following is to prove that the RHS of eqs. 6.2.1 and 6.2.3 are the same. We start with 6.2.3. The first derivative can be written as

$$\frac{\partial Z(B)}{\partial B} = \text{Trace} \left[ \frac{\partial}{\partial B} \exp \left\{ -\beta (\mathcal{H} + BS_d^z) \right\} \right] = \text{Trace} \left[ -\beta S_d^z \exp \left\{ -\beta (\mathcal{H} + BS_d^z) \right\} \right] \quad (6.2.4)$$

which means the first term becomes

$$\lim_{B \rightarrow 0} -\frac{1}{Z(B)^2} \left( \frac{\partial Z(B)}{\partial B} \right)^2 = - \left( \beta \frac{1}{\text{Trace} [\exp \{-\beta \mathcal{H}\}]} \text{Trace} [S_d^z \exp \{-\beta \mathcal{H}\}] \right)^2 = -\beta^2 \langle S_d^z \rangle^2 \quad (6.2.5)$$

The second derivative is

$$\frac{\partial^2 Z(B)}{\partial B^2} = \text{Trace} \left[ -\beta S_d^z \frac{\partial}{\partial B} \exp \left\{ -\beta (\mathcal{H} + BS_d^z) \right\} \right] = \text{Trace} \left[ \beta^2 (S_d^z)^2 \exp \left\{ -\beta (\mathcal{H} + BS_d^z) \right\} \right] \quad (6.2.6)$$

so the second term becomes

$$\lim_{B \rightarrow 0} \frac{1}{Z(B)} \frac{\partial^2 Z(B)}{\partial B^2} = \beta^2 \frac{1}{\text{Trace} [\exp \{-\beta \mathcal{H}\}]} \text{Trace} [(S_d^z)^2 \exp \{-\beta \mathcal{H}\}] = \beta^2 \langle (S_d^z)^2 \rangle \quad (6.2.7)$$

The full thing becomes

$$\begin{aligned} \lim_{B \rightarrow 0} \frac{1}{\beta} \left[ \frac{1}{Z(B)} \frac{\partial^2 Z(B)}{\partial B^2} - \frac{1}{Z(B)^2} \left( \frac{\partial Z(B)}{\partial B} \right)^2 \right] &= \frac{1}{\beta} \left( -\beta^2 \langle S_d^z \rangle^2 + \beta^2 \langle (S_d^z)^2 \rangle \right) \\ &= \beta \left( \langle (S_d^z)^2 \rangle - \langle S_d^z \rangle^2 \right) \end{aligned} \quad (6.2.8)$$

This completes the proof.

To calculate the impurity susceptibility, we take the zero bandwidth Hamiltonian  $\mathcal{H}_{IR}$  and insert a magnetic field to obtain the Hamiltonian in eq. (6.2.2). For a particular regime of  $U$ , only one of  $J$  or  $K$  will be non-zero. We then numerically diagonalise this Hamiltonian to obtain the partition function  $Z(B)$  and its derivatives. The spin susceptibility can then be calculated using eq. (6.2.3). The results for  $U > 0$  are shown in fig. 6.1.

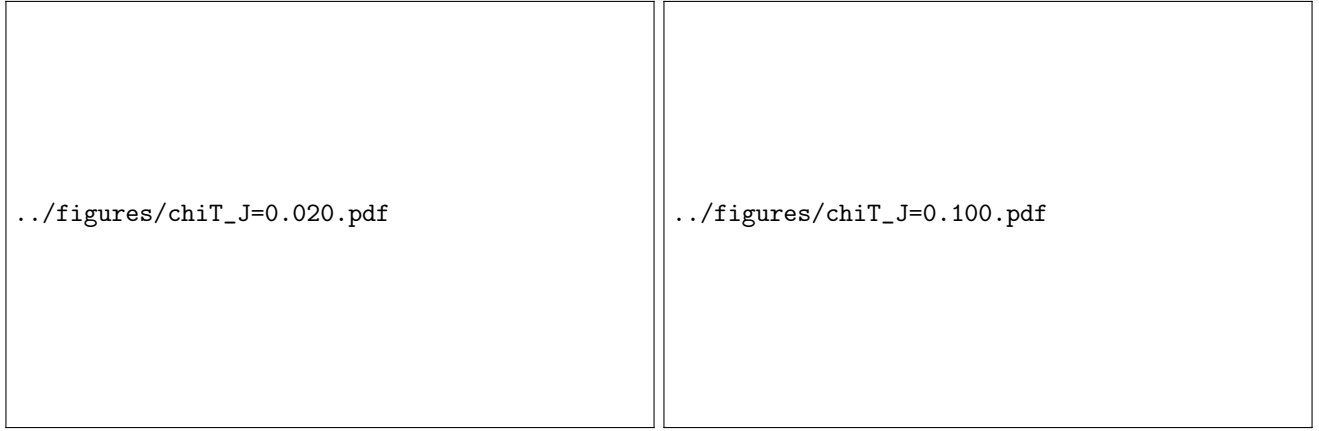


Figure 6.1: Spin susceptibility of the impurity times temperature, for two sets of bare parameters, in  $U > 0$ . At low temperatures, it becomes linear because  $\chi$  itself becomes constant (screening), while at high temperatures,  $\chi \times T$  becomes constant because of the paramagnetic  $\sim 1/T$  form of  $\chi$ . For the right panel with a larger value of the spin-exchange coupling, the  $\chi$  tries to go towards the local moment value of  $1/4$  but eventually drops back to the free orbital value of  $1/8$ .

### 6.2.2 Charge susceptibility

We can similarly define the charge susceptibility as

$$\chi(\beta) = \beta \left( \left\langle (C_d^z)^2 \right\rangle - \langle C_d^z \rangle^2 \right) = \lim_{B_c \rightarrow 0} \frac{1}{\beta} \left[ \frac{1}{Z(B_c)} \frac{\partial^2 Z(B_c)}{\partial B_c^2} - \frac{1}{Z(B_c)^2} \left( \frac{\partial Z(B_c)}{\partial B_c} \right)^2 \right] \quad (6.2.9)$$

where  $B_c$  is now a field that couples to the impurity charge-isospin:

$$\mathcal{H}'(B_c) = \mathcal{H} + B_c C_d^z \quad (6.2.10)$$

The charge susceptibility for  $U < 0$  is shown in fig. 6.2.

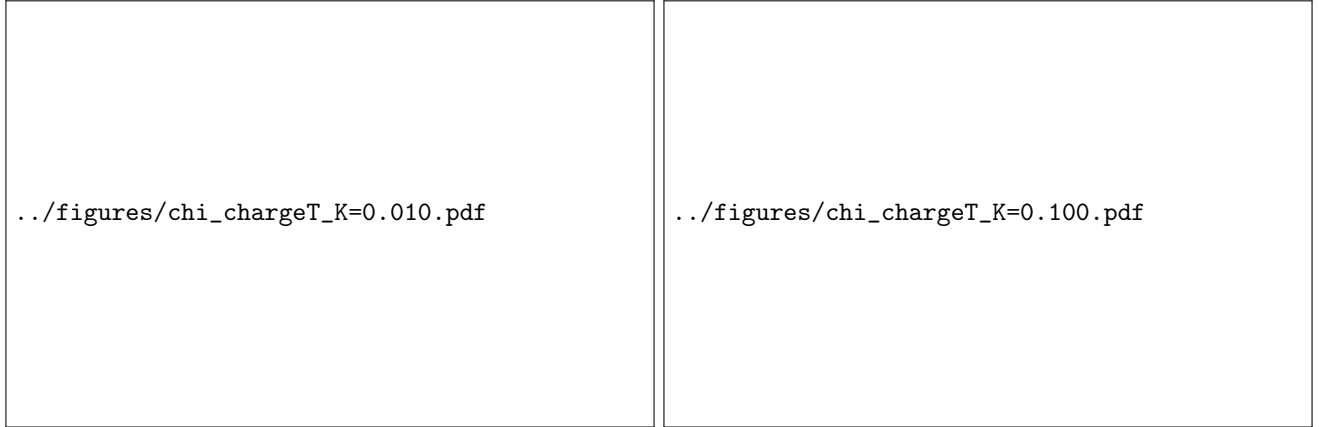


Figure 6.2: Charge susceptibility for the impurity at  $U < 0$ , for two sets of bare parameters. The physics is very similar to that of the spin susceptibility in  $U > 0$ .

It is interesting to look at the behaviour of the charge susceptibility in the positive  $U$  regime, fig. 6.3. It is seen that for  $J_0 < V_0$ , the charge susceptibility is very similar to the spin susceptibility, with a reduced saturation value. This is because, for that range of bare values, the ground state consists of a comparable mixture of the spin and charge states (see fig. 5.5). This means that the magnetic field term in eq. (6.2.10) can couple to the charge component of the ground state, and give a non-zero charge susceptibility at zero temperature. On the other hand,

for  $J_0 > V_0$ , we see that  $\chi_c$  vanishes at low temperatures. This can again be understood from the ground state. For that range of bare values, the ground state can be approximated by purely the singlet, because the charge fraction  $c_-^c$  becomes very small. This means that the field  $B_c$  has nothing to couple with. Alternatively, it can be said that since the ground state has only terms with  $\hat{n}_d = 1$ , no number fluctuation is possible, and the impurity isospin is not susceptible at all to charge polarisation.

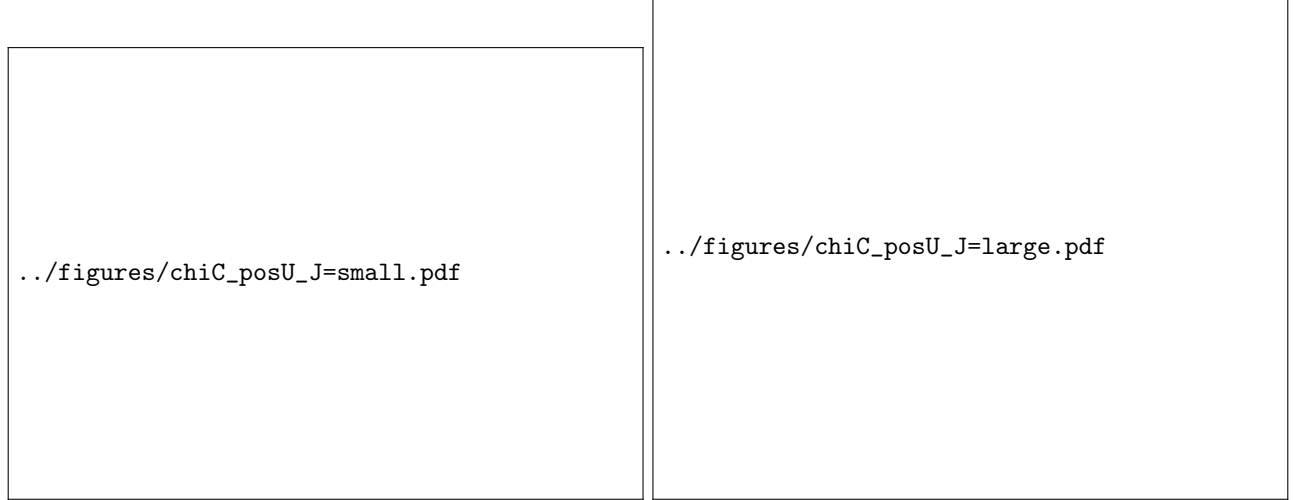


Figure 6.3: Charge susceptibility of the impurity in the positive  $U$  regime, for two values of  $J_0$ . The smaller bare value leads to a spin+charge mixed ground state, and hence a non-zero  $\chi_c$  at zero temperature. The larger  $J_0$ , however, leads to a purely spin ground state without any number fluctuation, and this gives vanishing  $\chi_c$  at zero temperature.

From eq. (5.12.1), we know that in the thermodynamic limit, the ground state of  $U > 0$  regime reduces to a screened local moment. That then implies that the charge susceptibility vanishes at low temperatures, owing to lack of any charge content in the ground state in the large bandwidth limit.

$$\lim_{D_0 \rightarrow \infty} \chi_c(U > 0, T \rightarrow 0) = 0 \quad (6.2.11)$$

### 6.3 Specific heat

The specific heat is calculated by diagonalizing the fixed point Hamiltonian, numerically. The obtained spectrum is denoted by  $\{\mathcal{E}_i\}$ . The total average energy of the impurity+cloud at temperature  $T$  is then

$$\langle \mathcal{E} \rangle = \frac{1}{Z} \sum_i \mathcal{E}_i e^{-\beta \mathcal{E}_i} \quad (6.3.1)$$

where  $Z = \sum_i e^{-\beta \mathcal{E}_i}$  is the partition function. The specific heat of this system is thus

$$\begin{aligned} C_V &= \frac{\partial \langle \mathcal{E} \rangle}{\partial T} \\ &= -\frac{1}{k_B T^2} \frac{\partial \langle \mathcal{E} \rangle}{\partial \beta} \\ &= \frac{1}{k_B T^2} \left[ \frac{1}{Z} \sum_i \mathcal{E}_i^2 e^{-\beta \mathcal{E}_i} - \left( \frac{1}{Z} \sum_i \mathcal{E}_i e^{-\beta \mathcal{E}_i} \right)^2 \right] \end{aligned} \quad (6.3.2)$$



In the absence of impurity, the eigenvalues of the Hamiltonian are  $\{\mathcal{E}_i^0\}$  with a partition function  $Z^0 = \sum_i e^{-\beta E_i^0}$ , so the bath specific heat is

$$C_V^0 = \frac{1}{k_B T^2} \left[ \frac{1}{Z_0} \sum_i \mathcal{E}_i^2 e^{-\beta \mathcal{E}_i^0} - \left( \frac{1}{Z_0} \sum_i \mathcal{E}_i^0 e^{-\beta \mathcal{E}_i^0} \right)^2 \right] \quad (6.3.3)$$

The impurity specific heat is the difference.

$$C_V^{\text{imp}} = C_V - C_V^0 \quad (6.3.4)$$

These values were calculated numerically and plotted against temperature in fig. 6.4.

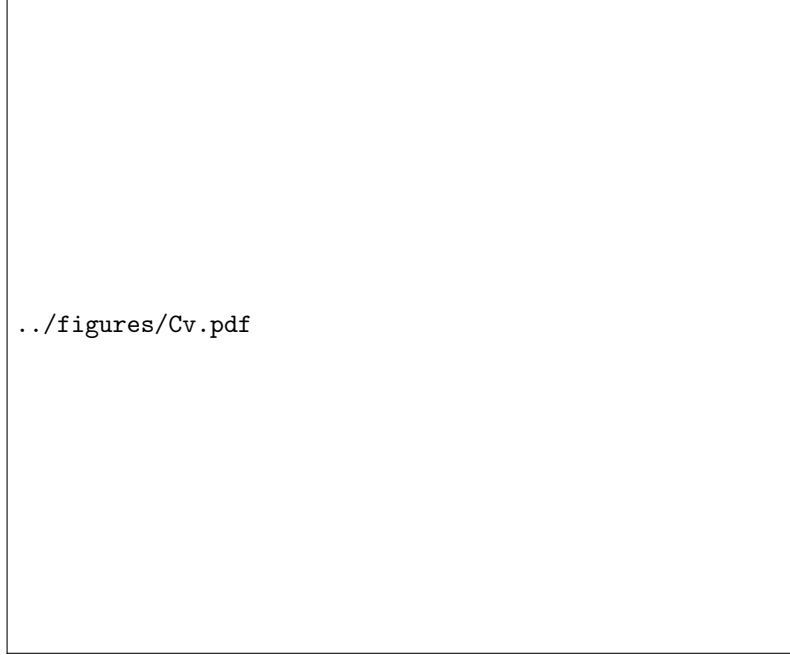


Figure 6.4: Impurity specific heat

## 6.4 Renormalization of impurity spectral function

In this section we will obtain the impurity spectral function, which is defined in terms of the impurity Green's function as

$$\mathcal{A}(\omega) = -\frac{1}{\pi} \text{Im} [G_{dd}^{\sigma}(\omega)] \quad (6.4.1)$$

The zero temperature retarded Green's function for the impurity, in the frequency domain, can be written as (see Appendix. A)

$$\mathcal{A}(\omega) = \frac{1}{d_0} \sum_{n,0} \left[ |\langle 0 | \mathcal{O}_{\sigma} | n \rangle|^2 \delta(\omega + E_0 - E_n) + |\langle n | \mathcal{O}_{\sigma} | 0 \rangle|^2 \delta(\omega - E_0 + E_n) \right] \quad (6.4.2)$$

where  $\mathcal{O}_{\sigma} = c_{d\sigma} + S_d^- c_{0\bar{\sigma}} + S_d^z c_{0\sigma}$  is the excitation whose spectral function we are interested in. The excitations defined in  $\mathcal{O}$  incorporates both single-particle excitations brought about by the hybridisation as well as two-particle spin excitations brought about by the spin-exchange term. Since this is in terms of the exact eigenstates, it is a discrete sum of delta-functions. In practice, we get a continuous distribution. To compare with experiment, we need to convert the discrete sum into a continuous function. Following [40], we replace the delta-functions at  $\pm x_n \equiv \pm(E_n - E_0)$  by normalized Gaussian functions

$$\delta(\omega \pm x_n) \rightarrow \frac{1}{\eta_n \sqrt{\pi}} e^{-\left(\frac{\omega \pm x_n}{\eta_n}\right)^2} \quad (6.4.3)$$

The parameter  $\eta_n$  determines the height and width of the Gaussian, and is chosen such that the higher energy poles are broader than the lower energy ones:

$$\eta_n = 4\Delta + \frac{1}{2}|x_n| \quad (6.4.4)$$

$\Delta = \pi\rho(0)V^2$  is the relevant energy scale for the non-interacting ( $U = 0$ ) problem,  $\rho(0)$  being the density of states of the conduction bath at the Fermi energy. As a result, the function that we will numerically compute and plot is

$$\mathcal{A}(\omega) = \sum_{n,0} \frac{1}{d_0\sqrt{\pi}\eta_n} \left[ \|\langle 0|c_{d\sigma}|n\rangle\|^2 e^{-\left(\frac{\omega-x_n}{\eta_n}\right)^2} + \|\langle n|c_{d\sigma}|0\rangle\|^2 e^{-\left(\frac{\omega+x_n}{\eta_n}\right)^2} \right] \quad (6.4.5)$$

From the results of Langreth [16], we know that the spectral function at zero frequency is fixed by the occupancy of the impurity. Since we are in the particle-hole symmetric regime, this occupancy is fixed at 1, and hence so is the spectral function height at  $\omega = 0$ . This result has been used to fix the spectral function height at the center during the computations. The fixed-point Hamiltonian  $H^*$  is diagonalized numerically to obtain  $\{E_n, |n\rangle\}$ , for various values of the couplings. The intention here is to get an idea of how the spectral function morphs under the RG. Doing an actual reverse RG (described in 6.10) would require us to diagonalize a huge Hamiltonian. We take the simpler route of tuning the  $U$  from zero to some large value. This should mimic the journey from the IR theory ( $U = 0$ ) to the UV theory ( $U \gg 0$ ).

The spectral function is plotted for three sets of values in fig. 6.5. For low values of  $U$ , the profile is that of a single peak at zero frequency. This is expected because at the low energy effective theory, the high energy Hubbard side bands have been integrated out. As  $U$  increases, shoulder-like structures appear on either side of the peak, which finally, at larger  $U$ , develop into two side-peaks. This is the microscopic theory, where high energy features are also relevant.



Figure 6.5: Impurity spectral function for multiple values of  $U$ . The increase in value of  $U$  is accompanied by the appearance of the side-peaks.

The physics of the three peaks can now be looked into. Since the central peak is at zero energy, it has to do with excitations that do not cost any energy. There are two such excitations: excitations within the spin sector and within the charge sector.

$$\begin{array}{cc} JS_d^- & KC_d^- \\ |\uparrow\rangle \xleftrightarrow{\quad} |\downarrow\rangle, & |\uparrow\rangle \xleftrightarrow{\quad} |\downarrow\rangle \\ JS_d^+ & KC_d^+ \end{array} \quad (6.4.6)$$

The thick arrow  $\uparrow$  represents the charge isospin. At particle-hole symmetry, both the spin configurations have energy of  $\epsilon_d$ , while the charge configurations have energy of  $2\epsilon_d + U = 0$  and  $0$ . Hence, no energy is required for these

excitations, which is why we see a macroscopic number of cloud electrons resonating with the impurity at the Fermi surface. Also note that if  $\hat{S}_i$  and  $\hat{C}_j$  are two operators of the spin and charge sector ( $i, j \in \{x, y, z\}$ ), then

$$\hat{S}_i \hat{C}_j = \hat{C}_j \hat{S}_i = 0 \quad (6.4.7)$$

We can see this by applying that operator on a basis state. Since the set of four states

$$|\hat{S}_i = \pm \frac{1}{2}, \hat{C}_j = 0\rangle, |\hat{S}_i = 0, \hat{C}_j = \pm \frac{1}{2}\rangle \quad (6.4.8)$$

are all independent, they form a basis. If we apply the operator on these states:

$$\begin{aligned} \hat{S}_i \hat{C}_j |\hat{S}_i\rangle &= 0, & \hat{C}_j \hat{S}_i |S_i\rangle &= S_i \hat{C}_j |S_i\rangle = 0 \\ \hat{C}_j \hat{S}_i |C_j\rangle &= 0, & \hat{S}_i \hat{C}_j |\hat{C}_j\rangle &= C_j \hat{S}_i |\hat{C}_j\rangle = 0 \end{aligned} \quad (6.4.9)$$

This shows that each operator acts only on its own subspace.  $S_i$  does not act on the charge sector, and vice-versa. There is no single-particle excitation here.

The physics of the side-peaks is that of single number fluctuations on the impurity. These are brought about by the term  $V c_{0\sigma}^\dagger c_{d\sigma} + \text{h.c.}$

$$(\epsilon_d) |\sigma\rangle \xrightleftharpoons[V c_{d\sigma}^\dagger / V c_{d\sigma}]{V c_{d\sigma}^\dagger / V c_{d\sigma}} |n_d = 2, 0\rangle (0) \quad (6.4.10)$$

These transitions involve energy transfer of the order of  $\epsilon_d$ . This is why, at very small  $U$ , they remain absorbed inside the central peak. These transitions do not involve any spin or charge-flip, rather they take the impurity between the spin and charge sectors.

## 6.5 Effective Hamiltonian for excitations of the Kondo cloud

To find an effective Hamiltonian for the excitations of the Kondo cloud, we will integrate out the impurity part of the wavefunction. The Schrodinger equation for the  $J > K$  ground state is

$$\begin{aligned} E_g & \left[ c_-^s (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + c_-^c (|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle) \right] \\ &= \mathcal{H} \left[ c_-^s (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + c_-^c (|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle) \right] \\ &= \mathcal{H}_0^* \left[ c_-^s (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + c_-^c (|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle) \right] \\ &+ V \sum_{\beta} \left[ c_{2\beta}^\dagger c_{1\beta} - c_{2\beta} c_{1\beta}^\dagger \right] \left[ c_-^s (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + c_-^c (|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle) \right] \\ &+ J \vec{S}_d \cdot \vec{s} \left[ c_-^s (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + c_-^c (|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle) \right] \\ &+ K \vec{C}_d \cdot \vec{c} \left[ c_-^s (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + c_-^c (|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle) \right] \end{aligned} \quad (6.5.1)$$

The last two lines gives

$$\begin{aligned} \frac{1}{2} J c_-^s & \left[ s^z (|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle) + s^+ |\downarrow, \downarrow\rangle - s^- |\uparrow, \uparrow\rangle \right] + \frac{1}{2} K c_-^c \left[ c^z (|\uparrow\downarrow, 0\rangle - |0, \uparrow\downarrow\rangle) + c^+ |0, 0\rangle \right. \\ & \left. + c^- |2, 2\rangle \right] \end{aligned} \quad (6.5.2)$$

The second line gives

$$\begin{aligned} & V c_{2\uparrow}^\dagger \left[ c_-^s (|0, \downarrow\rangle) + c_-^c (|\downarrow, 0\rangle) \right] + V c_{2\downarrow}^\dagger \left[ c_-^s (-|0, \uparrow\rangle) + c_-^c (|\uparrow, 0\rangle) \right] \\ & - V c_{2\uparrow} \left[ c_-^s (-|\uparrow\downarrow, \uparrow\rangle) + c_-^c (|\uparrow, \uparrow\downarrow\rangle) \right] - V c_{2\downarrow} \left[ c_-^s (-|\uparrow\downarrow, \downarrow\rangle) + c_-^c (|\downarrow, \uparrow\downarrow\rangle) \right] \end{aligned} \quad (6.5.3)$$

We will now write down four equations by comparing the coefficients of  $|\uparrow\rangle, |\downarrow\rangle, |0\rangle$  and  $|2\rangle$  of the impurity sector:

$$\begin{aligned}
 (E_g - H_0^*) c_-^s |\downarrow\rangle &= V c_-^c (c_{2\downarrow}^\dagger |0\rangle - c_{2\uparrow} |2\rangle) + \frac{1}{2} J c_-^s (s^z |\downarrow\rangle - s^- |\uparrow\rangle) & [\text{eq. from } |\uparrow\rangle] \\
 (-E_g + H_0^*) c_-^s |\uparrow\rangle &= V c_-^c (c_{2\uparrow}^\dagger |0\rangle - c_{2\downarrow}^\dagger |2\rangle) + \frac{1}{2} J c_-^s (s^z |\uparrow\rangle + s^+ |\downarrow\rangle) & [\text{eq. from } |\downarrow\rangle] \\
 (E_g - H_0^*) c_-^c |2\rangle &= V c_-^s (c_{2\uparrow}^\dagger |\downarrow\rangle - c_{2\downarrow}^\dagger |\uparrow\rangle) + \frac{1}{2} K c_-^c (-c^z |2\rangle + c^+ |0\rangle) & [\text{eq. from } |0\rangle] \\
 (E_g - H_0^*) c_-^c |0\rangle &= V c_-^s (c_{2\uparrow} |\uparrow\rangle + c_{2\downarrow} |\downarrow\rangle) + \frac{1}{2} K c_-^c (c^z |0\rangle + c^- |2\rangle) & [\text{eq. from } |2\rangle]
 \end{aligned} \tag{6.5.4}$$

These can be rearranged into

$$\begin{aligned}
 \left(E_g - H_0^* - \frac{1}{2} J s^z\right) |\downarrow\rangle &= V \lambda^{-1} (c_{2\downarrow}^\dagger |0\rangle - c_{2\uparrow} |2\rangle) - \frac{1}{2} J s^- |\uparrow\rangle \\
 \left(E_g - H_0^* + \frac{1}{2} J s^z\right) |\uparrow\rangle &= V \lambda^{-1} (c_{2\downarrow} |2\rangle - c_{2\uparrow}^\dagger |0\rangle) - \frac{1}{2} J s^+ |\downarrow\rangle \\
 \left(E_g - H_0^* + \frac{1}{2} K c^z\right) |2\rangle &= V \lambda (c_{2\uparrow}^\dagger |\downarrow\rangle - c_{2\downarrow}^\dagger |\uparrow\rangle) + \frac{1}{2} K c^+ |0\rangle \\
 \left(E_g - H_0^* - \frac{1}{2} K c^z\right) |0\rangle &= V \lambda (c_{2\uparrow} |\uparrow\rangle + c_{2\downarrow} |\downarrow\rangle) + \frac{1}{2} K c^- |2\rangle
 \end{aligned} \tag{6.5.5}$$

where  $\lambda = \frac{c_-^s}{c_-^c}$ . We want to find the effective Hamiltonian in the subspace of  $|\downarrow\rangle$ . We first eliminate the charge sector from these equations:

$$\begin{aligned}
 |0\rangle &= V \lambda \left[ \frac{1}{A_-^K} c_{2\uparrow} + \frac{K}{2} \frac{1}{A_-^K} c^- \frac{1}{A_+^K - \left(\frac{K}{2}\right)^2 c^+ \frac{1}{A_-^K} c^-} \left( \frac{K}{2} c^+ \frac{1}{A_-^K} c_{2\uparrow} - c_{2\downarrow}^\dagger \right) \right] |\uparrow\rangle \\
 &+ V \lambda \left[ \frac{1}{A_-^K} c_{2\downarrow} + \frac{K}{2} \frac{1}{A_-^K} c^- \frac{1}{A_+^K - \left(\frac{K}{2}\right)^2 c^+ \frac{1}{A_-^K} c^-} \left( c_{2\uparrow}^\dagger + \frac{K}{2} c^+ \frac{1}{A_-^K} c_{2\downarrow} \right) \right] |\downarrow\rangle \\
 |2\rangle &= \frac{V \lambda}{A_+^K - \left(\frac{K}{2}\right)^2 c^+ \frac{1}{A_-^K} c^-} \left[ \left( c_{2\uparrow}^\dagger + \frac{K}{2} c^+ \frac{1}{A_-^K} c_{2\downarrow} \right) |\downarrow\rangle + \left( \frac{K}{2} c^+ \frac{1}{A_-^K} c_{2\uparrow} - c_{2\downarrow}^\dagger \right) |\uparrow\rangle \right]
 \end{aligned} \tag{6.5.6}$$

where

$$A_{\pm}^K = E_g - H_0^* \pm \frac{1}{2} K c^z \tag{6.5.7}$$

For ease of labeling, we will think of these equations as

$$|0\rangle = a_0^\uparrow |\uparrow\rangle + a_0^\downarrow |\downarrow\rangle, |2\rangle = a_2^\uparrow |\uparrow\rangle + a_2^\downarrow |\downarrow\rangle \tag{6.5.8}$$

The remaining two equations can then be written as

$$\begin{aligned}
 A_-^J |\downarrow\rangle &= \frac{V}{\lambda} \left[ c_{2\downarrow}^\dagger (a_0^\uparrow |\uparrow\rangle + a_0^\downarrow |\downarrow\rangle) - c_{2\uparrow} (a_2^\uparrow |\uparrow\rangle + a_2^\downarrow |\downarrow\rangle) \right] - \frac{J}{2} s^- |\uparrow\rangle \\
 A_+^J |\uparrow\rangle &= \frac{V}{\lambda} \left[ c_{2\downarrow} (a_2^\uparrow |\uparrow\rangle + a_2^\downarrow |\downarrow\rangle) - c_{2\uparrow}^\dagger (a_0^\uparrow |\uparrow\rangle + a_0^\downarrow |\downarrow\rangle) \right] - \frac{J}{2} s^+ |\downarrow\rangle
 \end{aligned} \tag{6.5.9}$$

where

$$A_{\pm}^J = E_g - H_0^* \pm \frac{1}{2} J s^z \tag{6.5.10}$$

Eliminating  $|\downarrow\rangle$  and solving for  $|\uparrow\rangle$  gives

$$\begin{aligned}
 A_+^J |\uparrow\rangle &= \frac{V}{\lambda} (c_{2\downarrow} a_2^\uparrow - c_{2\uparrow}^\dagger a_0^\uparrow) |\uparrow\rangle + \left( \frac{V}{\lambda} c_{2\downarrow} a_2^\downarrow - \frac{V}{\lambda} c_{2\uparrow}^\dagger a_0^\downarrow - \frac{J}{2} s^+ \right) |\downarrow\rangle \\
 &= \frac{V}{\lambda} (c_{2\downarrow} a_2^\uparrow - c_{2\uparrow}^\dagger a_0^\uparrow) |\uparrow\rangle \\
 &\quad + \left[ \frac{V}{\lambda} (c_{2\downarrow} a_2^\downarrow - c_{2\uparrow}^\dagger a_0^\downarrow) - \frac{J}{2} s^+ \right] \frac{1}{A_-^J - \frac{V}{\lambda} (c_{2\downarrow}^\dagger a_0^\downarrow - c_{2\uparrow} a_2^\downarrow)} \left[ \frac{V}{\lambda} (c_{2\downarrow}^\dagger a_0^\uparrow - c_{2\uparrow} a_2^\uparrow) - \frac{J}{2} s^- \right] |\uparrow\rangle
 \end{aligned} \tag{6.5.11}$$

The effective Hamiltonian for the  $|\uparrow\rangle$  state is

$$\begin{aligned}
 H_0^* - \frac{J}{2} s^z + \frac{V}{\lambda} (c_{2\downarrow} a_2^\uparrow - c_{2\uparrow}^\dagger a_0^\uparrow) &+ \left[ \frac{V}{\lambda} (c_{2\downarrow} a_2^\downarrow - c_{2\uparrow}^\dagger a_0^\downarrow) - \frac{J}{2} s^+ \right] \frac{1}{A_-^J - \frac{V}{\lambda} (c_{2\downarrow}^\dagger a_0^\downarrow - c_{2\uparrow} a_2^\downarrow)} \\
 &\times \left[ \frac{V}{\lambda} (c_{2\downarrow}^\dagger a_0^\uparrow - c_{2\uparrow} a_2^\uparrow) - \frac{J}{2} s^- \right]
 \end{aligned} \tag{6.5.12}$$

To get a clearer picture of this effective Hamiltonian, we will keep up to two-particle interactions. We first write down the full forms of  $a_{0,2}^\sigma$ :

$$\begin{aligned}
 a_0^\sigma &= V\lambda \left[ \frac{1}{A_-^K} c_{2\sigma} + \frac{K}{2} \frac{1}{A_-^K} c^- \frac{1}{A_+^K - \left(\frac{K}{2}\right)^2 c^+ \frac{1}{A_-^K} c^-} \left( \frac{K}{2} c^+ \frac{1}{A_-^K} c_{2\sigma} - \sigma c_{2\sigma}^\dagger \right) \right] \\
 a_2^\sigma &= \frac{V\lambda}{A_+^K - \left(\frac{K}{2}\right)^2 c^+ \frac{1}{A_-^K} c^-} \left( -\sigma c_{2-\sigma}^\dagger + \frac{K}{2} c^+ \frac{1}{A_-^K} c_{2\sigma} \right)
 \end{aligned} \tag{6.5.13}$$

We will first look at the special case of  $K = 0$ . There, the above expressions simplify to

$$\begin{aligned}
 a_0^\sigma &= V\lambda \frac{1}{A_-^K} c_{2\sigma} = \frac{V\lambda}{E_g} \left[ 1 + \frac{1}{E_g} (H_0^*) + \frac{1}{E_g^2} (H_0^*)^2 \right] c_{2\sigma} + \mathcal{O}(H_0^{*3}) \\
 a_2^\sigma &= -\sigma V\lambda \frac{1}{A_+^K} c_{2-\sigma}^\dagger = -\sigma \frac{V\lambda}{E_g} \left[ 1 + \frac{1}{E_g} (H_0^*) + \frac{1}{E_g^2} (H_0^*)^2 \right] c_{2-\sigma}^\dagger + \mathcal{O}(H_0^{*3})
 \end{aligned} \tag{6.5.14}$$

We will make use of the following commutators:

$$\begin{aligned}
 [(H_0^*)^m, c_{2\sigma}] &= -\sum_k \frac{\epsilon_k^m}{\sqrt{N^*}} c_{k\sigma}, & [(H_0^*)^m, c_{2\sigma}^\dagger] &= \sum_k \frac{\epsilon_k^m}{\sqrt{N^*}} c_{k\sigma}^\dagger, & m &= 1, 2 \\
 [(H_0^*)^m, s^+] &= \sum_{kk'} (\epsilon_k^m - \epsilon_{k'}^m) c_{k\beta}^\dagger c_{k'\beta}, & & & m &= 1, 2 \\
 [(s^z)^m, c_{2\sigma}] &= -\left(\frac{\sigma}{2}\right)^m c_{2\sigma}, & [(s^z)^m, c_{2\sigma}^\dagger] &= \left(\frac{\sigma}{2}\right)^m c_{2\sigma}^\dagger, & m &= 1, 2 \\
 [(c^z)^m, c_{2\sigma}] &= -\left(\frac{1}{2}\right)^m c_{2\sigma}, & [(c^z)^m, c_{2\sigma}^\dagger] &= \left(\frac{1}{2}\right)^m c_{2\sigma}^\dagger, & m &= 1, 2
 \end{aligned} \tag{6.5.15}$$

Now we evaluate the various terms in the effective Hamiltonian.

$$\begin{aligned}
 c_{2\downarrow} a_2^\uparrow &= -\frac{V\lambda}{E_g} c_{2\downarrow} \left[ 1 + \frac{1}{E_g} (H_0^*) + \frac{1}{E_g^2} (H_0^*)^2 \right] c_{2\downarrow}^\dagger \\
 &= -\frac{V\lambda}{E_g} \left[ c_{2\downarrow} + \frac{1}{E_g} (H_0^*) c_{2\downarrow} + \sum_k \frac{\epsilon_k}{E_g \sqrt{N^*}} c_{k\downarrow} + \frac{1}{E_g^2} (H_0^*)^2 c_{2\downarrow} + \sum_k \frac{\epsilon_k^2}{E_g^2 \sqrt{N^*}} c_{k\downarrow} \right] c_{2\downarrow}^\dagger
 \end{aligned}$$

$$\begin{aligned}
&= -\frac{V\lambda}{E_g} \left[ 1 + \frac{H_0^*}{E_g} + \left( \frac{H_0^*}{E_g} \right)^2 \right] c_{2\downarrow} c_{2\downarrow}^\dagger - \frac{V\lambda}{E_g N^*} \sum_{kk'} \left( \frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2} \right) c_{k\downarrow} c_{k'\downarrow}^\dagger \\
c_{2\uparrow} a_2^\downarrow &= -\frac{V\lambda}{E_g} \left[ 1 + \frac{H_0^*}{E_g} + \left( \frac{H_0^*}{E_g} \right)^2 \right] c_{2\uparrow} c_{2\uparrow}^\dagger - \frac{V\lambda}{E_g N^*} \sum_{kk'} \left( \frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2} \right) c_{k\uparrow} c_{k'\uparrow}^\dagger \\
c_{2\uparrow}^\dagger a_0^\uparrow &= c_{2\uparrow}^\dagger \frac{V\lambda}{E_g} \left[ 1 + \frac{1}{E_g} (H_0^*) + \frac{1}{E_g^2} (H_0^*)^2 \right] c_{2\uparrow} \\
&= \frac{V\lambda}{E_g} \left[ 1 + \frac{H_0^*}{E_g} + \left( \frac{H_0^*}{E_g} \right)^2 \right] c_{2\uparrow}^\dagger c_{2\uparrow} - \frac{V\lambda}{E_g N^*} \sum_{kk'} \left( \frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2} \right) c_{k\uparrow}^\dagger c_{k'\uparrow} \\
c_{2\downarrow}^\dagger a_0^\downarrow &= \frac{V\lambda}{E_g} \left[ 1 + \frac{H_0^*}{E_g} + \left( \frac{H_0^*}{E_g} \right)^2 \right] c_{2\downarrow}^\dagger c_{2\downarrow} - \frac{V\lambda}{E_g N^*} \sum_{kk'} \left( \frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2} \right) c_{k\downarrow}^\dagger c_{k'\downarrow} \\
c_{2\downarrow} a_2^\downarrow &= \frac{V\lambda}{E_g} c_{2\downarrow} \left[ 1 + \frac{1}{E_g} (H_0^*) + \frac{1}{E_g^2} (H_0^*)^2 \right] c_{2\uparrow}^\dagger \\
&= \frac{V\lambda}{E_g} \left[ 1 + \frac{1}{E_g} (H_0^*) \right] c_{2\downarrow} c_{2\uparrow}^\dagger + \frac{V\lambda}{E_g N^*} \sum_{kk'} \left( \frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2} \right) c_{k\downarrow} c_{k'\uparrow}^\dagger \\
c_{2\uparrow} a_2^\uparrow &= -\frac{V\lambda}{E_g} \left[ 1 + \frac{1}{E_g} (H_0^*) \right] c_{2\uparrow}^\dagger c_{2\downarrow} - \frac{V\lambda}{E_g N^*} \sum_{kk'} \left( \frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2} \right) c_{k\uparrow}^\dagger c_{k'\downarrow} \\
c_{2\uparrow}^\dagger a_0^\downarrow &= \frac{V\lambda}{E_g} \left[ 1 + \frac{H_0^*}{E_g} \right] c_{2\uparrow}^\dagger c_{2\downarrow} - \frac{V\lambda}{E_g N^*} \sum_{kk'} \left( \frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2} \right) c_{k\uparrow}^\dagger c_{k'\downarrow} \\
c_{2\downarrow}^\dagger a_0^\uparrow &= \frac{V\lambda}{E_g} \left[ 1 + \frac{H_0^*}{E_g} \right] c_{2\downarrow}^\dagger c_{2\uparrow} - \frac{V\lambda}{E_g N^*} \sum_{kk'} \left( \frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2} \right) c_{k\downarrow}^\dagger c_{k'\uparrow} \\
c_{2\downarrow} a_2^\uparrow - c_{2\uparrow}^\dagger a_0^\uparrow &= -\frac{V\lambda}{E_g} \left[ 1 + \frac{H_0^*}{E_g} + \left( \frac{H_0^*}{E_g} \right)^2 \right] \times 2 + \frac{V\lambda}{E_g N^*} \sum_{kk'} \left( \frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2} \right) (c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow} c_{k'\downarrow}^\dagger) \\
c_{2\downarrow} a_2^\downarrow - c_{2\uparrow}^\dagger a_0^\downarrow &= \frac{V\lambda}{E_g} \left[ 1 + \frac{1}{E_g} (H_0^*) \right] c_{2\downarrow} c_{2\uparrow}^\dagger \times 2 + \frac{V\lambda}{E_g N^*} \sum_{kk'} \left( \frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2} \right) (c_{k\downarrow} c_{k'\uparrow}^\dagger + c_{k\uparrow}^\dagger c_{k'\downarrow}) \\
c_{2\downarrow}^\dagger a_0^\downarrow - c_{2\uparrow} a_2^\downarrow &= \frac{V\lambda}{E_g N^*} \sum_{kk'} \left( \frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2} \right) (c_{k\uparrow} c_{k'\uparrow}^\dagger - c_{k\downarrow}^\dagger c_{k'\downarrow}) \\
c_{2\downarrow}^\dagger a_0^\uparrow - c_{2\uparrow} a_2^\uparrow &= \frac{V\lambda}{E_g N^*} \sum_{kk'} \left( \frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2} \right) (c_{k\uparrow} c_{k'\downarrow}^\dagger - c_{k\downarrow}^\dagger c_{k'\uparrow})
\end{aligned}$$

In all the expressions, we have dropped terms that have more than 4 operators in product. Also, in the last four equations, we have substituted  $\hat{n}_{2\uparrow} - \hat{n}_{2\downarrow} = 1$ , because this is the effective Hamiltonian for the state with  $s^z = \frac{1}{2}$ .

We now substitute these expressions into the effective Hamiltonian:

$$\begin{aligned}
 H_0^* - \frac{J}{2} s^z - \frac{2V^2}{E_g} \left[ 1 + \frac{H_0^*}{E_g} + \left( \frac{H_0^*}{E_g} \right)^2 \right] + \frac{V^2}{E_g N^*} \sum_{kk'} \xi_k \left( c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow} c_{k'\downarrow}^\dagger \right) \\
 + \left[ \frac{V}{\lambda} \left( c_{2\downarrow} a_2^\dagger - c_{2\uparrow}^\dagger a_0^\dagger \right) \right] \frac{1}{A_-^J - \frac{V^2}{E_g N^*} \sum_{kk'} \xi_k \left( c_{k\uparrow} c_{k'\uparrow}^\dagger - c_{k\downarrow}^\dagger c_{k'\downarrow} \right)} \left[ \frac{V}{\lambda} \left( c_{2\downarrow}^\dagger a_0^\dagger - c_{2\uparrow} a_2^\dagger \right) \right] \\
 + \left[ \frac{V}{\lambda} \left( c_{2\downarrow} a_2^\dagger - c_{2\uparrow}^\dagger a_0^\dagger \right) \right] \frac{1}{A_-^J - \frac{V^2}{E_g N^*} \sum_{kk'} \xi_k \left( c_{k\uparrow} c_{k'\uparrow}^\dagger - c_{k\downarrow}^\dagger c_{k'\downarrow} \right)} \left[ -\frac{J}{2} s^- \right] \\
 + \left[ -\frac{J}{2} s^+ \right] \frac{1}{A_-^J - \frac{V^2}{E_g N^*} \sum_{kk'} \xi_k \left( c_{k\uparrow} c_{k'\uparrow}^\dagger - c_{k\downarrow}^\dagger c_{k'\downarrow} \right)} \left[ \frac{V}{\lambda} \left( c_{2\downarrow}^\dagger a_0^\dagger - c_{2\uparrow} a_2^\dagger \right) \right] \\
 + \frac{J^2}{4} \left[ s^+ \right] \frac{1}{A_-^J - \frac{V^2}{E_g N^*} \sum_{kk'} \xi_k \left( c_{k\uparrow} c_{k'\uparrow}^\dagger - c_{k\downarrow}^\dagger c_{k'\downarrow} \right)} \left[ s^- \right]
 \end{aligned} \tag{6.5.16}$$

where  $\xi_k = \frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2}$ . We first consider only zeroth order terms of the central propagator.

$$\begin{aligned}
 H_0^* - \frac{J}{2} \underbrace{s^z}_{\frac{1}{2}} - \frac{2V^2}{E_g} \left[ 1 + \frac{H_0^*}{E_g} + \left( \frac{H_0^*}{E_g} \right)^2 \right] + \frac{V^2}{E_g N^*} \sum_{kk'} (\xi_k) \left( c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow} c_{k'\downarrow}^\dagger \right) \\
 + \frac{V^4}{E_g^2 N^{*2} \left( E_g + \frac{J}{4} \right)} \sum_{kk'} (\xi_{k'} + 2 - \xi_k) c_{k\uparrow}^\dagger c_{k'\downarrow} \sum_{kk'} (\xi_k + \xi_{k'}) c_{k\downarrow}^\dagger c_{k'\uparrow} \\
 + \frac{V^2 J}{2 E_g \left( E_g + \frac{J}{4} \right) N^*} \sum_{kk'} (\xi_{k'} + 2 - \xi_k) c_{k\uparrow}^\dagger c_{k'\downarrow} \sum_{kk'} c_{k\downarrow}^\dagger c_{k'\uparrow} \\
 + \frac{J V^2}{2 E_g \left( E_g + \frac{J}{4} \right) N^*} \sum_{kk'} c_{k\uparrow}^\dagger c_{k'\downarrow} \sum_{kk'} (\xi_k + \xi_{k'}) c_{k\downarrow}^\dagger c_{k'\uparrow} \\
 + \frac{J^2}{4 \left( E_g + \frac{J}{4} \right)} \underbrace{s^+ s^-}_{s^z + \frac{1}{2} = 1}
 \end{aligned} \tag{6.5.17}$$

We have set  $s^z = -\frac{1}{2}$  in the denominator, hence the  $E_g = \frac{J}{4}$ . If we also consider the first and second order terms from the central propagator, note that they will produce terms of more than quartic interactions in the first three terms. For the last term, we get

$$\frac{J^2}{4 \left( E_g + \frac{J}{4} \right)} s^+ \left[ \frac{H_0^*}{E_g + \frac{J}{4}} + \left( \frac{H_0^*}{E_g + \frac{J}{4}} \right)^2 \right] s^- \tag{6.5.18}$$

Using the commutator of  $H_0^*$  with  $s^+$  to bring  $H_0^*$  to the left, and using  $s^+ s^- = s^z + \frac{1}{2} = 1$ , we get

$$\frac{J^2}{4 \left( E_g + \frac{J}{4} \right)} \left[ \frac{H_0^*}{E_g + \frac{J}{4}} + \left( \frac{H_0^*}{E_g + \frac{J}{4}} \right)^2 - \sum_{kk'qq'} \left( \xi_k^J - \xi_{k'}^J \right) c_{k\uparrow}^\dagger c_{k'\downarrow} c_{q\downarrow}^\dagger c_{q'\uparrow} \right] \tag{6.5.19}$$

where  $\xi_k^J = \frac{\epsilon_k}{E_g + \frac{J}{4}} + \frac{\epsilon_k^2}{(E_g + \frac{J}{4})^2}$ . The full effective Hamiltonian, for  $K = 0$ , up to quartic interactions, is

$$\begin{aligned} H_0^* + \frac{J}{4} \left( \frac{J}{E_g + \frac{J}{4}} - 1 \right) - \frac{2V^2}{E_g} + \frac{V^2}{E_g N^*} \sum_{kk'} (\xi_k) (c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow} c_{k'\downarrow}^\dagger) - \frac{2V^2}{E_g} \left[ \frac{H_0^*}{E_g} + \left( \frac{H_0^*}{E_g} \right)^2 \right] \\ + \frac{J^2}{4 \left( E_g + \frac{J}{4} \right)} \left[ \frac{H_0^*}{E_g + \frac{J}{4}} + \left( \frac{H_0^*}{E_g + \frac{J}{4}} \right)^2 \right] + \sum_{kk'qq'} F_{kk'qq'} c_{k\uparrow}^\dagger c_{k'\downarrow} c_{q\downarrow}^\dagger c_{q'\uparrow} \end{aligned} \quad (6.5.20)$$

The coefficient  $F_{kk'qq'}$  is

$$\begin{aligned} F_{kk'qq'} = \frac{V^2}{E_g N^* (E_g + \frac{J}{4})} \left[ \frac{V^2}{E_g N^*} (\xi_{k'} + 2 - \xi_k) (\xi_q + \xi_{q'}) + \frac{J}{2} (\xi_{k'} + 2 - \xi_k + \xi_q + \xi_{q'}) \right] \\ + \frac{J^2}{4 \left( E_g + \frac{J}{4} \right)} (\xi_{k'}^J - \xi_k^J) \end{aligned} \quad (6.5.21)$$

There are two main types of interactions that gets generated upon integrating out the impurity. One is the Fermi liquid type interactions arising from the  $H_0^{*2}$  terms. The Fermi liquid part of the Hamiltonian is

$$\begin{aligned} \left[ \frac{J^2}{4 \left( E_g + \frac{J}{4} \right)^2} - \frac{2V^2}{E_g^2} \right] H_0^* + \left[ \frac{J^2}{4 \left( E_g + \frac{J}{4} \right)^2} - \frac{2V^2}{E_g^3} \right] H_0^{*2} \\ = \left[ \frac{J^2}{4 \left( E_g + \frac{J}{4} \right)^2} - \frac{2V^2}{E_g^2} \right] \left[ H_0^* + \sum_{kk'\sigma\sigma'} f_{kk'} \hat{n}_{k\sigma} \hat{n}_{k'\sigma'} \right] \end{aligned} \quad (6.5.22)$$

where the Landau parameter is given by

$$f_{kk'} = \left[ \frac{J^2}{4 \left( E_g + \frac{J}{4} \right)^2} - \frac{2V^2}{E_g^2} \right]^{-1} \left[ \frac{J^2}{4 \left( E_g + \frac{J}{4} \right)^3} - \frac{2V^2}{E_g^3} \right] \epsilon_k \epsilon_{k'} \quad (6.5.23)$$

The more interesting interaction is the off-diagonal term

$$\sum_{kk'qq'} F_{kk'qq'} c_{k\uparrow}^\dagger c_{k'\downarrow} c_{q\downarrow}^\dagger c_{q'\uparrow} \quad (6.5.24)$$

This interaction arises from the enhanced entanglement between the impurity and the conduction electrons; removing the impurity from the singlet and the triplet generates these off-diagonal scatterings. As such, this is an indicator of the macroscopic entanglement of the singlet formed at the IR fixed point, and plotted in fig. 6.8.

We also wish to point out that this scattering is a signature of the change in Luttinger's count in going from the free orbital or local moment fixed point to the strong-coupling fixed point, as shown in eq. (6.9.28). Both this off-diagonal scattering as well as the change in Luttinger's count are a direct consequence of the non-number conserving term  $V c_k^\dagger c_d$  in the full Hamiltonian. The topological change of Luttinger's count is concomitant with the presence of the off-diagonal scattering term in the effective Hamiltonian. *Just the Fermi liquid piece in eq. (6.5.23) will give neither the enhanced mutual information nor the change in Luttinger's count.*

## 6.6 Obtaining the real space low energy Hamiltonian: the local Fermi liquid

The next step is to obtain the lowest excitations of the fixed point Hamiltonian, in real space. We will work in the  $U > 0$  regime. For  $V, J \gg 1$ , the impurity couples very strongly with the zeroth site, and at zeroth order, it



suffices to say that the zeroth site decouples from the rest of the lattice. This zeroth Hamiltonian then consists of two sites interacting with each other through  $V$  and  $J$  (the two site problem analysed before).

$$H_0^* = \sum_{\sigma} \left( V^* c_{0\sigma}^{\dagger} c_{d\sigma} + \text{h.c.} \right) + J^* \vec{S}_d \cdot \vec{s} - \frac{1}{2} U^* \left( \hat{n}_{d\uparrow} - \hat{n}_{d\downarrow} \right)^2 \quad (6.6.1)$$

$$|\Psi\rangle_1 = c_s \frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + c_c \frac{1}{\sqrt{2}} (|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle), \quad E_1 = -V^* \sqrt{\gamma^2 + 4} - \frac{1}{4} U^* - \frac{3}{8} J^* \quad (6.6.2)$$

These were obtained in eq. (5.11.5). The quantities  $\gamma$  and  $c_{s,c}$  were defined in and around eq. (5.11.6).

We start with the ground state  $|\Psi\rangle_1$  and the star graph as the zeroth level ground state and Hamiltonian, and then add a nearest-neighbour hopping term as a perturbation of the zeroth Hamiltonian. We know that the ground state for the interacting part is predominantly the spin-singlet (it was shown while calculating the ground states of the effective zero-mode Hamiltonian that the ground state is a mixture of singlet and triplet, and the triplet part dies out at large system sizes, see eq. (5.12.1)), so we will take that as our reference state and treat the hopping part that connects the origin to the first site,

$$H_X = t \sum_{\vec{r}_1, \sigma} c_{0\sigma}^{\dagger} c_{\vec{r}_1, \sigma} + \text{h.c.} \equiv v^{\dagger} + v \quad (6.6.3)$$

as a weak perturbation.  $\vec{r}_1$  here sums over the sites that are nearest to the origin. Once this perturbation is taken care of up to a certain order, we will have a decoupled singlet formed by the impurity and the zeroth site, and the rest of the lattice formed by  $N - 1$  sites along with the interaction induced by the perturbation. To be precise, the goal is to integrate out the perturbation and generate an effective Hamiltonian in the subspace of the minimal energy states of the two site Hamiltonian, and this effective Hamiltonian will therefore describe the lowest excitations on top of the ground state  $|\Psi\rangle_1$ . The minimal energy subspace is given by the states:

$$|\Phi\rangle_i = |\Psi\rangle_1 \otimes |\hat{n}_{1\uparrow}, \hat{n}_{1\downarrow}\rangle, \quad \text{where } i \in \begin{cases} 0 : & \hat{n}_{1\uparrow} = \hat{n}_{1\downarrow} = 0 \\ 1 : & 1 - \hat{n}_{1\uparrow} = \hat{n}_{1\downarrow} = 0 \\ 2 : & \hat{n}_{1\uparrow} = 1 - \hat{n}_{1\downarrow} = 0 \\ 3 : & 1 - \hat{n}_{1\uparrow} = 1 - \hat{n}_{1\downarrow} = 0 \end{cases} \quad (6.6.4)$$

The effective Hamiltonian will be calculated using perturbation theory in  $\frac{H_X^n}{H_0^{*n-1}}$ . Since an odd number of scattering processes cannot bring the initial state back to itself, such orders will be absent from the effective Hamiltonian.

### 6.6.1 Second order effective Hamiltonian

We first consider the case of  $n = 2$ . The renormalisation of the effective Hamiltonian in the ground state subspace, at this order, is given by

$$\Delta H = \sum_{ij, n} |\Phi\rangle_i \langle \Phi_i| H_X |\Psi\rangle_n \frac{1}{E_{\text{gs}} - E_n} \langle \Psi|_n H_X |\Phi\rangle_j \langle \Phi_j| = \sum_{ij} |\Phi\rangle_i \langle \Phi_j| \langle \Phi_i| v + v^{\dagger} |\Psi\rangle_n \frac{1}{E_{\text{gs}} - E_n} \langle \Psi|_n v + v^{\dagger} |\Phi\rangle_j. \quad (6.6.5)$$

Here,  $|\Psi\rangle_n$  are the eigenstates of the two site problem, with eigenvalue  $E_n$ . The total scattering process can be described as  $H_X$  acting on  $|\Phi\rangle_j$  to excite to  $|\Psi\rangle_n$ , and then a subsequent  $H_X$  acting on  $|\Psi\rangle_n$  to decay back to  $|\Phi\rangle_j$  and into the ground state manifold. Since  $|\Phi\rangle_{i,j}$  are eigenstates of the two site Hamiltonian, they are all eigenstates of the total number operator  $\hat{n}_{d0} = \sum_{\sigma} (\hat{n}_{d\sigma} + \hat{n}_{0\sigma})$  for the two site model, with eigenvalue 2. Since we are to finally return to the ground state manifold, only those processes in  $H_X^2$  are allowed that conserve  $\hat{n}_{d0}$ . These processes are  $v, v^{\dagger}$  and  $v^{\dagger}, v$ . This also means that the total number of particles on site 1 will remain constant in the process, and we will have  $|\Phi\rangle_i = |\Phi\rangle_j$ .

$$\Delta H = \sum_i |\Phi\rangle_i \langle \Phi_i| \frac{1}{E_{\text{gs}} - E_n} \left( \langle \Phi_i| v^{\dagger} |\Psi\rangle_n \langle \Psi|_n v |\Phi\rangle_i + \langle \Phi_i| v |\Psi\rangle_n \langle \Psi|_n v^{\dagger} |\Phi\rangle_i \right). \quad (6.6.6)$$

If we define the matrix element  $v_{ni} \equiv \langle \Psi|_n v |\Phi\rangle_i$  of  $v$  and the excitation energy  $\delta E_n = E_n - E_{\text{gs}}$ , we can write the renormalisation as

$$\Delta H = \sum_{i, n} \frac{|v_{ni}|^2 + |v_{in}|^2}{-\delta E_n} |\Phi\rangle_i \langle \Phi_i|. \quad (6.6.7)$$

We now look at each  $|\Phi_i\rangle$  separately. For  $|\Phi_i\rangle = |\Phi\rangle_0 = |\Psi\rangle_1 \otimes |0, 0\rangle$ , we can write

$$v^\dagger |\Phi\rangle_i = 0, \quad v |\Phi\rangle_i = \frac{t}{\sqrt{2}} \sum_{\sigma} \bar{\sigma} \left( c_s^- |\sigma, 0\rangle + c_c^- |0, \sigma\rangle \right) |\bar{\sigma}\rangle \quad (6.6.8)$$

The first relation gives  $v_{in} = \langle \Phi |_i v |\Psi\rangle_n = \left( \langle \Psi |_n v^\dagger |\Phi\rangle_i \right)^* = 0$ . The set of states that give non-zero  $v_{in}^\dagger$  are specific elements of the set of eigenstates that have a total of either 1 or 3 electrons on the impurity and zeroth sites:

$$|\Psi\rangle_n = |\Psi\rangle_{\pm, \sigma}^{s, p} = -\sqrt{2} \left( a_{1, \pm} |\sigma, p\rangle + a_{2, \pm} |p, \sigma\rangle \right) \otimes |s\rangle, \quad \sigma = \uparrow, \downarrow, \quad E_{\pm, \sigma}^{s, p} = -\frac{U}{4} \pm \frac{1}{2} \Delta; \quad (6.6.9)$$

here,  $s$  is a string from the set  $\{0, \uparrow, \downarrow, 2\}$  and represents the configuration of the first site  $|s\rangle$  in direct product with the impurity and zeroth site entangled composite state, and  $p$  is either 2 or 0 such that  $p+1 (= 1 \text{ or } 3)$  represents the total number of electrons on the impurity and zeroth sites. For  $|\Phi\rangle_0$ , only  $s = \bar{\sigma}$  and  $p = 0$  give non-zero inner product. The coefficients are defined as  $a_{1, \pm} = \frac{4V}{\sqrt{2}\mathcal{N}_{\pm}}, a_{2, \pm} = \frac{U \pm 2\Delta}{\sqrt{2}\mathcal{N}_{\pm}}$ . The inner product is

$$v_{\pm \sigma, i} = \langle \Psi_{\pm, \sigma}^{\bar{\sigma}, 0} | v |\Phi_i\rangle = \sigma t \left[ a_{1, \pm} c_s^- + a_{2, \pm} c_c^- \right] \quad (6.6.10)$$

$\mathcal{N}_{\pm} = \sqrt{16V^2 + (U \pm 2\Delta)^2}$  is the normalisation factor and  $\Delta = \frac{1}{2} \sqrt{U^2 + 16V^2}$ . The renormalisation for this value of  $i$  then becomes

$$(\Delta H)_{i=0} = |\Phi\rangle_0 \langle \Phi |_0 \sum_n \frac{|v_{ni}|^2}{-\delta E_n} = |\Phi\rangle_0 \langle \Phi |_0 \sum_{\sigma, \pm} \frac{|v_{\pm \sigma, i}|^2}{-\delta E_{\pm}^{\sigma}} = -|\Phi\rangle_0 \langle \Phi |_0 2t^2 \sum_{\pm} \frac{\left[ a_{1, \pm} c_s^- + a_{2, \pm} c_c^- \right]^2}{\delta E_{\pm}^{\sigma}} \quad (6.6.11)$$

where  $\delta E_{\pm}^{\sigma} = E_{\pm}^{\sigma} - E_{\text{gs}}$ .

For  $i = 1$ , we have  $|\Phi\rangle_1 = |\Psi\rangle_1 \otimes |\uparrow\rangle$ . Carrying out a similar calculation above, we get

$$v |\Phi\rangle_1 = t \frac{1}{\sqrt{2}} \left( c_s^- |\uparrow, 0, 2\rangle + c_c^- |0, \uparrow, 2\rangle \right), \quad |\psi\rangle_n = |\Psi\rangle_{\pm, \uparrow}^{2, 0}, \quad v_{ni} = -t \left( c_s^- a_{1, \pm} + c_c^- a_{2, \pm} \right) \quad (6.6.12)$$

$$v^\dagger |\Phi\rangle_1 = t \frac{1}{\sqrt{2}} \left( c_s^- |\uparrow, 2, 0\rangle - c_c^- |2, \uparrow, 0\rangle \right), \quad |\psi\rangle_n = |\Psi\rangle_{\pm, \uparrow}^{0, 2}, \quad v_{in} = -t \left( c_s^- a_{1, \pm} - c_c^- a_{2, \pm} \right) \quad (6.6.13)$$

$$(\Delta H)_{i=1} = -|\Phi\rangle_1 \langle \Phi |_1 2t^2 \sum_{\pm} \frac{a_{1, \pm}^2 c_s^{-2} + a_{2, \pm}^2 c_c^{-2}}{\delta E_{\pm}^{\sigma}} \quad (6.6.14)$$

The total Hamiltonian  $H_0^* + H_X$  is invariant under the transformations  $c_\sigma^\dagger \rightarrow c_\sigma, t \rightarrow -t$ . Since the renormalisation only involves even powers of  $t$ , we can conclude that the renormalisation for  $i = 2$  and  $i = 3$  will be the same as that of  $i = 1$  and  $i = 0$  respectively. The total renormalisation at second order is

$$\begin{aligned} \Delta H &= -\sum_{i=0}^3 |\Phi\rangle_i \langle \Phi |_i 2t^2 \sum_{\pm} \frac{a_{1, \pm}^2 c_s^{-2} + a_{2, \pm}^2 c_c^{-2}}{\delta E_{\pm}^{\sigma}} - \left( |\Phi\rangle_0 \langle \Phi |_0 + |\Phi\rangle_3 \langle \Phi |_3 \right) 4t^2 \sum_{\pm} \frac{a_{1, \pm} a_{2, \pm} c_s^- c_c^-}{\delta E_{\pm}^{\sigma}} \\ &= -\sum_{i=0}^3 |\Phi\rangle_i \langle \Phi |_i t^2 \sum_{\pm} \frac{1}{\mathcal{N}_{\pm}^2} \frac{\left( 4V c_s^- \right)^2 + (U \pm 2\Delta)^2 c_c^{-2}}{\delta E_{\pm}^{\sigma}} - \left( |\Phi\rangle_0 \langle \Phi |_0 + |\Phi\rangle_3 \langle \Phi |_3 \right) \sum_{\pm} \frac{t^2}{\mathcal{N}_{\pm}^2} \frac{8V c_s^- (U \pm 2\Delta) c_c^-}{\delta E_{\pm}^{\sigma}} \end{aligned} \quad (6.6.15)$$

Since the  $|\hat{n}_{1\sigma}, \hat{n}_{1\bar{\sigma}}\rangle$  form a complete set, we have  $\sum_{i=0}^3 |\Phi\rangle_i \langle \Phi |_i = |\Psi\rangle_1 \langle \Psi |_1$ , and the first term becomes a constant. The second term is a local Fermi liquid term on the first site:

$$\begin{aligned} \Delta H &= |\Psi\rangle_1 \langle \Psi |_1 \left[ \text{constant} - \left\{ \hat{n}_{1\uparrow} \hat{n}_{1\downarrow} + \left( 1 - \hat{n}_{1\uparrow} \right) \left( 1 - \hat{n}_{1\downarrow} \right) \right\} \sum_{\pm} \frac{t^2}{\mathcal{N}_{\pm}^2} \frac{8V c_s^- (U \pm 2\Delta) c_c^-}{\delta E_{\pm}^{\sigma}} \right] \\ &= |\Psi\rangle_1 \langle \Psi |_1 \left[ \text{constant} + \left( \hat{n}_{1\uparrow} - \hat{n}_{1\downarrow} \right)^2 \sum_{\pm} \frac{t^2}{\mathcal{N}_{\pm}^2} \frac{8V c_s^- (U \pm 2\Delta) c_c^-}{\delta E_{\pm}^{\sigma}} \right] \end{aligned} \quad (6.6.16)$$

In the strong-coupling regime, we have  $J, V \gg U$ , and we can then approximate:

$$\delta E_{\pm}^{\sigma} \simeq \frac{3J}{8} + \sqrt{4V^2 - \left(\frac{3J}{8}\right)^2} \mp V, \quad U \pm 2\Delta \simeq \pm 4V, \quad \text{and} \quad \mathcal{N}_{\pm}^2 \simeq 32V^2 \quad (6.6.17)$$

Substituting this gives

$$\Delta H = |\Psi\rangle_1 \langle \Psi|_1 \left[ \text{constant} - \left(\hat{n}_{1\uparrow} - \hat{n}_{1\downarrow}\right)^2 \frac{2t^2 V c_s^- c_c^-}{2 \left(\frac{3J}{8}\right)^2 + 3V^2 + \frac{3J}{4} \sqrt{4V^2 + \left(\frac{3J}{8}\right)^2}} \right] \quad (6.6.18)$$

### 6.6.2 Fourth order effective Hamiltonian

Using fourth order perturbation theory, we can write the effective Hamiltonian renormalisation at that order in the form

$$\begin{aligned} \Delta H &= - \sum_i |\Phi\rangle_i \langle \Phi|_i \left[ \sum_{lmn} \frac{\langle \Phi_i | H_X | \Psi_l \rangle \langle \Psi_l | H_X | \Psi_m \rangle \langle \Psi_m | H_X | \Psi_n \rangle \langle \Psi_n | H_X | \Phi_i \rangle}{\delta E_l \delta E_m \delta E_n} + \Delta^{(2)} H \sum_n \frac{|\langle \Psi_n | H_X | \Phi_i \rangle|^2}{(\delta E_n)^2} \right], \\ &= - \sum_i |\Phi\rangle_i \langle \Phi|_i \left[ \sum_m \frac{1}{\delta E_m} \left\| \sum_n \frac{1}{\delta E_n} (H_X)_{mn} (H_X)_{ni} \right\|^2 + \Delta^{(2)} H \sum_n \frac{1}{(\delta E_n)^2} \left\| (H_X)_{ni} \right\|^2 \right]. \end{aligned} \quad (6.6.19)$$

We can have at most two successive  $v^\dagger$  or two successive  $v$  act on a particular state. Any more would lead to  $c_\sigma^\dagger |\hat{n}_\sigma = 2\rangle = 0$ . This limits the possible scattering processes (in the first term) to the following channels:

$$a. vv^\dagger vv^\dagger, \quad b. v^\dagger vv^\dagger v, \quad c. vvv^\dagger v^\dagger, \quad d. v^\dagger v^\dagger vv. \quad (6.6.20)$$

We start with  $i = 0$ . Out of the four channels  $a$  through  $d$ , only  $b$  and  $d$  survive. For  $i = 0$ , we already know the relevant  $|\Psi\rangle_n$  and hence the  $(H_X)_{ni} = v_{ni}$ , from eq. (6.6.10).

$$v_{\pm\sigma,i} = \langle \Psi_{\pm,\sigma}^{\bar{\sigma},0} | v | \Phi_i \rangle = \sigma t \left[ a_{1,\pm} c_s^- + a_{2,\pm} c_c^- \right] = \sigma t \mathcal{S}_{\pm}^- \quad (6.6.21)$$

where we have defined the sum and difference  $\mathcal{S}_{\pm}^{\pm} = a_{1,\pm} c_s^{\pm} + a_{2,\pm} c_c^{\pm}$ ,  $\mathcal{D}_{\pm}^{\pm} = a_{1,\pm} c_s^{\pm} - a_{2,\pm} c_c^{\pm}$ . For channel  $b$ , we then proceed as follows:

$$|\Psi\rangle_{\pm,\sigma}^{\bar{\sigma},0} = -\sqrt{2} \left( a_{1,\pm} |\sigma, 0\rangle + a_{2,\pm} |0, \sigma\rangle \right) \otimes |\bar{\sigma}\rangle \quad (6.6.22)$$

$$v^\dagger |\Psi\rangle_n = v^\dagger |\Psi\rangle_{\pm,\sigma}^{\bar{\sigma},0} = \sqrt{2} t \left( a_{1,\pm} |\sigma, \bar{\sigma}\rangle + a_{2,\pm} |0, \sigma \bar{\sigma}\rangle \right) \otimes |0\rangle \quad (6.6.23)$$

$$|\Psi\rangle_m = \begin{cases} \frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle) \otimes |0\rangle \\ \frac{1}{\sqrt{2}} (|2, 0\rangle - |0, 2\rangle) \otimes |0\rangle \\ \left[ \frac{c_s^+}{\sqrt{2}} (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + \frac{c_c^+}{\sqrt{2}} (|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle) \right] \otimes |0\rangle \end{cases} \implies (H_X)_{m,\pm\sigma} = \begin{cases} ta_{1\pm} \\ \bar{\sigma} ta_{2\pm} \\ \sigma t (a_{1\pm} c_s^+ + a_{2\pm} c_c^+) = \sigma t \mathcal{S}_{\pm}^+ \end{cases} \quad (6.6.24)$$

$$\frac{1}{\delta E_m} \left\| \sum_n \frac{1}{\delta E_n} (H_X)_{mn} (H_X)_{ni} \right\|^2 = \begin{cases} \frac{1}{\delta E_{\text{ST}}} \left( \sum_{\sigma,\pm} \frac{t^2}{\delta E_{\pm}} \sigma a_{1\pm} \mathcal{S}_{\pm}^- \right)^2 = 0 \\ \frac{1}{\delta E_{\text{CS}}} \left( \sum_{\pm,\sigma} \frac{t^2}{\delta E_{\pm}} a_{2\pm} \mathcal{S}_{\pm}^- \right)^2 = \frac{4t^4}{\delta E_{\text{CS}}} \left( \sum_{\pm} \frac{1}{\delta E_{\pm}} a_{2\pm} \mathcal{S}_{\pm}^- \right)^2 \\ \frac{1}{\delta E_2} \left( - \sum_{\pm,\sigma} \frac{t^2}{\delta E_{\pm}} \mathcal{S}_{\pm}^+ \mathcal{S}_{\pm}^- \right)^2 = \frac{4t^4}{\delta E_2} \left( \sum_{\pm} \frac{1}{\delta E_{\pm}} \mathcal{S}_{\pm}^+ \mathcal{S}_{\pm}^- \right)^2 \end{cases} \quad (6.6.25)$$

$E_{\text{ST}}, E_{\text{CS}}$  and  $E_2$  are the energies of the spin triplet zero, charge singlet and spin singlet+charge triplet excited states of the set  $|\Psi\rangle_m$  in eq. (6.6.24).

We now turn to channel  $d$ :

$$v|\Psi\rangle_n = v|\Psi\rangle_{\pm,\sigma}^{\bar{\sigma},0} = \sqrt{2}t\sigma a_{2\pm}|0,0\rangle \otimes |2\rangle, \quad |\Psi\rangle_m = |0,0,2\rangle, \quad (H_X)_{m,\pm\sigma} = \sqrt{2}t\sigma a_{2\pm} \quad (6.6.26)$$

$$\frac{1}{\delta E_m} \left\| \sum_n \frac{1}{\delta E_n} (H_X)_{mn} (H_X)_{ni} \right\|^2 = \frac{8t^4}{\delta E_{00}} \left( \sum_{\pm} \frac{1}{\delta E_{\pm}} a_{2\pm} \mathcal{S}_{\pm}^- \right)^2 \quad (6.6.27)$$

$E_{00}$  is the energy of the state  $|0,0,2\rangle$ .

Having accounted for both channels, we will calculate the second part of the effective Hamiltonian in eq. (6.6.19), the part involving  $\Delta^{(2)}H$ . We already know, from eq. (6.6.11), that

$$\Delta^{(2)}H_{i=0} = -2t^2 \sum_{\pm} \frac{1}{\delta E_{\pm}} (\mathcal{S}_{\pm}^-)^2 \quad (6.6.28)$$

Also, from the expression of  $v_{\pm\sigma,i}$ , we get

$$\sum_n \frac{1}{(\delta E_n)^2} \left\| (H_X)_{ni} \right\|^2 = \sum_{\pm} \frac{2t^2}{(\delta E_{\pm})^2} (\mathcal{S}_{\pm}^-)^2 \quad (6.6.29)$$

Combining it all, the total renormalisation in  $i=0$  is

$$-|\Phi\rangle_0 \langle \Phi|_0 4t^4 \left[ \left( \frac{1}{\delta E_{CS}} + \frac{2}{\delta E_{00}} \right) \left( \sum_{\pm} \frac{a_{2\pm} \mathcal{S}_{\pm}^-}{\delta E_{\pm}} \right)^2 + \frac{1}{\delta E_2} \left( \sum_{\pm} \frac{\mathcal{S}_{\pm}^+ \mathcal{S}_{\pm}^-}{\delta E_{\pm}} \right)^2 - \sum_{\pm} \frac{(\mathcal{S}_{\pm}^-)^2}{\delta E_{\pm}} \sum_{\pm} \left( \frac{\mathcal{S}_{\pm}^-}{\delta E_{\pm}} \right)^2 \right] \quad (6.6.30)$$

We now come to  $i=1$ :  $|\Phi\rangle_1 = |\Psi\rangle_1 \otimes |\uparrow\rangle$ . Channels  $a$  and  $b$  are non-zero here. We start with channel  $b$ :  $v^\dagger v v^\dagger v$ . We already know, from eq. (6.6.12), that

$$v|\Phi\rangle_1 = t \frac{1}{\sqrt{2}} \left( c_s^- |\uparrow, 0, 2\rangle + c_c^- |0, \uparrow, 2\rangle \right), \quad |\psi\rangle_n = |\Psi\rangle_{\pm,\uparrow}^{2,0} = -\sqrt{2} \left( a_{1,\pm} |\uparrow, 0\rangle + a_{2,\pm} |0, \uparrow\rangle \right) \otimes |2\rangle, \quad (H_X)_{ni} = -t \mathcal{S}_{\pm}^- \quad (6.6.31)$$

Moving forward:

$$v^\dagger |\Psi\rangle_n = \sqrt{2}t \left( a_{1,\pm} |\uparrow, \uparrow\rangle \otimes |\downarrow\rangle - a_{1,\pm} |\uparrow, \downarrow\rangle \otimes |\uparrow\rangle - a_{2,\pm} |0, 2\rangle \otimes |\uparrow\rangle \right) \quad (6.6.32)$$

$$|\Psi\rangle_m = \begin{cases} \frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle) \otimes |\uparrow\rangle \\ \frac{1}{\sqrt{2}} (|2, 0\rangle - |0, 2\rangle) \otimes |\uparrow\rangle \\ \left[ \frac{c_s^+}{\sqrt{2}} (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + \frac{c_c^+}{\sqrt{2}} (|\uparrow, 0\rangle + |0, \uparrow\rangle) \right] \otimes |\uparrow\rangle \\ |\uparrow, \uparrow\rangle \otimes |\downarrow\rangle \end{cases} \implies (H_X)_{m,\pm} (H_X)_{\pm,i} = \begin{cases} t^2 a_{1\pm} \mathcal{S}_{\pm}^- \\ -t^2 a_{2\pm} \mathcal{S}_{\pm}^- \\ t^2 \mathcal{S}_{\pm}^+ \mathcal{S}_{\pm}^- \\ -\sqrt{2}t^2 a_{1\pm} \mathcal{S}_{\pm}^- \end{cases} \quad (6.6.33)$$

$$\frac{1}{\delta E_m} \left\| \sum_n \frac{1}{\delta E_n} (H_X)_{mn} (H_X)_{ni} \right\|^2 = \begin{cases} \frac{t^4}{\delta E_{ST}} \left( \sum_{\pm} \frac{1}{\delta E_{\pm}} a_{1\pm} \mathcal{S}_{\pm}^- \right)^2 \\ \frac{t^4}{\delta E_{CS}} \left( \sum_{\pm} \frac{1}{\delta E_{\pm}} a_{2\pm} \mathcal{S}_{\pm}^- \right)^2 \\ \frac{t^4}{\delta E_2} \left( \sum_{\pm} \frac{1}{\delta E_{\pm}} \mathcal{S}_{\pm}^+ \mathcal{S}_{\pm}^- \right)^2 \\ \frac{2t^4}{\delta E_{\uparrow\uparrow}} \left( \sum_{\pm} \frac{1}{\delta E_{\pm}} a_{1\pm} \mathcal{S}_{\pm}^- \right)^2 \end{cases} \quad (6.6.34)$$

$E_{\uparrow\uparrow}$  is the energy of the upwards polarised state  $|\uparrow, \uparrow\rangle \otimes |\downarrow\rangle$ .

Next is channel  $a$ :  $vv^\dagger vv^\dagger$ . Using eq. (6.6.13) and following the same steps as above, we get:

$$v^\dagger |\Phi\rangle_1 = t \frac{1}{\sqrt{2}} \left( c_s^- |\uparrow, 2, 0\rangle - c_c^- |2, \uparrow, 0\rangle \right), \quad |\Psi\rangle_n = |\Psi\rangle_{\pm,\uparrow}^{0,2} = -\sqrt{2} \left( a_{1,\pm} |\uparrow, 2\rangle + a_{2,\pm} |2, \uparrow\rangle \right) \otimes |0\rangle, \quad (H_X)_{ni} = -t \mathcal{D}_{\pm}^- \quad (6.6.35)$$

$$v|\Psi\rangle_n = \sqrt{2}t \left( a_{1,\pm} |\uparrow, \uparrow\rangle \otimes |\downarrow\rangle - a_{1,\pm} |\uparrow, \downarrow\rangle \otimes |\uparrow\rangle + a_{2,\pm} |2, 0\rangle \otimes |\uparrow\rangle \right) \quad (6.6.36)$$

$$|\Psi\rangle_m = \begin{cases} \frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle) \otimes |\uparrow\rangle \\ \frac{1}{\sqrt{2}} (|2, 0\rangle - |0, 2\rangle) \otimes |\uparrow\rangle \\ \left[ \frac{c_s^+}{\sqrt{2}} (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + \frac{c_e^+}{\sqrt{2}} (|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle) \right] \otimes |\uparrow\rangle \\ |\uparrow, \uparrow\rangle \otimes |\downarrow\rangle \end{cases} \implies (H_X)_{m,\pm} (H_X)_{\pm,i} = \begin{cases} t^2 a_{1\pm} \mathcal{D}_{\pm}^- \\ -t^2 a_{2\pm} \mathcal{D}_{\pm}^- \\ t^2 \mathcal{D}_{\pm}^+ \mathcal{D}_{\pm}^- \\ -\sqrt{2} t^2 a_{1\pm} \mathcal{D}_{\pm}^- \end{cases} \quad (6.6.37)$$

$$\frac{1}{\delta E_m} \left\| \sum_n \frac{1}{\delta E_n} (H_X)_{mn} (H_X)_{ni} \right\|^2 = \begin{cases} \frac{1}{\delta E_{ST}} \left( \sum_{\pm} \frac{t^2}{\delta E_{\pm}} a_{1\pm} \mathcal{D}_{\pm}^- \right)^2 \\ \frac{t^4}{\delta E_{CS}} \left( \sum_{\pm} \frac{1}{\delta E_{\pm}} a_{2\pm} \mathcal{D}_{\pm}^- \right)^2 \\ \frac{t^4}{\delta E_2} \left( \sum_{\pm} \frac{1}{\delta E_{\pm}} \mathcal{D}_{\pm}^+ \mathcal{D}_{\pm}^- \right)^2 \\ \frac{2t^4}{\delta E_{\uparrow\uparrow}} \left( \sum_{\pm} \frac{1}{\delta E_{\pm}} a_{1\pm} \mathcal{D}_{\pm}^- \right)^2 \end{cases} \quad (6.6.38)$$

For the final part, we again use  $\Delta^{(2)} H_{i=1} = -t^2 \sum_{\pm} \frac{1}{\delta E_{\pm}} \left[ (\mathcal{S}_{\pm}^-)^2 + (\mathcal{D}_{\pm}^-)^2 \right]$ . Also, since  $(H_X)_{ni} = (v + v^\dagger)_{ni}$ , we have

$$\sum_n \frac{1}{(\delta E_n)^2} \left\| (H_X)_{ni} \right\|^2 = t^2 \sum_{\pm} \left[ \left( \frac{\mathcal{S}_{\pm}^-}{\delta E_{\pm}} \right)^2 + \left( \frac{\mathcal{D}_{\pm}^-}{\delta E_{\pm}} \right)^2 \right] \quad (6.6.39)$$

Combining all the terms, we get

$$\begin{aligned} -|\Phi\rangle_1 \langle \Phi|_1 4t^4 & \left[ \left( \frac{1}{\delta E_{ST}} + \frac{2}{\delta E_{\uparrow\uparrow}} \right) \left\{ \left( \frac{1}{2} \sum_{\pm} \frac{a_{1\pm} \mathcal{S}_{\pm}^-}{\delta E_{\pm}} \right)^2 + \left( \frac{1}{2} \sum_{\pm} \frac{a_{1\pm} \mathcal{D}_{\pm}^-}{\delta E_{\pm}} \right)^2 \right\} + \frac{1}{\delta E_{CS}} \left\{ \left( \frac{1}{2} \sum_{\pm} \frac{a_{2\pm} \mathcal{S}_{\pm}^-}{\delta E_{\pm}} \right)^2 \right. \right. \\ & \left. \left. + \left( \frac{1}{2} \sum_{\pm} \frac{a_{2\pm} \mathcal{D}_{\pm}^-}{\delta E_{\pm}} \right)^2 \right\} + \frac{1}{\delta E_2} \left\{ \left( \frac{1}{2} \sum_{\pm} \frac{\mathcal{S}_{\pm}^+ \mathcal{S}_{\pm}^-}{\delta E_{\pm}} \right)^2 + \left( \frac{1}{2} \sum_{\pm} \frac{\mathcal{D}_{\pm}^+ \mathcal{D}_{\pm}^-}{\delta E_{\pm}} \right)^2 \right\} \right. \\ & \left. - \sum_{\pm} \frac{1}{\delta E_{\pm}} \frac{1}{2} \left\{ (\mathcal{S}_{\pm}^-)^2 + (\mathcal{D}_{\pm}^-)^2 \right\} \sum_{\pm} \frac{1}{2} \left\{ \left( \frac{\mathcal{S}_{\pm}^-}{\delta E_{\pm}} \right)^2 + \left( \frac{\mathcal{D}_{\pm}^-}{\delta E_{\pm}} \right)^2 \right\} \right] \quad (6.6.40) \end{aligned}$$

If we define some quantities:  $F_{(1,2)} = \sum_{\pm} \frac{a_{(1,2)\pm} \mathcal{S}_{\pm}^-}{\delta E_{\pm}}$ ,  $G_{(1,2)} = \sum_{\pm} \frac{a_{(1,2)\pm} \mathcal{D}_{\pm}^-}{\delta E_{\pm}}$ ,  $P = \sum_{\pm} \frac{\mathcal{S}_{\pm}^+ \mathcal{S}_{\pm}^-}{\delta E_{\pm}}$ ,  $Q = \sum_{\pm} \frac{\mathcal{D}_{\pm}^+ \mathcal{D}_{\pm}^-}{\delta E_{\pm}}$ ,  $X_n = \sum_{\pm} \frac{(\mathcal{S}_{\pm}^-)^2}{(\delta E_{\pm})^n}$ ,  $Y_n = \sum_{\pm} \frac{(\mathcal{D}_{\pm}^-)^2}{(\delta E_{\pm})^n}$ , the total renormalisation from second and fourth order can be written as

$$\begin{aligned} & -(|\Phi\rangle_0 \langle \Phi|_0 + |\Phi\rangle_3 \langle \Phi|_3) 4t^4 \left[ \frac{1}{2t^2} X_1 + \left( \frac{1}{\delta E_{CS}} + \frac{2}{\delta E_{00}} \right) F_2^2 + \frac{1}{\delta E_2} P^2 - X_1 X_2 \right] \\ & -(|\Phi\rangle_1 \langle \Phi|_1 + |\Phi\rangle_2 \langle \Phi|_2) t^4 \left[ \frac{1}{t^2} (X_1 + Y_1) + \left( \frac{1}{\delta E_{ST}} + \frac{2}{\delta E_{\uparrow\uparrow}} \right) (F_1^2 + G_1^2) + \frac{1}{\delta E_{CS}} (F_2^2 + G_2^2) \right. \\ & \left. + \frac{1}{\delta E_2} (P^2 + Q^2) - (X_1 + Y_1) (X_2 + Y_2) \right] \quad (6.6.41) \end{aligned}$$

The excitation energies are given by

$$\delta E_{CS} = \delta E_{00} = \frac{3J}{8} + \frac{U}{4} + \alpha, \quad \delta E_{\uparrow\uparrow} = \delta E_{ST} = -\frac{U}{4} + \frac{5J}{8} + \alpha, \quad \delta E_2 = 2\alpha, \quad \delta E_{\pm} = \frac{3J}{8} + \alpha \pm \frac{1}{2} \Delta, \quad \alpha \equiv \sqrt{V^2 \gamma^2 + 4V^2} \quad (6.6.42)$$

where  $V\gamma = \frac{3J}{8} + \frac{U}{4}$  and  $\Delta = \sqrt{\frac{U^2}{4} + 4V^2}$ . The effective Hamiltonian can be expressed in the general form

$$H_{\text{eff}} = |\Psi\rangle_1 \langle \Psi|_1 \otimes \left[ \text{constant} + \alpha_{\text{spin}} \hat{\mathcal{P}}_{\text{spin}} + \alpha_{\text{charge}} \hat{\mathcal{P}}_{\text{charge}} \right] \quad (6.6.43)$$

$\hat{\mathcal{P}}_{\text{charge}}$  and  $\hat{\mathcal{P}}_{\text{spin}}$  are projection operators for, respectively, the charge ( $\hat{n}_1 \neq 1$ ) and spin ( $\hat{n}_1 = 1$ ) sectors of the first site. Since  $\hat{\mathcal{P}}_{\text{charge}} + \hat{\mathcal{P}}_{\text{spin}} = 1$ , we can eliminate one of the terms and rewrite the effective Hamiltonian in the simpler form

$$H_{\text{eff}} = |\Psi\rangle_1 \langle \Psi|_1 \otimes \left[ \text{constant} + \mathcal{F} \hat{\mathcal{P}}_{\text{charge}} \right] \quad (6.6.44)$$

where  $\mathcal{F} \equiv \alpha_{\text{charge}} - \alpha_{\text{spin}}$  is the net energy of the charge sector above the spin sector.

We will now look at the extreme strong-coupling regime  $J \gg V \gg U, t$ . There, all the expressions simplify:

$$\begin{aligned} V\gamma &\simeq \frac{3J}{8}, \quad \Delta \simeq 2V, \quad \alpha \simeq \frac{3J}{8}, \quad c_s^+ = -c_c^- \simeq 0, \quad c_s^- = c_c^+ \simeq 1, \quad \mathcal{N}_{\pm} \simeq 4\sqrt{2}V, \quad a_{1,\pm} \simeq \frac{1}{2}, \quad a_{2,\pm} \simeq \pm \frac{1}{2}, \\ \delta E_{\pm} &= \delta E_{\text{CS}} = \delta E_{00} = \delta E_2 \simeq \frac{3J}{4}, \quad \delta E_{\text{ST}} = \delta E_{\uparrow\uparrow} \simeq J, \quad \mathcal{S}_{\pm}^- = \mathcal{D}_{\pm}^- \simeq \frac{1}{2}, \quad \mathcal{S}_{\pm}^+ = -\mathcal{D}_{\pm}^+ \simeq \pm \frac{1}{2}, \\ F_1 &= G_1 \simeq \frac{2}{3J}, \quad F_2 = G_2 \simeq 0, \quad P = Q \simeq 0, \quad X_1 = Y_1 \simeq \frac{2}{3J}, \quad X_2 = Y_2 \simeq \frac{8}{9J^2} \end{aligned} \quad (6.6.45)$$

The effective Hamiltonian becomes

$$\begin{aligned} & - \left( |\Phi\rangle_0 \langle \Phi|_0 + |\Phi\rangle_3 \langle \Phi|_3 \right) \frac{4t^2}{3J} \left[ 1 - \frac{16t^2}{9J^3} \right] - \left( |\Phi\rangle_1 \langle \Phi|_1 + |\Phi\rangle_2 \langle \Phi|_2 \right) \frac{4t^2}{3J} \left[ 1 + \frac{2t^2}{9J^2} \right] \\ &= - \frac{4t^2}{3J} \sum_i |\Phi\rangle_i \langle \Phi|_i + \left( |\Phi\rangle_0 \langle \Phi|_0 + |\Phi\rangle_3 \langle \Phi|_3 \right) \frac{64t^4}{27J^3} - \left( |\Phi\rangle_1 \langle \Phi|_1 + |\Phi\rangle_2 \langle \Phi|_2 \right) \frac{8t^4}{27J^3} \\ &= |\Psi\rangle_1 \langle \Psi|_1 \left[ \text{constant} + \frac{64t^4}{27J^3} \mathcal{P}_{\text{charge}} - \frac{8t^4}{27J^3} \mathcal{P}_{\text{spin}} \right] \end{aligned} \quad (6.6.46)$$

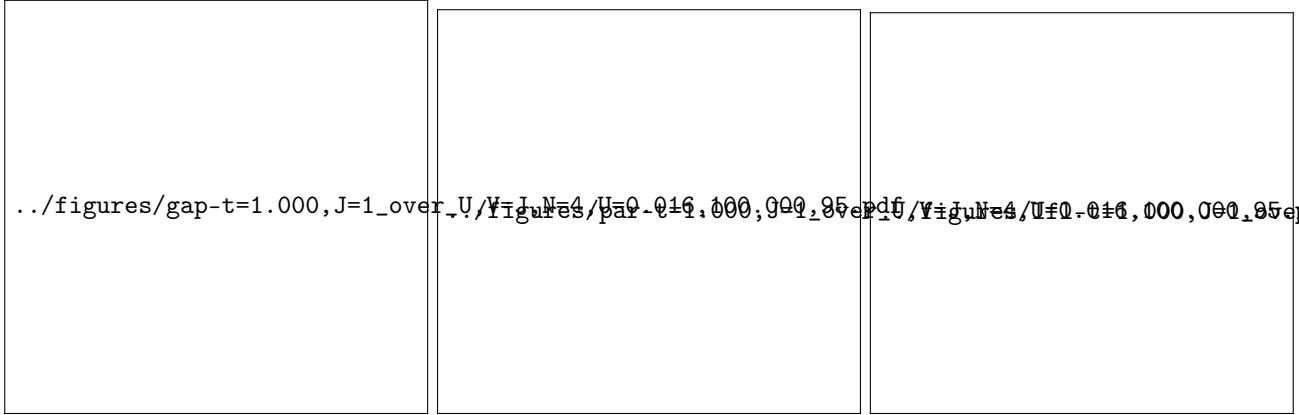
$\mathcal{P}_{\text{spin}}$  and  $\mathcal{P}_{\text{charge}}$  project, respectively, onto the spin and charge sectors of the first site. The fact that the charge sector comes with a positive factor means that the holon-doublon states are repulsive, and this renormalisation of the states generates an effective particle-hole symmetric Fermi liquid interaction on the first site - also known as the local Fermi liquid (LFL) [41].

## 6.7 Destruction of the Abrikosov-Suhl resonance: transition from strong-coupling to local moment

We will now tune the parameters of the fixed point Hamiltonian and study the variation of quantities related to the effective Hamiltonian like the local FL strength  $\mathcal{F}$ , the gap in the spectrum of the zeroth Hamiltonian  $H_0^*$  and the value of the small parameter  $t^2/\delta E$ , as well as various measures of entanglement like entanglement entropy, mutual information and spin-spin correlations between various sets of members of the real-space impurity+lattice construction. We will trace a specific path through the space of values of fixed point couplings: we will start from the strong-coupling regime  $U \ll J, V$  and go towards the local moment regime  $U \gg J, V$ . The context of this study is that the technique of dynamical mean-field theory (DMFT) obtains a metal-insulator transition in the 2D Hubbard model by studying the Anderson impurity model as the auxiliary system for the Hubbard; there, the local moment regime of the impurity corresponds to the insulator in the bulk. Our goal here is to study what precisely happens in the effective Hamiltonian in the journey from the metal to the insulator, and draw a concrete connection between this modification of the effective Hamiltonian, and the simultaneous change of the impurity spectral function in fig. 6.5.

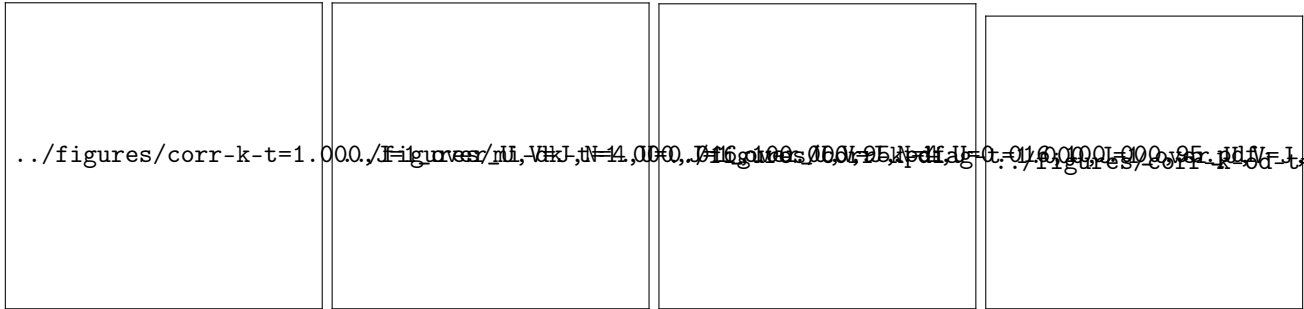
### 6.7.1 Generalised SIAM

#### Behaviour of $\mathcal{F}$ , the gap and the small parameter



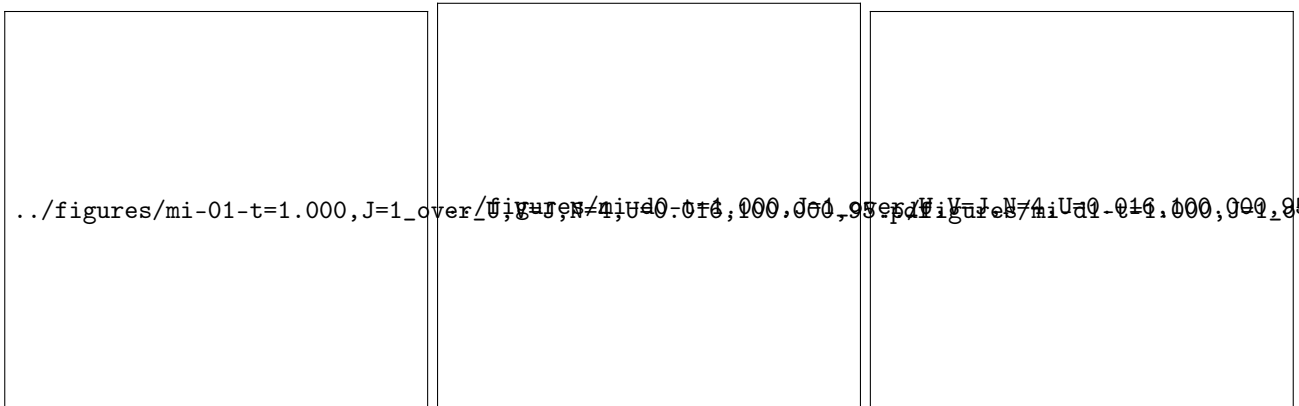
The vanishing of the gap and the growth of the small parameter indicates the breakdown of perturbation theory around the singlet; this simply shows that there is a degeneracy in the local moment regime, and the effective Hamiltonian will have to be obtained using degenerate perturbation theory. The presence of degeneracy also suggests that the effective Hamiltonian will be of the non-Fermi liquid type.

#### Behaviour of correlation within the Kondo cloud



The vanishing of the Kondo cloud at large  $U/J$  is clear indication of the destruction of the Kondo cloud and the breakdown of screening. Non-zero mutual information indicates an (impurity-mediated) interaction between the  $k$ -states of the conduction bath; seen differently, it is this interaction that is responsively for the screening of the impurity. The disappearance of the mutual information is indicative of the disappearance of this interaction.

#### Behaviour of mutual information between various real space members



The impurity-zeroth site mutual information  $I(d : 0)$  remains unchanged at the maximum for an appreciable range of values, and this shows the stability of the singlet. Meanwhile, the mutual information between the zeroth site and the site nearest to it ( $I(0 : 1)$ ) grows, because when the singlet weakens, the zeroth site is able to entangle more with the other sites. It finally saturates to its maximum value, which is the value produced as result of the tight-binding hopping. The mutual information between the impurity and sites beyond the zeroth site ( $I(d : 1)$ ) show a non-monotonic behaviour; it first increases as the entanglement that was initially restricted to just the impurity and the zeroth sites begins "seeping" into the other sites as well. Beyond a critical value of  $U/J$ ,  $I(d : 1)$  starts dropping, because the entanglement has now mostly shifted out of the zero mode and into the conduction bath.

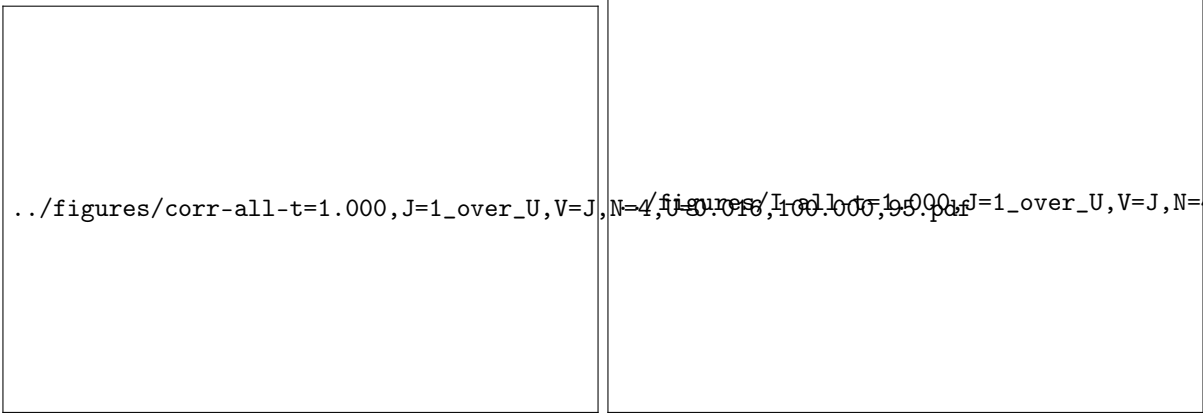
### Behaviour of impurity entanglement entropy and spin-spin correlations



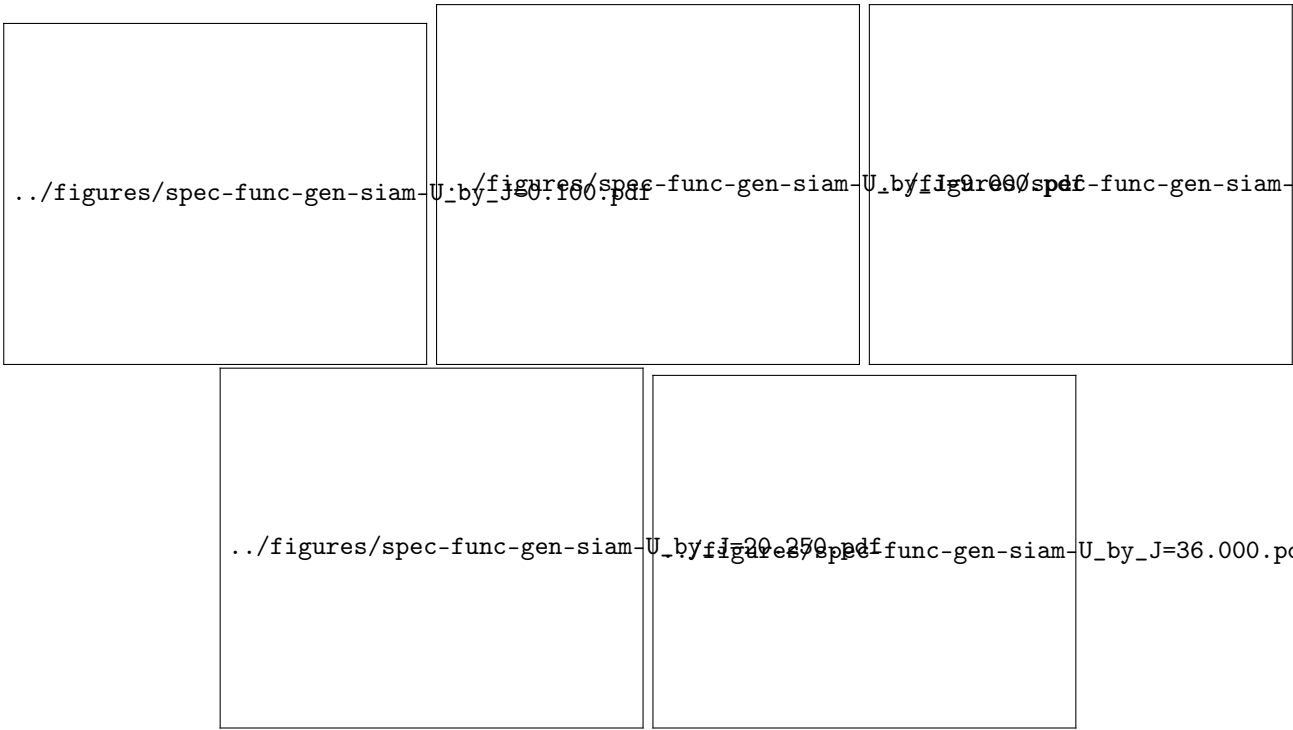
The von-Neumann entanglement entropy  $S(d)$  of the impurity shows pretty straightforward behaviour. It is maximum for  $U \ll J$  because it is in a singlet configuration. For  $U \gg J$ , the singlet weakens and the impurity begins to decouple from the bath, leading to a reduction in  $S(d)$ . At sufficiently low values of  $J/U$ , the impurity decouples from the zeroth site and the total system can be factorised into a local moment in product with a tight-binding chain, so that the impurity site will now have zero entanglement entropy.





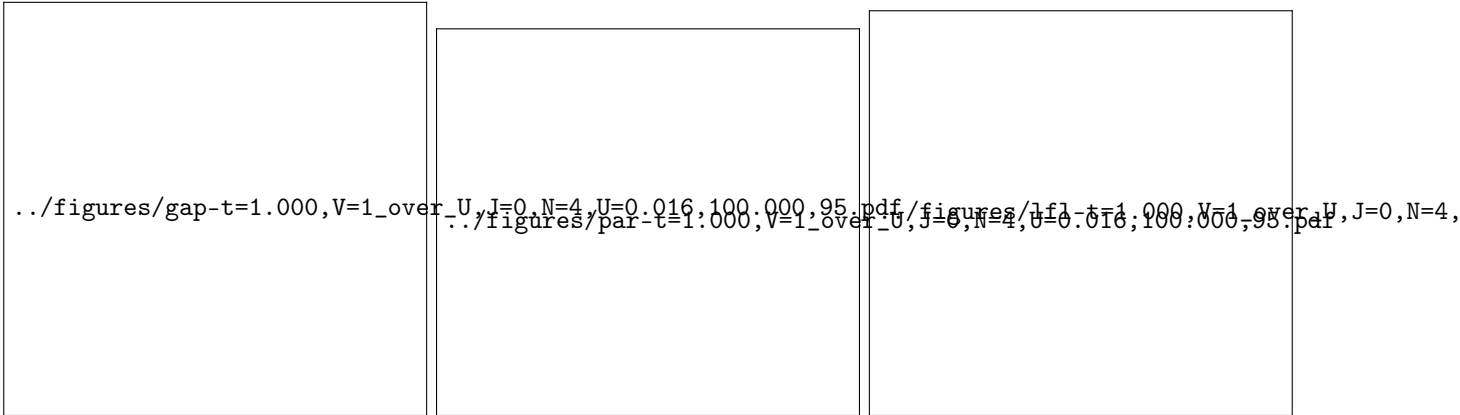


**Behaviour of  $A(\omega)$**

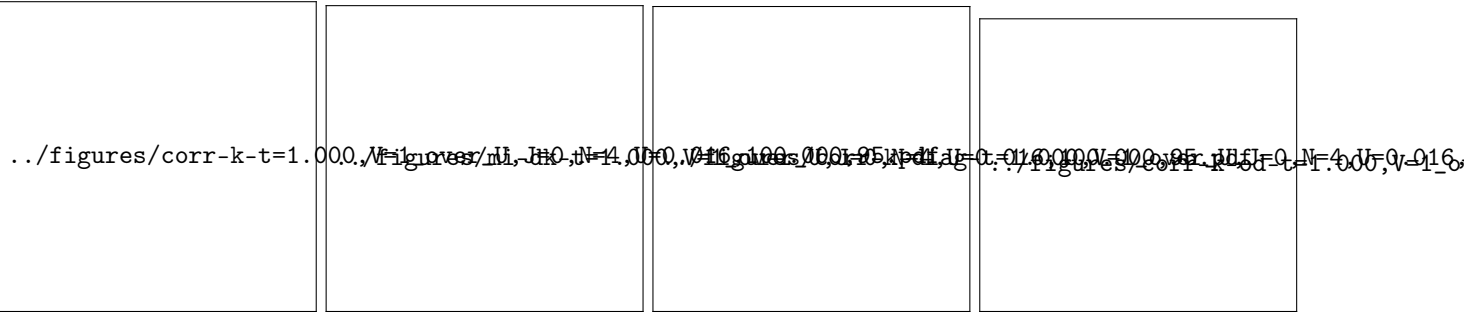


6.7.2 Pure SIAM

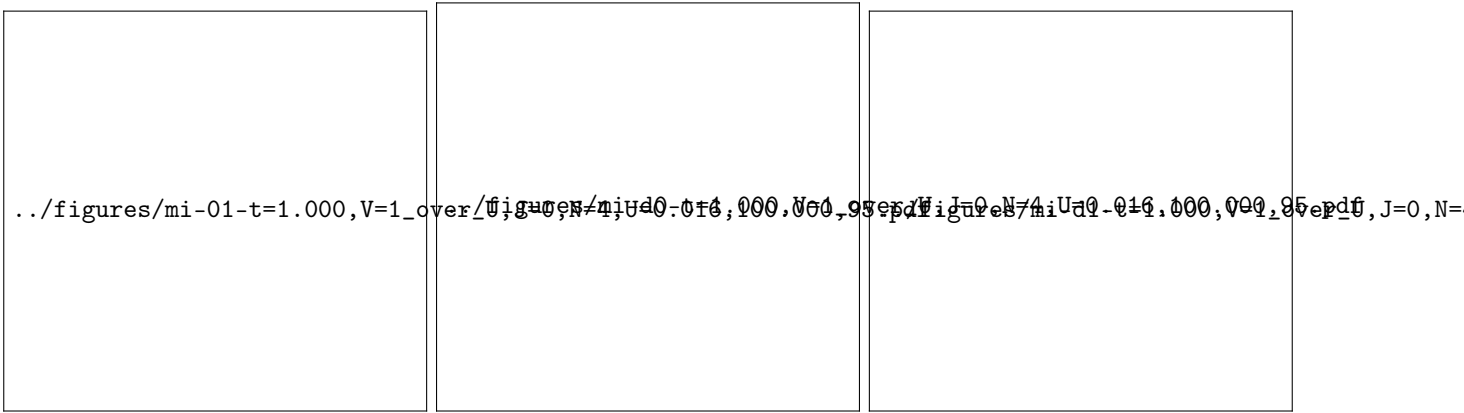
Behaviour of  $\mathcal{F}$ , the gap and the small parameter



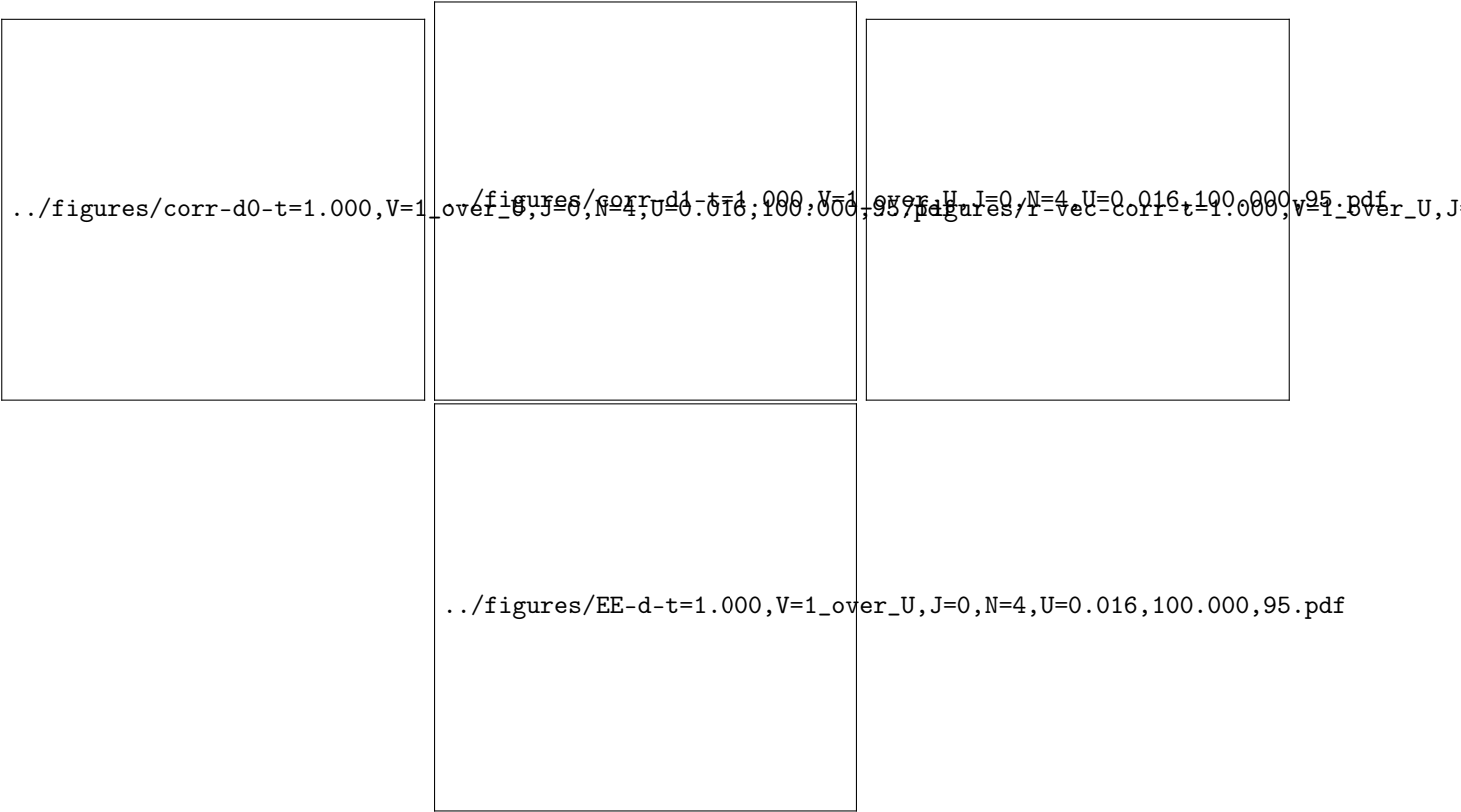
Behaviour of correlation within the Kondo cloud



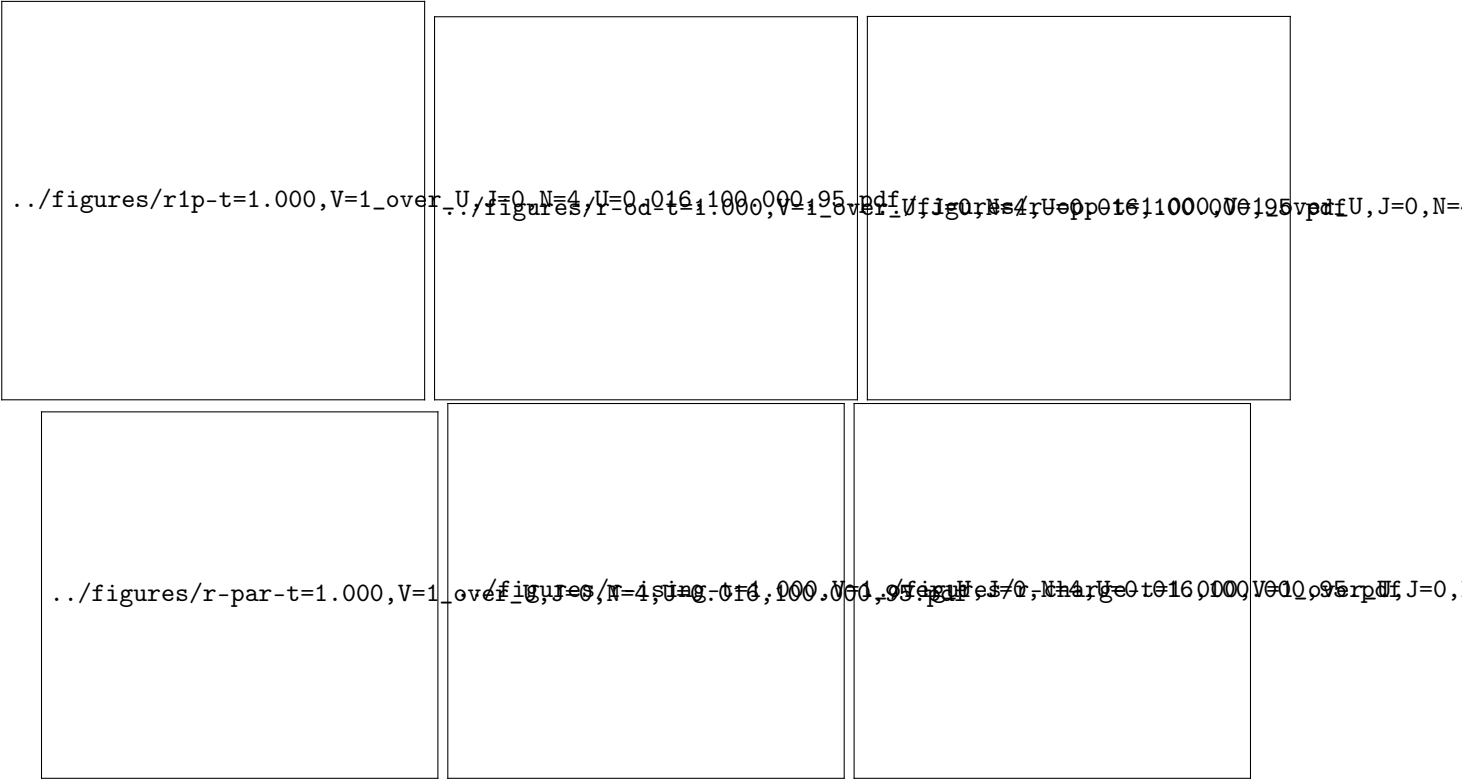
Behaviour of mutual information between various real space members



Behaviour of impurity entanglement entropy and spin-spin correlations



Behaviour of real-space correlations



Behaviour of real-space correlations as function of distance



Behaviour of  $A(\omega)$



## 6.8 Calculating the $T = 0$ Wilson ratio from low energy excitations

The total system now consists of two decoupled parts - the singlet composed of the impurity and the zeroth site, and the remaining lattice composed of  $N-1$  sites with a tight-binding dispersion and a local interaction at the 1-th site. The effective Hamiltonian for the remaining lattice is

$$\sum_{\sigma} \sum_{i=1}^{\infty} t \left( c_{i\sigma}^{\dagger} c_{i+1\sigma} + c_{i+1\sigma}^{\dagger} c_{i\sigma} \right) + u \hat{n}_{1\uparrow} \hat{n}_{1\downarrow} \quad (6.8.1)$$

We have rewritten the holon term in terms of the spin and doublon operators. We will now invoke the mean-field

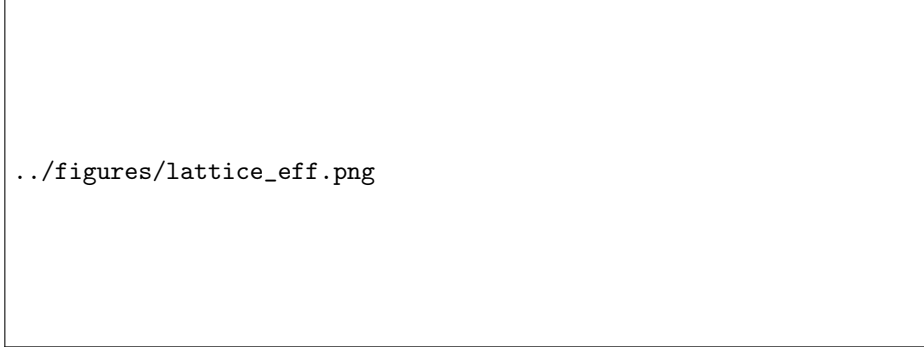


Figure 6.6: *Left*: The nearest-neighbor hopping described by the effective Hamiltonian. The red circle is the impurity. The black cloud at the center demarcates the collection of electrons at the origin of the lattice (which couple to the impurity). The green circles represent lattice sites that are nearest to the origin. The blue circles represent next-nearest sites. *Right*: After treating the hopping between origin and its nearest neighbors as perturbation, we get a system consisting of two decoupled parts: one part is the impurity+cloud singlet, the other part is the rest of the lattice sites. The effect of the hopping between the origin and the green sites is a repulsion term on the green sites.

approximation in simplifying this term. We will be dealing with thermodynamic quantities soon, so the operators will be replaced by their thermodynamic values, that is, the values that minimize the free energy functional.

$$\hat{n}_{1\uparrow} \hat{n}_{1\downarrow} \rightarrow \langle \hat{n}_{1\uparrow} \hat{n}_{1\downarrow} \rangle = \langle \delta n_{1\uparrow} \delta n_{1\downarrow} \rangle + \langle n_{1\uparrow} \rangle \langle n_{1\downarrow} \rangle \quad (6.8.2)$$

where  $\delta n_{1\sigma} \equiv n_{1\sigma} - \langle n_{1\sigma} \rangle$  is the fluctuation of the particle number above the ground state. The mean-field approximation then involves dropping the first term which is a quadratic fluctuation - since we are interested in values of quantities at  $T \rightarrow 0$ , this quadratic fluctuation is very small. The interaction we are left with is

$$u \langle n_{1\uparrow} \rangle \langle n_{1\downarrow} \rangle = \sum_{kq\sigma} f_{kq} \langle n_{k\sigma} \rangle \langle n_{q\bar{\sigma}} \rangle \quad (6.8.3)$$

This interaction converts the problem to that of a Landau Fermi liquid, with the quasiparticle energy functional being given by

$$\epsilon_{k\sigma} = \epsilon_k + \sum_q f_{kq} \langle \hat{n}_{q\bar{\sigma}} \rangle \quad (6.8.4)$$

From the form of the quasiparticle energy functional, we can see that there is no spin-parallel term, so we can write

$$f_{kk'\sigma\sigma} = 0, f_{kk'\sigma\bar{\sigma}} = f_{kk'} \quad (6.8.5)$$

We will now use this Fermi liquid form to extract the Wilson ratio. We will make use of the following definitions/results:

$$dn_{k\sigma} = \frac{\partial n}{\partial \epsilon_{k\sigma}} (d\epsilon_{k\sigma} - d\mu) \quad [\text{follows from differentiating FD distribution}] \quad (6.8.6)$$

$$C_V = \frac{d\epsilon}{dT}, \quad \chi^{s,c} = \frac{d}{d(B, \mu)} (n_{\uparrow} \mp n_{\downarrow}), \quad 2f_0^{s,a} = \sum_k \left( f_{kk'\uparrow\uparrow} \pm f_{kk'\uparrow\downarrow} \right), \quad F_0^{s,a} = \rho(0) f_0^{s,a} \quad (6.8.7)$$

### 6.8.1 Low- $T$ Specific heat

$$\begin{aligned}
 C &= \frac{d}{dT} \sum_{k\sigma} \epsilon_{k\sigma} n_{k\sigma} \\
 &\approx \sum_{k\sigma} \epsilon_{k\sigma}^0 \frac{dn_{k\sigma}}{dT} \quad [\text{no quasiparticles at ground state}] \\
 &\approx \sum_{k\sigma} \epsilon_{k\sigma}^0 \frac{dn_{k\sigma}}{dT} \quad [\text{same expression as Fermi gas but with modified distribution function}] \\
 &= \rho(0)T
 \end{aligned} \tag{6.8.8}$$

where  $\rho$  is the total quasiparticle DOS with contributions from conduction bath and impurity.

$$\rho \sim \text{Im Trace} [G] = \text{Im} \sum_{d\sigma} G_{dd}^\sigma + \text{Im} \sum_{k\sigma} G_{kk}^\sigma = \rho_0 + \rho_{\text{imp}} \tag{6.8.9}$$

which gives

$$C_{\text{imp}} \equiv C - C_0 = \rho_{\text{imp}}(0)T \tag{6.8.10}$$

### 6.8.2 Low- $T$ Charge Susceptibility

$$\chi^c = \frac{dN}{d\mu} \tag{6.8.11}$$

Due to change in chemical potential,  $\delta\epsilon_{k\sigma}$  is isotropic and SU(2)-symmetric. Hence

$$\begin{aligned}
 d\epsilon_{k\sigma} &= \sum_{k'\sigma'} f_{kk'\sigma\sigma'} dn_{k'\sigma'} \\
 &= dn \sum_{k'} \left( f_{kk'\uparrow\uparrow} + f_{kk'\uparrow\downarrow} \right) \quad [dn = dn_{k'\uparrow} = dn_{k\downarrow}] \\
 &= 2dn f_0^s
 \end{aligned} \tag{6.8.12}$$

Therefore,

$$\begin{aligned}
 dN &= \sum_{k\sigma} dn_{k\sigma} = \sum_{k\sigma} \frac{\partial n}{\partial \epsilon_{k\sigma}} (d\epsilon_{k\sigma} - d\mu) = \sum_{k\sigma} -\frac{1}{2}\rho (2dn f_0^s - d\mu) = -\rho(0)dN f_0^s + d\mu\rho(0) \\
 &\approx d\mu\rho(0) - \rho(0)f_0^s d\mu\rho(0) \quad [\text{substitute } dN \text{ back into itself}] \\
 \implies \frac{dN}{d\mu} &= \rho(0) (1 - \rho(0)f_0^s) \implies \chi_{\text{imp}}^c = \rho(0)_{\text{imp}} - \rho(0)f_0^s
 \end{aligned} \tag{6.8.13}$$

At an intermediate state, we substituted  $dN$  back into itself and kept only the leading order term. This is justified because  $f_{kk'}$  goes as  $\frac{1}{NJ}$ . At the fixed point and for a thermodynamically large system, both  $J$  and  $N$  are very large, so keeping only the leading order suffices.

From a previous calculation, we know that the charge susceptibility at  $T = 0$  is zero (eq. (6.2.9)), so we can write down the following relation:

$$f_0^s = \frac{\rho(0)_{\text{imp}}}{\rho(0)} \tag{6.8.14}$$

### 6.8.3 Low- $T$ Spin Susceptibility

$$\chi^s = \frac{dm}{d\mu} \tag{6.8.15}$$

Due to change in magnetic field, change in  $\epsilon_{k\sigma}$  should be isotropic and SU(2)-antisymmetric. Hence

$$\begin{aligned}
 d\epsilon_{k\sigma} &= -\frac{1}{2}dB\sigma + \sum_{k'\sigma'} f_{kk'\sigma\sigma'} dn_{k'\sigma'} \\
 &= -\frac{1}{2}dB\sigma + dn_\sigma \sum_{k'} \left( f_{kk'\uparrow\uparrow} - f_{kk'\uparrow\downarrow} \right) \quad [dn_{k'\uparrow} = -dn_{k\downarrow}] \\
 &= -\frac{1}{2}dB\sigma + 2dn_\sigma f_0^a
 \end{aligned} \tag{6.8.16}$$

Since the total number remains constant,  $\mu = 0$ . Therefore,

$$\begin{aligned}
 dm &= \sum_k (dn_{k\uparrow} - dn_{k\downarrow}) = -\frac{1}{2} \sum_k \rho (d\epsilon_{k\uparrow} - d\epsilon_{k\downarrow}) = -\frac{1}{2} \sum_k \rho (-dB + 2f_0^a (dn_{k\uparrow} - dn_{k\downarrow})) \\
 &= dB\rho(0) - dm\rho(0)f_0^a \approx dB\rho(0) - \rho(0)f_0^a B\rho(0) \quad [\text{substitute } dm \text{ back into itself}] \\
 \implies \frac{dm}{dB} &= \rho(0) (1 - \rho(0)f_0^a) \implies \chi_{imp}^s = \rho(0)_{imp} - \rho(0)f_0^a
 \end{aligned} \tag{6.8.17}$$

### 6.8.4 Wilson ratio

The Wilson ratio for the impurity is defined as

$$R = \frac{\chi_{imp}^s}{\frac{C_{imp}}{T}} \tag{6.8.18}$$

From eq. (6.8.5), we have  $f_0^s = -f_0^a$ , which, when combined with eq. (6.8.14), gives

$$\chi_{imp}^s = 2\rho(0)_{imp} \tag{6.8.19}$$

The Wilson ratio becomes

$$R = \frac{2\rho(0)_{imp}}{\rho(0)_{imp}} = 2 \tag{6.8.20}$$

## 6.9 Luttinger's and Friedel's sum rules

The subsequent discussions are for the first quadrant where  $U^* = 0$  and  $J^* > K^*$ . At high temperatures, we see that the impurity susceptibility attains the value of

$$\frac{1}{8k_B T} \tag{6.9.1}$$

which implies that the impurity behaves as a free orbital in this limit, having no coupling with the bath. We can write down the following effective Hamiltonian for such a limit:

$$\mathcal{H}_{\text{high-T}} = \tilde{\epsilon}_d \hat{n}_d + \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} \tag{6.9.2}$$

Since the impurity is decoupled from the bath, we can immediately write down the Hamiltonian just for the impurity:

$$\mathcal{H}_{\text{high-T, imp}} = \tilde{\epsilon}_d \hat{n}_d \tag{6.9.3}$$

We consider the resonant-level model:

$$\mathcal{H}_{\text{res}} = \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \epsilon_d \hat{n}_d + \sum_{k\sigma} \left( V_k c_{k\sigma}^\dagger c_{d\sigma} + \text{h.c.} \right) \tag{6.9.4}$$

The total Green's function is

$$G(z) = \frac{1}{z - \mathcal{H}_{\text{res}}} \tag{6.9.5}$$

The impurity diagonal Green's function is

$$G_{dd}(z) = \frac{1}{z - \epsilon_d - \Sigma_d(z)}, \quad G_d(z) = G_{dd} |d\rangle \langle d| \tag{6.9.6}$$

where  $\Sigma_d(z)$  is in general complex and is zero at the free orbital fixed point. The conduction electron Green's function is

$$G_{kk}(z) = G_k^0(z) + \left[ G_k^0(z) V_k \right]^2 G_{dd}(z), \quad G_c(z) \equiv \sum_k |k\rangle \langle k| G_{kk}(z), \quad G_{c0}(z) \equiv \sum_k G_{kk}^0(z) |k\rangle \langle k| \tag{6.9.7}$$



The total Green's function can be written as

$$\begin{aligned}
 G(z) &= \left( \sum_k |k\rangle \langle k| + |d\rangle \langle d| \right) G \left( \sum_k |k\rangle \langle k| + |d\rangle \langle d| \right) \\
 &= \sum_k |k\rangle \langle k| G_{kk}(z) + G_{dd}(z) |d\rangle \langle d| + \text{off-diagonal terms} \\
 &= G_c(z) + G_d(z) + \text{off-diagonal terms}
 \end{aligned} \tag{6.9.8}$$

The total number of electrons is given by

$$\begin{aligned}
 N &= \oint \frac{dz}{2\pi i} n_F(z) \text{Tr} [G(z)] \\
 &= \oint \frac{dz}{2\pi i} n_F(z) \text{Tr} [G_d(z) + G_c(z)]
 \end{aligned} \tag{6.9.9}$$

The contour  $\Gamma$  counts all the singularities of  $\text{Tr} G(z)$ , and thus encloses only the real axis of the complex plane (since  $G(z)$  comes from a Hermitian matrix  $\mathcal{H}_{\text{res}}$ , all its singularities are real). At this point, we can use an identity:

$$\begin{aligned}
 \text{Tr} [G_d(z)] &= \text{Tr} \left[ \frac{|d\rangle \langle d|}{z - \epsilon_d - \Sigma_d(z)} \right] = \text{Tr} \left[ \frac{|d\rangle \langle d|}{z - \epsilon_d - \Sigma_d(z)} \frac{\partial(z - \epsilon_d)}{\partial z} \right] = \text{Tr} \left[ |d\rangle \langle d| G_{dd} \frac{\partial \{G_{dd}^{-1}(z) + \Sigma_d(z)\}}{\partial z} \right] \\
 &= \text{Tr} \left[ G_d(z) \frac{\partial G_d^{-1}(z)}{\partial z} \right] + \text{Tr} \left[ G_d(z) \frac{\partial \Sigma_d(z)}{\partial z} \right] = \frac{\partial}{\partial z} [\ln \text{Det} G_d^{-1}(z)] + \text{Tr} \left[ G_d(z) \frac{\partial \Sigma_d(z)}{\partial z} \right]
 \end{aligned} \tag{6.9.10}$$

In the last step, we converted the trace to a determinant using

$$\text{Tr} \left[ A \frac{\partial A^{-1}}{\partial z} \right] = \frac{\partial}{\partial z} \text{Tr} \ln A^{-1} = \frac{\partial}{\partial z} \sum_i \ln \lambda_i = \frac{\partial}{\partial z} \ln \prod_i \lambda_i = \frac{\partial}{\partial z} \ln \text{Det} A^{-1} \tag{6.9.11}$$

where  $\lambda_i$  are the eigenvalues of  $A^{-1}$ . Substituting  $\text{Tr} [G_d(z)]$  into the total number of particles gives

$$N = \oint \frac{dz}{2\pi i} n_F(z) \left[ \frac{\partial}{\partial z} \ln \text{Det} \{G_d^{-1}(z)\} + \text{Tr} \left( G_d(z) \frac{\partial}{\partial z} \Sigma_d(z) \right) + \text{Tr} G_c(z) \right] \tag{6.9.12}$$

The conduction electron part can also be simplified:

$$\text{Tr} G_c(z) = \text{Tr} \left[ G_{c0}(z) + \sum_k \left\{ G_k^0(z) V_k \right\}^2 G_{dd}(z) |k\rangle \langle k| \right] = \text{Tr} [G_{c0}(z)] + \sum_k \left[ G_k^0(z) V_k \right]^2 G_{dd}(z) \tag{6.9.13}$$

Since  $G_{c0}^{-1}(z) = z - \sum_k \epsilon_k \hat{n}_k$ , we can write  $\text{Tr} [G_{c0}(z)] = \text{Tr} \left[ G_{c0}(z) \frac{\partial}{\partial z} G_{c0}^{-1} \right]$  and hence

$$\text{Tr} G_c(z) = \frac{\partial}{\partial z} [\ln \text{Det} G_{c0}^{-1}(z)] + \sum_k \left[ G_k^0(z) V_k \right]^2 G_{dd}(z) \tag{6.9.14}$$

Updating the total particles with this leads to

$$N = \oint \frac{dz}{2\pi i} n_F(z) \left[ \frac{\partial}{\partial z} \ln \text{Det} \{G_d^{-1}(z)\} + \frac{\partial}{\partial z} \ln \text{Det} \{G_{c0}^{-1}(z)\} + \text{Tr} \left( G_d(z) \frac{\partial}{\partial z} \Sigma_d(z) \right) + \sum_k \left( V_k G_k^0 \right)^2 G_{dd}(z) \right] \tag{6.9.15}$$

For the resonant-level model, we have

$$\Sigma_d = \sum_k V_k^2 G_k^0 = \sum_k \frac{V_k^2}{z - \epsilon_k} \tag{6.9.16}$$

such that

$$\text{Tr} \left( G_d(z) \frac{\partial}{\partial z} \Sigma_d(z) \right) = -G_{dd}(z) \sum_k \left( V_k G_k^0 \right)^2 \quad (6.9.17)$$

which allows us to write

$$N = \oint \frac{dz}{2\pi i} n_F(z) \left[ \frac{\partial}{\partial z} \ln \text{Det} \left\{ G_d^{-1}(z) \right\} + \frac{\partial}{\partial z} \ln \text{Det} \left\{ G_{c0}^{-1}(z) \right\} \right] \quad (6.9.18)$$

At  $T = 0$ ,  $n_F$  is defined as 1 below the FS,  $\frac{1}{2}$  at the FS and 0 above it.

$$N = \left[ \oint_{\Gamma_{<}} + \frac{1}{2} \oint_{\Gamma_0} \right] \frac{dz}{2\pi i} \left[ \frac{\partial}{\partial z} \ln \text{Det} \left\{ G_d^{-1}(z) \right\} + \frac{\partial}{\partial z} \ln \text{Det} \left\{ G_{c0}^{-1}(z) \right\} \right] \quad (6.9.19)$$

Following Seki and Yunoki, we can define a winding number for a Green's function  $G(z)$ :

$$n_{\text{Det } G^{-1}(C)} = \oint_C \frac{dz}{2\pi i} \frac{\partial \ln \text{Det } G^{-1}(z)}{\partial z} = \oint_{\text{Det } G^{-1}(C)} \frac{d \text{Det } G^{-1}}{\text{Det } G^{-1}} \quad (6.9.20)$$

Since  $n_{\text{Det } G^{-1}(C)}$  counts the number of times the curve  $\text{Det } G^{-1}(C)$  winds around the origin, it is integer-valued and topological. Seki and Yunoki also show that this number is given by

$$n_{\text{Det } G^{-1}(C)} = P_{\text{Det } G}(C) - Z_{\text{Det } G}(C) \quad (6.9.21)$$

where  $P_{f(z)}(C)$  is the number of poles of  $f(z)$  enclosed by the contour  $C$ , and  $Z$  is the corresponding number of zeros. The total number of particles in the resonant level model can thus be written as

$$N = P_{\text{Det } G_d}(\Gamma_{<}) - Z_{\text{Det } G_d}(\Gamma_{<}) + \frac{1}{2} \left[ P_{\text{Det } G_d}(\Gamma_0) - Z_{\text{Det } G_d}(\Gamma_0) \right] + P_{\text{Det } G_{c0}}(\Gamma_{<}) - Z_{\text{Det } G_{c0}}(\Gamma_{<}) \\ + \frac{1}{2} \left[ P_{\text{Det } G_{c0}}(\Gamma_0) - Z_{\text{Det } G_{c0}}(\Gamma_0) \right] \quad (6.9.22)$$

The average number of particles can thus be expressed purely in terms of the number of poles and zeros of the impurity and the conduction electron Green's functions. As shown by Seki and Yunoki, the second line gives the Luttinger volume  $V_L$ :

$$N = P_{\text{Det } G_d}(\Gamma_{<}) - Z_{\text{Det } G_d}(\Gamma_{<}) + \frac{1}{2} \left[ P_{\text{Det } G_d}(\Gamma_0) - Z_{\text{Det } G_d}(\Gamma_0) \right] + V_L \quad (6.9.23)$$

If we start from a non-interacting model ( $V_k = 0$ ), we can write

$$N = \mathcal{N}_{imp}^0 + V_L^0 \quad (6.9.24)$$

where  $\mathcal{N}_{imp}^0$  is simply the number of singularities of  $G_d$  on the real axis, for the non-interacting case. We now turn up the interaction  $V_k$ , keeping the total number of particles conserved at  $N$ . With a non-zero  $V_k$ , the impurity self-energy can be written (assuming a constant density of states) as

$$\Sigma_d(z) = \Sigma_d^{\text{real}}(z) - i\Delta \quad (6.9.25)$$

so that the impurity Greens function becomes

$$G_d(z) = \frac{1}{z - \epsilon_d - \Sigma_d^{\text{real}}(z) + i\Delta} \quad (6.9.26)$$

We can see that the presence of an imaginary part lifts the pole of  $G_d(z)$  off the real axis, and since the contour  $\Gamma_0$  encloses only the real axis, this will count as a loss in the number of poles of  $G_d(z)$ . Also, if we specialize to the case where the renormalized impurity site energy  $\epsilon_d^* = \epsilon_d + \Sigma_d^{\text{real}} = 0$ , this loss will happen at the Fermi surface, and will hence be multiplied by a factor of half. We can therefore write

$$N = \mathcal{N}_{imp} + V_L = \mathcal{N}_{imp}^0 - \frac{1}{2} + V_L \implies V_L = V_L^0 + \frac{1}{2} \quad (6.9.27)$$

../figures/luttinger\_top\_change.png

If we take into account the spin-degeneracy and redefine  $V_L$  to mean the Luttinger volume for both momentum and spin degrees of freedom, we get

$$V_L = V_L^0 + 1 \quad (6.9.28)$$

This is a specific case of the more general result for Kondo lattices obtained by Oshikawa using flux-insertion arguments in [42]. One can now ask what happens to this result once we also incorporate the spin-exchange interaction  $J\vec{S}_d \cdot \vec{s}$ ; we can expect that it will complicate the self-energy of the impurity. It cannot, however, preclude the loss of the real pole, nor can it create a new singularity - to do so would require the self-energy to diverge, and we are working with finite systems here. This suggests that the eq. (6.9.28) would still hold.

We have also not accounted for the RG flow from the local moment fixed point to the strong-coupling fixed point. The local moment fixed point is characterized by a decoupled quantum top:

$$\mathcal{H}_{\text{LM}} = \epsilon_d \hat{n}_d + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \quad (6.9.29)$$

It can be shown that the single-particle Green's function for this effective Hamiltonian is similar to the one at the free-orbital fixed point. We will use the equation of motion technique to solve for the Green's function. The time-domain retarded Green's function is defined as

$$G_{d\sigma}(t, t') = -i\theta(t - t') \left\langle \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger(t') \right\} \right\rangle \quad (6.9.30)$$

Since the Hamiltonian is time-translation invariant, we can drop one of the instants:

$$G_{d\sigma}(t, 0) = -i\theta(t) \left\langle \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle \quad (6.9.31)$$

The time derivative is

$$\begin{aligned} \partial_t G_{d\sigma} &= -i \left[ \partial_t \theta(t) \left\langle \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle + \theta(t) \partial_t \left\langle \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle \right] \\ &= -i \left[ \delta(t) \left\langle \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle + \theta(t) \left\langle \left\{ \partial_t c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle \right] = -i\delta(t) - i\theta(t) \left\langle \left\{ \partial_t c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle \end{aligned} \quad (6.9.32)$$

From the Heisenberg equations of motion, we get

$$i\partial_t c_{d\sigma}(t) = [c_{d\sigma}(t), \mathcal{H}_{\text{LM}}(t)] = [\epsilon_d + U \hat{n}_{d\bar{\sigma}}(t)] c_{d\sigma}(t) \quad (6.9.33)$$

Substituting this into the time-derivative gives

$$\partial_t G_{d\sigma} = -i\delta(t) - i\theta(t) \left\langle \left\{ -i [\epsilon_d + U \hat{n}_{d\bar{\sigma}}(t)] c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle = -i\delta(t) - i\epsilon_d G_{d\sigma} - U\theta(t) \left\langle \hat{n}_{d\bar{\sigma}}(t) \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle \quad (6.9.34)$$

We define another Greens function

$$G' = -i\theta(t) \left\langle \hat{n}_{d\bar{\sigma}}(t) \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle \quad (6.9.35)$$

which satisfies the equation of motion

$$\partial_t G' = -i\delta(t) - i\theta(t) \left\langle \left\{ \partial_t \hat{n}_{d\bar{\sigma}}(t) c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle - i\theta(t) \left\langle \left\{ \hat{n}_{d\bar{\sigma}}(t) \partial_t c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle \quad (6.9.36)$$

The second term vanishes because  $[\hat{n}_{d\bar{\sigma}}, \mathcal{H}_{LM}] = 0$  and hence  $\partial_t \hat{n}_{d\bar{\sigma}} = 0$ . Also,

$$\hat{n}_{d\bar{\sigma}}(t) \partial_t c_{d\sigma}(t) = -i\hat{n}_{d\bar{\sigma}}(t) [\epsilon_d + U \hat{n}_{d\bar{\sigma}}(t)] c_{d\sigma}(t) = -i [\epsilon_d + U] \hat{n}_{d\bar{\sigma}}(t) c_{d\sigma}(t) \quad (6.9.37)$$

Therefore,

$$\partial_t G' = -i\delta(t) \langle \hat{n}_{d\bar{\sigma}}(0) \rangle - [\epsilon_d + U] \theta(t) \left\langle \left\{ \hat{n}_{d\bar{\sigma}}(t) c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle = -i\delta(t) - i(\epsilon_d + U) G' \quad (6.9.38)$$

Changing all quantities to frequency-domain:

$$\begin{aligned} G'(t) &= \int_{-\infty}^{\infty} d\omega e^{-i\omega t} G'(\omega) \\ \partial_t G'(t) &= - \int_{-\infty}^{\infty} d\omega i\omega e^{-i\omega t} G'(\omega) \\ \delta(t) &= \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \end{aligned} \quad (6.9.39)$$

Substituting these forms in the equation and comparing the coefficients of  $e^{i\omega t}$  gives

$$\omega G'(\omega) = \langle \hat{n}_{d\bar{\sigma}}(0) \rangle + (\epsilon_d + U) G'(\omega) \implies G'(\omega) = \frac{\langle \hat{n}_{d\bar{\sigma}}(0) \rangle}{\omega - \epsilon_d - U} \quad (6.9.40)$$

The equation of motion  $G_{d\sigma}$  can now be solved

$$\begin{aligned} \partial_t G_{d\sigma}(t) &= -i\delta(t) - i\epsilon_d G_{d\sigma}(t) - iU G'_{d\sigma}(t) \implies \omega G_{d\sigma}(\omega) = 1 + \epsilon_d G_{d\sigma}(\omega) + U \frac{\langle \hat{n}_{d\bar{\sigma}}(0) \rangle}{\omega - \epsilon_d - U} \\ \implies G_{d\sigma}(\omega) &= \frac{1}{\omega - \epsilon_d} + \frac{U \langle \hat{n}_{d\bar{\sigma}}(0) \rangle}{(\omega - \epsilon_d)(\omega - \epsilon_d - U)} \end{aligned} \quad (6.9.41)$$

For a particle-hole symmetric system, we can substitute  $\epsilon_d = -|\epsilon_d|$  and  $\epsilon_d + U = |\epsilon_d|$ .

$$G_{d\sigma}(\omega) = \frac{1}{\omega + |\epsilon_d|} + \frac{U \langle \hat{n}_{d\bar{\sigma}}(0) \rangle}{(\omega + |\epsilon_d|)(\omega - |\epsilon_d|)} \quad (6.9.42)$$

which reveals two poles at  $\pm|\epsilon_d|$ , one above and one below the Fermi surface. Since the RHS of eq. (6.9.23) counts the number of poles on or below the FS, we will still count one pole for  $G_{d\sigma}$ . Thus, this Green's function is topological similar to the free-orbital one at  $T = 0$ .

The scattering phase shift suffered by the conduction electrons at the Fermi surface, off the impurity, can be calculated from the impurity occupancy, using the Friedel sum rule. From the ground state wavefunction, we can calculate the average number of particles on the impurity:

$$\langle n_d \rangle = \langle \Psi | \sum_{\sigma} \hat{n}_{d\sigma} | \Psi \rangle_1 \quad (6.9.43)$$

$|\Psi\rangle_1$  is the lower energy state in eq. (5.11.5). Performing the inner product gives

$$\langle n_d \rangle = \left(c_s^-\right)^2 + \left(c_c^-\right)^2 = 1 \quad (6.9.44)$$

The phase shift is thus

$$\frac{1}{\pi} \sum_{\sigma} \delta_{\sigma}(0) = \langle n_d \rangle \implies \delta_{\sigma}(0) = \frac{\pi}{2} \quad (6.9.45)$$

There we used  $\delta_{\uparrow} = \delta_{\downarrow}$  because the model is SU(2)-symmetric. This line of arguments was first presented for the Kondo model in [25].

The change in Luttinger's number also allows us to calculate the Wilson ratio of the system, from eq. (2.7.7).

$$R = 1 + \sin^2 \left( \frac{\pi}{2} \Delta N_L \right) = 1 + \sin^2 \frac{\pi}{2} = 2 \quad (6.9.46)$$

## 6.10 Reverse RG analysis

The goal here is to chart the journey starting from the IR fixed point towards the UV regime, by following one particular wavefunction. We will start with a very simple IR ground state wavefunction, and then go back towards the UV ground state by applying the inverse unitary operator  $U^\dagger$ :

$$\begin{aligned} U : \underbrace{|1, 2, \dots, N\rangle}_{\text{UV ground state}} &\rightarrow |1, 2, \dots, N-1\rangle |N\rangle \rightarrow \dots \rightarrow \underbrace{|1, 2, \dots, N^*\rangle |N^*+1\rangle \dots |N\rangle}_{\text{IR ground state}} \\ U^\dagger : \underbrace{|1, 2, \dots, N^*\rangle |N^*+1\rangle \dots |N\rangle}_{\text{IR ground state}} &\rightarrow |1, 2, \dots, N^*+1\rangle |N^*+2\rangle \dots |N\rangle \rightarrow \dots \rightarrow \underbrace{|1, 2, \dots, N\rangle}_{\text{UV ground state}} \end{aligned}$$

The first process is the forward RG which we used to obtain the scaling equations. The second process is the reverse RG which we will undertake now. In general, we start with an IR wavefunction that consists a certain number of momentum states  $n_1$  still entangled with the impurity, and the remaining momentum states  $n_2$  disentangled from the impurity. The former are said to be part of the emergent Kondo cloud, while the latter are said to be part of the integrals of motion (IOMs) and appear in direct product with the cloud+impurity system in the ground state wavefunction. Each momentum state is tagged with two conduction bath levels, one above the Fermi surface and one below. These will be represented as  $k, \pm$ . If we represent the emergent cloud momentum states as  $\{k_i\}$  and the IOM states as  $\{q_i\}$ , the ground state wavefunction can be written as

$$|\Psi\rangle_0 = \left( \otimes_{i=1}^{n_2} |q_i, -, \uparrow\rangle |q_i, -, \downarrow\rangle \right) |\Phi\rangle_{\text{cloud}} \left( \otimes_{i=1}^{n_1} |q_i, +, \uparrow\rangle |q_i, +, \downarrow\rangle \right) \quad (6.10.1)$$

Throughout, we have assumed that the IOMs below the Fermi surface are occupied while those above are unoccupied. This means:

$$|\Psi\rangle_0 = \left( \otimes_{i=1}^{n_2} |\hat{n}_{q_i, -, \uparrow} = 1\rangle |\hat{n}_{q_i, -, \downarrow} = 1\rangle \right) |\Phi\rangle_{\text{cloud}} \left( \otimes_{i=1}^{n_1} |\hat{n}_{q_i, +, \uparrow} = 0\rangle |\hat{n}_{q_i, +, \downarrow} = 0\rangle \right) \quad (6.10.2)$$

$|\Phi\rangle_{\text{cloud}}$  will be obtained by diagonalising a small system of  $n_1$  conduction bath  $k$  states. This completes the construction of the IR ground state  $|\Psi\rangle_0$ . The algorithm of reverse RG then involves applying unitary transformations on this IR wavefunction; the unitary transformations will be the inverse of those that were applied during the forward RG algorithm. Since the forwards RG transformations decoupled  $k$  states and transformed them into the IOMs, the inverse transformations will take the momentum states in the IOMs and re-entangle them with the impurity+cloud system, one at a time. This is shown in fig. 6.7.

The next step is to write down the unitaries that will take us from the IR ground state to the UV ground state. In the forward RG, we used the following unitary for decoupling the shell  $\epsilon_q$  and spin  $\beta$  is

$$U_{q\beta} = \frac{1}{\sqrt{2}} \left[ 1 + \eta_{0\beta} + \eta_{1\beta}^\dagger \right]. \quad (6.10.3)$$

Here, the subscripts 0 and 1 indicate it decouples an electron above and below the Fermi surface respectively. The inverse transformation for re-entangling  $q\beta$  is

$$U_{q\beta}^\dagger = \frac{1}{\sqrt{2}} \left[ 1 + \eta_{0\beta}^\dagger + \eta_{1\beta} \right]. \quad (6.10.4)$$

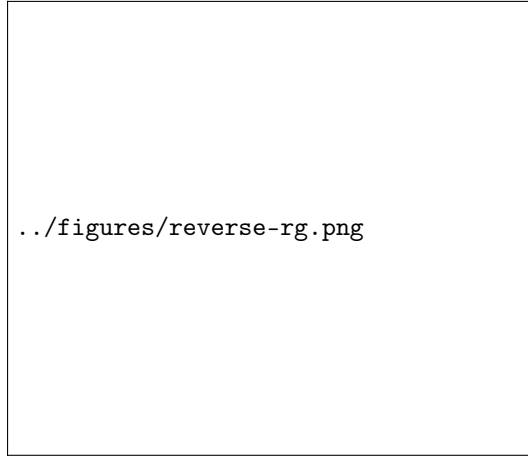


Figure 6.7: We start with a Hamiltonian with an impurity site (red) coupled with two conduction electrons (dark green), with four other decoupled electrons (bright green). The dotted rectangle represents the emergent window  $(-\Lambda_j, \Lambda_j)$  at each step; the electrons inside that rectangle are still entangled with the impurity, while the ones inside have been decoupled. The next step of reverse RG involves applying the inverse transformation on the Hamiltonian, which will couple two more electrons from the IOMS (hence four dark green circles in the second step), leading to an enlargement of the emergent window. The unitary varies for each step, hence the notation  $U_j$ .

In the  $U > 0$  regime, the  $\eta$ s are given by

$$\begin{aligned}\eta_{0\beta}^\dagger &= V \left[ \frac{1}{d_0} \left( 1 - \hat{n}_{d\bar{\beta}} \right) + \frac{1}{d_1} \hat{n}_{d\bar{\beta}} \right] c_{q\beta}^\dagger c_{d\beta} + \frac{1}{d_2} \frac{J}{2} \sum_k \left( S_d^z \beta c_{q\beta}^\dagger c_{k\beta} + c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\bar{\beta}} \right), \\ \eta_{1\beta} &= V \left[ \frac{1}{d_1} \left( 1 - \hat{n}_{d\bar{\beta}} \right) + \frac{1}{d_0} \hat{n}_{d\bar{\beta}} \right] c_{d\beta}^\dagger c_{q\beta} + \frac{1}{d_2} \frac{J}{2} \sum_k \left( S_d^z \beta c_{k\beta}^\dagger c_{q\beta} + c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \right); \end{aligned} \quad (6.10.5)$$

since  $K$  is irrelevant, we have set  $K = 0$  here. The denominators have already been defined in eq. (5.9.5).

$$d_0 = \omega - \frac{D}{2} - \frac{U}{2} + \frac{K}{4}, \quad d_1 = \omega - \frac{D}{2} + \frac{U}{2} + \frac{J}{4}, \quad d_2 = \omega - \frac{D}{2} + \frac{J}{4}, \quad d_3 = \omega - \frac{D}{2} + \frac{K}{4} \quad (6.10.6)$$

The wavefunction after reversing one step of the RG will thus be

$$|\Psi\rangle_1 = U_{q\uparrow}^\dagger U_{q\downarrow}^\dagger |\Psi\rangle_0 \quad (6.10.7)$$

Here,  $q$  is the first momentum state immediately outside the emergent cloud. Re-entangling further momentum states using their respective unitaries lead to the sequence of wavefunctions  $|\Psi\rangle_2, |\Psi\rangle_3$  and so on.

The results of the reverse RG study are depicted in the following plots. We have used two types of quantities in the process - mutual information and correlation functions. The mutual information between two subsystems  $A$  and  $B$  in a wavefunction with many subsystems is defined as

$$I(A : B) = S_A + S_B - S_{AB} \quad (6.10.8)$$

where  $S_{ij..q}$  is the von-Neumann entropy of the reduced density matrix obtained after tracing out all degrees of freedom except those in the subscript of  $S$ .

The mutual information between two electrons inside the entangled cloud increases as we go towards the IR fixed point. This can be understood in the following manner; as the wavefunction flows towards a smaller sized emergent cloud, the entanglement between those electrons gets distilled out.

We have also computed some correlation functions. All of them increase towards the IR fixed point. The increase in the correlation function  $\langle \hat{n}_{k_1\uparrow} \hat{n}_{k_2\downarrow} \rangle$  arises from the crystallization of the spin singlet at the fixed point. The increase in the correlation function  $\langle \hat{n}_{k\uparrow} \hat{n}_{k\downarrow} \rangle$  arises from the charge triplet content of the wavefunction, showing the increase of the charge contribution on the momenta. The increase in the off-diagonal correlation function



Figure 6.8: *Left*: Mutual information between two conduction electrons inside the cloud. *Right*: Mutual information between a conduction electron inside the cloud and an impurity electron. Both the measures increase towards the strong-coupling fixed point, because of the distillation of the Kondo cloud brought about by the RG flow.

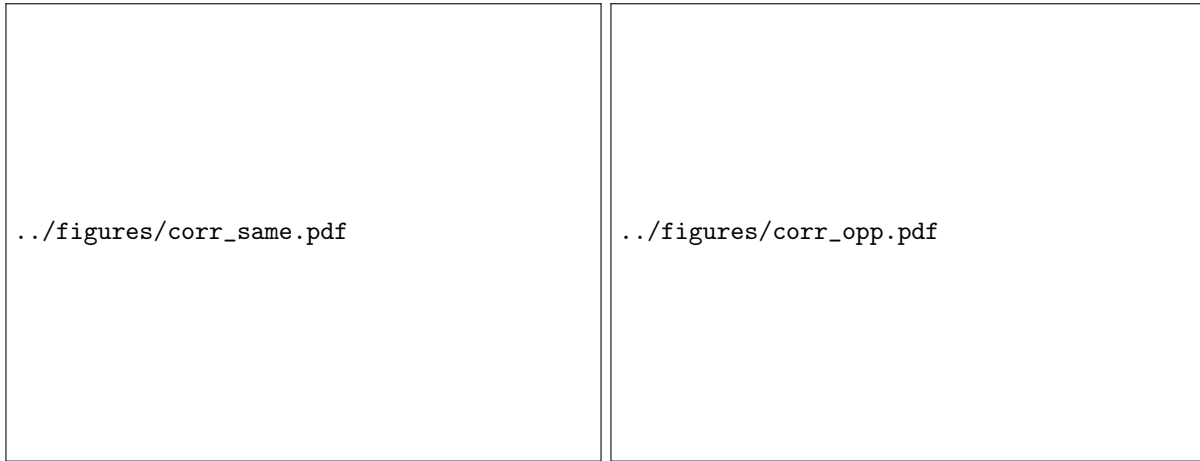


Figure 6.9: Increase in the diagonal correlation functions between cloud electrons under RG flow towards the strong-coupling fixed point. This is consistent with the Fermi liquid pieces generated in the  $k$ -space effective Hamiltonian of the Kondo cloud.

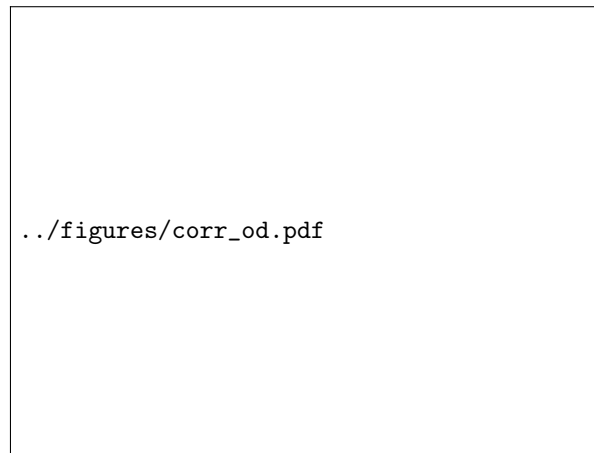


Figure 6.10: Growth of the off-diagonal correlation function between Kondo cloud electrons towards the strong-coupling fixed point. This is the direct cause of the screening of the impurity spin, and is a reflection of the off-diagonal two-particle scattering terms in the  $k$ -space effective Hamiltonian of the Kondo cloud.

$\langle c_{k\uparrow}^\dagger c_{k'\downarrow} c_{q\downarrow}^\dagger c_{q'\uparrow} \rangle$  shows that there is a large and non-trivial interaction between the electrons of the cloud that is being mediated by the impurity electron. This interaction is not of the Fermi liquid type, but instead was obtained in the effective Hamiltonian for the Kondo cloud.



## Chapter 7

# Conclusions and Future Directions

In this work, we have seen that the fate of the SIAM at low temperatures is a growth in the spin, charge and hybridisation couplings  $J, K$  and  $V$ . This confirms the NRG and Bethe ansatz result that the low energy behavior is that of a screened impurity. We stress that the spin or the charge exchange coupling,  $J$  or  $K$ , is necessary to screen the corresponding degree of freedom on the impurity. The ground state wavefunction for the low energy theory is primarily a spin-singlet with some charge-triplet content in the spin-Kondo regime. In the charge-Kondo regime, we find a charge-singlet instead. The susceptibility is seen to increase as we go to lower temperatures, signaling increased spin-flip scattering and providing a justification for the increase in resistivity after the Kondo temperature  $T_K$ . At high temperatures the susceptibility saturates to  $\frac{1}{8}$ , mimicking a four-fold degenerate object because at high temperatures, the impurity energy scales become blurred. We encountered a maximum in the susceptibility vs temperature plot which is not present in NRG or Bethe Ansatz plots, and we believe it can be attributed to the approximation made in working with a zero mode Hamiltonian. We also calculated the specific heat, and it shows two peaks.

We also obtain a Hamiltonian for the Kondo cloud (the set of electrons which screen the impurity) - it has a Fermi liquid number diagonal term as well as an off-diagonal non-Fermi liquid piece. It is this off-diagonal piece that is responsible for the strong entanglement between the impurity and the conduction electrons. This contribution is found to increase as we move towards the infrared fixed point. Higher order scattering processes will give more complicated terms in the effective Hamiltonian. We also calculate information-theoretic quantities like mutual information between impurity and conduction electrons. They show that the conduction electrons become more strongly-entangled as we move towards the infrared fixed point. They also reveal an increase in off-diagonal correlations between conduction electrons which is indicative of an increase in the off-diagonal scattering content in the effective Hamiltonian of the Kondo cloud. We also find the value of the zero-temperature Wilson ratio to be 2 in the Kondo regime. Closely related to this is the result that the Luttinger's volume at the fixed point accommodates the impurity site into the Fermi volume such that Luttinger's count increases by 1 compared to the value at the free-orbital or local moment fixed points. The renormalization of the impurity spectral across the RG shows the emergence of the central resonance at the strong-coupling fixed point.

This work still leaves some problems untouched. Some new questions and interesting prospects have also emerged. We discuss them now.

- Can we obtain an analytical expression for the finite temperature Wilson ratio? The zero temperature value was obtained using low temperature approximations, so a finite temperature calculation would need to be non-perturbative. In other words, the full effect of the conduction bath will most probably come into play.
- The spectral function of the impurity is another interesting quantity to explore. It is not yet completely certain which parts of the effective Hamiltonian for the cloud lead to which features of the spectral function. It would be interesting to check whether the Fermi liquid part gives the central peak and the non-Fermi liquid the side humps, or something else altogether. We also intend to explore the bath spectral function and its variation under the RG.
- In Chapter 4, we find that the URG renormalization in Hamiltonian has a form similar to that of URG - a generalized double-bracket form. This suggests that URG might have uses in linear algebra as well. It is well-known that transformations of the double-bracket form are unitary and can be used in minimization and sorting problems [14]. It has also been shown that the unitary flows correspond to motion along a geodesic if

a suitable manifold is defined. This suggests that we can look for a quantity which is minimized by URG in the journey towards the fixed point and see if it can be used to provide a faster and more robust algorithm for optimization problems.

- One can also look into the lattice versions of these models - the Kondo lattice and the Anderson lattice problems which involve two interacting bands - one for the impurity and the other for the conduction electrons [43]. Since there is a macroscopic number of impurity electrons, such a model shows phase transitions. One big project for the future can be to look into such models, map the phase diagram and search for superconducting phases or non-Fermi liquid phases.
- We have seen that the zero-mode of the low-energy effective Hamiltonian is essentially a two-site Anderson model (a.k.a Anderson dimer), which can be solved exactly. An interesting endeavor in this context could be to see if there is a unitary transformation that converts the Anderson dimer to a two-site Hubbard model (Hubbard dimer). The point of this exercise would be to shed some light on the inner workings of DMFT. The imposition of the self-consistency requirement in DMFT introduces a translational invariance into the Anderson model and converts it into the Hubbard model. If we could figure out a transformation that does the same (albeit, between dimers and not the full-fledged models), it might lead to new insights into DMFT). This might allow us to see a metal-insulator phase transition. With the single-impurity Anderson model, it is not possible to see such a transition because the impurity can always tunnel into the conduction bath through the origin of the lattice. The central peak of the spectral disappears only at  $U \rightarrow \infty$ . However, if one introduces correlation into the bath, the impurity electron will find it harder to disperse, leading to the possibility that we end up with an insulator at some critical value of the onsite repulsion. An interesting project could be to redo the URG of the SIAM with more complicated baths (by inserting non-trivial self-energies into the bath), and see if the phase-diagram changes. As it stands now, there is no provision for a phase transition in the SIAM because there is only one stable phase. If the inclusion of a non-trivial bath brings about a phase-transition in the impurity phase diagram, that is essentially a mirror of the phase transition happening in the Hubbard model. The importance of this potential discovery is that the self-energies that we wish to insert into the bath have been obtained from a URG treatment of the Hubbard model, and the appearance of the phase transition would then show that URG can be used to do much of the work that DMFT does, and it provides an avenue for improving/remodeling DMFT.

# Appendices

## Appendix A

# Zero temperature Greens function in frequency domain

The impurity retarded Green's function (assuming the Hamiltonian to be time-independent, which it is) is defined as

$$G_{dd}^\sigma(t) = -i\theta(t) \left\langle \left\{ \mathcal{O}_\sigma(t), \mathcal{O}_\sigma^\dagger \right\} \right\rangle \quad (\text{A.0.1})$$

where the average  $\langle \rangle$  is over a canonical ensemble at temperature  $T$ , and  $\mathcal{O}_\sigma = c_{d\sigma} + S_d^- c_{0\bar{\sigma}} + S_d^z c_{0\sigma}$  is the excitation whose spectral function we are interested in. The excitations defined in  $\mathcal{O}$  incorporates both single-particle excitations brought about by the hybridisation as well as two-particle spin excitations brought about by the spin-exchange term. What follows is a standard calculation where we write the Green's function in the Lehmann representation. The ensemble average for an arbitrary operator  $\hat{M}$  can be written in terms of the exact eigenstates of the fixed point Hamiltonian:

$$H^* |n\rangle = E_n^* |n\rangle, \quad \langle \hat{M} \rangle \equiv \frac{1}{Z} \sum_n \langle n | \hat{M} | n \rangle e^{-\beta E_n^*} \quad (\text{A.0.2})$$

where  $Z = \sum_n e^{-\beta E_n^*}$  is the fixed point partition function and  $\{|n\rangle\}$  is the set of eigenfunctions of the fixed point Hamiltonian. We can therefore write

$$\begin{aligned} & \left\langle \left\{ \mathcal{O}_\sigma(t), \mathcal{O}_\sigma^\dagger \right\} \right\rangle \\ &= \frac{1}{Z} \sum_m e^{-\beta E_m} \langle m | \left\{ \mathcal{O}_\sigma(t), \mathcal{O}_\sigma^\dagger \right\} | m \rangle \\ &= \frac{1}{Z} \sum_{m,n} e^{-\beta E_m} \langle m | \left( \mathcal{O}_\sigma(t) | n \rangle \langle n | \mathcal{O}_\sigma^\dagger + \mathcal{O}_\sigma^\dagger | n \rangle \langle n | \mathcal{O}_\sigma(t) \right) | m \rangle \quad \left[ \sum_n |n\rangle \langle n| = 1 \right] \\ &= \frac{1}{Z} \sum_{m,n} e^{-\beta E_m} \langle m | \left( e^{iH^*t} \mathcal{O}_\sigma e^{-iH^*t} | n \rangle \langle n | \mathcal{O}_\sigma^\dagger + \mathcal{O}_\sigma^\dagger | n \rangle \langle n | e^{iH^*t} \mathcal{O}_\sigma e^{-iH^*t} \right) | m \rangle \\ &= \frac{1}{Z} \sum_{m,n} e^{-\beta E_m} \left( e^{i(E_m - E_n)t} \langle m | \mathcal{O}_\sigma | n \rangle \langle n | \mathcal{O}_\sigma^\dagger | m \rangle + e^{i(E_n - E_m)t} \langle m | \mathcal{O}_\sigma^\dagger | n \rangle \langle n | \mathcal{O}_\sigma | m \rangle \right) \\ &= \frac{1}{Z} \sum_{m,n} e^{i(E_m - E_n)t} \|\langle m | \mathcal{O}_\sigma | n \rangle\|^2 \left( e^{-\beta E_m} + e^{-\beta E_n} \right) \end{aligned} \quad (\text{A.0.3})$$

The time-domain impurity Green's function can thus be written as (this is the so-called Lehmann representation)

$$G_{dd}^\sigma = -i\theta(t) \frac{1}{Z} \sum_{m,n} e^{i(E_m - E_n)t} \|\langle m | \mathcal{O}_\sigma | n \rangle\|^2 \left( e^{-\beta E_m} + e^{-\beta E_n} \right) \quad (\text{A.0.4})$$

We are interested in the frequency domain form.

$$\begin{aligned} G_{dd}^\sigma(\omega) &= \int_{-\infty}^{\infty} dt e^{i\omega t} G_{dd}^\sigma(t) \\ &= \frac{1}{Z} \sum_{m,n} \|\langle m | \mathcal{O}_\sigma | n \rangle\|^2 \left( e^{-\beta E_m} + e^{-\beta E_n} \right) (-i) \int_{-\infty}^{\infty} dt \theta(t) e^{i(\omega + E_m - E_n)t} \end{aligned} \quad (\text{A.0.5})$$

To evaluate the time-integral, we will use the integral representation of the Heaviside function:

$$\theta(t) = \frac{1}{2\pi i} \lim_{\eta \rightarrow 0^+} \int_{-\infty}^{\infty} \frac{1}{x - i\eta} e^{ixt} dx \quad (\text{A.0.6})$$

With this definition, the integral in  $G_{dd}^\sigma(\omega)$  becomes

$$\begin{aligned} (-i) \int_{-\infty}^{\infty} dt \theta(t) e^{i(\omega + E_m - E_n)t} &= (-i) \frac{1}{2\pi i} \lim_{\eta \rightarrow 0^+} \int_{-\infty}^{\infty} dx \frac{1}{x - i\eta} \int_{-\infty}^{\infty} dt e^{i(\omega + E_m - E_n + x)t} \\ &= (-i) \frac{1}{2\pi i} \lim_{\eta \rightarrow 0^+} \int_{-\infty}^{\infty} dx \frac{1}{x - i\eta} 2\pi \delta(\omega + E_m - E_n + x) \\ &= (-i) \frac{1}{i} \lim_{\eta \rightarrow 0^+} \frac{-1}{\omega + E_m - E_n - i\eta} \\ &= \frac{1}{\omega + E_m - E_n} \end{aligned} \quad (\text{A.0.7})$$

The frequency-domain Green's function is thus

$$G_{dd}^\sigma(\omega) = \frac{1}{Z} \sum_{m,n} \|\langle m | \mathcal{O}_\sigma | n \rangle\|^2 \left( e^{-\beta E_m} + e^{-\beta E_n} \right) \frac{1}{\omega + E_m - E_n} \quad (\text{A.0.8})$$

The zero temperature Green's function is obtained by taking the limit of  $\beta \rightarrow \infty$ . In both the partition function as well as inside the summation, the only term that will survive is the exponential of the ground state energy  $E_0$ .

$$Z \equiv \sum_m e^{-\beta E_m} \implies \lim_{\beta \rightarrow \infty} Z = d_0 e^{-\beta E_0}, \quad E_0 \equiv \min \{E_n\}$$

where  $d_0$  is the degeneracy of the ground state. The Greens function then simplifies to

$$\begin{aligned} G_{dd}^\sigma(\omega, \beta \rightarrow \infty) &= \frac{1}{d_0 e^{-\beta E_0}} \sum_{m,n} \|\langle m | \mathcal{O}_\sigma | n \rangle\|^2 \left[ e^{-\beta E_m} \delta_{E_m, E_0} + e^{-\beta E_n} \delta_{E_n, E_0} \right] \frac{1}{\omega + E_m - E_n} \\ &= \frac{1}{d_0} \sum_{n,0} \left[ \|\langle 0 | \mathcal{O}_\sigma | n \rangle\|^2 \frac{1}{\omega + E_0 - E_n} + \|\langle n | \mathcal{O}_\sigma | 0 \rangle\|^2 \frac{1}{\omega - E_0 + E_n} \right] \end{aligned} \quad (\text{A.0.9})$$

The label 0 sums over all states  $|0\rangle$  with energy  $E_0$ . The spectral function is the imaginary part of this Green's function. To extract the imaginary part, we insert an infinitesimal imaginary part in the denominator:

$$G_{dd}^\sigma(\omega, \eta) = \frac{1}{d_0} \lim_{\eta \rightarrow 0^-} \sum_{n,0} \left[ \|\langle 0 | \mathcal{O}_\sigma | n \rangle\|^2 \frac{1}{\omega + E_0 - E_n + i\eta} + \|\langle n | \mathcal{O}_\sigma | 0 \rangle\|^2 \frac{1}{\omega - E_0 + E_n + i\eta} \right] \quad (\text{A.0.10})$$

The spectral function at zero temperature can then be written as

$$\begin{aligned} \mathcal{A}(\omega) &= -\frac{1}{\pi} \text{Im} [G_{dd}^\sigma(\omega)] \\ &= \frac{1}{d_0} \frac{1}{\pi} \text{Im} \left[ \lim_{\eta \rightarrow 0^-} \sum_{n,0} \left( \frac{-i\eta \|\langle 0 | \mathcal{O}_\sigma | n \rangle\|^2}{(\omega + E_0 - E_n)^2 + \eta^2} + \frac{-i\eta \|\langle n | \mathcal{O}_\sigma | 0 \rangle\|^2}{(\omega - E_0 + E_n)^2 + \eta^2} \right) \right] \\ &= \frac{1}{d_0} \frac{1}{\pi} \sum_{n,0} \left[ \|\langle 0 | \mathcal{O}_\sigma | n \rangle\|^2 \pi \delta(\omega + E_0 - E_n) + \|\langle n | \mathcal{O}_\sigma | 0 \rangle\|^2 \pi \delta(\omega - E_0 + E_n) \right] \\ &= \frac{1}{d_0} \sum_{n,0} \left[ \|\langle 0 | \mathcal{O}_\sigma | n \rangle\|^2 \delta(\omega + E_0 - E_n) + \|\langle n | \mathcal{O}_\sigma | 0 \rangle\|^2 \delta(\omega - E_0 + E_n) \right] \end{aligned} \quad (\text{A.0.11})$$

## Appendix B

# URG Equations for Generalised SIAM in Presence of Bath Correlation

We will include a local particle-hole symmetric correlation of strength  $U_b$  on the origin of the lattice:

$$\mathcal{H} = \sum_{k\sigma} \epsilon_k \tau_{k\sigma} + \epsilon_d \left( \hat{n}_{d\uparrow} - \hat{n}_{d\downarrow} \right)^2 + \sum_{k\sigma} \left( V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right) + J \vec{S}_d \cdot \vec{s} + K \vec{C}_d \cdot \vec{C} - U_b \left( \hat{n}_{0\uparrow} - \hat{n}_{0\downarrow} \right)^2 \quad (\text{B.0.1})$$

To treat this under RG, we first Fourier transform this term to  $k$ -space. In  $k$ -space, the diagonal contribution (to  $H_D$ ) coming from this term is the single-particle self-energy  $-U_b \left( \hat{n}_{q\beta} \right)^2$  which can be made particle-hole symmetric in the form:

$$-U_b \left( \tau_{q\beta} \right)^2 \quad (\text{B.0.2})$$

where  $q$  is the  $k$ -state being decoupled and  $\tau \equiv \hat{n} - 1/2$ . In the initial state  $|\Psi\rangle_i$ , we have  $\langle \hat{n}_{q\beta} \rangle = 1/2 \implies \tau_{q\beta} = 0$ , so the contribution of  $U_b$  to that state is 0. For both hole excitations  $c_{q\beta} |\Psi\rangle_i$  as well as particle excitations  $c_{q\beta}^\dagger |\Psi\rangle_i$ , the intermediate state energy lowers to  $-U_b/4$ .

The off-diagonal part is

$$-\frac{U_b}{2} \sum_{kk'\sigma} c_{k\sigma}^\dagger c_{k'\sigma} + U_b \sum_{k_1, k_2, k'_1, k'_2} c_{k_1\uparrow}^\dagger c_{k_2\uparrow} c_{k'_1\downarrow}^\dagger c_{k'_2\downarrow} \quad (\text{B.0.3})$$

We ignore the potential scattering arising from the first term.

### B.1 Renormalisation of $U_b$

$U_b$  can renormalise only via itself. The relevant renormalisation term in the particle sector is

$$U_b^2 \sum_{q\beta} \sum_{k_1, k_2, k_3, k'_1, k'_2, k'_3} c_{q\beta}^\dagger c_{k_1\beta} c_{k_3\beta}^\dagger c_{k'_1\beta} \frac{1}{\omega - H_D} c_{k'_2\beta}^\dagger c_{k'_3\beta} c_{k_2\beta}^\dagger c_{q\beta} \quad (\text{B.1.1})$$

In order to renormalise  $U_b$ , we need to contract one more pair of momenta. There are two choices. The first is by setting  $k_3 = k'_3 = q$ . The two internal states, then, are  $q\beta$  and  $q\bar{\beta}$ . As discussed above, the intermediate state energy is  $-U_b/4$ . We therefore have

$$\frac{U_b^2 n_j}{\omega - D/2 + U_b/4} \sum_{\beta} \sum_{k_1, k_2, k'_1, k'_2} c_{k_1\beta} c_{k'_1\bar{\beta}} c_{k'_2\bar{\beta}}^\dagger c_{k_2\beta}^\dagger = \frac{U_b^2 n_j}{\omega - D/2 + U_b/4} \sum_{\beta} \sum_{k_1, k_2, k'_1, k'_2} c_{k'_2\bar{\beta}}^\dagger c_{k'_1\bar{\beta}} c_{k_2\beta}^\dagger c_{k_1\beta} \quad (\text{B.1.2})$$

Another way to contract the momenta is by setting  $k'_1 = k'_2 = q$ , which gives a renormalisation of

$$\frac{U_b^2 n_j}{\omega - D/2 + U_b/4} \sum_{\beta} \sum_{k_1, k_2, k_3, k'_3} c_{k_1\beta} c_{k_3\bar{\beta}}^\dagger c_{k_3\bar{\beta}} c_{k_2\beta}^\dagger = -\frac{U_b^2 n_j}{\omega - D/2} \sum_{\beta} \sum_{k_1, k_2, k_3, k'_3} c_{k_3\bar{\beta}}^\dagger c_{k_3\bar{\beta}} c_{k_2\beta}^\dagger c_{k_1\beta} \quad (\text{B.1.3})$$

The two contributions cancel each other. The same cancellation happens in the hole sector as well.

## B.2 Renormalisation of $U$

$U_b$  does not have any new renormalisation term on account of  $U_b$ .  $U_b$  does however modify the existing RG equation for  $U$ , by shifting the denominator. The existing RG equation is

$$\Delta U = -4V^2 n_j \left( \frac{1}{\omega - \frac{D}{2} + \epsilon_d + \frac{K}{4}} - \frac{1}{\omega - \frac{D}{2} - \epsilon_d + \frac{J}{4}} \right) - n_j \left( \frac{J^2}{\omega - \frac{D}{2} + \frac{J}{4}} - \frac{K^2}{\omega - \frac{D}{2} + \frac{K}{4}} \right). \quad (\text{B.2.1})$$

On accounting for the contribution of  $U_b$  to the denominator, we get

$$\Delta U = -4V^2 n_j \left( \frac{1}{\omega - \frac{D}{2} + \frac{U_b}{4} + \epsilon_d + \frac{K}{4}} - \frac{1}{\omega - \frac{D}{2} + \frac{U_b}{4} - \epsilon_d + \frac{J}{4}} \right) - n_j \left( \frac{J^2}{\omega - \frac{D}{2} + \frac{U_b}{4} + \frac{J}{4}} - \frac{K^2}{\omega - \frac{D}{2} + \frac{U_b}{4} + \frac{K}{4}} \right). \quad (\text{B.2.2})$$

## B.3 Renormalisation of $V$

The single-particle hybridisation  $V$  renormalises through terms of  $VU_b$  and  $U_bV$  kind. The first term gives

$$\begin{aligned} & \sum_{q\beta} \sum_k U_b V c_{q\beta}^\dagger c_{k\beta} \hat{n}_{q\bar{\beta}} \frac{1}{\omega - H_D} c_{d\beta}^\dagger c_{q\beta} \\ &= n_j U_b V \sum_{k\beta} c_{k\beta} \left[ \frac{\hat{n}_{d\bar{\beta}}}{2} \left( \frac{1}{\omega_1 - E_1} + \frac{1}{\omega'_1 - E_1} \right) + \frac{1 - \hat{n}_{d\bar{\beta}}}{2} \left( \frac{1}{\omega_0 - E_0} + \frac{1}{\omega'_0 - E_0} \right) \right] c_{d\beta}^\dagger \end{aligned} \quad (\text{B.3.1})$$

$E_1$  and  $E_0$  are the intermediate state energies for  $\hat{n}_{d\bar{\beta}} = 1$  and 0 respectively.  $\omega_{1,0}$  are the quantum fluctuation scales for the corresponding initial states.  $\omega'_{1,0}$  are the fluctuation scales for the corresponding final states. The intermediate energies are  $E_1 = D/2 - U_b/4$ ,  $E_0 = D/2 - U_b/4 - U/2 - J/4$ . The fluctuation scales are  $\omega_1 = \omega - U/2 = \omega'_0$ ,  $\omega'_1 = \omega = \omega_0$ . Substituting these gives

$$-n_j U_b V \sum_{k\beta} c_{d\beta}^\dagger c_{k\beta} \left[ \frac{\hat{n}_{d\bar{\beta}}}{2} \left( \frac{1}{\omega - \frac{D}{2} - \frac{U}{2} + \frac{U_b}{4}} + \frac{1}{\omega - \frac{D}{2} + \frac{U_b}{4}} \right) + \frac{1 - \hat{n}_{d\bar{\beta}}}{2} \left( \frac{1}{\omega - \frac{D}{2} + \frac{U_b}{4} + \frac{U}{2} + \frac{J}{4}} + \frac{1}{\omega - \frac{D}{2} + \frac{U_b}{4} + \frac{J}{4}} \right) \right] \quad (\text{B.3.2})$$

The second term is of the form

$$\sum_{q\beta} \sum_k U_b V c_{q\beta}^\dagger c_{d\beta} \frac{1}{\omega - H_D} \hat{n}_{q\bar{\beta}} c_{k\beta}^\dagger c_{q\beta} \quad (\text{B.3.3})$$

and this is just the Hermitian conjugate of the previous term, so these two terms together lead to

$$\begin{aligned} & -n_j U_b V \sum_{k\beta} \left( c_{d\beta}^\dagger c_{k\beta} + \text{h.c.} \right) \left[ \frac{\hat{n}_{d\bar{\beta}}}{2} \left( \frac{1}{\omega - \frac{D}{2} - \frac{U}{2} + \frac{U_b}{4}} + \frac{1}{\omega - \frac{D}{2} + \frac{U_b}{4}} \right) \right. \\ & \quad \left. + \frac{1 - \hat{n}_{d\bar{\beta}}}{2} \left( \frac{1}{\omega - \frac{D}{2} + \frac{U_b}{4} + \frac{U}{2} + \frac{J}{4}} + \frac{1}{\omega - \frac{D}{2} + \frac{U_b}{4} - \frac{U}{2} + \frac{J}{4}} \right) \right] \end{aligned} \quad (\text{B.3.4})$$

In the hole sector, we have

$$\begin{aligned} & \sum_{q\beta} \sum_k U_b V \hat{n}_{q\bar{\beta}} c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega - H_D} c_{q\beta}^\dagger c_{d\beta} \\ &= n_j U_b V \sum_{k\beta} c_{k\beta}^\dagger \left[ \frac{\hat{n}_{d\bar{\beta}}}{2} \left( \frac{1}{\omega_1 - E_1} + \frac{1}{\omega'_1 - E_1} \right) + \frac{1 - \hat{n}_{d\bar{\beta}}}{2} \left( \frac{1}{\omega_0 - E_0} + \frac{1}{\omega'_0 - E_0} \right) \right] c_{d\beta} \end{aligned} \quad (\text{B.3.5})$$

$E_1 = D/2 - U_b/4 - U/2 - J/4$ ,  $E_0 = D/2 - U_b/4$ . The fluctuation scales are  $\omega_1 = \omega = \omega'_0$ ,  $\omega'_1 = \omega - U/2 = \omega_0$ . Substituting these gives

$$n_j U_b V \sum_{k\beta} c_{d\beta}^\dagger c_{k\beta} \left[ \frac{1 - \hat{n}_{d\bar{\beta}}}{2} \left( \frac{1}{\omega - \frac{D}{2} - \frac{U}{2} + \frac{U_b}{4}} + \frac{1}{\omega - \frac{D}{2} + \frac{U_b}{4}} \right) + \frac{\hat{n}_{d\bar{\beta}}}{2} \left( \frac{1}{\omega - \frac{D}{2} + \frac{U_b}{4} + \frac{U}{2} + \frac{J}{4}} + \frac{1}{\omega - \frac{D}{2} + \frac{U_b}{4} + \frac{J}{4}} \right) \right]$$

(B.3.6)



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