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# Unitary Renormalization Group Solution of The Single-Impurity Anderson Model

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## MS Project Report

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*by*

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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[6], 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[7] 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[8] 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 [9, 10] 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 [5]. Their calculations were again supported by later Bethe ansatz calculations by Wiegmann and Tsvelick[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 chaining.

- *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 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 ?? 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 ?? contains the URG analysis of the SIAM and its generalizations, obtained by adding spin-spin and charge-charge interactions to the SIAM. They lay out the foundation for the URG treatment on the full model with both charge and spin fluctuations. We derive the RG equations for these separate models in detail and briefly observe how the couplings flow in certain symmetric settings. Chapter ?? performs the URG on the full generalized SIAM, obtains the RG equations and writes down a low-energy effective Hamiltonian for the fixed point theory in the symmetric case. We study the flow of the

couplings and identify various fixed points. We also determine how the fixed point values behave with system size. The low-energy effective zero-mode Hamiltonian is solved and the ground state wavefunctions are obtained for both the spin and charge-dominated regimes of the model. We show that a phase transition occurs at some critical value of the couplings, between the spin singlet and the charge singlet. Chapter ?? 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 [6, 15, 16, 17] 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  $\epsilon_F$ :

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

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]

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

## 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. 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.

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

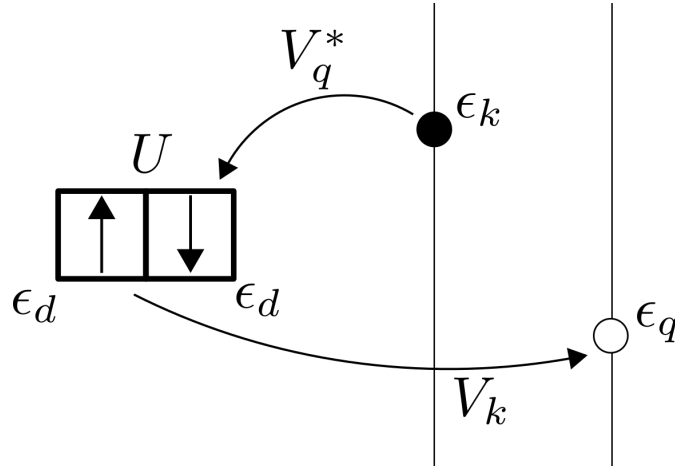


Figure 2.1: The single-impurity Anderson model Hamiltonian

The SIAM involves the following energy scales:

- the onsite energy:  $\epsilon_d$
- the onsite repulsion:  $U$
- the energy scale generated by the hybridisation:  $\Delta = \pi t^2 \sum_k \rho(\epsilon_k) \rightarrow$ . 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 dynamic of the model, we can consider the very simple atomic limit ( $V = 0$ ).

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

Since we are not interested in the Fermi sea and since there is no interaction between that and the impurity, we can choose to look only at the impurity:

$$H_{\text{atomic}} = \epsilon_d n_d + U n_{d\uparrow} n_{d\downarrow} \quad (2.3.3)$$

For a magnetic solution, we need

$$(\epsilon_{\uparrow} = \epsilon_{\downarrow}) \epsilon_d < (\epsilon_0, \epsilon_{\uparrow\downarrow}) 0, 2\epsilon_d + U \quad (2.3.4)$$

Assuming  $\epsilon_d = -|\epsilon_d|$ , this is equivalent to

$$\epsilon_d > -U \quad (2.3.5)$$

### 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.

$$H_{\text{non-int}} = \epsilon_d n_d + \sum_k \epsilon_k n_k + \sum_{k\sigma} t \left( c_{k\sigma}^\dagger c_{d\sigma} + c_{d\sigma}^\dagger c_{k\sigma} \right) \quad (2.3.6)$$

#### Green's function of impurity site:

We want to write down the *Green's function*  $G_d$  for the impurity site. In the absence of the hybridisation, this quantity is

$$G_d^0(E) = \frac{1}{E - \epsilon_d} \quad (2.3.7)$$

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  $E$ . The first is the bare Green's function. This is the situation when the impurity site electron has not scattered. Next is the case that there is an excitation with energy  $E$  ( $G_d^0(E)$ ) followed by a scattering to the conduction band at some momentum  $k$ . The probability of the scattering is  $t$ . The Greens function for creating the electron  $k$  is  $G_k^0 = \frac{1}{E - \epsilon_k}$ , and the probability of again scattering back to the impurity site is  $t$ , with the Greens function for this final excitation being  $G_d^0$ . The total Greens function contribution for this case is

$$G_d^0 \Sigma_c G_d^0, \text{ where } \Sigma_c = t \left( \sum_k G_k^0 \right) t = \sum_k \frac{t^2}{E - \epsilon_k} \quad (2.3.8)$$

Considering higher scatterings lead to terms like  $G_d^0 \Sigma_c G_d^0 \Sigma_c G_d^0$ ,  $G_d^0 \Sigma_c G_d^0 \Sigma_c G_d^0 \Sigma_c G_d^0$  and so on. The total Greens function is

$$\begin{aligned} G_d(E) &= G_d^0 + G_d^0 \Sigma_c G_d^0 + G_d^0 \Sigma_c G_d^0 \Sigma_c G_d^0 + G_d^0 \Sigma_c G_d^0 \Sigma_c G_d^0 \Sigma_c G_d^0 + \dots \\ &= G_d^0 \left[ 1 + \left( \Sigma_c G_d^0 \right)^2 + \dots \right] = G_d^0 \frac{1}{1 - \Sigma_c G_d^0} = \frac{1}{E - \epsilon_d - \Sigma_c(E)} \end{aligned} \quad (2.3.9)$$

Now,

$$\frac{1}{t^2} \Sigma_c(E) = \sum_k \frac{1}{E - \epsilon_k} = \lim_{\eta \rightarrow 0} \int_{-W}^W d\epsilon \rho(\epsilon) \frac{1}{E - \epsilon + i\eta} \quad (2.3.10)$$

$$\Rightarrow \frac{1}{t^2} \text{Re} [\Sigma_c(E)] = \int_{-W}^W d\epsilon \rho(\epsilon) \frac{1}{E - \epsilon}, \text{ and} \quad (2.3.11)$$

$$\frac{1}{t^2} \text{Im} [\Sigma_c(E)] = \int_{-W}^W d\epsilon \rho(\epsilon) (-i\pi) \delta(E - \epsilon) \quad (2.3.12)$$

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

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

Therefore,

$$G_d(E) = \frac{1}{E - \epsilon_d + i\Delta} \quad (2.3.14)$$

The difference from  $G_d^0$  can be seen by computing the density of states for both the bare and the interacting ones:

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

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

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:

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

**Phase shift of conduction electron due to scattering off the impurity:**

$T$ -matrix is defined by

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

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

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

Noting that

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

we have

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

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

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

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  $\delta(0) = \frac{\pi}{2}$ .



### Coulomb blockade

This section follows the discussion in reference [18]. A quantum dot is a set of electrons that are localized in a sufficiently small region so that their spectrum is quantized. The localization means that double occupation will come at a cost of  $U$ .

$$H_{\text{dot}} = \sum_{m\sigma} \epsilon_m n_{m\sigma} + U \frac{N(N+1)}{2} \quad (2.3.29)$$

$\epsilon_m$  are the single-particle energy levels.  $N = \sum_{m\sigma} n_{m\sigma}$  is the total number of electrons. Switching on a voltage  $V$  across the dot shifts the energy levels, creating the possibility of conduction.

$$H_{\text{dot}} = \sum_{m\sigma} (\epsilon_m - eV) n_{m\sigma} + U \frac{N(N+1)}{2} \quad (2.3.30)$$

$e$  is positive. The energy difference between  $n_N = 1$  and  $n_N = 2$  levels is

$$\Delta E = UN + \epsilon_N - eV \quad (2.3.31)$$

Tuning the voltage can make these two levels degenerate.

$$eV^* = UN + \epsilon_N \quad (2.3.32)$$

At this voltage, the two levels have the same energy and double occupancy becomes possible. Electrons can flow from the source to the sink via double occupation on the dot. For a non-interacting resonance, the conductance can be calculated as follows. The conductance for perfect transmission is given by the quantum of conductance  $G_0 = \frac{2e^2}{h}$ . In this case, the transmission is not perfect, but is modulated by the density of states of the dot at the Fermi surface. Hence,

$$G(V) = G_0 \rho(0) = \frac{2e^2}{h} \frac{\Delta^2}{(\epsilon_m - eV)^2 + \Delta^2} \quad (2.3.33)$$

The conductance is maximum whenever  $\epsilon_m = eV$ .

### 2.3.2 Total Hamiltonian: Mean field treatment

$$n_{d\uparrow} n_{d\downarrow} \approx n_{d\uparrow} \langle n_{d\downarrow} \rangle + n_{d\downarrow} \langle n_{d\uparrow} \rangle + \text{constant} \quad (2.3.34)$$

$$H \approx \sum_k \epsilon_k n_k + \sum_{\sigma} [\epsilon_d + U \langle n_{d\bar{\sigma}} \rangle] n_{d\sigma} + t \sum_{k\sigma} (c_{k\sigma}^\dagger c_{d\sigma} + c_{d\sigma}^\dagger c_{k\sigma}) \quad (2.3.35)$$

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

$$\rho_{d\sigma} = \frac{1}{\pi} \frac{\Delta}{(E - \epsilon_{d\sigma})^2 + \Delta^2} \implies \langle n_{d\sigma} \rangle = \int \rho_{d\sigma} = \frac{1}{\pi} \cot^{-1} \left( \frac{\epsilon_{d\sigma}}{\Delta} \right) \quad (2.3.36)$$

An alternative way of writing that is

$$\frac{\epsilon_{d\sigma}}{\Delta} = \frac{\epsilon_d + U \langle n_{d\sigma} \rangle}{\Delta} = \cot(\pi \langle n_{d\sigma} \rangle) \implies \langle n_{d\sigma} \rangle = \frac{\Delta}{U} \left[ \cot(\pi \langle n_{d\sigma} \rangle) - \frac{\epsilon_d}{\Delta} \right] \quad (2.3.37)$$

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

$$\begin{aligned} \langle n_{d\uparrow} - n_{d\downarrow} \rangle \equiv m &= \frac{\Delta}{U} \left[ \cot \left( \pi \langle n_{d\downarrow} \rangle \right) - \cot \left( \pi \langle n_{d\uparrow} \rangle \right) \right] \\ &= \frac{\Delta}{U} \left[ \cot \frac{\pi}{2} (n_d - m) - \cot \frac{\pi}{2} (n_d + m) \right] \end{aligned} \quad (2.3.38)$$

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

$$\cot(a + x) \approx \cot a - x (\sin a)^{-2} \implies \cot(a - x) - \cot(a + x) \approx 2x (\sin a)^{-2} \quad (2.3.39)$$

we get

$$m = \frac{\Delta}{U} \left[ -\pi \frac{m}{\sin^2 \frac{\pi}{2} n_d} \right] \implies 1 = \lim_{m \rightarrow 0} \frac{U}{\pi \Delta} \frac{1}{1 + \cot^2 \frac{\pi n_d}{2}} \quad (2.3.40)$$

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. 2.3.40,

$$1 = \frac{U_c}{\pi} \frac{\Delta}{\Delta^2 + \left( \frac{U_c n_d}{2} + \epsilon_d \right)^2} \quad (2.3.41)$$

Magnetism will prevail for  $U \geq U_c$ . Comparing with eq. 2.3.37,

$$1 = U_c \rho_d(E = 0) \quad (2.3.42)$$

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

$$U_c = \pi \Delta \quad (2.3.43)$$

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

$$\langle n_{d\uparrow} \rangle = \frac{1 + m}{2} \quad (2.3.44)$$

$$\langle n_{d\downarrow} \rangle = \frac{1 - m}{2} \quad (2.3.45)$$

$$\epsilon_{d\sigma} = \epsilon_d + U \langle n_{d\bar{\sigma}} \rangle = \epsilon_d + \frac{U}{2} \pm \frac{U}{2} m = \pm \frac{U}{2} m \quad (2.3.46)$$

$$\rho_d = \rho_{d\uparrow} + \rho_{d\downarrow} = \frac{\Delta}{\pi} \left[ \frac{1}{\Delta^2 + \left( E - \frac{Um}{2} \right)^2} + \frac{1}{\Delta^2 + \left( E + \frac{Um}{2} \right)^2} \right] \quad (2.3.47)$$

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

### 2.3.3 Some conclusions and observations

- The mean field solution predicts that local moments are sustained in the limit of large  $U$  and small  $|\epsilon_d|$ . However, this treatment becomes faulty at low temperatures.
- 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  $Vc_k^\dagger c_d + \text{h.c.}$ . 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 [19]. 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 [17] is shown in ???. The space of the impurity electron can be divided into low energy and high energy subspaces:

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

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

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

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

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

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

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

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

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

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

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,

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

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

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

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. 2.3.36,

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

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,

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

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

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

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

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

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

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

$$g_1 = NJ_z, g_2 = NJ_T \quad (2.4.150)$$

the equations become

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

$$\frac{dg_2}{dD} = -\frac{2g_1g_2}{D} \quad (2.4.152)$$

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

$$\begin{aligned} T_2 &= \sum_{q \in \{D-|\delta D|\}, \lambda, \sigma''} \langle q\lambda, k'\beta, \sigma' | V | k'\beta, k\alpha, \sigma'' \rangle \langle k'\beta, k\alpha, \sigma'' | V | q\lambda, k\alpha, \sigma \rangle \frac{1}{E - (E_k + E_{k'} - E_q)} \\ &\approx -J^2 (S_d^a S_d^b)_{\sigma'\sigma} (\sigma^b \sigma^a)_{\beta\alpha} \frac{N|\delta D|}{E - D} \end{aligned} \quad (2.4.165)$$

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

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

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

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

Therefore,

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

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

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

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

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

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

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

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

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

This gives a better estimate of the Kondo temperature

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

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

$$k_B T_K = Dy(g) \tag{2.4.174}$$

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

$$\frac{dT_K}{dD} = 0 \tag{2.4.175}$$

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

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

This gives almost the same solution as eq. 2.4.173:

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

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

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

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

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

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

$$C_V = \gamma T \tag{2.4.180}$$

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

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

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

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,

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



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 [12] 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  $n_k^0$ ,

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

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

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

$\mathcal{N}(0) = \left. \frac{\partial n}{\partial E} \right|_{\epsilon_F}$  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 [21] 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

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

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  $\bar{H}_N$ ,

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

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 [22] 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

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

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:

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

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

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

The function  $\frac{e^{\beta\epsilon_{k\sigma}}}{(e^{\beta\epsilon_{k\sigma}} + 1)^2}$  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.

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

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

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

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

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

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

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

we can write

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

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

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

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,

$$1 - U\rho_d(0) = 0 \implies U\rho_d(0) = 1\tag{2.6.36}$$

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

$$R = 1 + \sin^2 \delta(0)\tag{2.6.37}$$

## 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:

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

From the optical theorem, we can write

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

This allows us to write [1]

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

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

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

From the work of Seki and Yunoki [23], 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  $\Delta V_L = -1 = -\tilde{N}$  [24] (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

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

Close to the Fermi surface, we also have

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

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

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

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  $\tilde{U}$ .

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

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

$$\tag{2.8.21}$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

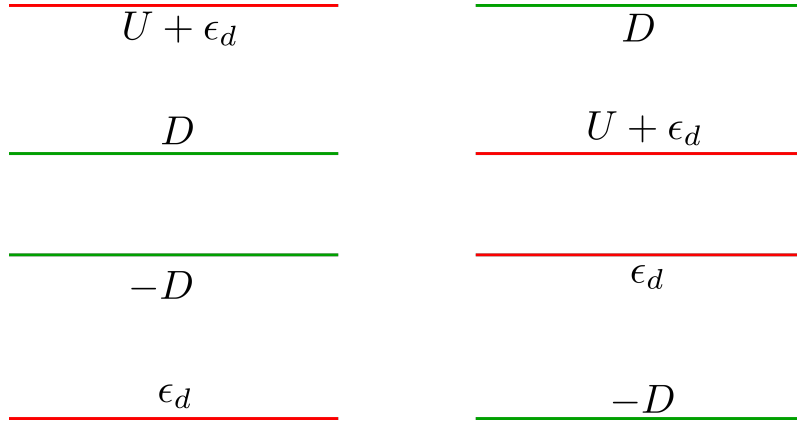


Figure 2.2: *Left*: Both impurity levels far outside the bandwidth. *Right*: Both impurity levels comfortably inside the bandwidth.

## 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

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

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.

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

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

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,

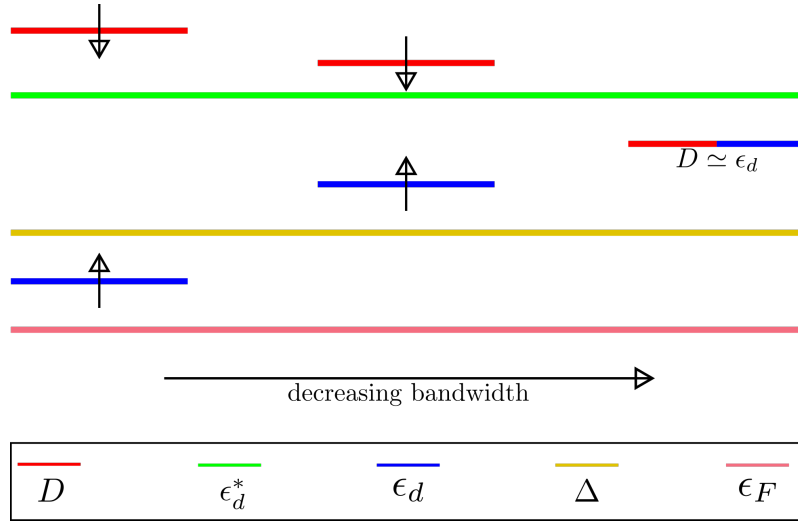
$$J = -\frac{V^2}{\epsilon_d} \quad (2.9.26)$$

$$g = J\rho = -\frac{\Delta}{\epsilon_d} \quad (2.9.27)$$

$$\implies T_K = D \sqrt{\frac{\Delta}{\epsilon_d}} \exp \left\{ \frac{\epsilon_d}{2\Delta} \right\} \quad (2.9.28)$$

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).



Figure 2.3: Renormalization in the energy levels when  $\epsilon_d^* \gg \Delta$ 

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

$$\bar{\epsilon}_d = \epsilon_d^* - \frac{\Delta}{\pi} \ln \frac{a\bar{\epsilon}_d}{\Delta} \quad (2.9.29)$$

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

$$\chi = \frac{1}{4T} \frac{2}{e^{\frac{\beta}{\beta^*}} + 2} + \frac{\Delta}{2\pi T^{*2}} \quad (2.9.57)$$

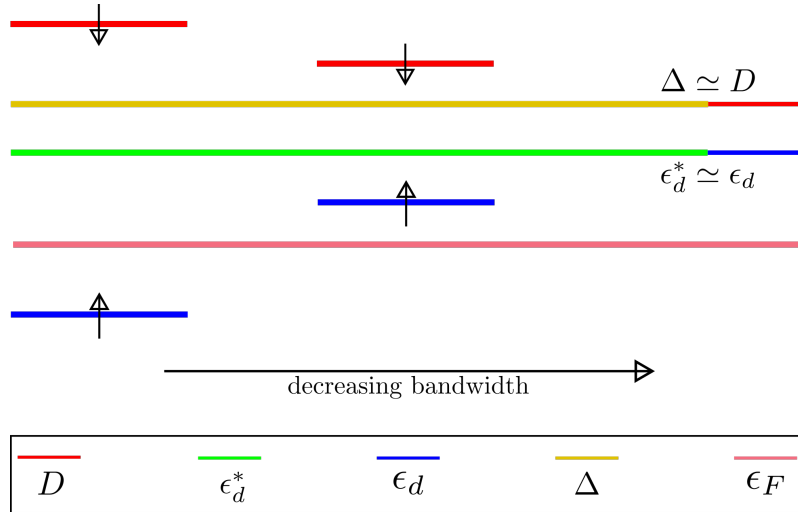
Below some temperature  $T_{FL} \ll T^*$ , the susceptibility reduces to

$$\chi \approx \frac{1}{4T} \frac{2}{e^{\frac{\beta}{\beta^*}}} + \frac{\Delta}{2\pi T^{*2}} \approx \frac{\Delta}{2\pi T^{*2}} \quad (2.9.58)$$

$$\implies \chi T \propto T \quad (2.9.59)$$

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  $T$ .

$$\begin{array}{lll} n_d = 1 & & n_d = \frac{2}{3} & & n_d = 0 \\ \chi T \sim \frac{1}{8} & \implies & \chi T \sim \frac{1}{6} & \implies & \chi T \sim T \\ T \gg U & & T \gg T^* & & T \ll T^* \end{array}$$

Figure 2.4: Renormalization in energy levels when  $|\epsilon_d^*| \lesssim \Delta$ 

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.

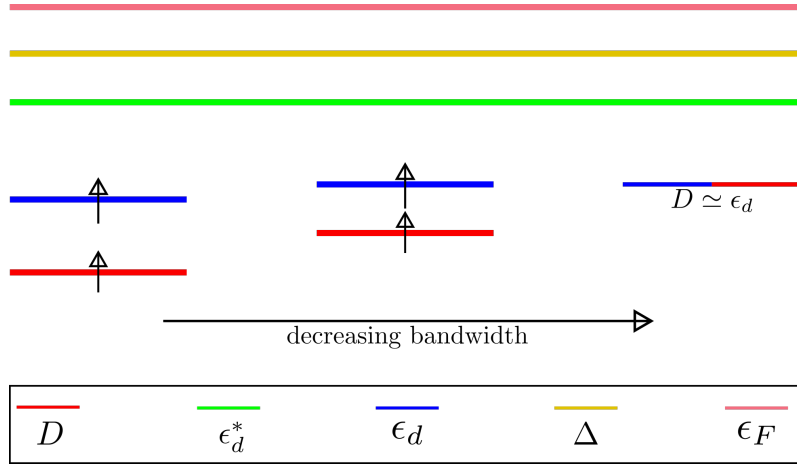
Since we have  $|\epsilon_d^*| \lesssim \Delta$ , as we renormalize, the decreasing cutoff will first match  $\Delta$  or  $k_B T$ , whichever is greater. From eq. 2.9.19, we know that if  $D$  comes close to  $\Delta$ , our analysis will break down because we can no longer ignore that term. Since that 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


 Figure 2.5: Renormalization in energy levels when  $\epsilon_d^* \ll -\Delta$ 

occur. These fluctuations, as well as 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.

$$\begin{array}{ccccccc}
 n_d = 1 & & n_d = \frac{2}{3} & & n_d = 1 & & n_d = 1 \\
 \chi T = \frac{1}{8} & \implies & \chi T = \frac{1}{6} & \implies & \chi T = \frac{1}{4} & \implies & \chi T \propto T \\
 \frac{1}{8}T \gg U & & T \gg \tilde{T} & & T \ll \tilde{T} & & T \ll \tilde{T}_K
 \end{array}$$

### Jefferson's calculation

Jefferson did a slightly more rigorous calculation to obtain the scaling equation. He divided the Hamiltonian into two parts

$$H = \sum_{k\sigma} \epsilon_{k\sigma} n_{k\sigma} + \epsilon_d n_d + \sum_{k\sigma} \left( V_{kd}^- c_{k\sigma}^\dagger c_{d\sigma} + V_{kd}^+ c_{d\sigma}^\dagger c_{k\sigma} \right) = H_0 + V \quad (2.9.62)$$

Before scaling,  $V^+ = V^- = V$ . The Schrödinger equation we want to solve is

$$H\psi = E\psi \quad (2.9.63)$$

We know the eigenstates  $\psi_0$  of  $H_0$ . They are the states  $\{|n_{k_i\sigma}, n_{d\sigma'}\rangle\}$ . These states of course span the entire Hilbert space. A subset of these states form the model subspace. We call these states  $\phi$ . For our case, that is the subspace with all conduction electrons inside  $D - \delta D$ . The projection operator for this subspace is

$$P = \sum |\phi\rangle \langle\phi| = \sum_{|k| < D - \delta D, \sigma = \pm 1, n_{d\sigma} = 0, 1} |n_{k\sigma}, n_{d\sigma'}\rangle \quad (2.9.64)$$

Its orthogonal subspace has a projection operator

$$Q = 1 - P = \sum_{D - \delta D < |k| < D, \sigma = \pm 1, n_{d\sigma} = 0, 1} |n_{k\sigma}, n_{d\sigma'}\rangle \quad (2.9.65)$$

If the dimension of model subspace is  $d$ , we can say that  $P$  takes  $d$  eigenstates  $\psi$  of the total Hamiltonian to  $d$  eigenstates in the model subspace:

$$P\{\psi\}_d = \{\phi\} \quad (2.9.66)$$

This is of course true in the non-interacting limit. There, the  $\psi_0$  are the exact eigenstates, and the action of  $P$  is basically

$$P\psi_0 \Big|_{|k| < D - \delta D} = \psi_0 \Big|_{|k| < D - \delta D} \quad (2.9.67)$$

Now, as we turn on the interactions adiabatically, it is safe to assume that these  $d$  non-interacting eigenstates flow into  $d$  interacting eigenstates. This means that we can define an inverse for the  $P$  operator which takes a non-interacting eigenstate from the model subspace into the interacting eigenstate:

$$\Omega\{\phi\} = \{\psi\} \quad (2.9.68)$$

Since  $\Omega$  can only act on states in the model subspace, we define

$$\Omega\{\phi\}^\perp = 0 \quad (2.9.69)$$

This allows us to write

$$\Omega P\phi = \Omega\phi \quad (2.9.70)$$

$$\Omega P\phi^\perp = \Omega \times 0 = 0 = \Omega\phi^\perp \quad (2.9.71)$$

In the first equation, I used  $P\phi = \phi$  because the projection of  $\phi$  into the model subspace is  $\phi$  itself. Together these two identities give

$$\Omega P = \Omega \quad (2.9.72)$$

With these definitions, we now change the problem a bit. We want to solve the Schrödinger equation only in the model subspace. To this end we write the Schrödinger equation as

$$H\Omega\phi = E\Omega\phi \quad (2.9.73)$$

Since we want to write down an equation only in the model subspace, the equation should operate only on the  $\phi$ . To remove the  $\Omega$  on the right side, operate on this equation with  $P$  from the left. This gives

$$PH\Omega\phi = EP\Omega\phi = E\phi \quad (2.9.74)$$

This is the effective Schrödinger equation in the model subspace. The effective Hamiltonian for the model subspace is

$$H_{\text{eff}} = PH\Omega = PH_0P + PV\Omega = PH_0P + PV\Omega \quad (2.9.75)$$

To solve for the  $\Omega$ , apply eq. 2.9.72 on the Schrödinger equation  $(E - H_0)\psi = V\psi$ :

$$\Omega V\psi = (E\Omega P - \Omega PH_0)\psi \quad (2.9.76)$$

Now, since  $P$  is made up of the eigenstates of  $H_0$ , those two will commute:  $[H_0, P] = 0$ . The equation then becomes

$$\Omega V\psi = (E - \Omega H_0 P)\psi \quad (2.9.77)$$

Subtracting the Schrödinger equation from the last equation gives

$$\begin{aligned} (\Omega - 1) V\psi &= (H_0 - \Omega H_0 P) \psi \\ \implies (\Omega - 1) V\Omega\phi &= (H_0 - \Omega H_0 P) \Omega\phi \\ \implies (\Omega - 1) V\Omega\phi &= (H_0\Omega - \Omega H_0) \phi \\ \implies (\Omega - 1) V\Omega &= [H_0, \Omega] \end{aligned} \quad (2.9.78)$$

This is the main equation. To make progress, we expand the operator  $\Omega$  in powers of the interaction  $V$ :

$$\Omega = \sum_n c_n V^n = \sum_n \Lambda_n \quad (2.9.79)$$

The zeroth term in the main equation becomes

$$[H_0, \Lambda_0] = 0 \implies \Lambda_0 = P \quad (2.9.80)$$

The first order equation is

$$[H_0, \Lambda_1] = (\Lambda_0 - 1) V\Lambda_0 = (P - 1) VP = -QVP \quad (2.9.81)$$

The second order equation is

$$[H_0, \Lambda_2] = -V\Lambda_1 + \Lambda_0 V\Lambda_1 + \Lambda_1 V\Lambda_0 = -QV\Lambda_1 + \Lambda_1 VP \quad (2.9.82)$$



These equations are of the form  $[H_0, \Lambda_n] = A_n$ , where  $A_n$  is an operator in terms of  $\Lambda_{n-1}$  and lower orders.

$$A_1 = -QVP \quad (2.9.83)$$

$$A_2 = -QV\Lambda_1 + \Lambda_1VP \quad (2.9.84)$$

Let  $|l\rangle$  and  $|h\rangle$  belong to the model subspace and its orthogonal subspace respectively. Then, taking matrix element between  $\langle h|$  and  $|l\rangle$  of the general form equation gives

$$\langle h| A_n |l\rangle = (E_h - E_l) \langle h| \Lambda_n |l\rangle \implies \langle h| \Lambda_n |l\rangle = \frac{\langle h| A_n |l\rangle}{E_h - E_l} \quad (2.9.85)$$

If we define an operator  $S$  by its action on a general operator  $A$  as

$$\langle h| SA |l\rangle = \frac{\langle h| A |l\rangle}{E_l - E_h} \quad (2.9.86)$$

we can write the solution

$$\Lambda_n = -S(A_n) \quad (2.9.87)$$

The expression of  $SA$  can be written as

$$\begin{aligned} SA &= \sum_{h,l} |h\rangle \langle l| \frac{\langle h| A |l\rangle}{E_l - E_h} \\ &= \sum_{h,l} \frac{1}{E_l - E_h} |h\rangle \langle h| A |l\rangle \langle l| \\ &= \sum_l \frac{1}{E_l - H_0} \left( \sum_h |h\rangle \langle h| \right) A |l\rangle \langle l| \\ &= \sum_l G_l A P_l \end{aligned} \quad (2.9.88)$$

where  $P_l = |l\rangle \langle l|$  and  $G_l = \frac{1}{E_l - H_0} Q$ .

$S$  has the property

$$\begin{aligned} \langle h| SQA |l\rangle &= \frac{\langle h| QA |l\rangle}{E_l - E_h} = \frac{\langle h| A |l\rangle}{E_l - E_h} = \langle h| SA |l\rangle \\ \implies S(QA) &= S(A) \end{aligned} \quad (2.9.89)$$

The lowest order solutions are thus

$$\Lambda_1 = S(QVP) = S(VP) \quad (2.9.90)$$

$$\Lambda_2 = S(QV\Lambda_1) - S(\Lambda_1VP) = S(VS(VP)) - S(S(VP)VP) \quad (2.9.91)$$

We can now expand the effective Hamiltonian in powers of  $V$ . From eq. 2.9.75, the interacting part of the effective Hamiltonian becomes

$$\begin{aligned} H_{\text{eff}} - PH_0P &= PV\Omega \\ &\approx PV(\Lambda_0 + \Lambda_1 + \Lambda_2) \\ &= PV [P + S(VP) + S(VS(VP)) - S(S(VP)VP)] \\ &= PVP + PVS(VP) + PVS(VS(VP)) - PVS(S(VP)VP) \end{aligned} \quad (2.9.92)$$

Therefore,

$$H_{\text{eff}} = PHP + PVS(VP) + PVS(VS(VP)) - PVS(S(VP)VP) \quad (2.9.93)$$

The first term is the obvious lowest approximation; you just project the entire Hamiltonian into the model subspace. The second term is

$$PVSVP = PV \sum_l G_l V P P_l = PV \sum_l G_l V P_l \quad (2.9.94)$$

where I used  $PP_l = \sum_{l'} |l'\rangle \langle l'| |l\rangle \langle l| = \sum_{l'} |l'\rangle \langle l'| \delta_{ll'} = P_l$ . The third term becomes

$$\begin{aligned} PVS V SVP &= PVS V \sum_l G_l V P_l = PV \sum_l S V G_l V P_l \\ &= PV \sum_{l,l'} G_{l'} V G_l V P_l P_{l'} = PV \sum_l G_l V G_l V P_l \end{aligned} \quad (2.9.95)$$

The fourth term is

$$\begin{aligned} PVS(S(VP)VP) &= PVS\left(\sum_l G_l V P P_l V P\right) = PV \sum_{l,l'} G_{l'} G_l V P_l V P P_{l'} \\ &= PV \sum_{l'} G_{l'} \left( \sum_l G_l V P_l \right) V P_{l'} \end{aligned} \quad (2.9.96)$$

The effective Hamiltonian up to third order in  $V$  is

$$\begin{aligned} H_{\text{eff}} &= PH_0P + PV \sum_l G_l V P_l + PV \sum_l G_l V G_l V P_l \\ &\quad - PV \sum_{l,l'} G_{l'} G_l V P_l V P_{l'} \end{aligned} \quad (2.9.97)$$

These results have been more or less general. We now need to write these in terms of the creation and annihilation operators of our Hamiltonian. The model subspace for our problem is the part of the conduction band up to  $D - \delta D$ . Here on,  $\sum$  represent sum over the model subspace momenta and  $\sum'$  represent sum over the remaining momenta. To facilitate writing the effective Hamiltonian in terms of the creation and annihilation operators, we change the projection operators from the bra-ket representation to operator representation:

$$|k_1\rangle \langle k_2| = c_{k_1}^\dagger c_{k_2} \quad (2.9.98)$$

$$P_k = |k, n_{d\sigma}\rangle \langle k, n_{d\sigma}| = c_k^\dagger c_k c_{d\sigma}^\dagger c_{d\sigma} = n_{k\sigma} n_{d\sigma} \quad (2.9.99)$$

The first term becomes

$$PH_0P = \sum_{k\sigma} \epsilon_{k\sigma} n_{k\sigma} + \epsilon_d n_d + \sum_{k\sigma} \left( V_{kd} c_{k\sigma}^\dagger c_{d\sigma} + \text{h.c.} \right) \quad (2.9.100)$$

The second term involves two potential terms that scatter from the model subspace to the high energy subspace and then back to the model subspace. Hence this term is

$$\begin{aligned}
PV \sum_l G_l V P_l &= V \sum_{q\sigma} \left( \frac{V_q}{\epsilon_d - \epsilon_q} c_{q\sigma}^\dagger c_{d\sigma} + \frac{V_q^*}{\epsilon_q - \epsilon_d} c_{d\sigma}^\dagger c_{q\sigma} \right) \\
&= \sum_{q\sigma}^+ \frac{|V_q|^2 c_{d\sigma}^\dagger c_{q\sigma} c_{q\sigma}^\dagger c_{d\sigma}}{\epsilon_d - \epsilon_q} + \sum_{q\sigma}^- \frac{|V_q|^2 c_{q\sigma}^\dagger c_{d\sigma} c_{d\sigma}^\dagger c_{q\sigma}}{\epsilon_q - \epsilon_d} \\
&= \sum_{q\sigma}^+ \frac{|V_q|^2 n_{d\sigma} (1 - n_{q\sigma})}{\epsilon_d - \epsilon_q} + \sum_{q\sigma}^- \frac{|V_q|^2 n_{q\sigma} (1 - n_{d\sigma})}{\epsilon_q - \epsilon_d}
\end{aligned} \tag{2.9.101}$$

In the high energy subspaces,  $n_q^+ = 1 - n_q^- = 0$ . Therefore,

$$\begin{aligned}
PV \sum_l G_l V P_l &= \sum_q^+ \frac{|V_q|^2 n_{d\sigma}}{\epsilon_d - \epsilon_q} + \sum_q^- \frac{|V_q|^2 (1 - n_{d\sigma})}{\epsilon_q - \epsilon_d} \\
&= n_d \left( \sum_q^+ \frac{|V_q|^2}{\epsilon_d - \epsilon_q} + 2 \sum_q^- \frac{|V_q|^2}{\epsilon_d - \epsilon_q} \right) \\
&= n_d \delta \epsilon_d
\end{aligned} \tag{2.9.102}$$

The third term is zero in our case. The part  $G_l V G_l V$  will do the following.

$$|k, n_{d\sigma}\rangle \rightarrow \begin{cases} |q_e, n_d = 0\rangle \rightarrow \begin{cases} |q_e, n_d = 1\rangle \\ |q_e, q'_h, n_d = 1\rangle \end{cases} \\ |q_h, n_d = 1\rangle \rightarrow \begin{cases} |q_h, q'_e, n_d = 0\rangle \\ |q_h, n_d = 0\rangle \end{cases} \end{cases} \tag{2.9.103}$$

None of the four final states belong to the model subspace, so this term is zero.

The fourth term involves a first scattering between two model states, followed by a scattering to a high energy subspace and then a scattering back to the model subspace. One way for going through such a process is

$$|k, n_d = 0\rangle \xrightarrow[\Delta E = \epsilon_k - \epsilon_q]{|n_d = 1\rangle} |q_e, n_d = 0\rangle \xrightarrow[\Delta E = \epsilon_q - \epsilon_d]{|k', n_d = 1\rangle} \tag{2.9.104}$$

Another way is to start with  $c_d$  instead of  $c_d^\dagger$

$$|n_{d\sigma} = 1\rangle \xrightarrow[\Delta E = \epsilon_k - \epsilon_q]{|k\sigma, n_d = 0\rangle} \begin{cases} |q_h \uparrow, n_{d\uparrow} = 1\rangle \\ |q_h \downarrow, n_{d\downarrow} = 1\rangle \end{cases} \xrightarrow[\Delta E = \epsilon_q - \epsilon_d]{|n_d = 0\rangle} \tag{2.9.105}$$

Combining the two processes gives

$$\begin{aligned}
\sum_q^+ \sum_{k\sigma} \frac{|V_q|^2 c_{d\sigma}^\dagger c_{q\sigma} c_{q\sigma}^\dagger c_{d\sigma} c_{d\sigma}^\dagger c_{k\sigma}}{(\epsilon_q - \epsilon_d)(\epsilon_k - \epsilon_q)} + \sum_{q\sigma'}^- \sum_{k\sigma} \frac{|V_q|^2 c_{q\sigma'}^\dagger c_{d\sigma'} c_{d\sigma'}^\dagger c_{q\sigma'} c_{k\sigma}^\dagger c_{d\sigma}}{(\epsilon_q - \epsilon_d)(\epsilon_k - \epsilon_q)} \\
= \sum_{k\sigma} \left( c_{k\sigma}^\dagger c_{d\sigma} \delta V_k^- + c_{d\sigma}^\dagger c_{k\sigma} \delta V_k^- \right)
\end{aligned} \tag{2.9.106}$$

where

$$\begin{aligned}
\delta V^+ &= \sum_q^+ \frac{|V_q|^2}{(\epsilon_q - \epsilon_d)(\epsilon_k - \epsilon_q)} \\
\delta V^- &= \sum_q^- 2 \frac{|V_q|^2}{(\epsilon_q - \epsilon_d)(\epsilon_k - \epsilon_q)}
\end{aligned} \tag{2.9.107}$$

The total Hamiltonian can be written in the form

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

We now evaluate the changes:

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

I used the approximation

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

Also,

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

We now make the following assumptions:

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

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

## 2.10 Numerical Renormalization Group Calculation of the symmetric SIAM

NRG calculations of the symmetric SIAM were carried out by H. R. Krishnamurthy, Wilkins and Wilson in ref. [5]. They identified three fixed points in the phase diagram. Two of them, the free-orbital and the local moment, are unstable while the strong-coupling fixed point is stable. These fixed points along with typical RG flows are marked in fig. 2.6. The free-orbital fixed point

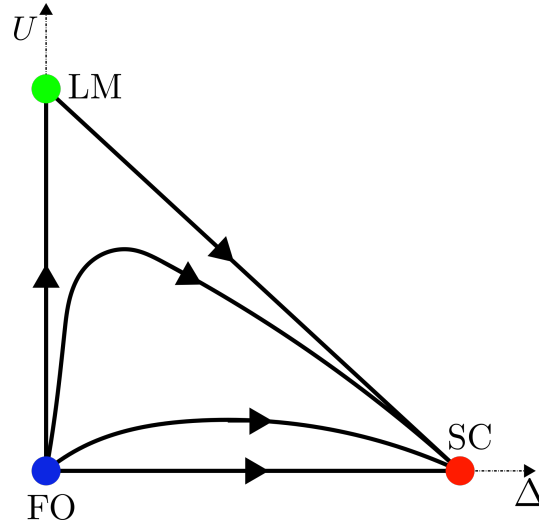


Figure 2.6: Schematic diagram of RG flows and fixed points of the symmetric SIAM, as obtained by ref.[5]. The y-axis is the impurity site repulsion  $U = -\frac{1}{2}\epsilon_d$  while the x-axis is the hybridisation parameter  $\Delta \sim \rho V^2$ . The abbreviations mark the three fixed-points: FO is free-orbital, LM is local moment and SC is strong-coupling. The fixed-points are described in the text.

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

# Chapter 3

## Unitary Renormalization Group Method

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 and Results

#### 3.1.1 Description of the problem

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

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

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

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

This gives

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

### 3.1.2 Obtaining the decoupling transformation

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

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

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  $\hat{\omega}_i = \hat{\omega}_i^1 \hat{n}_{q\beta} + \hat{\omega}_i^0 (1 - \hat{n}_{q\beta})$ . 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  $\omega_i^{1,0}$ :

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

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:

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

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

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

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

$$\begin{aligned} |\psi_1\rangle &= |1\rangle |\phi_1^i\rangle + |0\rangle |\phi_0^i\rangle = (1 + \eta) |1\rangle |\phi_1^i\rangle \\ |\psi_0\rangle &= \left(1 + \eta^\dagger\right) |0\rangle |\phi_0^i\rangle \end{aligned} \quad (3.1.18)$$

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

$$U_1 = 1 + \eta \quad (3.1.19)$$



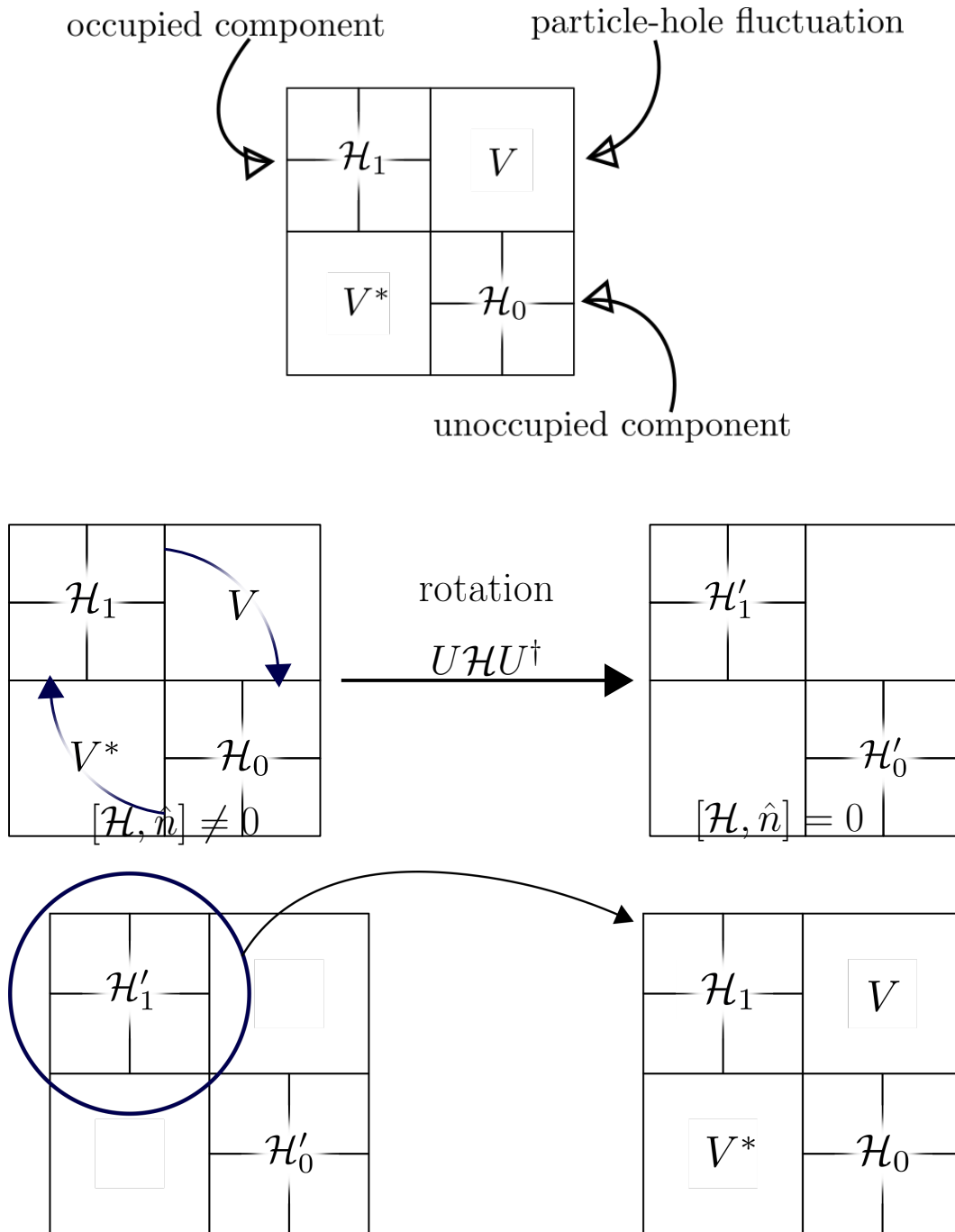


Figure 3.1: Three steps of the URG: Decompose the Hamiltonian in a  $2 \times 2$  matrix, apply the unitary operator to rotate it, then repeat these steps with one of the rotated blocks.

### 3.1.3 Properties of the many-body transition operators

The operators  $\eta$  have some important properties. First is the Fermionic nature:

$$\eta^2 = \eta^{\dagger 2} = 0 \quad [c^{\dagger 2} = c^2 = 0] \quad (3.1.20)$$

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. [25] 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,

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

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

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

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

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

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,

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

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

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

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

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:

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

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

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

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

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

It can also be shown that

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

Putting it all together,

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

The renormalizing in the Hamiltonian is

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

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

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

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

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

$$\begin{aligned} \left[ \tilde{\mathcal{H}}, \hat{n}_{q\beta} \right] &= \left[ \left[ c_{q\beta}^\dagger T, \eta \right], \hat{n}_{q\beta} \right] \\ &= \left[ c_{q\beta}^\dagger T \eta, \hat{n}_{q\beta} \right] - \left[ \eta c_{q\beta}^\dagger T, \hat{n}_{q\beta} \right] \\ &= c_{q\beta}^\dagger T \eta \hat{n}_{q\beta} - \hat{n}_{q\beta} c_{q\beta}^\dagger T \eta \quad \left[ 2^{\text{nd}} [ \cdot ] \text{ is } 0, \because c_{q\beta}^\dagger \hat{n}_{q\beta} = \hat{n}_{q\beta} \eta = 0 \right] \\ &= c_{q\beta}^\dagger T \eta - c_{q\beta}^\dagger T \eta \\ &= 0 \end{aligned} \quad (3.1.48)$$

### 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  $[c^\dagger T, \eta]$  in this case. That form will be non-Hermitian. The correct form is obtained from the more general form  $[\eta^\dagger - \eta, \mathcal{H}_X]$ :

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

### 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

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

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  $\eta$ :

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

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

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

Since the two unitaries should give the same effective Hamiltonian, we require  $U_1 = U_0$ . That requires  $\eta_1 = -\eta_0$ . Comparing the expressions of the  $\eta$ 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 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  $\eta(\omega_i^0) = (\eta^\dagger(\omega_i^1))^\dagger$  (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.

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

The first two come from  $\eta(\omega_i^0) = \left(\eta^\dagger(\omega_i^1)\right)^\dagger$  while the last comes from  $\eta(\omega_0^j) = -\eta(\omega_1^j)$ . These are the only independent relations. Other relations like the one between  $\omega_1^0$  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

$$\Delta\mathcal{H} = c_{q\beta}^\dagger \text{Tr} \left( \mathcal{H} c_{q\beta} \right) \eta_1 + \text{Tr} \left( c_{q\beta}^\dagger \mathcal{H} \right) c_{q\beta} \eta_0^\dagger \quad (3.2.7)$$

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 [7, 26]. Writing down the forms of  $\eta$  and  $\eta^\dagger$  explicitly, we get

$$\Delta\mathcal{H} = c_{q\beta}^\dagger \text{Tr} \left( \mathcal{H} c_{q\beta} \right) \frac{1}{\omega_1^0 - \mathcal{H}_0^d} \text{Tr} \left( c_{q\beta}^\dagger \mathcal{H} \right) c_{q\beta} + \text{Tr} \left( c_{q\beta}^\dagger \mathcal{H} \right) c_{q\beta} \frac{1}{\omega_0^1 - \mathcal{H}_1^d} c_{q\beta}^\dagger \text{Tr} \left( \mathcal{H} c_{q\beta} \right) \quad (3.2.8)$$

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

$$\Delta\mathcal{H} = \sum_{q\beta} \left[ c_{q\beta}^\dagger \text{Tr} \left( \mathcal{H} c_{q\beta} \right) \frac{1}{\omega_1^0 - \mathcal{H}_0^d} \text{Tr} \left( c_{q\beta}^\dagger \mathcal{H} \right) c_{q\beta} + \text{Tr} \left( c_{q\beta}^\dagger \mathcal{H} \right) c_{q\beta} \frac{1}{\omega_0^1 - \mathcal{H}_1^d} c_{q\beta}^\dagger \text{Tr} \left( \mathcal{H} c_{q\beta} \right) \right] \quad (3.2.9)$$

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

### 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. [27]. 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.

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

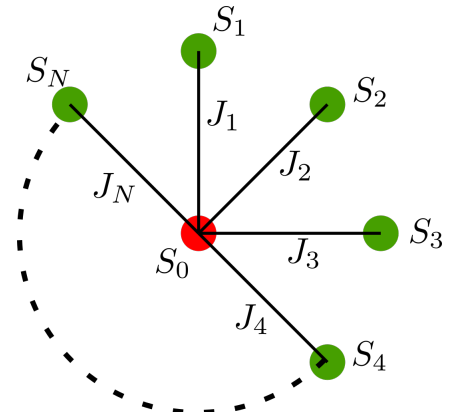


Figure 3.2: Star Graph model

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

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

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

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

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

The RG involves decoupling the nodes  $N$  through 1, and looking at the resultant renormalization in  $\epsilon_i$  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

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

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

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

### 3.3.1 Calculation of Renormalization

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

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

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

$$\Delta \mathcal{H} = [S_N^+ T, \eta] \quad (3.3.7)$$

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

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

and

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

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

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

and

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

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

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

To compare  $\omega$  and  $\omega'$ , we will write down their Poor Man' Scaling counterparts.

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

So, the renormalization becomes

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

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

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

We can now read off the renormalizations in  $\epsilon_N$  and  $\epsilon_0$ .

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

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

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

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

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

Our goal here is to look for a fixed-point condition such that the denominator vanishes at some point of the RG. If we start with a bare of  $\epsilon_0$  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  $\epsilon_0$  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 the other  $\omega$  in the URG formalism. Recall that  $\eta$  and  $\eta^\dagger$  will, in general, have different  $\omega$ , eq. 3.1.14.

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

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

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

Substituting this in eq. 3.3.17 gives

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

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

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

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 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

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

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.

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

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

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

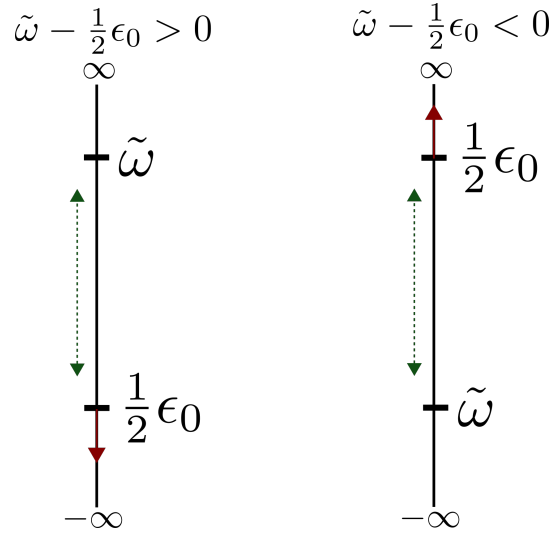


Figure 3.3: RG flow for the two cases. The green line is the distance between the bare values of the two couplings, and hence also the magnitude of the denominator. The red arrow denotes the direction in which  $\epsilon_0$  will flow. Upward flow is increase. In both cases, the flow is such that the 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.

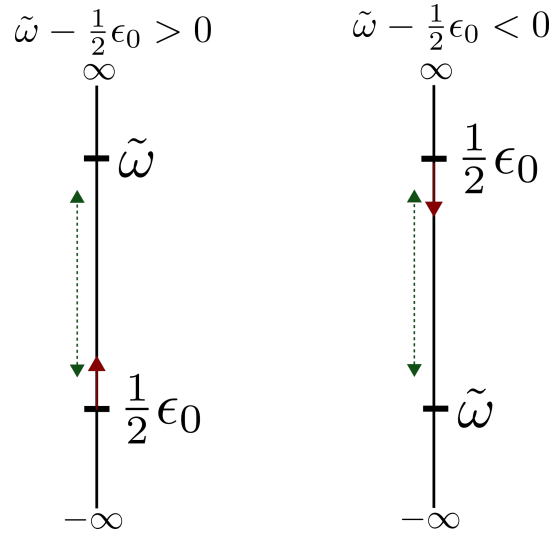


Figure 3.4: RG flow for the two cases with the new  $-\tilde{\omega} = \omega' - \frac{1}{2}\epsilon + \frac{1}{4}J$ . Now we can see that in both cases, the flow is such that the distance (green dotted line) between the couplings decreases. A fixed point is reached when this distance vanishes.

### 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. 3.5. The second kind are those where the two couplings have different signs, and so  $\epsilon_0$  flows to 0. These are shown in fig. 3.6.

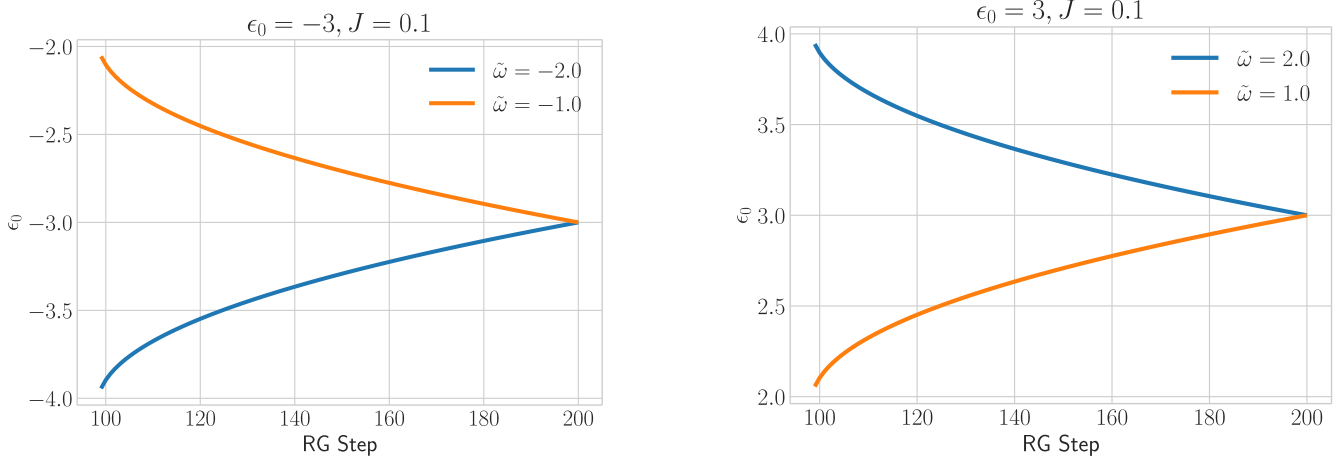


Figure 3.5: Flows where  $\epsilon_0$  and  $\tilde{\omega}$  have same sign. The left and right panels show flows starting from negative and positive values respectively. The two plots in each panel correspond to different values of  $\tilde{\omega}$ , one greater than the bare  $\epsilon_0$ , the other less than that. The fixed point value is  $2\tilde{\omega}$ .

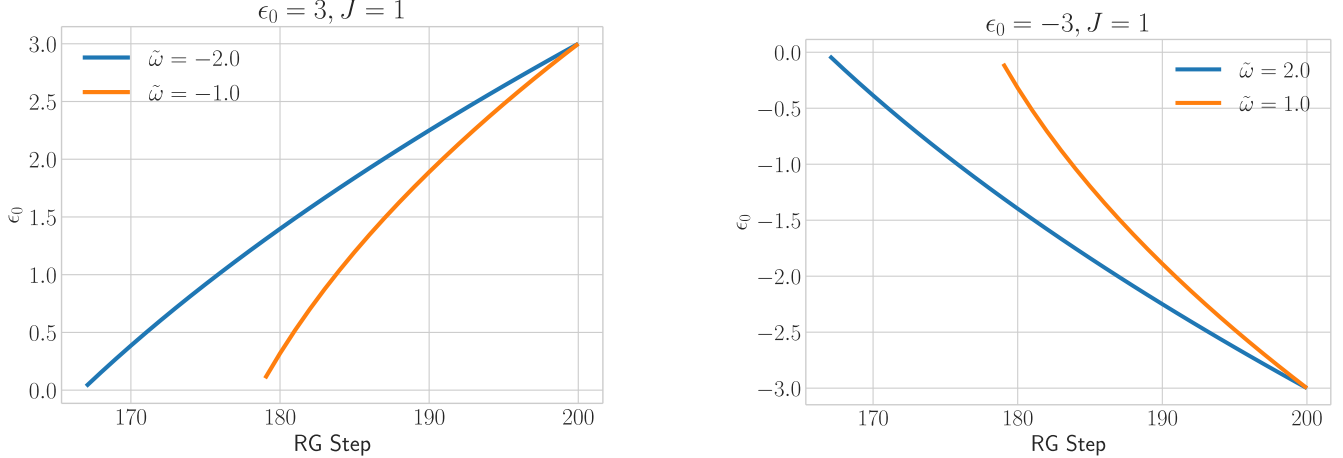


Figure 3.6: Flows where  $\epsilon_0$  and  $\tilde{\omega}$  have opposite sign. The left and right panels show flows starting from negative and positive values respectively. The two plots in each panel correspond to different values of  $\tilde{\omega}$ , one greater than the bare  $\epsilon_0$ , the 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 is first carried out in ref. [13]. The model is of course described by the Hamiltonian

$$\mathcal{H} = \sum_{k\alpha} \epsilon_k \hat{n}_{k\alpha} + J_z \sum_{k,k'} S_d^z \left( c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow} \right) + J_t \sum_{k,k'} \left( S_d^+ c_{k\downarrow}^\dagger c_{k'\uparrow} + S_d^- c_{k\uparrow}^\dagger c_{k'\downarrow} \right) \quad (3.4.1)$$

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

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

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

$$\mathcal{H}_d = \epsilon_q \tau_{q\beta} + J_z S_d^z \beta \hat{n}_{q\beta} \quad (3.4.3)$$

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

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

$$\mathcal{H}^I = J_z \sum_k S_d^z \beta \left( c_{k\beta}^\dagger c_{q\beta} + c_{q\beta}^\dagger c_{k\beta} \right) + J_t \sum_k \left( c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} + c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\bar{\beta}} \right) \quad (3.4.4)$$

These are the terms that come in the numerator.

### 3.4.1 Particle sector

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

$$c_{q\beta}^\dagger T \eta \quad (3.4.5)$$

where

$$\begin{aligned} \eta &= \frac{1}{\omega - \mathcal{H}_d} \left[ J_z \sum_k \beta S_d^z c_{k\beta}^\dagger c_{q\beta} + J_t \sum_k c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \right] \\ &= \sum_k \left[ \frac{1}{\hat{\omega}_1 - \hat{E}_1} J_z S_d^z \beta c_{k\beta}^\dagger c_{q\beta} + \frac{1}{\omega_3 - E_3} J_t c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \right] \end{aligned} \quad (3.4.6)$$

Noting that  $\beta S_d^z = \frac{1}{2} (\hat{n}_{d\beta} - \hat{n}_{d\bar{\beta}}) = \frac{1}{2} \hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}}) - \frac{1}{2} \hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta})$ , we can write the  $\eta$  as

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

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

$$E_3 = \frac{1}{2} \epsilon_q - \frac{1}{2} J_z \quad (3.4.8)$$

For the first two term, note that these terms do not flip the spin; hence, the denominator should reflect that. The total magnetization for the spin  $\beta$  in the initial state is  $\hat{n}_\beta = \hat{n}_{q\beta} = 1$ , because of the  $q\beta$ . It is also 1 in the intermediate state, because of the spin  $k\beta$ :  $\hat{n}_\beta = \hat{n}_{k\beta} = 1$ . This holds for



both  $E_1$  and  $E_2$ . The impurity magnetization is however 1 in the first term but  $-1$  in the second term. Hence,

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

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

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

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

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

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

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

Therefore,

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

The renormalization is therefore

$$\begin{aligned} &\frac{1}{\xi} \sum_{kk'} \left[ J_z \beta S_d^z c_{q\beta}^\dagger c_{k'\beta} \times J_z \beta S_d^z c_{k\beta}^\dagger c_{q\beta} + J_t c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\bar{\beta}} \times J_t c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \right. \\ &\quad \left. + J_t c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\bar{\beta}} \times J_z \beta S_d^z c_{k\beta}^\dagger c_{q\beta} + J_z \beta S_d^z c_{q\beta}^\dagger c_{k'\beta} \times J_t c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \right] \end{aligned} \quad (3.4.14)$$

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

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

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

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

and

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

The renormalization then becomes

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

### 3.4.2 Hole sector

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

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

where  $\eta_0$  is defined in eq. 3.1.57.

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

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

$$\eta_0^\dagger = \sum_k \left[ \frac{J_z \frac{1}{2} \hat{n}_{d\beta} \left( 1 - \hat{n}_{d\bar{\beta}} \right) c_{q\beta}^\dagger c_{k\beta}}{\xi'_1} - \frac{J_z \frac{1}{2} \hat{n}_{d\bar{\beta}} \left( 1 - \hat{n}_{d\beta} \right) c_{q\beta}^\dagger c_{k\beta}}{\xi'_2} + \frac{J_t c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\bar{\beta}}}{\xi'_3} \right] \quad (3.4.21)$$

Calculating the energies gives

$$\begin{aligned} E'_1 &= \frac{1}{2} \epsilon_q + \frac{1}{2} J_z \\ E'_2 &= \frac{1}{2} \epsilon_q - \frac{1}{2} J_z = E'_3 \\ \omega'_1 &= -\frac{1}{2} \epsilon_q + \frac{1}{2} J_z = \omega + J_z \\ \omega'_2 &= \omega'_3 = -\frac{1}{2} \epsilon_q - \frac{1}{2} J_z = \omega \\ \xi'_i &= \omega - \frac{1}{2} \epsilon_q + \frac{1}{2} J_z = \xi \end{aligned} \quad (3.4.22)$$

Evaluating the terms similar to the particle sector gives

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

### 3.4.3 Scaling equations

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

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

Summing over  $\beta$  and  $q$  gives

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

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

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

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

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

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

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

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

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

$$\Delta J \approx J^2 \sum_q \frac{1}{\epsilon_q} \quad (3.4.29)$$

### 3.4.4 Numerical Solutions

The symmetric scaling equation 3.4.28 was solved numerically with the choice  $\omega = -\frac{\epsilon_q}{2}$ , for both positive and negative bare values of  $J$ . For sufficiently low values of  $\omega$ , 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. 3.8

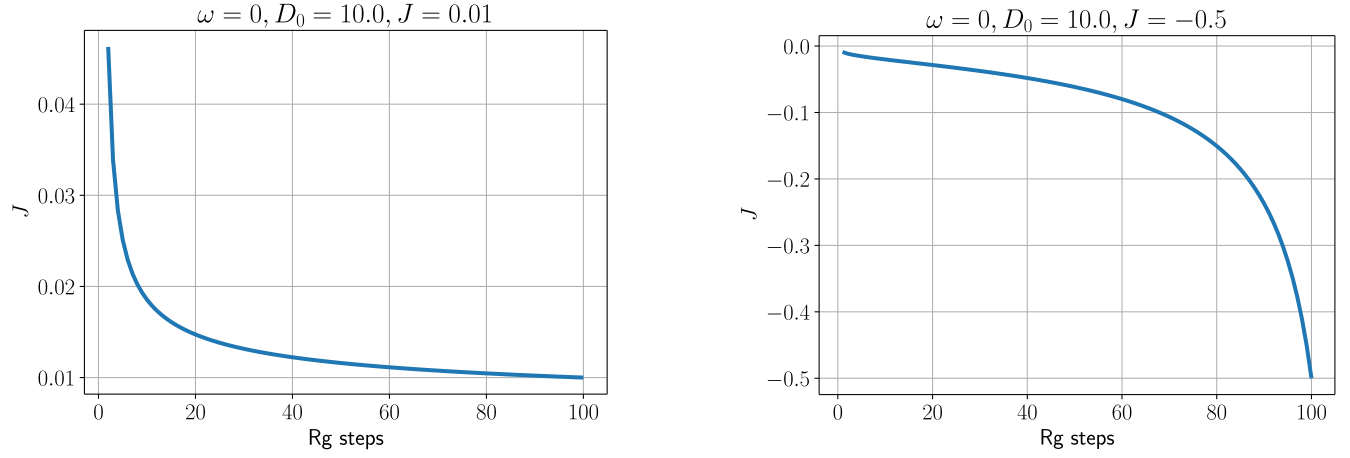


Figure 3.7: Flow of  $J$  towards the strong-coupling fixed point (right) and the weak coupling saddle-point (left). The x-axis indicates the index of the energy shell being decoupled. The largest value (UV) is the first step, and we go towards the left (IR).

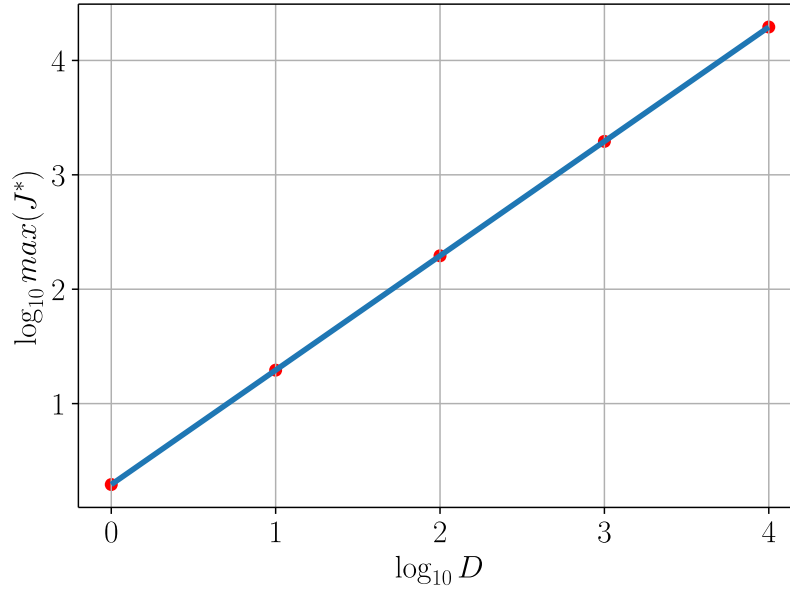


Figure 3.8: Variation of the fixed point value  $J^*$  against the bare bandwidth, in log scale.

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