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Chapter 1

Introduction

1.1 Summary of the problem

¹⁶ The single-impurity Anderson model (SIAM) is one of the most well-studied models in condensed matter physics and ⁴⁴ is the prototypical model for magnetism. It shows how strong correlations between electrons give rise to a residual local moment. Friedel[1], 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 ³² would correspond to the local moment. Taking inspiration from this, P.W.Anderson[2] 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 ⁷¹ 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 ¹⁰ its 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 ⁸³ in-spin interaction. This model can be related to the SIAM through a canonical transformation followed by ⁸³ projection to the low energy subspace. In 1964, Jun Kondo[3] found ¹⁰² 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 ²⁶; 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 [4, 5] corroborated Wilson's findings.

A similar sequence of events also happened in the context of the Anderson model. In 1977 and 1978, Jeffereson 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 [10]), 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 [6]. Their calculations were again supported by later Bethe ansatz calculations by Wiegmann and Tsvelick[7].

¹⁶ 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, putting 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[8].
- What is the nature of the Kondo cloud that screens the spin(charge) 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 [9] 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 ω :* The URG process involves a parameter ω 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 ω , 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 Δ . We then derive the Kondo model from the [S₂₂M](#) 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 ω and show that the URG actually diagonalizes the Hamiltonian. We derive many-body creation and annihilation operators η^\dagger and η which rotate the full Hamiltonian into successively more block-diagonal form.

Chapter 4 is closely tied to the formalism chapter and develops the connections between URG and other canonical

transformations in the literature. We first define and setup each of the other transformations - the Schrieffer-Wolff transformation (SWT), Poor Man's scaling (PMS) and the Continuous Unitary Transformation (CUT) RG. We show that all of these are in some sense perturbative derivatives of URG. A byproduct of the discussion is a demonstration of the fact that PMS and SWT are exactly identical and differ only in the contexts in which they are applied. We also discuss the differences between URG and CUT-RG, and show that URG behaves like a generalized double-bracket flow [10].

Chapter 5 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 6 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 7 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 ω , signaling strong-coupling fixed points.

¹² 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 χ_{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, χ_{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.

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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

2.1 Some important results of scattering theory

2.1.1 T-matrix and S-matrix

T -matrix is defined as[11]

$$V |\Psi\rangle = T |\Phi\rangle \quad (2.1.1)$$

where $|\Psi\rangle$ is the total scattered wavefunction and $|\Phi\rangle$ is the incoming (non-interacting) wavefunction. This equation is supposed to hold for all eigenkets $|\Phi\rangle$ of the Hamiltonian H_0 .

The kets $|\Psi\rangle$ and $|\Phi\rangle$ satisfy the Schrodinger equations

$$H_0 |\Phi\rangle = E |\Phi\rangle \quad (2.1.2)$$

$$(H_0 + V) |\Psi\rangle = E |\Psi\rangle \quad (2.1.3)$$

We will also define an S -matrix- it is the unitary operator that relates the non-interacting eigenstate to the interacting one:

$$|\Psi\rangle = S |\Phi\rangle \quad (2.1.4)$$

Since we are assuming elastic scattering, both $|\Psi\rangle$ and $|\Phi\rangle$ have the same energy. The Schrodinger equation for $|\Psi\rangle$ can be rearranged into

$$|\Psi\rangle = |\Phi\rangle + G_0 V |\Psi\rangle \quad (2.1.5)$$

where $G_0^{-1}(\omega) = \omega - H_0$ is then on-interacting Greens function. This is also called the Lippmann-Schwinger equation. Multiplying with the interacting operator V from the left gives

$$\begin{aligned} V |\Psi\rangle &= V |\Phi\rangle + V G_0 V |\Psi\rangle \\ \Rightarrow T |\Phi\rangle &= V |\Phi\rangle + V G_0 T |\Phi\rangle \quad [\text{eq. 2.1.1}] \end{aligned} \quad (2.1.6)$$

Since the last equation should hold for all $|\Phi\rangle$, and since the set of $|\Phi\rangle$ form a complete set, we can extract the operator equation

$$T = V + V G_0 T \quad (2.1.7)$$

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

$$T = V + V G_0 V + V G_0 V G_0 V + \dots \quad (2.1.8)$$

We can relate this T -matrix with the total (interacting) Green's function

$$G = \frac{1}{\omega - H_0 - V} \quad (2.1.9)$$

That definition can be massaged into the following identity:

$$\begin{aligned} G^{-1} &= G_0^{-1} - V \\ \Rightarrow G_0 G^{-1} G &= G_0 G_0^{-1} G - G_0 V G \\ \Rightarrow G &= G_0 + G_0 V G \end{aligned} \quad (2.1.10)$$

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

$$\begin{aligned} G &= G_0 + G_0 V (G_0 + G_0 V G) = G_0 + G_0 V G_0 + G_0 V G_0 V G_0 + \dots \\ &= G_0 + G_0 (V + V G_0 V + \dots) G_0 \end{aligned} \quad (2.1.11)$$

By comparing with eq. 2.1.8, we can recognize the term inside the brackets as the T -matrix, and write

$$G = G_0 + G_0 T G_0 \quad (2.1.12)$$

By substituting $|\Psi\rangle = S|\Phi\rangle$ into the L-S equation, we can also extract a relation between S and T , and hence between S and G . Combining eqs. 2.1.1, 2.1.4 and 2.1.5, we get

$$S|\Phi\rangle = |\Phi\rangle + G_0 T |\Phi\rangle \quad (2.1.13)$$

$$\Rightarrow S = 1 + G_0 T \quad (2.1.14)$$

$$\Rightarrow S G_0 = G_0 + G_0 T G_0 = G \quad [\text{eq. 2.1.12}] \quad (2.1.15)$$

$$\Rightarrow S = G G_0^{-1} \quad (2.1.16)$$

³² It is a standard result in scattering theory that the total scattered wavefunction can be written as the sum of the incoming plane wave and an outgoing spherical wave:

$$\Psi(x) = (2\pi)^{-\frac{3}{2}} \left[e^{ikx} + f(k', k) \frac{e^{ikr}}{r} \right] \quad (2.1.17)$$

where the amplitude of the outgoing wave, $f(k', k)$, quantifies the amount of scattering and is given by

$$f(k', k) = -\frac{(2\pi)^3}{4\pi} \frac{2m}{\hbar^2} \langle k' | V | \Psi \rangle \quad (2.1.18)$$

Using the definition of T , we get

$$f(k', k) = -\frac{(2\pi)^3}{4\pi} \frac{2m}{\hbar^2} \langle k' | T | \Phi \rangle = -\frac{(2\pi)^3}{4\pi} \frac{2m}{\hbar^2} \langle k' | T | k \rangle \quad (2.1.19)$$

where we chose the non-interacting eigenkets to be the momentum eigenkets ($|\Phi\rangle = |k\rangle$). By expanding in terms of the eigenstates of L^2 and L_z , this can be written as

$$f(k', k) = -\frac{\pi}{k} \sum_l (2l+1) P_l(\cos \theta) T_l(\epsilon_k) \equiv \sum_l (2l+1) P_l(\cos \theta) f_l(k) \quad (2.1.20)$$

where we have chosen \vec{k} to be the z-direction and θ is the angle between k and k' . The last part of the equation defines $f_l(k)$:

$$f_l(k) = -\frac{\pi}{k} T_l(\epsilon_k) \quad (2.1.21)$$

This enables us to write

$$\Psi(x) = (2\pi)^{-\frac{3}{2}} \left[e^{ikx} + \sum_l (2l+1) P_l(\cos \theta) f_l(k) \frac{e^{ikr}}{r} \right] \quad (2.1.22)$$

Writing the plane wave in terms of incoming and outgoing spherical waves and expanding the spherical waves in terms of the spherical harmonics gives

$$\Psi(x) = (2\pi)^{-\frac{3}{2}} \sum_l (2l+1) \frac{1}{2ik} P_l \left[(1 + 2ik f_l) \frac{e^{ikr}}{r} - e^{-i(kr-l\pi)} \frac{1}{r} \right] \quad (2.1.23)$$

From conservation of probabilities, we know that the amplitude squared of the incoming and outgoing waves must be equal. Assuming a spherically symmetric scattering center means the probabilities will be conserved separately for each value of l . This means that the coefficient

$$S_l(k) \equiv 1 + 2ikf_l(k) \quad (2.1.24)$$

can, at most, be a phase:

$$S_l(k) \equiv 1 + 2ikf_l(k) = e^{2i\delta_l(k)} \quad (2.1.25)$$

From the definition of f_l in terms of T_l , we can relate $S_l(k)$ with the T-matrix $T(\epsilon_k)$:

$$S_l(k) = 1 + 2ikf_l = 1 - 2\pi iT_l(\epsilon_k) \quad (2.1.26)$$

53 We can express the LHS in terms of energy:

$$\begin{aligned} S_l(\omega) &= \langle \omega | S_l | \omega \rangle \\ &= \int d\vec{k} \stackrel{36}{\langle \omega |} |\vec{k}\rangle \langle \vec{k}| S_l |\vec{k}\rangle \langle \vec{k}| |\omega \rangle \\ &= \int d\vec{k} \delta(\omega - \epsilon_k) S_l(\vec{k}) \\ &= \int d\vec{k} \delta(\omega - \epsilon_k) [1 - 2\pi iT_l(\epsilon_k)] \\ &= 1 - 2\pi i \int d\vec{k} \delta(\omega - \epsilon_k) T_l(\epsilon_k) \\ &= 1 - 2\pi i \int g(k) dk \delta(\omega - \epsilon_k) T_l(\epsilon_k) \\ &= 1 - 2\pi i \int g(\epsilon_k) d\epsilon_k \delta(\omega - \epsilon_k) T_l(\epsilon_k) \\ &= 1 - 2\pi i g(\omega) T_l(\omega) \end{aligned} \quad (2.1.27)$$

19 where $g(k)$ is the density of states at momentum magnitude $k = |\vec{k}|$ and $g(\epsilon_k)$ is the density of states at that energy. Note that these are the non-interacting density of states: they count energy states that match with the kinetic energy ϵ_k and do not take into account any self-energy term that may come from some interaction. The relation between S and T is thus

$$S_l(\omega) = 1 - 2\pi i g(\omega) T_l(\omega) \quad (2.1.28)$$

2 The scattering phase shifts can be expressed in terms of T :

$$\begin{aligned} T_l(\omega) &= \frac{1}{2\pi i g(\omega)} [1 - S_l(\omega)] \\ &= \frac{1}{2\pi i g(\omega)} [1 - \exp(2i\delta_l(\omega))] \\ &= \frac{1}{2\pi i g(\omega)} \exp(i\delta_l(\omega)) [\exp(-i\delta_l(\omega)) - \exp(i\delta_l(\omega))] \end{aligned} \quad (2.1.29)$$

Converting the exponentials inside the box brackets to sines gives

$$T_l(\omega) = -\frac{1}{\pi g(\omega)} \exp(i\delta_l(\omega)) \sin \delta_l(\omega) \quad (2.1.30)$$

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

$$\delta_l(\omega) = \arg[T_l(\omega)] \quad (2.1.31)$$

Since the total T -matrix will be

$$T(\omega) = \sum_{lm\sigma} T_l(\omega) \quad (2.1.32)$$

the determinant of $T(\omega)$ will be the product of the eigenvalues $T_l(\omega)$, so we can write

$$\text{Det} [T(\omega)] = \prod_{lm\sigma} T_l = \exp \left[i \sum_{lm\sigma} \delta_l(\omega) \right] \prod_{lm\sigma} \left(-\frac{1}{\pi g(\omega)} \right) \sin \delta_l(\omega) \quad (2.1.33)$$

and the argument of this function will be the total scattering phase shift:

$$\arg \left[\text{Det} [T(\omega)] \right] = \sum_{lm\sigma} \delta_l(\omega) \equiv \delta(\omega) \quad (2.1.34)$$

³ $\delta(\omega)$ is the total scattering phase shift suffered by the scattering states due to scattering off the potential, at energy ω .

Summing equation 2.1.28 over l also relates the total S with the total T :

$$S(\omega) = 1 - 2\pi i g(\omega) T(\omega) \quad (2.1.35)$$

2.1.2 The Friedel sum-rule

This is a very ¹⁰⁶ general and important theorem that will come up quite often throughout the calculations. It states that the ^{ch}₁₀₆ in the number of states of a Hamiltonian on introduction of a localized scattering center is equal to the sum of the scattering phase shifts suffered by the conduction electrons at the Fermi surface as they scatter off the scattering center. We can obtain a clearer picture by looking at a simple derivation of this result [12].

Consider a Hamiltonian

$$\mathcal{H} = H_0 + V \quad (2.1.36)$$

where $H_0 = \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma}$. We will define the ⁿ₃₄umber 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

$$G(\omega) = \lim_{\eta \rightarrow 0} \frac{1}{\omega - \mathcal{H} + i\eta} = \frac{1}{\omega - \mathcal{H}} - i\pi\delta(\omega - \mathcal{H}) \quad (2.1.37)$$

The non-interacting Greens function is then

$$G_0(\omega) = \frac{1}{\omega - H_0} - i\pi\delta(\omega - H_0) \quad (2.1.38)$$

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

$$\begin{aligned} \rho(\omega) &= \sum_{\epsilon} \delta(\omega - \epsilon) = \text{Tr} [\delta(\omega - \mathcal{H})] = -\frac{1}{\pi} \text{ImTr} [G(\omega)] \\ \rho_0(\omega) &= -\frac{1}{\pi} \text{ImTr} [G_0(\omega)] \\ N &= \int_{-\infty}^{\epsilon_F} \rho(\omega) d\omega = - \int_{-\infty}^{\epsilon_F} \frac{1}{\pi} \text{ImTr} [G(\omega)] d\omega \\ N_0 &= - \int_{-\infty}^{\epsilon_F} \frac{1}{\pi} \text{ImTr} [G_0(\omega)] d\omega \end{aligned} \quad (2.1.39)$$

Note that $\rho_0(\omega)$ is nothing but ⁵⁴the $g(\omega)$ that appears in eq. 2.1.28. The quantity N ¹⁷counts 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

$$\Delta\rho(\omega) = \rho(\omega) - \rho_0(\omega) = -\frac{1}{\pi} \text{ImTr} [G(\omega) - G_0(\omega)] \quad (2.1.40)$$

We can rewrite the trace of Green's function as

$$\begin{aligned}
 \text{Tr} [G(\omega)] &= \sum_i \frac{1}{\omega - E_i} \\
 &= \sum_i \frac{\partial}{\partial \omega} \ln (\omega - E_i) \\
 &= \frac{\partial}{\partial \omega} \ln \prod_i (\omega - E_i) \\
 &= -\frac{\partial}{\partial \omega} \ln \text{Det} [G(\omega)]
 \end{aligned} \tag{2.1.41}$$

such that

$$\begin{aligned}
 -\text{Tr} [G(\omega) - G_0(\omega)] &= \frac{\partial}{\partial \omega} \ln \left\{ \text{Det} [G] \left(\text{Det} [G_0] \right)^{-1} \right\} \\
 &= \frac{\partial}{\partial \omega} \ln \text{Det} [G(\omega) G_0^{-1}(\omega)] \\
 &= \frac{\partial}{\partial \omega} \ln \text{Det} [G_0^{-1}(\omega) G(\omega)]
 \end{aligned} \tag{2.1.42}$$

which works because $\text{Det} [AB] = \text{Det} [BA]$. From eq. 2.1.12, we can write $G_0^{-1}(\omega)G(\omega) = 1 + G_0T$, which means

$$\begin{aligned}
 -\text{Tr} [G(\omega) - G_0(\omega)] &= \frac{\partial}{\partial \omega} \ln \text{Det} [1 + G_0T] \\
 &= \frac{\partial}{\partial \omega} \ln \text{Det} [V^{-1}T] \quad [\text{eq. 2.1.7}] \\
 &= \frac{\partial}{\partial \omega} \ln \text{Det} [V^{-1}] \text{Det} [T] \\
 &= \frac{\partial}{\partial \omega} \left(\ln \text{Det} [V^{-1}] + \ln \text{Det} [T] \right)
 \end{aligned} \tag{2.1.43}$$

Since V is independent of ω , the first term will vanish under the derivative.

$$-\text{Tr} [G(\omega) - G_0(\omega)] = \frac{\partial}{\partial \omega} \ln \text{Det} [T] \tag{2.1.44}$$

The change in the dos becomes

$$\begin{aligned}
 \Delta\rho(\omega) &= \frac{1}{\pi} \text{Im} \left(\frac{\partial}{\partial \omega} \ln \text{Det} [T] \right) \\
 &= \frac{1}{\pi} \frac{\partial}{\partial \omega} \text{Im} (\ln \text{Det} [T])
 \end{aligned} \tag{2.1.45}$$

Note that while the $\text{Det} [T]$ will have both an argument and an amplitude (as a general complex number), the \ln followed by the $\text{Im}()$ will pick out just the argument:

$$\text{Im} (\ln(re^{i\phi})) = \text{Im} (\ln r + i\phi) = \phi \tag{2.1.46}$$

Hence,

$$\Delta\rho(\omega) = \frac{1}{\pi} \frac{\partial}{\partial \omega} \text{arg} \text{Det} [T] \tag{2.1.47}$$

From eq. 2.1.34, we get

$$\Delta\rho(\omega) = \frac{1}{\pi} \frac{\partial}{\partial \omega} \delta(\omega) \tag{2.1.48}$$

The ⁵ change in the total number of states is obtained simply by integrating the dos from $-\infty$ to the chemical potential ϵ_F :

$$\begin{aligned}
 \Delta N &= \frac{1}{\pi} \int_{-\infty}^{\epsilon_F} \frac{\partial}{\partial \omega} \delta(\omega) d\omega \\
 &= \frac{1}{\pi} [\delta(\epsilon_F) - \delta(-\infty)]
 \end{aligned} \tag{2.1.49}$$

For $\omega \rightarrow -\infty$, we can write $\omega - \mathcal{H} \rightarrow \omega - H_0$ such that $G(\omega) \rightarrow G_0(\omega)$ and hence $S(\omega) \rightarrow 1$, which means that $S(\omega)$ becomes real and $\delta(\omega) \rightarrow 0$. Making this substitution, we get the spherically symmetric case of the Friedel sum rule

$$\Delta N = \frac{1}{\pi} \delta(\epsilon_F) \quad (2.1.50)$$

2.1.3 An identity

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

$$HA = A(\lambda + H) \quad (2.1.51)$$

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

$$(E - H)A = AE - A(\lambda + H) = A(E - \lambda - H) \quad (2.1.52)$$

$$\Rightarrow A(E - \lambda - H)^{-1} = (E - H)^{-1}A \quad (2.1.53)$$

2.2 Landau's theory of Fermi liquids

Since we will be using some results and concepts of Fermi liquids, its best to discuss the relevant details briefly. This section is adapted from ref. [13].

A ideal Fermi gas is a collection of non-interacting Fermions. Since they are non-interacting, the eigenstates of the complete system are just the collections of the eigenstates of the particles and holes. The eigenstate will be of the form $\{n_{k_1\uparrow}, n_{k_1\downarrow}, n_{k_2\uparrow}, n_{k_2\downarrow}, n_{k_3\uparrow}, n_{k_3\downarrow}, \dots\}$, where $n_{k\sigma} \in \{0, 1\}$ is the number of particles with momentum k and spin σ . In the ground state,

$$n_{k\sigma} = \begin{cases} 1 & k \leq k_F \\ 0 & k > k_F \end{cases} \quad (2.2.1)$$

Excitations involve adding an electron above k_F or removing an electron below k_F . The former is called a *particle* while the latter is called a *hole*. A general excited state of the total system is a collection of particle and hole excitations.

We next consider interacting systems, but very specific ones. That is, we consider interacting systems whose excitations can be mapped one-to-one with the excitations of the ideal system, provided the interactions are turned on sufficiently slowly. Alternatively, there exists a sufficiently slow rate of turning off the interactions such that any interacting excited state Ψ^* continuously flows into some excited state Φ of the ideal system as the interactions flow to 0.

$$\Psi^* \xrightarrow{\text{turn interactions off}} \Phi \quad (2.2.2)$$

$$\Phi^* \xrightarrow{\text{turn interactions off}} \Psi \quad (2.2.3)$$

If some state Γ^* , instead of flowing into an ideal excited state, gets lost while the interactions are being turned off, then we are not considering that system. All excited states must flow into some ideal state and vice-versa. This means that the interacting excited states can be labeled by the same good quantum numbers \vec{k} and σ . That is, if some eigenstate of the interacting system flows into the ideal eigenstate $\{n_{k\sigma}\}$, we can just as well use the distribution $\{n_{k\sigma}\}$ to label the interacting eigenstate. The particle and hole excitations of the ideal system might flow into some very complicated state of the interacting system, which we call a quasiparticle/quasihole. In other words, a system (ideal ground state + particle of momentum k) goes to (interacting ground state + quasiparticle of momentum k). If an interacting eigenstate corresponds to the state $\{n_{k\sigma}\}$, then $\{n_{k\sigma}\}$ is said to be the quasiparticle distribution function for that interacting state. Just as we denote eigenstates of the total ideal system using the collection of particles and holes, similarly we use the quasiparticle and quasiholes to describe eigenstates of the interacting system. Let $k_+ > k_F$ and $k_- < k_F$. Then,

$$|IGS\rangle \otimes |k_+\rangle \xrightarrow{\text{turn interactions on}} |RGS\rangle \otimes |k_+\rangle^* \quad (2.2.4)$$

$$|IGS\rangle \otimes |k_-\rangle \xrightarrow{\text{turn interactions on}} |RGS\rangle \otimes |k_-\rangle^* \quad (2.2.5)$$

$$(2.2.6)$$

$| \rangle^*$ denotes a quasi-ket. "IGS" and "RGS" are ideal and real(interacting) ground states. Another way of putting this is

$$c_{k+}^\dagger |IGS\rangle \xrightarrow{\text{turn interactions on}} \eta_{k+}^\dagger |RGS\rangle \quad (2.2.7)$$

$$c_{k-} |IGS\rangle \xrightarrow{\text{turn interactions on}} \eta_{k-} |RGS\rangle \quad (2.2.8)$$

η^\dagger is the creation operator for the quasiparticle. n_k gives the distribution of momentum k quasiparticles. If n_k^0 is the distribution in the ground state, the excitation can be measured as

$$\delta n_k = n_k - n_k^0 \quad (2.2.9)$$

In general, the total energy \mathcal{E} of the system will be a functional of the distribution function n_k . For the ideal system, this function is very simple.

$$\mathcal{E}^0[n_k] = \sum_k n_k \epsilon_k \quad (2.2.10)$$

The functional in case of the interacting system might be very complex. Up to first order in the functional, we can write

$$\mathcal{E}[n_k] = \mathcal{E}[n_k^0] + \sum_k \frac{\partial \mathcal{E}}{\partial n_k} \delta n_k \quad (2.2.11)$$

The first order variation in \mathcal{E} is thus

$$\delta \mathcal{E} \equiv \mathcal{E}[n_k] - \mathcal{E}[n_k^0] = \sum_k \xi_k \delta n_k \quad (2.2.12)$$

where $\xi_k = \frac{\partial \mathcal{E}}{\partial n_k}$. ξ_k is the energy of the quasiparticles(hole) or momentum k . To see this, note that if $\mathcal{E}[n_k^1]$ and $\mathcal{E}[n_k^2]$ are the energies before and after adding a quasiparticle of momentum q , we have

$$n_k^2 - n_k^1 = \begin{cases} 0 & k \neq q \\ 1 & k = q \end{cases} \quad (2.2.13)$$

Then, up to first order,

$$\mathcal{E}[n_k^2] - \mathcal{E}[n_k^1] = \sum_k \xi_k (n_k^2 - n_k^1) = \xi_q \quad (2.2.14)$$

This shows that the effect of adding a quasiparticle of momentum q is to raise the total energy by ξ_q . It is thus sensible to call that the energy of the quasiparticle. ξ_k itself might depend on whether other quasiparticles are present; there might be interactions among them. This effectively means that ξ_k itself is, in general, a functional of n_k . Consequently, we expand it up to first order.

$$\xi_k = \xi_k^0 + \sum_q \frac{\partial \xi_k}{\partial n_q} \delta n_q \quad (2.2.15)$$

Eq. 2.2.12 then becomes

$$\delta \mathcal{E} = \sum_k \xi_k^0 \delta n_k + \sum_{k,q} f(k, q) \delta n_k \delta n_q \quad (2.2.16)$$

where $f(k, q) = \frac{\partial \xi_k}{\partial n_q} = \frac{\partial^2 \mathcal{E}}{\partial n_k \partial n_q}$ is the interaction between two quasiparticles of momenta k and q . The first term is the self energy of the quasiparticles, the other they would have had even if no other quasiparticle was present. Its sort of like their kinetic energy. The second term is the interaction energy between all the quasiparticles. Hence, the term $f(k_1, k_2)$ comes into play only when $\delta n_{k_1} \neq 0$ and $\delta n_{k_2} \neq 0$, that is when both the quasiparticles are present.

Since the quasiparticles are in direct correspondence with the Fermionic particles, they must also be fermions. This allows us to write down the probability of finding a quasiparticle at energy ξ ,

$$f(\xi) = \left[e^{(\xi - \mu)\beta} + 1 \right]^{-1} \quad (2.2.17)$$

where $\mu = \mathcal{E}_F(N+1) - \mathcal{E}_F(N) = \frac{\partial \mathcal{E}_0}{\partial N}$ is the change in ground state energy on adding one quasiparticle. There is a subtlety here though. Since ξ itself depends on the occupancy, and the occupancy also depends on ξ through the probability distribution, there is a feedback effect in action here. If any perturbation or field modifies the occupation $n_{k\sigma}$, it will produce a feedback effect on all the occupations, through the ξ .

A temperature-dependent free energy can be concocted using

$$F[\delta n_k] = \delta \mathcal{E}[\delta n_k] - TS[\delta n_k] \quad (2.2.18)$$

Minimizing this gives an expectation value of the excitation distribution $\langle \delta n_k \rangle$. This in turn gives a temperature-dependent quasiparticle energy

$$\xi_k(T) = \xi_k^0 + \sum_q f(k, q) \langle \delta n_q \rangle \quad (2.2.19)$$

where $\langle \delta n_q \rangle$ is obtained by

$$\left. \frac{dF}{d\delta n_q} \right|_{\delta n_q = \langle \delta n_q \rangle} = 0 \quad (2.2.20)$$

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 ϵ_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.

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

The SIAM involves the following energy scales:

Figure 2.1: The single-impurity Anderson model Hamiltonian

- the onsite energy: ϵ_d
- the double-occupation cost: U
- the energy scale generated by the hybridisation: $\Delta = \pi t^2 \sum_k \rho(\epsilon_k) \rightarrow$. The rate of hybridisation is $\frac{2\Delta}{h}$.

We can have the following situations regarding dominance of various energy scales:

- $U \gg \epsilon_d \gg \Delta$: Double occupation is not possible. Δ being small means very small hybridisation. So, d-site is either up or down, hence magnetic.
- $U \gg \Delta \gg \epsilon_d$: Double occupation is still not possible, but now hybridisation will allow the up and down spins to fluctuate on the d-site, leading to zero average magnetization.
- $\Delta \gg U \gg \epsilon_d$: Hybridisation now fluctuates the up and down spins, leading to zero average magnetization.

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.

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

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

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

Now,

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

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

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

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 ⁷ 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 ϵ_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:

²⁴ T -matrix is defined by

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

We also have

$$\begin{aligned} G &= G_0 + G_0 V G = G_0 + G_0 T \frac{1}{1 + GT} G \\ &= G_0 + G_0 T (1 - GT + \dots) (G_0 + G_0 V G_0 + \dots) \\ &= G_0 + G_0 T G_0 \end{aligned} \quad (2.3.19)$$

The conduction electron Green's function can be calculated as ¹

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

Noting that

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

we have ⁵⁷

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

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

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

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

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

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 δ , 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 π , 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 Fried ³ 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 [14]. 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 .

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

ϵ_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

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

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

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

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.

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

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

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

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

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

2.3.3 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 [49] 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 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 ∞ 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_{eff} flows to ∞ under poor man's scaling as $T \rightarrow 0$. Thus, the singlet phase shift at ϵ_F approaches $\frac{\pi}{2}$ as $T \rightarrow 0$.

2.4 The Kondo model

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

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

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

2.4.1 Derivation of the Kondo Hamiltonian

Deriving the Kondo Hamiltonian involves separating the impurity spinon subspace ($\hat{n}_{d\uparrow} \neq \hat{n}_{d\downarrow}$) from the doublon and holon subspaces ($\hat{n}_{d\uparrow} = \hat{n}_{d\downarrow}$). ¹⁸ The canonical (pun intended) way of doing this is via a Schrieffer-Wolff transformation [15]. 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 [14]. An alternate derivation via a projector operator method due to [12] is shown in 4.2.1.

The space of the impurity electron can be divided into low energy and high energy subspaces:

$$\begin{aligned} \text{low energy (L)} &\rightarrow \left\{ \begin{array}{l} |\uparrow\rangle \\ |\downarrow\rangle \end{array} \right. \\ \text{high energy (H)} &\rightarrow \left\{ \begin{array}{l} |\rangle \\ |\uparrow\downarrow\rangle \end{array} \right. \end{aligned} \quad (2.4.2)$$

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

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

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 $i \in H, j \in L$.

$$[V, S] = \begin{pmatrix} 0 & v^\dagger \\ v & 0 \end{pmatrix} \begin{pmatrix} 0 & -s^\dagger \\ s & 0 \end{pmatrix} \stackrel{\text{37}}{=} \begin{pmatrix} 0 & -s^\dagger \\ s & 0 \end{pmatrix} \begin{pmatrix} 0 & v^\dagger \\ v & 0 \end{pmatrix} \stackrel{\text{37}}{=} \begin{pmatrix} v^\dagger s + s^\dagger v & 0 \\ 0 & -v s^\dagger - s v^\dagger \end{pmatrix} \quad (2.4.11)$$

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 $|H_{12}\rangle$ 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

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

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,

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

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 $c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger = \delta_{\sigma_1, \sigma_2} \delta_{k_1, k_2} - c_{k_1\sigma_1}^\dagger c_{k_2\sigma_2}$. The δ 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 [16]. 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:

$$T = V + VG_0V \quad (2.4.33)$$

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

First order scattering

$$|k \uparrow, d_\sigma\rangle \rightarrow |q \uparrow, d_\sigma\rangle \left. \right\} \text{non-spin-flip}$$

$$|k \uparrow, d_\downarrow\rangle \rightarrow |q \downarrow, d_\uparrow\rangle \left. \right\} \text{pro-spin-flip}$$

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 $\rho(0)$.

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

For spin-flip, the matrix element is

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

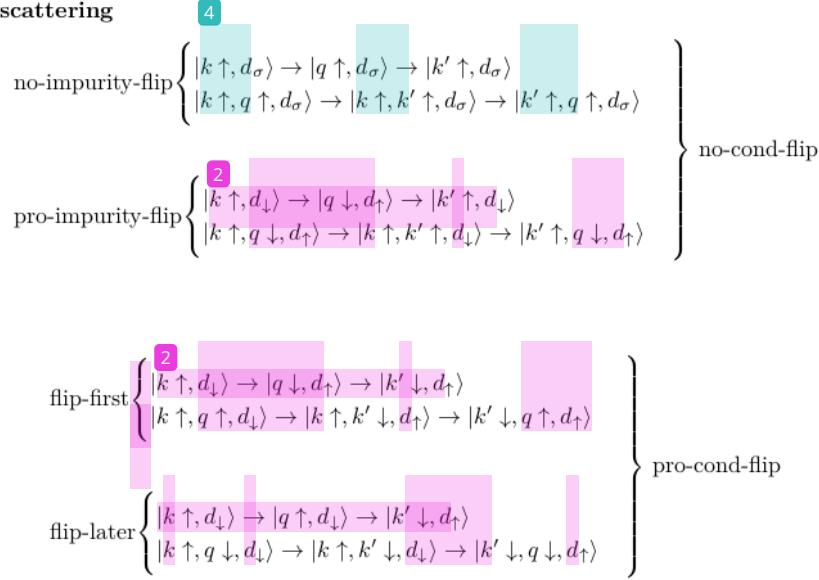
where $\lambda_\pm = \langle m_d \pm 1 | S_d^\pm | m_d \rangle = \sqrt{s_d(s_d+1) - m_d(m_d \pm 1)}$. The probability for this scattering is hence

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

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



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:

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

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 $\langle qk'|V|k'k\rangle \sim \langle qk'|c_q^\dagger c_k|k'k\rangle = -\langle qk'|c_q^\dagger c_k|kk'\rangle = -1$. 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

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

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 $\epsilon_k = \epsilon_F$.

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

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

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

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

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

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 5th to 8th),

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

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

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

$$J \vec{S}_d \cdot \vec{\sigma}_e = 2J \vec{S}_d \cdot \vec{S}_e = J \left(S^2 - S_d^2 - S_e^2 \right) = J \left(s(s+1) - \frac{3}{2} \right) = \begin{cases} -\frac{3J}{2} & (\text{singlet}) \\ \frac{J}{2} & (\text{triplet}) \end{cases} \quad (2.4.64)$$

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, α will encounter a zero in its denominator, because the integral in α is outside the Fermi surface. On the other hand, the integral in γ is inside the Fermi surface, so the denominator in γ 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. 2.1.30, 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,

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

For $n_c = 1$ (half-filling), the mean field value is less than the one obtained from the spin- $\frac{1}{2}$ 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

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

$\alpha + \gamma$ can be calculated as

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

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

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

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

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

Since

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

we can write

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

Similarly,

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

giving

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

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

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

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

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

This scattered wave is thus another radial wave but its phase is shifted by an amount $\Delta r = \frac{\delta_d}{k_F}$. For a positive Δr (and hence a positive δ_d), the wave will be drawn inward. Hence, the singlet channel having a positive δ 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 ϵ_d . This self energy can be Taylor-expanded about $E = 0$:

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

Defining

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

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 Δ 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 ϵ_d^* and Δ^* 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

⁶⁹

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 singlet 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

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

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

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

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

$$E_b = De^{-\frac{2}{3JN(0)J}} \quad (2.4.110)$$

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

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

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 ΔV . 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 ΔV 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

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

Using eq. 2.1.53, we can write

$$(E - H_0)^{-1} c_{q\downarrow}^\dagger c_{k\uparrow} = c_{q\downarrow}^\dagger c_{k\uparrow} (E - \lambda - H_0)^{-1} \quad (2.4.116)$$

where λ 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,

$$T_1 = J_T^2 S_d^- S_d^+ \sum_q c_{k'\uparrow}^\dagger c_{q\downarrow} c_{q\downarrow}^\dagger c_{k\uparrow} (E - \epsilon_q + \epsilon_k - H_0)^{-1} \quad (2.4.117)$$

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

$$T_1 = J_T^2 S_d^- S_d^+ c_{k'\uparrow}^\dagger c_{k\uparrow} \sum_q (E - \epsilon_q + \epsilon_k - H_0)^{-1} \quad (2.4.118)$$

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

$$\sum_q (E - \epsilon_q + \epsilon_k - H_0)^{-1} = N |\delta D| \frac{1}{E - D + \epsilon_k} \quad (2.4.119)$$

N is the density of states. Also,

$$S^- S^+ = (S^x - iS^y) (S^x + iS^y) = \frac{1}{2} + i [S^x, S^y] = \frac{1}{2} - S^z \quad (2.4.120)$$

Putting it all together,

$$T_1 = J_T^2 \left(\frac{1}{2} - S_d^z \right) N |\delta D| c_{k'\uparrow}^\dagger c_{k\uparrow} \frac{1}{E - D + \epsilon_k} \quad (2.4.121)$$

For the second possible scattering,

$$q \downarrow k \uparrow d \uparrow \rightarrow k' \uparrow k \uparrow d \downarrow \rightarrow k' \uparrow q \downarrow d \uparrow \quad (2.4.122)$$

we get

$$T_2 = J_T^2 \sum_q S_d^+ S_d^- c_{q\downarrow}^\dagger c_{k\uparrow} \frac{1}{E - H_0} c_{k'\uparrow}^\dagger c_{q\downarrow} \quad (2.4.123)$$

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

$$\begin{aligned} T_2 &= J_T^2 \left(\frac{1}{2} + S_d^z \right) N |\delta D| c_{k\uparrow} c_{k'\uparrow}^\dagger \frac{1}{E - D - \epsilon_{k'}} \\ &= -J_T^2 \left(\frac{1}{2} + S_d^z \right) N |\delta D| c_{k'\uparrow}^\dagger c_{k\uparrow} \frac{1}{E - D - \epsilon_{k'}} \end{aligned} \quad (2.4.124)$$

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 :

$$\begin{array}{c} \textcolor{red}{2} \\ \textcolor{purple}{k} \downarrow, d \uparrow \rightarrow q \uparrow d \downarrow \rightarrow k' \downarrow \textcolor{red}{d} \uparrow \end{array} \quad (2.4.125)$$

$$q \uparrow k \downarrow d \downarrow \rightarrow k' \downarrow k \downarrow \textcolor{red}{d} \uparrow \rightarrow k' \downarrow q \uparrow d \downarrow \quad (2.4.126)$$

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

$$T_3 = J_T^2 \left(\frac{1}{2} + S_d^z \right) N |\delta D| c_{k'\downarrow}^\dagger c_{k\downarrow} \frac{1}{E - D + \epsilon_k} \quad (2.4.127)$$

$$T_4 = -J_T^2 \left(\frac{1}{2} - S_d^z \right) N |\delta D| c_{k'\downarrow}^\dagger c_{k\downarrow} \frac{1}{E - D - \epsilon_{k'}} \quad (2.4.128)$$

The total second order contribution is

$$T^{(2)} = -J_T^2 S_d^z N |\delta D| \left(\frac{1}{E - D + \epsilon_k} + \frac{1}{E - D - \epsilon_{k'}} \right) \left(\textcolor{red}{1} \right) \left(c_{k'\uparrow}^\dagger c_{k\uparrow} - c_{k'\downarrow}^\dagger c_{k\downarrow} \right) \quad (2.4.129)$$

Comparing this with the S_d^z term in the Hamiltonian

$$J_z S_d^z \left(\textcolor{red}{1} \right) \left(c_{k'\uparrow}^\dagger c_{k\uparrow} - c_{k'\downarrow}^\dagger c_{k\downarrow} \right) \quad (2.4.130)$$

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

$$\delta J_d^z = -J_T^2 N |\delta D| \left(\frac{1}{E - D + \epsilon_k} + \frac{1}{E - D - \epsilon_{k'}} \right) \quad (2.4.131)$$

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

$$\frac{d J_d^z}{d D} = -J_T^2 N \frac{2}{D} \quad (2.4.132)$$

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

Renormalization of J_T

Consider the scattering

$$k \uparrow d \downarrow \rightarrow q \downarrow d \uparrow \rightarrow k' \downarrow d \uparrow \quad (2.4.133)$$

$$T_1 = -J_T J_z S_d^z S_d^+ N |\delta D| c_{k'\downarrow}^\dagger c_{k\uparrow} \frac{1}{E - D + \epsilon_k} \quad (2.4.134)$$

The minus sign at the front comes from the term

$$-S_d^z c_{k'\downarrow}^\dagger c_{q\downarrow} \quad (2.4.135)$$

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

$$T_1 = -J_T J_z \frac{S_d^+}{2} N |\delta D| c_{k'\downarrow}^\dagger c_{k\uparrow} \frac{1}{E - D + \epsilon_k} \quad (2.4.136)$$

The second process is

$$\begin{array}{c} \textcolor{blue}{95} \\ q \uparrow k \uparrow d \downarrow \rightarrow k' \downarrow k \uparrow d \uparrow \rightarrow q \uparrow k' \downarrow d \uparrow \end{array} \quad (2.4.137)$$

$$T_2 = -J_T J_z \frac{S_d^+}{2} N |\delta D| c_{k'\downarrow}^\dagger c_{k\uparrow} \frac{1}{E - D - \epsilon_{k'}} \quad (2.4.138)$$

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

$$+S_d^z c_{k'\uparrow}^\dagger c_{q\uparrow} \quad (2.4.139)$$

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

$$-S_d^z c_{k'\downarrow}^\dagger c_{q\downarrow} \quad (2.4.140)$$

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 proces.

$$T_3 = T_1 \quad (2.4.141)$$

$$T_4 = T_2 \quad (2.4.142)$$

The total contribution is

$$T^{(2)} = -J_T J_z S_d^+ N |\delta D| c_{k'\downarrow}^\dagger c_{k\uparrow} \left(\frac{1}{E - D - \epsilon_{k'}} + \frac{1}{E - D + \epsilon_k} \right) \quad (2.4.143)$$

Comparing with the S_d^+ term in the Hamiltonian

$$J_T S_d^+ c_{k'\downarrow}^\dagger c_{k\uparrow} \quad (2.4.144)$$

we can write

$$\delta J_T = -J_T J_z N |\delta D| \left(\frac{1}{E - D - \epsilon_{k'}} + \frac{1}{E - D + \epsilon_k} \right) \quad (2.4.145)$$

Again neglecting the terms in the denominator, we get

$$\frac{dJ_T}{dD} = -J_T J_z N \frac{2}{D} \quad (2.4.146)$$

This is the scaling equation for J_T .

Flow of the couplings

Switching to the dimensionless couplings

$$g_1 = NJ_z, g_2 = NJ_T \quad (2.4.147)$$

the equations become

$$\frac{dg_1}{dD} = -\frac{2g_2^2}{D} \quad (2.4.148)$$

$$\frac{dg_2}{dD} = -\frac{2g_1 g_2}{D} \quad (2.4.149)$$

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

$$\frac{dg_1}{dg_2} = \frac{g_2}{g_1} \implies g_1^2 - g_2^2 = \text{constant} \quad (2.4.150)$$

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

$$\begin{aligned} g(D') &= \frac{g_0}{1 - 2g_0 \ln \frac{D}{D'}} \\ \implies 2g(D') &= \frac{1}{\ln \frac{D'}{T_K}} \end{aligned} \quad (2.4.151)$$

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.

$$g(D') = \frac{g_0}{1 - 2g_0 \ln \frac{D}{D'}} = -\frac{|g_0|}{1 + 2|g_0| \ln \frac{D}{D'}} \quad (2.4.152)$$

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

$$\Delta H_{ll'} = \frac{1}{2} [T_{ll'}(E_l) + T_{ll'}(E_{l'})] \quad (2.4.153)$$

where the transition matrix T is

$$T_{ll'}(E) = \sum_H \frac{V_{lH} V_{Hl'}}{E - E_H} \quad (2.4.154)$$

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

$$V = J \vec{S}_d \cdot \sum_{k, k', \alpha, \alpha'} c_{k\alpha}^\dagger \vec{\sigma}_{\alpha\alpha'} c_{k'\alpha'} \quad (2.4.155)$$

The first process is

$$k\alpha \xrightarrow{\sigma^b} q\lambda \xrightarrow{\sigma^a} k'\beta \quad (2.4.156)$$

$$d\sigma \xrightarrow{S_d^b} d\sigma'' \xrightarrow{S_d^a} d\sigma' \quad (2.4.157)$$

The transition matrix element is

$$\begin{aligned} T_1 &= \sum_{q \in \{D - \delta D\}, \lambda, \sigma''} \langle k'\beta, \sigma' | V | q\lambda, \sigma'' \rangle \langle q\lambda, \sigma'' | V | k\alpha, \sigma \rangle \frac{1}{E - E_q} \\ &= J^2 \sum_{\sigma''} (S_d^a)_{\sigma'\sigma''} (S_d^b)_{\sigma''\sigma} \sum_{\lambda} (\sigma^a)_{\beta\lambda} (\sigma^b)_{\lambda\alpha} \sum_{q \in \{D - \delta D\}} \frac{1}{E - E_q} \\ &\approx J^2 (S_d^a S_d^b)_{\sigma'\sigma} (\sigma^a \sigma^b)_{\beta\alpha} \frac{N|\delta D|}{E - D} \end{aligned} \quad (2.4.158)$$

The second process is

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

$$q\lambda \xrightarrow{\sigma^b} k'\beta \longrightarrow k'\beta \quad (2.4.160)$$

$$d\sigma \xrightarrow{S_d^b} d\sigma'' \xrightarrow{S_d^a} d\sigma' \quad (2.4.161)$$

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

$$\begin{aligned} T_2 &= \sum_{q \in \{D - |\delta D|\}, \lambda, \sigma''} \langle q\lambda, k' \beta, \sigma' | V | k' \beta, k\alpha, \sigma'' \rangle \langle k' \beta, k\alpha, \sigma'' | V | q\lambda, k\alpha, \sigma \rangle \frac{1}{E - (E_k + E_{k'} - E_q)} \\ &\approx -J^2 (S_d^a S_d^b)_{\sigma' \sigma} (\sigma^b \sigma^a)_{\beta \alpha} \frac{N|\delta D|}{E - D} \end{aligned} \quad (2.4.162)$$

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

$$\begin{aligned} T &= \frac{J^2 N |\delta D|}{D} (S_d^a S_d^b)_{\sigma' \sigma} [\sigma^b, \sigma^a]_{\beta \alpha} \\ &= \frac{J^2 N |\delta D|}{2D} [S_d^a, S_d^b]_{\sigma' \sigma} [\sigma^b, \sigma^a]_{\beta \alpha} \end{aligned} \quad (2.4.163)$$

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

$$\begin{aligned} [S_d^a, S_d^b]_{\sigma' \sigma} [\sigma^b, \sigma^a]_{\beta \alpha} &= -[S_d^a, S_d^b]_{\sigma' \sigma} [\sigma^a, \sigma^b]_{\beta \alpha} \\ &= -i\epsilon_{abc} S_{\sigma \sigma'}^c 2i\epsilon_{abd} \sigma_{\beta \alpha}^d \\ &= 4\delta_{cd} S_{\sigma \sigma'}^c \sigma_{\beta \alpha}^d \\ &= 4\vec{S}_{\sigma \sigma'} \cdot \vec{\sigma}_{\beta \alpha} \end{aligned} \quad (2.4.164)$$

Therefore,

$$T = \frac{2J^2 N |\delta D|}{D} \vec{S}_{\sigma \sigma'} \cdot \vec{\sigma}_{\beta \alpha} \quad (2.4.165)$$

The correction to the coupling J can be read off:

$$J(D - \delta D) = J(D) - \frac{2J^2 N \delta D}{D} \quad (2.4.166)$$

This gives the same scaling equations we found earlier.

2.4.7 Universality

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

$$\frac{\partial g}{\partial \ln D} = -2g^2 + 2g^3 \quad (2.4.167)$$

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

$$\ln \frac{D'}{D} = - \int_{g_0}^{g'} \frac{dg}{2g^2 - 2g^3} = - \int_{g_0}^{g'} \frac{dg}{2g^2} (1 + g) \quad (2.4.168)$$

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

$$\begin{aligned} \ln \frac{k_B T_K}{D} &= - \int_{g_0}^1 \frac{dg}{2g^2} (1 + g) = -\frac{1}{2g_0} + \frac{1}{2} \ln g_0 + O(1) \\ &= -\frac{1}{2g_0} + \frac{1}{2} \ln 2g_0 + O(1) \end{aligned} \quad (2.4.169)$$

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This gives a better estimate of the Kondo temperature

$$T_K = \frac{D}{k_B} \sqrt{2g_0} \exp\left(-\frac{1}{2g_0}\right) \quad (2.4.170)$$

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

$$k_B T_K = D y(g) \quad (2.4.171)$$

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

$$\frac{dT_K}{dD} = 0 \quad (2.4.172)$$

Substituting the form of T_K , eq. 2.4.171, in this equation gives

$$\begin{aligned} y(g) + D \frac{dy(g)}{dD} &= 0 \\ \implies y + D \frac{dy}{dg} \frac{dg}{dD} &= 0 \\ \implies y - 2g^2 \frac{dy}{dg} &= 0 \\ \implies y &= e^{-\frac{1}{2g}} \end{aligned} \quad (2.4.173)$$

This gives almost the same solution as eq. 2.4.170:

$$T_K = \frac{D}{k_B} e^{-\frac{1}{2g}} \quad (2.4.174)$$

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. 2.4.151, up to second order, we can write

$$g(D') = g_0 \left(1 + 2g_0^2 \ln \frac{D}{D'} \right) \quad (2.4.175)$$

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

$$g_0 \rightarrow g = g_0 \left(1 + 2g_0 \ln \frac{T_F}{T} \right) \quad (2.4.176)$$

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 Method of pseudo-fermions

Spin operators, unlike fermionic creation and annihilation operators, do not satisfy Wick's theorem. To remedy this, they can be factorised into fermionic operators [17]. For example,

$$S^z = \frac{\sigma^z}{2} = \sum_{ij} c_i^\dagger \frac{\sigma^z_{ij}}{2} c_j = \frac{1}{2} (c_\uparrow^\dagger c_\uparrow - c_\downarrow^\dagger c_\downarrow) \quad (2.4.177)$$

Similarly,

$$\begin{aligned} S^x &= \frac{1}{2} (c_\uparrow^\dagger c_\downarrow + c_\downarrow^\dagger c_\uparrow) \\ S^y &= \frac{-i}{2} (c_\uparrow^\dagger c_\downarrow - c_\downarrow^\dagger c_\uparrow) \end{aligned} \quad (2.4.178)$$

Now, the state $|\uparrow\rangle$ can be represented as

$$|\uparrow\rangle = c_{\uparrow}^{\dagger} |0\rangle \quad (2.4.179)$$

This however means that we get two other states in the Hilbert space, $|0\rangle$ and $|\uparrow\downarrow\rangle$, which are not allowed physically. To remove them, we can do the following. We can modify the Hamiltonian H , by introducing a complex chemical potential [18]

$$\mu = -i\frac{\pi}{2}k_B T \quad (2.4.180)$$

The new Hamiltonian is

$$\tilde{H} = H - \mu(n_d - 1) \quad (2.4.181)$$

The new partition function is then allowed to run over the entire Hilbert space, including the unphysical states. The actual partition function for the original Hamiltonian H is

$$Z = \text{Tr} \left[\exp(-\beta H) \right] = \sum_{\sigma_d=\uparrow,\downarrow} \sum_k \left[\exp(-\beta H) \right] \quad (2.4.182)$$

⁵⁶ The modified partition function is

$$\begin{aligned} \tilde{Z} &= \text{Tr} \left[\exp \left(-\beta (H - \mu(n_d - 1)) \right) \right] \\ &= \text{Tr} \left[\exp \left(-\beta H - i\frac{\pi}{2}(n_d - 1) \right) \right] \\ &= \sum_{\sigma_d=\uparrow,\downarrow} \sum_k \left[\exp(-\beta H) \right] + \sum_k \exp \left(-\beta H + i\frac{\pi}{2} \right) + \sum_k \exp \left(-\beta H - i\frac{\pi}{2} \right) \\ &= Z \Big|_{n_d=1} + iZ \Big|_{n_d=0} - iZ \Big|_{n_d=0} \end{aligned} \quad (2.4.183)$$

Since the Hamiltonian involves the impurity electrons only as spin operators, and since $S_d(0) = 0 = S_d(\uparrow\downarrow)$, we have

$$Z \Big|_{n_d=0} = Z \Big|_{n_d=0} \quad (2.4.184)$$

Hence,

$$\tilde{Z} = Z \quad (2.4.185)$$

Thus, we are able to retain the correct partition function because of the introduction of the complex chemical potential.

This method can also be used to determine the higher order corrections to the susceptibility. The zeroth order diagrams are

The dotted lines are the impurity Greens function, so that diagram gives the impurity contribution to the susceptibility. Similarly, the solid lines are the conduction electron Greens function. The first diagram gives

$$\chi_c = -k_B T \sum_{k,\omega_n,\phi_0} \langle \phi_0 | \sigma^a G(k, i\omega_n) \sigma^b G_k(i\omega_n) | \phi_0 \rangle \quad (2.4.186)$$

The sum over the ground states $|\phi_0\rangle$ constitutes a trace, so we can write it as

$$\begin{aligned}
 \chi_c &= -k_B T \sum_{k, \omega_n} \text{Tr} [\sigma^a G(k, i\omega_n) \sigma^b G(k, i\omega_n)] \\
 &= -2k_B T \sum_{k, \omega_n} G^2(k, i\omega_n) \\
 &= -2k_B T \sum_{k, \omega_n} (i\omega_n - \epsilon_k)^{-2} \\
 &= 2 \sum_k \frac{d}{d\epsilon_k} k_B T \sum_{\omega_n} (i\omega_n - \epsilon_k)^{-1}
 \end{aligned} \tag{2.4.187}$$

Now, it can be shown that

$$k_B T \sum_{\omega_n} (i\omega_n - \epsilon_k)^{-1} = f(\epsilon_k) - \frac{1}{2} \tag{2.4.188}$$

where $f(\epsilon_k)$ is the FD-distribution at ϵ_k . Therefore,

$$\chi_c = 2 \sum_k \frac{df(\epsilon_k)}{d\epsilon_k} = 2 \sum_k \rho(\epsilon_k) = 2N(0) \tag{2.4.189}$$

The second diagram gives

$$\chi_d^{(0)} = -k_B T \sum_{\omega_n} \text{Tr} [\sigma^a G_d(i\omega_n) \sigma^b G_d(i\omega_n)] \tag{2.4.190}$$

In the Popov-Fedotov scheme, we replace the impurity Greens function with

$$G_d = \frac{1}{i\omega_n - \lambda_d} \tag{2.4.191}$$

where $\lambda_d = i\pi \frac{1}{2\beta}$ is the imaginary chemical potential introduced. Since this is, for mathematical purposes, the same as the conduction Greens function with λ_d replacing ϵ_k , we again get

$$\chi_d^{(0)} = 2 \frac{df(\lambda_d)}{d\lambda_d} = -2\beta \frac{e^{\beta\lambda_d}}{(1 + e^{\beta\lambda_d})^2} = \beta \tag{2.4.192}$$

The first order diagrams are The first diagram gives

$$\chi^{(1)} = \chi_c \left(-\frac{J}{2} \right) \chi_d = -\beta J N(0) \tag{2.4.193}$$

The second one gives

$$\chi_d^{(1)} = \chi_d \left(-\frac{J}{2} \right) \chi_c = -\beta J N(0) \tag{2.4.194}$$

The total susceptibility is

$$\chi_d = \chi_d^{(0)} + \chi_d^{(1)} = \beta (1 - 2J N(0)) \tag{2.4.195}$$

2.4.9 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

$$C_V = \gamma T \tag{2.4.196}$$

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

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

$$E_g = J [2\vec{S}_e \cdot \vec{S}_d] = J [S^2 - S_d^2 - S_e^2] = J \left[s(s+1) - \frac{3}{2} \right] = -\frac{3J}{2} \tag{2.4.197}$$

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

$$\frac{|0_\uparrow, d\downarrow\rangle - |0_\downarrow, d\uparrow\rangle}{\sqrt{2}} \quad (2.4.198)$$

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

$$E_1 = -\frac{3}{2}J + \frac{3}{2}J = 0 \quad (2.4.199)$$

because the new electron would have the spin opposite to the other electron on the 0th 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 [8] 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

$$\psi \sim \frac{\sin [kr + \delta(E_k)]}{r} \quad (2.4.200)$$

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.

$$n = \sum_{\sigma} \frac{\delta}{\pi} \implies 1 = \frac{2\delta}{\pi} \implies \delta = \frac{\pi}{2} \quad (2.4.201)$$

²⁵ 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. 2.4.200, by substituting $k = k_F$ and noting that the isolation of the 0th site means all wavefunctions should shift by $\Delta r = a$:

$$k_F a = \delta(0) \implies \delta(0) = \frac{\pi}{2a} 2 = \frac{\pi}{2} \quad (2.4.202)$$

where the formula for k_F was used.

In a Fermi gas, the energy levels are separated by

$$\Delta\epsilon = \frac{\partial\epsilon}{\partial k} \Delta k \quad (2.4.203)$$

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

$$\Delta\epsilon = \frac{\partial\epsilon}{\partial k} \frac{\pi}{L} \quad (2.4.204)$$

However, this changes in the presence of the impurity. Because of eq. 2.4.200, the boundary condition becomes

$$k_n L + \delta(\epsilon_k) = n\pi \implies k_n = \frac{n\pi}{L} - \frac{\delta}{L} = k_n^0 - \frac{\delta(\epsilon_k)}{L} \quad (2.4.205)$$

The energy becomes

$$\begin{aligned}\epsilon(k) &= \epsilon(k^0) + \frac{\partial\epsilon}{\partial k}(k - k_0) \\ &= \epsilon_k - \frac{\partial\epsilon}{\partial k} \frac{\delta(\epsilon_k)}{L}\end{aligned}\quad (2.4.206)$$

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

$$\tilde{\epsilon}_\sigma(k) = \epsilon_k - \frac{\partial\epsilon}{\partial k} \frac{\delta_\sigma(\epsilon_k, \{n_{q\sigma}\})}{L} \quad (2.4.207)$$

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 ,

$$\begin{aligned}\tilde{\epsilon}_p &= \underbrace{\epsilon_F}_{\text{Fermi gas}} + \overbrace{\frac{p_F^*}{m}(p - p_F)}^{\text{linear contribution for } p \text{ close to } p_F} \\ &\quad + \underbrace{\sum_{q\sigma} f(p, q)(n_q - n_q^0)}_{\text{interacting between two quasiparticles at momenta } p \text{ and } q}\end{aligned}\quad (2.4.208)$$

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,

$$\delta_\sigma(\tilde{\epsilon}, \{n_{q\sigma}\}) = \delta_\sigma(\tilde{\epsilon} = \epsilon_F, n_k = n_k^0) + \alpha(\tilde{\epsilon} - \epsilon_F) + \Phi \sum_{q\sigma'} (n_{q\sigma'} - n_{q\sigma'}^0) \quad (2.4.209)$$

This is just a Taylor expansion of δ_σ around $\tilde{\epsilon} = \epsilon_F$ and $n_q = n_q^0$. Φ and α play the same role as f and $\frac{p_F^*}{m}$ in eq. 2.4.208. Specifically, Φ represents the onsite interaction between quasiparticles of opposite spin and

$$\alpha = \frac{d\delta_\sigma}{dE} \quad (2.4.210)$$

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

$$\delta_\sigma(\tilde{\epsilon}, \{n_{q\sigma}\}) = \delta_\sigma(\tilde{\epsilon} = \epsilon_F, n_k = n_k^0) + \alpha(\tilde{\epsilon} - \epsilon_F) + \Phi \sum_q \delta n_{q,-\sigma} \quad (2.4.211)$$

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,

$$\delta_\uparrow^0 = \frac{\pi}{2} + \Phi \sum_q \delta n_{q,\downarrow}^0 \quad (2.4.212)$$

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

$$\delta_\uparrow^0 = \frac{\pi}{2} \quad (2.4.213)$$

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

$$N(\mu = 0) = N^0 \quad (2.4.214)$$

$$N(E' = E + \mu) = N(E' = E) + \frac{dN}{dE'} (E' - E) = N^0 + \rho \Delta\mu \quad (2.4.215)$$

$$\Rightarrow \sum_q \delta n_q = N - N^0 = \rho \Delta\mu \quad (2.4.216)$$

Hence, from eq. 2.4.211,

$$\begin{aligned}\delta_{\uparrow} &= \frac{\pi}{2} + \alpha (\epsilon'_F - \epsilon_F) + \Phi \sum_q \delta n_{q\downarrow} \\ &= \delta_{\uparrow}^0 + \alpha \Delta \mu + \Phi \rho \Delta \mu\end{aligned}\quad (2.4.217)$$

Hence the change in the phase is

$$0 = \Delta \delta_{\uparrow} = \Delta \mu (\alpha + \Phi \rho) \implies \alpha = -\Phi \rho \quad (2.4.218)$$

This shows that the interaction term Φ 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

$$n_{\sigma} = \frac{kL}{\pi} + \frac{\delta_{\sigma}(E)}{\pi} = n^0 + \frac{\delta_{\sigma}(E)}{\pi} \quad (2.4.219)$$

Hence,

$$\begin{aligned}\rho &= \frac{dn_{\sigma}}{dE} = \rho^0 + \frac{1}{\pi} \frac{d\delta_{\sigma}}{dE} \\ \implies \rho &= \rho^0 + \frac{1}{\pi} \alpha\end{aligned}\quad (2.4.220)$$

ρ^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

$$C_v^0 = \gamma T = \frac{\pi^2 k_B^2}{3} \mathcal{N}(0) T \quad (2.4.221)$$

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

$$\begin{aligned}C_v &= \frac{\pi^2 k_B^2}{3} (\rho_{\uparrow} + \rho_{\downarrow}) T \\ &= \frac{2\alpha}{\pi} \frac{\pi^2 k_B^2}{3} T\end{aligned}\quad (2.4.222)$$

In presence of a magnetic field B , the magnetization is

$$m = \delta n \times \mu \quad (2.4.223)$$

where μ is the magnetic moment

$$\mu = -\frac{g}{2} \mu_B \quad (2.4.224)$$

and δn is the difference in number between up and down electrons

$$\delta n = \langle n_{\uparrow} \rangle - \langle n_{\downarrow} \rangle = \frac{1}{\pi} (\delta_{\uparrow} - \delta_{\downarrow}) \quad (2.4.225)$$

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

$$E_{\sigma}^B = E - \sigma \frac{g\mu_B}{2} B \quad (2.4.226)$$

Hence,

$$\sum_k \delta n_{k\sigma} = N_{\sigma}(E_{\sigma}^B) - N(E) = \frac{dN}{dE^B} (E^B - E) = -\rho \frac{g\mu_B}{2} \sigma B \quad (2.4.227)$$

This modifies the phase shift at the Fermi surface,

$$\begin{aligned}\delta_\sigma(\epsilon_F) &= \frac{\pi}{2} + \alpha \left(\epsilon_F - \frac{g\mu_B}{2} \sigma B - \epsilon_F \right) + \Phi \sum_q \delta n_{q,-\sigma} \\ &= \frac{\pi}{2} - \sigma \frac{g\mu_B}{2} \alpha B + \Phi \rho \frac{g\mu_B}{2} \sigma B \\ &= \frac{\pi}{2} - 2\alpha \frac{g\mu_B}{2} \sigma B\end{aligned}\quad (2.4.228)$$

Hence,

$$\delta n = \frac{1}{\pi} (\delta_\uparrow - \delta_\downarrow) = -\frac{4\alpha B}{\pi} \frac{g\mu_B}{2} \quad (2.4.229)$$

The susceptibility is

$$\chi = \frac{\partial m}{\partial B} = \frac{\partial}{\partial B} \mu \delta n = \frac{4\alpha}{\pi} \left(\frac{g\mu_B}{2} \right)^2 \quad (2.4.230)$$

The susceptibility for an ideal Fermi gas can be calculated similarly. The additional energy of an electron with spin σ 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 μ is the magnetic moment

$$\mu = -\frac{g}{2} \mu_B \quad (2.4.231)$$

and δn is the difference in number between up and down electrons

$$\delta n = n_\uparrow(0) - n_\downarrow(0) = n_\uparrow(\epsilon_F - \frac{g}{2} \mu_B B) - n_\downarrow(\epsilon_F + \frac{g}{2} \mu_B B) = -\frac{1}{2} \mathcal{N}(0) g B \mu_B \quad (2.4.232)$$

26 $\mathcal{N}(0) = \frac{\partial n}{\partial E} \Big|_{\epsilon_F}$ 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,

$$m = \delta n \times \mu = \mathcal{N}(0) \left(\frac{g}{2} \mu_B \right)^2 B \quad (2.4.233)$$

The magnetic susceptibility comes out to be

$$\chi^0 = \frac{\partial m}{\partial B} \Big|_{B \rightarrow 0} = \mathcal{N}(0) \left(\frac{g}{2} \mu_B \right)^2 \quad (2.4.234)$$

The Wilson ratio R can now be computed,

$$R = \frac{\chi/\chi_0}{C_v/C_v^0} = \frac{4\alpha/\pi \mathcal{N}(0)}{2\alpha/\pi \mathcal{N}(0)} = 2 \quad (2.4.235)$$

2.5 Numerical renormalization group calculation

Wilson's idea [19] 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

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

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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 γ_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

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

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^{th} interval $k \in [\Lambda^{-(n+1)}, \Lambda^{-n}]$,

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

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 $-k \in [\Lambda^{-(n+1)}, \Lambda^{-n}]$.

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

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

Then,

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

Summing over n involves summing over all momenta.

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

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

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

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 \overline{H}_{N+1} and \overline{H}_N ,

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

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

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

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

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

The next Hamiltonian is then

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

This is the same equation as eq. 2.5.26, with \overline{H}_{N+1} 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 [16]: 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 [20] 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 ϵ_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,

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

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 ϵ_F , the number of excitations is given usually:

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

where n_k^p stands for the number of particles. For states below ϵ_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, eq. 2.2.19, 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. 2

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

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

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

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 χ

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

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

2 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

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

4 Relation between the density of states and scattering phase shift

The Green's function is of the general form

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

3 Close to the Fermi surface, the imaginary part of the self energy goes as ω^2 . Therefore, up to first order in ω , 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 :

$$\begin{aligned}G &= \overset{43}{G^{(0)}} + G^{(0)} V G_d^{(0)} V G^{(0)} + \overset{43}{G^{(0)} V G_d^{(0)} V G^{(0)} V G_d^{(0)} V G^{(0)}} + \dots \\ &= G^{(0)} + G^{(0)} V \left[G_d^{(0)} + G_d^{(0)} V G^{(0)} V G_d^{(0)} \right] V G^{(0)} \\ &= G^{(0)} + G^{(0)} V^2 G_d G^{(0)}\end{aligned}\quad (2.6.26)$$

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 point¹, 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 the⁵ particle-hole symmetry intact (by suitably shifting the impurity levels), the resonance¹⁰⁵ 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 Δn_\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

⁸ From the Friedel sum rule[21], 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 [22]

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

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 [4] 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 ΔV_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 [8].

2.8 Renormalized perturbation theory

⁴⁸ 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 quasi-particle 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.

⁴⁹ 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 \sim represents the renormalised quantities

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

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

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

The Anderson hamiltonian

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

3 can be written in the form

$$H = \tilde{H}_{qp} - \tilde{H}_c\tag{2.8.7}$$

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

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

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

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

$$\tilde{c}_d^\dagger = \sqrt{z} c_d^\dagger\tag{2.8.10}$$

$$\tilde{c}_d = \sqrt{z} c_d\tag{2.8.11}$$

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

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

where

$$\lambda_1 = z\Sigma(0, 0)\tag{2.8.13}$$

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

93 \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

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

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

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

This is the third constraint. The perturbation expansion is in powers of the renormalised interaction \tilde{U} . The parameters that are determined by the expansion are λ_1, λ_2, z . Hence, they should be expanded in powers of \tilde{U} .

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

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

$$(2.8.21)$$

The expansion is about the ³ non-interacting quasiparticle Hamiltonian. The corresponding Green's function is

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

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

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

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

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

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

³ The first order Feynman diagram for the self-energy is of the Hartree type. They give a contribution

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

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

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

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

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

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

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

We can recognize that

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

Therefore,

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

Up to first order, we can write

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

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

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

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

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

Substituting in to the parent equation, we get

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

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.

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

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

Multiplying both equations throughout by Z , we get

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

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

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

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

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

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

These can be used to prove the mean-field results regarding specific heat and the susceptibilities. Similar to the mean field treatment, close to $T = 0$, the effects of the self energy vanish, and the specific heat linear term, γ , 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,

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

2.9 ⁴² 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 fig. 2.2a. 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 ϵ_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 fig. 2.2b 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 hybridise 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

(a)	(b)
Sub-	Sub-
cap-	cap-
tion	tion
1	1

is the following. We are working with the asymmetric Anderson model, that is, $U + \epsilon_d \gg D \gg |\epsilon_d|, \Delta$. The total Hamiltonian is

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

⁴⁴ 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

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

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

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

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 $|1_{d\sigma}\rangle$. 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 ϵ_d , and not the hybridisation coupling V_{kd} . To find the renormalization in the site energies ϵ_0 and ϵ_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 ϵ_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 $E \in \{-D, D\}$.

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

The change in ϵ_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 ϵ_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 ϵ_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 ϵ_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 ϵ_0 and ϵ_1 discussed earlier.

We do not yet know whether Δ is a function of the cutoff D . To find the renormalization of Δ , 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 Δ , 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 ϵ_1 and ϵ_0 will change equally and there won't be any scaling in ϵ_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 ϵ_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 ϵ_d with $\tilde{\epsilon}_d$ in eq. 2.4.26. For simplicity set $U = \infty$. Then,

$$\tilde{J} = -\frac{|V|^2}{\tilde{\epsilon}_d} = \frac{a|V|^2}{D} \quad (2.9.24)$$

Figure 2.2: Renormalization in the energy levels when $\epsilon_d^* \gg \Delta$

We can then do the poor man's scaling with this coupling. From eq. 2.4.170,

$$\begin{aligned} T_K &\sim D \sqrt{\tilde{J}N(0)^2} \exp\left(-\frac{1}{2\tilde{J}N(0)^2}\right) = \sqrt{\Delta D} \exp\left(-\frac{D}{2\Delta}\right) \\ &\sim D \sqrt{\frac{\Delta}{D}} \exp\left(\frac{\epsilon_d}{2\Delta}\right) \end{aligned} \quad (2.9.25)$$

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, fig. 2.2a. Assuming $U \rightarrow \infty$ and ϵ_d outside the conduction band, we can do a SWT and the T_K obtained is q. 2.4.170,

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

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

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

The two forms of the Kondo temperature show that the prefactor is not a universal function; it depends on the starting conditions (the microscopic Hamiltonian from which we start the scaling). But the universal fact is that in the local moment regime ($U \rightarrow \infty$), all physical quantities will involve only one energy scale, T_K . This T_K itself might be different based on the starting Hamiltonian.

For $\epsilon_d^* \gg \Delta$, the renormalization will stop at $D \sim \epsilon_d$. Note that we had assumed $D \gg \epsilon_d$. That was the starting condition, that is, ϵ_d deep inside the Fermi surface. During the renormalization, D will keep on decreasing and ϵ_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 $\overline{D} = a\epsilon_d(\overline{D}) \equiv \bar{\epsilon}_d$ 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 \overline{D} . We can hence substitute $D = a\bar{\epsilon}_d$, $\epsilon_d = \bar{\epsilon}_d$. With this in mind, the susceptibility becomes

$$\begin{aligned} \chi_d &= \frac{\Delta}{2\pi} \left(\frac{g\mu_B}{\bar{\epsilon}_d} \right)^2 \left[1 + \frac{2\Delta}{\pi\bar{\epsilon}_d} \ln a + \dots \right] \\ &= \frac{\Delta}{2\pi} \left(\frac{g\mu_B}{\bar{\epsilon}_d} \right)^2 \left[1 + O\left(\frac{2\Delta}{\pi\bar{\epsilon}_d}\right) \right] \end{aligned} \quad (2.9.31)$$

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 Δ . From eq. 2.9.29, we can drop the π 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 Δ 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 ϵ_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 χT .

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

$$\chi T = \frac{1}{2D} \quad (2.9.49)$$

where $Z(h=0) = 2 + 2 = 4 = D$ is the degeneracy.

Similarly, for the triplet case (ϵ_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 $Z(h=0) = 1 + 2 = 3 = D$.

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 Δ . 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

$$m^{(1)} = \frac{g\mu_B}{2} (n_\uparrow - n_\downarrow) = \frac{g\mu_B}{2\pi} \left[\tan^{-1} \frac{\Delta}{k_B T^* - h} - \tan^{-1} \frac{\Delta}{k_B T^* + h} \right] \quad (2.9.54)$$

Figure 2.3: Renormalization in energy levels when $|\epsilon_d^*| \lesssim \Delta$

80 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

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

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

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

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

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 .

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

Next we consider the mixed valence regime, described by $|\epsilon_d^*| < \Delta$. It is clear that since the impurity level is within an interval of the hybridisation from the Fermi 37 face, 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 Δ or $k_B T$, whichever is greater. From eq. 2.9.19, we know that if D comes close to Δ , 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

$$(\epsilon_d)_{MV} = \epsilon_d^* \quad (2.9.60)$$

Figure 2.4: Renormalization in energy levels when $\epsilon_d^* \ll -\Delta$

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 Δ , for $\epsilon_d \gg \Delta$, this transition will not be possible. However, in the mixed valence regime, because $\epsilon_d \sim \Delta$, these excitations do occur. These fluctuations, as well as 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.

$$\begin{array}{lll} n_d = 1 & n_d = \frac{2}{3} & n_d = \text{fractional} \\ \chi T = \frac{1}{8} & \Rightarrow \chi T = \frac{1}{6} & \Rightarrow \chi T \propto T \\ T \gg U & T \gg \Delta & T \ll \Delta \end{array}$$

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.

$$\begin{array}{lll} n_d = 1 & n_d = \frac{2}{3} & n_d = 1 \\ \chi T = \frac{1}{8} & \Rightarrow \chi T = \frac{1}{6} & \Rightarrow \chi T = \frac{1}{4} \\ T \gg U & T \gg \tilde{T} & T \ll \tilde{T} \\ & & T \ll T_K \end{array}$$

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 ψ_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 ϕ . 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 if d , we can say that P takes d eigenstates ψ 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 ψ_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 Ω 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 ϕ into the model subspace is ϕ itself. Together these two identities give

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

With these definitions, we no ¹⁹ 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 ϕ . To remove the Ω 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 Ω , 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 Ω 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

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

The second order equation is

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

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

$$A_1 = -Q V P \quad (2.9.83)$$

$$A_2 = -Q V \Lambda_1 + \Lambda_1 V P \quad (2.9.84)$$

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

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

we can write the solution

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

1 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

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

The lowest order solutions are thus

$$\Lambda_1 = S(Q V P) = S(V P) \quad (2.9.90)$$

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

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

$$\begin{aligned} H_{\text{eff}} - PH_0P &= PV\Omega \\ &\approx P \overset{36}{45} \Lambda_0 + \Lambda_1 + \Lambda_2 \\ &= PV [P + S(VP) + S(VS(VP)) - S(S(VP)VP)] \\ &= PVP + PV S(VP) + PV S(VS(VP)) - PV S(S(VP)VP) \end{aligned} \quad (2.9.92)$$

Therefore,

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

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

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

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

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

The fourth term is

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

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

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

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

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

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

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

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

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

The total Hamiltonian can be written in the form

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

We now evaluate the changes:

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

I used the approximation

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

Also,

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

We now make the following assumptions:

- ϵ_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. Krishna ⁴² rthy, Wilkins and Wilson in ref. [6]. 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. The ⁴³ fixed points along with typical RG flows are marked in fig. 2.5. The free-orbital fixed point is described by $U = V = 0$. The local moment fixed point is described by

Figure 2.5: Schematic diagram of RG flows and fixed points of the symmetric SIAM, as obtained by ref.[6]. The y-axis is the impurity site repulsion $U = -\frac{1}{2}\epsilon_d$ [26] 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.

$U \rightarrow \infty, V = 16$ [92] 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

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 : $[\mathcal{H}, \hat{n}_k] \neq 0$. k labels any set of quantum numbers depending on the system. For spin-less Fermions it can be the momentum of the particle, while for spin-full Fermions it can be the set of momentum and spin. There are terms that scatter electrons from one quantum number k to another quantum number k' .

We take a general Hamiltonian,

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

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

$$\mathcal{H} = \begin{pmatrix} |1\rangle & |0\rangle \\ H_1 & T \\ T^\dagger & H_0 \end{pmatrix} \quad (3.1.2)$$

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

$$\tilde{\mathcal{H}} \equiv U\mathcal{H}U^\dagger = \begin{pmatrix} |1\rangle & |0\rangle \\ \tilde{H}_1 & 0 \\ 0 & \tilde{H}_0 \end{pmatrix} \quad (3.1.3)$$

U_q is defined by

$$\tilde{\mathcal{H}} = U_q \mathcal{H} U_q^\dagger \text{ such that } [\tilde{\mathcal{H}}, n_q] = 0 \quad (3.1.4)$$

It is clear that U is the diagonalizing matrix for \mathcal{H} . Hence we can frame this problem as an eigenvalue equation as well. Let $|\psi_1\rangle, |\psi_0\rangle$ be the basis in which the original Hamiltonian \mathcal{H} has no off-diagonal terms corresponding to $q\beta$. Hence, we can write

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

Since $|\psi_i\rangle$ is the set of eigenstates of \mathcal{H} and $|i\rangle$ is the set of eigenstates in which $U\mathcal{H}U^\dagger$ has no off-diagonal terms corresponding to $q\beta$, we can relate $|\psi_i\rangle$ and $|i\rangle$ by the same transformation : $|\psi_i\rangle = U^\dagger|i\rangle$. We can expand the state $|\psi_i\rangle$ in the subspace of $q\beta$:

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

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

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

The diagonal parts $H_e = \text{tr} [\mathcal{H} \hat{n}_{q\beta}]$ 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,

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

This gives

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

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

$$c_{q\beta}^\dagger T |0\rangle |\phi_0^i\rangle = (\omega_i^1 - \mathcal{H}^d) |1\rangle |\phi_1^i\rangle \quad (3.1.12)$$

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

$$T^\dagger c_{q\beta} |1\rangle |\phi_1^i\rangle = (\omega_i^0 - \mathcal{H}^d) |0\rangle |\phi_0^i\rangle \quad (3.1.13)$$

We now define two many-particle transition operators:

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

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

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

where $\hat{\omega}_i = \omega_i^0 (1 - \hat{n}_{q\beta}) + \omega_i^1 \hat{n}_{q\beta} = \begin{pmatrix} \omega_i^1 & \\ & \omega_i^0 \end{pmatrix}$ is a 2x2 matrix and $\mathcal{H}^d = \mathcal{H}_0^d (1 - \hat{n}_{q\beta}) + \mathcal{H}_1^d \hat{n}_{q\beta}$ and $G = (\hat{\omega} - \mathcal{H}^d)^{-1}$. It is easy to check that this reproduces the previous forms of η_0 and η_1^\dagger . We will later find that it

is important to demand that these two be Hermitian conjugates of each other; that constraint is imposed on the denominators:

$$\eta^\dagger(\omega_i^0) = \eta^\dagger(\omega_i^1) \implies \frac{1}{\omega_i^1 - \mathcal{H}^d} c_{q\beta}^\dagger T = c_{q\beta}^\dagger T \frac{1}{\omega_i^0 - \mathcal{H}^d} \quad (3.1.16)$$

Henceforth we will assume that this constraint has been imposed.

In terms of these operators, eq. 3.1.13 becomes

$$\begin{aligned} |1\rangle |\phi_1^i\rangle &= \eta^\dagger |0\rangle |\phi_0^i\rangle \\ |0\rangle |\phi_0^i\rangle &= \eta |1\rangle |\phi_1^i\rangle \end{aligned} \quad (3.1.17)$$

These allow us to write

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

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

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

rotation

$$U \mathcal{H} U^\dagger$$

$$[\mathcal{H}, \hat{n}] \neq 0 \quad [\mathcal{H}, \hat{n}] = 0$$

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

3.1.3 Properties of the many-body transition operators

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

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

Second is:

$$\begin{aligned} |1\rangle |\phi_1^i\rangle &= \eta^\dagger |0\rangle |\phi_0^i\rangle = \eta^\dagger \eta |1\rangle |\phi_1^i\rangle \stackrel{66}{\implies} \eta^\dagger \eta = \hat{n}_{q\beta} \\ |0\rangle |\phi_0^i\rangle &= \eta |1\rangle |\phi_1^i\rangle = \eta \eta^\dagger |0\rangle |\phi_0^i\rangle \implies \eta \eta^\dagger = 1 - \hat{n}_{q\beta} \end{aligned} \quad (3.1.21)$$

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.

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

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^ω , there exists a unitary transformation e^G where

$$G = \tanh^{-1} (\omega - \omega^\dagger) \quad (3.1.25)$$

Applying that to the problem at hand gives

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

Let $x = \tanh y$. Then,

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

Therefore,

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

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

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

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

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

There we used

$$\stackrel{15}{\left(\eta^\dagger - \eta\right)^2} = \eta^{\dagger 2} + \eta^2 - \left\{\eta^\dagger, \eta\right\} = -1 \quad \left[\because \eta^2 = \eta^{\dagger 2} = 0\right] \quad (3.1.31)$$

and hence

$$\stackrel{19}{\left(\eta^\dagger - \eta\right)^3} = -1 \left(\eta^\dagger - \eta\right) \quad (3.1.32)$$

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,

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

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

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

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

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

$$\eta\mathcal{H}\eta = \eta c_q^\dagger T \eta \quad (3.1.35)$$

and

$$\eta^\dagger\mathcal{H}\eta^\dagger = \eta^\dagger T^\dagger c_q \eta^\dagger \quad (3.1.36)$$

Group 2 becomes

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

To simplify this, we use the relation

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

which gives

$$\eta c_q^\dagger T \eta = T^\dagger c_q \quad (3.1.39)$$

Taking the Hermitian conjugate of eq. 3.1.39 gives

$$\eta^\dagger T^\dagger c_q \eta^\dagger = c_q^\dagger T \quad (3.1.40)$$

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

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

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

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

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

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

Putting it all together,

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

The renormalizing in the Hamiltonian is

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

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

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

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

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

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

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

3.1.7 Multiple off-diagonal terms

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

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

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 $\eta = (\eta^\dagger)^\dagger$ 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 ω_i .

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

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

$$\omega_i^0 - \omega_i^1 = E_i^0 - E_i^1 \quad (3.1.53)$$

and so

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

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 $[\eta^\dagger - \eta, \mathcal{H}_X]$:

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

3.1.8 Equivalence of the two unitaries and preservation of partial trace

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

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

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

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

This η will however be different from the η in eq. 3.1.29. The reason is, in order to get U_1 , we must start from the eigenvalue equation $\mathcal{H}|\psi_1\rangle = \tilde{H}_1|\psi_1\rangle$. This means that the corresponding $\hat{\omega}$ will be defined as $\hat{\omega}_1 = \tilde{H}_1 - \mathcal{H}^i$. On the other hand, in order to get U_0 we must start with $\mathcal{H}|\psi_0\rangle = \tilde{H}_0|\psi_0\rangle$, and hence this $\hat{\omega}$ will be $\hat{\omega}_0 = \tilde{H}_0 - \mathcal{H}^i$. This difference in the $\hat{\omega}$ will define two different sets of η :

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

The ω_j^i eigenvalues have both upper and lower indices. The upper index i signifies which eigenstate it relates to - $\omega_j|i\rangle = \omega_j^i|i\rangle$. The lower index refers to the exact eigenstate we started with - starting with $\mathcal{H}|\psi_j\rangle = \tilde{H}_j|\psi_j\rangle$ leads to ω_j . The two unitaries are

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

Since the two unitaries should give the same effective Hamiltonian, we require $U_1 = U_0$. That requires $\eta_1 = -\eta_0$. Comparing the expressions of the η 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 ω_i^j

At a particular step of the URG, there are two quantum fluctuation energy scales associated with each sector. If we rotate $|\psi_1\rangle$ to $|1\rangle$ (particle/occupied sector), the corresponding unitary will be a function of $\omega_1^{0,1}$. If we, on the other hand, rotate $|\psi_0\rangle$ to $|0\rangle$ (hole/unoccupied sector), the unitary will be a function of $\omega_0^{0,1}$. The superscript j signifies whether this particular ω_i^j is an eigenvalue corresponding to $|1, \phi_i\rangle$ or $|0, \phi_i\rangle$. ω_i^0 occurs in the many-body transition operator η , because η is preceded by c and hence it picks out the eigenstate $|0, \phi_i\rangle$. On the other hand, ω_i^1 occurs in the many-body transition operator η^\dagger , because that is preceded by c^\dagger . This constrains these two values, because we must have $\eta(\omega_i^0) = (\eta^\dagger(\omega_i^1))^\dagger$ (eq. 3.1.16), for each value of i , giving us two constraints in total. The subscript i signifies whether ω_i^j is a part of the particle sector unitary $U_1(\omega_1^j)$ or the hole sector unitary $U_0(\omega_0^j)$. As mentioned in the previous section, since both ways are equivalent, we must have $U_1 = U_0$ which leads to the constraints $\eta(\omega_0^j) = -\eta(\omega_1^j)$. All the independent constraints are listed below.

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

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

3.2 Prescription

Given a Hamiltonian

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

the goal is to look at the renormalization of the various couplings in the Hamiltonian as we decouple high energy electron states. Typically we have a shell of electrons at some energy D . During the process, we make one simplification. We assume that there is only one electron on that shell at a time, say with quantum numbers q, σ , and calculate the renormalization of the various couplings due to this electron. We then sum the momentum q over the shell and the spin β , and this gives the total renormalization due to decoupling the entire shell.

From eq. 3.1.45, the first two terms in the rotated Hamiltonian are just the diagonal parts of the bare Hamiltonian; they are unchanged in that part. The renormalization comes from the third term. For one electron $q\beta$ on the shell, the renormalization is

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

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

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

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*.

$$\Delta_1 \mathcal{H} = c_{q\beta}^\dagger \text{Tr}(\mathcal{H} c_{q\beta}) \eta_1\tag{3.2.4}$$

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

$$\Delta_0 \mathcal{H} = -\eta_1 c_{q\beta}^\dagger \text{Tr}(\mathcal{H} c_{q\beta})\tag{3.2.5}$$

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:

$$\Delta\mathcal{H} = c_{q\beta}^\dagger \text{Tr}(\mathcal{H}c_{q\beta}) \eta_1 + \eta_0 c_{q\beta}^\dagger \text{Tr}(\mathcal{H}c_{q\beta}) \quad (3.2.6)$$

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

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

This form of the total renormalization is identical to the one we use in the "Poor Man's scaling"-type of renormalization that was used to get the scaling equations in the Kondo and Anderson models [2, 26]. Writing down the forms of η and η^\dagger explicitly, we get

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

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

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

These equations will now need to be simplified. For example, in the particle sector, we can set $\hat{n}_{q\beta} = 0$ in the numerator, because there is no such excitation in the initial state. Similarly, in the hole sector, we can set $\hat{n}_{q\beta} = 1$ because that state was occupied in the initial state. Another simplification we typically employ is that $\mathcal{H}_{0,1}^d$ will, in general, have the energies of all the electrons. But we consider only the energy of the on-shell electrons in the denominator. After integrating out these electrons, we can rearrange the remaining operators to determine which term in the Hamiltonian it renormalizes and what is the renormalization.

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

3.3 Star Graph URG

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

Figure 3.2: Star Graph model

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

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

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

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 ϵ_i and J_i . As a simplification, we will ignore the lower nodes in the denominator and keep only the node currently being decoupled, ie node N . Since node 0 is connected to node N , we will keep node 0 in the denominator as well. Making this simplification gives

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

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

91 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_N^- . η 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 η , and the opposite values in the denominator of η_0^\dagger , because there is $S_0^+ S_N^- (S_N^+ S_0^-)$ in front of the Greens function of η (η_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 ω and ω' , we will write down their Poor Man's 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

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

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

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

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 ϵ_N and ϵ_0 .

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

3.3.2 Nature of flows

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

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

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 ϵ_0 such that $\tilde{\omega} - \frac{1}{2}\epsilon_0 > 0$, the denominator will be positive and the RG equation will be irrelevant. This means that ϵ_0 will keep on decreasing, and the denominator will keep on becoming more and more positive, meaning there cannot be a fixed point in this situation.

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

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

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

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

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

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

3.3.3 Effective Hamiltonians

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

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

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

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

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

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

3.3.4 Fixed points

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

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

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

3.4 Kondo Model URG

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

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

The goal is to disentangle an electron $q\beta$ from the Hamiltonian, q being the momentum and β 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 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

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

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

$$\begin{aligned} \eta &= \frac{1}{\omega - \mathcal{H}_d} \left[J_z \sum_k \beta S_d^z c_{k\beta}^\dagger c_{q\beta} + J_t \sum_k c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \right] \\ &= \sum_k \left[\frac{1}{\hat{\omega}_1 - E_1} J_z S_d^z \beta c_{k\beta}^\dagger c_{q\beta} + \frac{1}{\omega_3 - E_3} J_t c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \right] \end{aligned} \quad (3.4.6)$$

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 η as

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

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

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

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

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

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

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

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

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

Therefore,

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

The renormalization is therefore

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

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

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

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

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

and

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

The renormalization then becomes

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

3.4.2 Hole sector

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

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

where η_0 is defined in eq. 3.1.57.

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

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

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

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

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

3.4.3 Scaling equations

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

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

Summing over β and q gives

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

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

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

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 ω , where the J is relevant and there is a flow to a strong-coupling fixed point.⁶

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

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

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

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

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

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

3.4.4 Numerical Solutions

The symmetric scaling equation 3.4.28 was solved numerically with the choice $\omega = -\frac{\epsilon_q}{2}$, for both positive and negative bare values of J . For sufficiently low values of ω , the Kondo coupling J flows to the strong-coupling limit. This limit, as obtained from the URG, is of course finite. This can be reconciled with the NRG result $J^* = \infty$ by noting the fact that increasing the bare bandwidth D does increase the value of URG J^* , such that in the thermodynamic limit $D \rightarrow \infty$, 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 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).³¹

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

Chapter 4

Connection between URG and Other Canonical Transformations

2.1 Poor Man's Scaling

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

$$\mathcal{H} |\Psi\rangle = E |\Psi\rangle \quad (4.1.1)$$

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

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

$$|\Psi\rangle = \sum_i |\phi_0^i\rangle + \sum_i |\phi_1^i\rangle \quad (4.1.2)$$

The Hamiltonian can also be split as

$$\mathcal{H} = H_0 + V_+ + V_- \quad (4.1.3)$$

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

$$\begin{aligned} V_+ \{|0\rangle\} &\mapsto \{|1\rangle\}, & V_+ |1\rangle &\rightarrow 0 \\ V_- \{|1\rangle\} &\mapsto \{|0\rangle\}, & V_- |0\rangle &\rightarrow 0 \end{aligned} \quad (4.1.4)$$

The Schrodinger equation can thus be split into

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

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

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

The effective Hamiltonian in this subspace is therefore

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

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

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

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

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

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

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

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

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

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

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

The second term similarly gives

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

The total renormalization becomes

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

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

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

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

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

Therefore,

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

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In summary, the prescription of replacing all ω with the initial state energy will be correct only if the initial and final states are the same. This happens when we are decoupling a single-electron state - then the total renormalization is of the form $c^\dagger T^\dagger c$ such that we start from an initial state, scatter to an intermediate state and then go back to the initial state so that the final state is the same as the initial state. However, if we are using PMS to decouple states in one-shot, each subspace will have multiple states and there might be terms where we do not end up at the initial state we started with. Then the correct prescription would be to use the mean of the initial and final state denominators.

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

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

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

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

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

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

Substituting eqs. 4.1.19 and 4.1.18 in eq. 4.1.1 gives

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

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

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

The second equation ⁴ can be written as

$$|\Psi_1\rangle = \eta^\dagger |\Psi_0\rangle \quad (4.1.22)$$

where

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

Substituting this in the first equation gives

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

This new Hamiltonian,

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

has the high energy mode removed; the scattering terms start from the low energy subspace ⁸⁹ and end at the low energy subspace as well. The renormalization in the low energy subspace scatterings is

$$\Delta V_0 = V_- \eta^\dagger \quad (4.1.26)$$

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

$$|\Psi_0\rangle = \eta |\Psi_1\rangle \quad (4.1.27)$$

where

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

, so

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

The renormalized Hamiltonian in the high energy subspace is thus

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

¹ If we want to keep both the high energy and low energy parts of the Hamiltonian, the new Hamiltonian is

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

The total renormalization is

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

It can be shown that if we define a unitary operator $U = 1 - \eta + \eta^\dagger$, the transformed Hamiltonian $U \mathcal{H} U^\dagger$ is the same as eq. 4.1.31. This, along with the properties of η , have been shown in section 3. The important feature of eq. 4.1.31 is that there is no term in the transformed Hamiltonian which scatters between $|\Psi_0\rangle$ and $|\Psi_1\rangle$ - the two subspaces have been truly decoupled.

$$[U \mathcal{H} U^\dagger, n_q] = 0 \quad (4.1.33)$$

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

$$\tilde{\mathcal{H}}_0 |\Psi_0\rangle = E |\Psi_0\rangle \quad (4.1.34)$$

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

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

$$\mathcal{H} |\Phi\rangle = \mathcal{H}' |\Phi\rangle \quad (4.1.35)$$

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

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

The operators η and its conjugate change accordingly:

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

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

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

The renormalization is again

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

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

$$U = 1 - \eta + \eta^\dagger, [\hat{n}_q, U\mathcal{H}U^\dagger] = 0 \quad (4.1.39)$$

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

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

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

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

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

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

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

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

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

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

The intermediate energy (at the propagator) is

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

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

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

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

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

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

Substituting this in ΔV_0 gives

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

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

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

The renormalization in the hole sector is

$$\begin{aligned} \Delta V_0 &= c_{q\beta}^\dagger c_{d\beta} \frac{1}{(E - V_0) - \hat{\mathcal{H}}_0^d} c_{d\beta}^\dagger c_{q\beta} \\ &= c_{q\beta}^\dagger c_{d\beta} \frac{1}{(E - V_0) - \sum_{k,\sigma} \epsilon_k \tau_{k\sigma} - \epsilon_d - (\epsilon_d + U) \hat{n}_{d\bar{\beta}}} c_{d\beta}^\dagger c_{q\beta} \end{aligned} \quad (4.1.48)$$

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

This time we substitute

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

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

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

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

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

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

Some conclusions:

- The *only* difference in the formalism of PMS and URG is that while PMS uses the exact energy eigenvalue E to parameterise the flow, URG uses a general intermediate decoupled Hamiltonian to do the same. Since the E is also, technically, an intermediate decoupled Hamiltonian (it is the final Hamiltonian), PMS can be seen as an URG but with a specific choice for the parameter.
- In practise, PMS replaces $E - V_0$ with the diagonal part of the initial state at the current step of the RG. We are talking about the energy of the initial state, not the intermediate state. This is because, from eq. 4.1.1, E is the energy of the initial state on which V_\pm act.
- The ideal solution would have been to substitute the exact energy and the total scattering term V , but since we do not know E and keeping the V would make the thing untractable, we use our current best guess (renormalised diagonal part). As the RG flows, both E_j and V flow, such that at the fixed point, V becomes zero (scattering terms get removed) and E_j morphs into the exact E .
- In practise, URG replaces the $\hat{\omega}$ with a guess for the final energy E . This however ignores the renormalization of $\hat{\omega}$. A better approach would be to replace it with E_j , following PMS. That would act like the one-particle renormalization of $\hat{\omega}$.

- PMS usually drops any diagonal component of the scattering from the denominator. For example, in the PMS of the Kondo model by Anderson [2] or that of the anisotropic power law Kondo model by Chenge et.al [28], they do not keep the term $J_z S_d^z s^z$ in the denominator although it is number(spin) conserving. Such terms are kept in the denominator of the URG though. It must be mentioned however that ref. [29] *does* bring a diagonal charge-charge interaction in the denominator in the PMS of the extended Anderson model.

4.2 Schrieffer-Wolff transformation

Formal Differences

We have a general Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_X \quad (4.2.1)$$

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

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

where H_1 is diagonal and H_2 is off-diagonal.

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

The decoupling condition is $H_2 = 0$.

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

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

The second order decoupling condition is thus

$$[S, \mathcal{H}_0] = -\mathcal{H}_X \quad (4.2.5)$$

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

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

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

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

There we used

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

and hence

$$(\eta^\dagger - \eta)^3 = -1 (\eta^\dagger - \eta) \quad (4.2.9)$$

and so on. This simplification allows us to write

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

and

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

The off-diagonal part now becomes

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

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

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

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

That gives

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

The decoupling condition becomes

$$[S, \mathcal{H}_0] = -\frac{\pi}{4} \mathcal{H}_X + \frac{4}{\pi} S \mathcal{H}_X S \quad (4.2.15)$$

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

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

The differences between the perturbative and non-perturbative ways are summarized in table 4.1. There appear to

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

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

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

Renormalization due to SWT and Comparison with PMS and URG

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

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

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

$$-\mathcal{H}_X = [S, H_0] = S H_0 - H_0 S \quad (4.2.18)$$

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

$$-\langle \phi_0^a | V + V^\dagger | \phi_1^b \rangle = \langle \phi_0^a | S H_0 - H_0 S | \phi_1^b \rangle \quad (4.2.19)$$

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

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

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

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

The renormalization is thus

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

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

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

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

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

where

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

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

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

SIAM URG vs SIAM SWT

²² The SWT for the single-impurity Anderson model is briefly sketched below. In order to decouple a state $q\beta$ from the SIAM ($\epsilon_q > 0$), we take an ansatz $S = (A + B\hat{n}_{d\bar{\beta}})(c_{q\beta}^\dagger c_{d\beta} - \text{h.c.})$. Plugging this into the decoupling condition gives

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

which gives

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

The remaining diagonal part constitutes the effective Hamiltonian.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

The diagonal part is the rest of the Hamiltonian.

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

Following eq. 3.1.47, the renormalization is

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

The transition operator η is

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

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

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

The renormalization is

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

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

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

We can now define two new energy scales:

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

The renormalization Δ_1 becomes

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

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

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

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

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

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

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

Similarly, for the second term, we get

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

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

where K_{kq} is yet another energy scale.

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

The third term gives

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

The total renormalization can thus be written as

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

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

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

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

4.3 CUT RG

Formalism

The following equation generates a family of unitary Hamiltonians.

$$\frac{d\mathcal{H}(l)}{dl} = [\mathcal{H}, \eta(l)] \quad (4.3.1)$$

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

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

This will give

$$\begin{aligned} \frac{d\mathcal{H}(l)}{dl} &= \frac{dU}{dl}\overset{2}{\mathcal{H}(0)}U^\dagger(l) + U\mathcal{H}(0)\frac{dU^\dagger}{dl} \\ &= \frac{dU}{dl}U^\dagger\mathcal{H}(l) + \mathcal{H}(l)U\frac{dU(l)^\dagger}{dl} \\ &= \eta(l)\mathcal{H}(l) - \mathcal{H}(l)\eta(l) \\ &= [\eta(l), \mathcal{H}(l)] \end{aligned} \quad (4.3.3)$$

This proves that the family of Hamiltonians $\mathcal{H}(l)$ satisfy the flow equation eq. 4.3.1. $\eta(l)$ is referred to as the generator of the flow equation. It is chosen so as to reduce the off-diagonal part of the Hamiltonian, either progressively or in one shot. In Schrieffer-Wolff transformation, the transformation is one-shot, and the η there is the S that sits on top of the exponential in the unitary transformation. In URG, the generator to decouple one electron $q\beta$ is $\eta_{q\beta}^\dagger - \eta_{q\beta}$.

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

$$\frac{d\mathcal{H}}{dl} = [[\mathcal{H}_d(l), \mathcal{H}_X(l)], \mathcal{H}(l)] \quad (4.3.4)$$

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

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

where $g_{ij}^* = g_{ji}$. The canonical generator then turns out to be

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

and the renormalization in the Hamiltonian is

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

The first commutator gives

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

The second commutator gives

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

The total renormalization is

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

The couplings renormalize as

$$\begin{aligned} \frac{d\epsilon_i}{dl} &= \sum_{k \neq i} 2|g_{ik}|^2 (\epsilon_i - \epsilon_k) \\ \frac{dg_{ij}}{dl} &= -g_{ij} (\epsilon_i - \epsilon_j)^2 + \sum_{k \neq i} g_{ik} g_{kj} (\epsilon_i + \epsilon_j - 2\epsilon_k) \end{aligned} \quad (4.3.11)$$

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

$$0 = \frac{d\text{Tr}(\mathcal{H})^2}{dl} = \sum_i \frac{d\epsilon_i^2}{dl} + \sum_{i \neq j} \frac{d|g_{ij}|^2}{dl} \Rightarrow \sum_{i \neq j} \frac{d|g_{ij}|^2}{dl} = - \sum_i \frac{d\epsilon_i^2}{dl} \quad (4.3.12)$$

From the flow equation, we can see that

$$\sum_i \frac{d\epsilon_i^2}{dl} = 2 \sum_{i \neq k} \epsilon_i \frac{d\epsilon_i}{dl} = 2 \sum_i |g_{ik}|^2 (\epsilon_i - \epsilon_k)^2 \geq 0 \quad (4.3.13)$$

Therefore,

$$\sum_{i \neq j} \frac{d|g_{ij}|^2}{dl} \leq 0 \quad (4.3.14)$$

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

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

$$\mathcal{H} = \mathcal{H}_d + \mathcal{H}_X \quad (4.3.15)$$

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

$$\sum_{kq} g_q b_{-q}^\dagger c_{k+q,\sigma}^\dagger c_{k\sigma} + \text{h.c.} \quad (4.3.16)$$

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

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

It is easy to compute the commutators.

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

Therefore,

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

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

$$\frac{d\mathcal{H}}{dl} = [\eta, \mathcal{H}] \quad (4.3.20)$$

The flow equation for the electron-phonon coupling is

$$\frac{dg_q}{dl} = -\xi^2 g_q \implies g_q(l) = g_q(0) \exp(-\xi^2 l) \quad (4.3.21)$$

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

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

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

CUT RG from URG

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

$$\Delta\mathcal{H}^0 = \frac{1}{2} [\eta^\dagger - \eta, \mathcal{H}] \quad (4.3.23)$$

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

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

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

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

In the last step, the extra $c^\dagger T$ and $T^\dagger c$ terms canceled out. In the second and third terms, we can bring the Greens function closer to the operators $c^\dagger T$ and $T^\dagger c$ because $(\omega_j - G_j^{-1}) G_j = G_j (\omega_j - G_j^{-1})$:

$$\begin{aligned}\eta^\dagger - \eta &= \frac{1}{\omega_1 - \omega_0} \left[G_1 (\omega_1 - G_1^{-1}) c^\dagger T - c^\dagger T G_0 (\omega_0 - G_0^{-1}) \right. \\ &\quad \left. - T^\dagger c G_1 (\omega_1 - G_1^{-1}) + G_0 (\omega_0 - G_0^{-1}) T^\dagger c \right] \\ &= \frac{1}{\omega_1 - \omega_0} \left[G_1 (\omega_1 - G_1^{-1}) c^\dagger T - G_1 c^\dagger T (\omega_0 - G_0^{-1}) \right. \\ &\quad \left. - G_0 T^\dagger c (\omega_1 - G_1^{-1}) + G_0 (\omega_0 - G_0^{-1}) T^\dagger c \right]\end{aligned}\tag{4.3.26}$$

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In the last step, we again used the constraint $G_1 c^\dagger T = c^\dagger T G_0$ and its partner. From the definition of the Green's function $G = (\omega - \mathcal{H}^d)^{-1}$, we can write $\omega_j - G_j^{-1} = \mathcal{H}_j^d$. Therefore,

$$\begin{aligned}\eta^\dagger - \eta &= \frac{1}{\omega_1 - \omega_0} \left[G_1 \mathcal{H}_1^d c^\dagger T - G_1 c^\dagger T \mathcal{H}_0^d - G_0 T^\dagger c \mathcal{H}_1^d + G_0 \mathcal{H}_0^d T^\dagger c \right] \\ &= \frac{1}{\omega_1 - \omega_0} \left[G \mathcal{H}^d c^\dagger T - G c^\dagger T \mathcal{H}^d - G T^\dagger c \mathcal{H}^d + G \mathcal{H}^d T^\dagger c \right] \\ &= \frac{1}{\omega_1 - \omega_0} G [\mathcal{H}^d, c^\dagger T + T^\dagger c]\end{aligned}\tag{4.3.27}$$

where $\mathcal{H}^d = \mathcal{H}_1^d \hat{n} + \mathcal{H}_0^d (1 - \hat{n})$ and $G = G_1 \hat{n} + G_0 (1 - \hat{n}) = (\hat{\omega} - \mathcal{H}^d)^{-1}$. For URG, the relevant off-diagonal part of the Hamiltonian for the current node is $\mathcal{H}^I = c^\dagger T + T^\dagger c$. Therefore,

$$\eta^\dagger - \eta = \frac{1}{\omega_1 - \omega_0} G [\mathcal{H}^d, \mathcal{H}^I] = \left[\mathcal{H}^d, \frac{1}{\omega_1 - \omega_0} G \mathcal{H}^I \right]\tag{4.3.28}$$

The last equality comes about because both G and \mathcal{H}^I are completely diagonal and hence commute. The renormalization in the Hamiltonian under URG, which is a function of both the quantum fluctuation scale ω and the running bandwidth D , can thus be written as

$$\Delta \mathcal{H}(\omega, D) = \left[[\mathcal{H}^d, \tilde{\mathcal{H}}^I], \mathcal{H} \right] - \mathcal{H}_X\tag{4.3.29}$$

The most obvious difference with the CUT version is the presence of the off-diagonal piece $-\mathcal{H}_X$. This is a result of the philosophical difference between URG and CUT-RG - while CUT-RG gradually suppresses the off-diagonal matrix elements, URG makes the off-diagonal components in each 2×2 block vanish completely. We can instead look at the renormalization in the diagonal part of the Hamiltonian under URG:

$$\Delta \mathcal{H}^0(\omega, D) = \left[[\mathcal{H}^d, \tilde{\mathcal{H}}^I], \mathcal{H} \right]\tag{4.3.30}$$

where $\tilde{\mathcal{H}}^I = \frac{1}{\omega_1 - \omega_0} G \mathcal{H}^I$. This can be compared to the analogous equation for CUT (eq. 4.3.4),

$$\Delta \mathcal{H}(\lambda) = \Delta \lambda [[\mathcal{H}_d, \mathcal{H}_X], \mathcal{H}]\tag{4.3.31}$$

Leaving aside the obvious differences in the philosophies (the presence of ω in URG or the fact that while URG decouples as a flow in the bandwidth, CUT uses a general parameter λ or the algorithmic difference that while URG decouples one specific node, CUT tries to make the Hamiltonian band-diagonal), the major physical difference is the presence of the total Green's function in the URG equation. It must be noted that while CUT employs the entire off-diagonal part in \mathcal{H}_X , the \mathcal{H}^I of URG contains only those parts that are off-diagonal with respect to the node being decoupled at this step.

To bring the URG form closer to CUT, we can make some approximations.

$$G = (\hat{\omega} - \mathcal{H}^d)^{-1} \approx -(\mathcal{H}^d)^{-1} \quad (4.3.32)$$

where we assumed that the quantum fluctuations are small and can be ignored w.r.t the diagonal contribution \mathcal{H}^d . This gives

$$\frac{\Delta\mathcal{H}^0(\omega, D)}{[\mathcal{H}_1^d(\omega_0 - \omega_1)]^{-1}} = [\mathcal{H}^d, \mathcal{H}^I], \mathcal{H} \quad (4.3.33)$$

We can thus make the connection,

$$\Delta\lambda \sim [\mathcal{H}_1^d(\omega_0 - \omega_1)]^{-1} \quad (4.3.34)$$

Note that in going from eq. 4.3.30 to the simplified form eq. 4.3.33, we had to drop all quantum fluctuations in the denominator and we lose the fixed point structure in the process. This results in the distinction that while URG can reach a fixed point theory in a finite number of steps, CUT cannot do so.

4.4 Comparison of the Canonical Transformations

2 We have considered three canonical transformations in this section: the Poor Man's scaling (PMS), the Schrieffer-Wolff transformation (SWT) and the continuous unitary transformation renormalization group (CUT-RG). PMS and SWT are more or less identical; they differ in the context in which they are used. PMS is used when there is an entire spectrum of energies in the model, ranging from a low energy limit to a high energy; it is then employed to decouple the highest energy modes in an iterative fashion. SWT is used when the Hamiltonian can be split into one high and one low energy part, and we need to decouple these two modes. It is clear when seen from this perspective that SWT is like a one-shot PMS; it decouples the UV from the IR in one step, compared to the iterative approach of PMS. However, as has been shown in the previous subsections, both PMS and SWT can be formalized in an identical fashion, so that one can be switched for the other in both contexts.

Now that we have established that PMS and SWT are formally identical, we can relate them to URG. URG is similar in philosophy to PMS in the fact that URG also successively decouples high energy modes from the low energy ones. The difference is that URG takes care of the quantum fluctuations, at least in principle, by introducing a new set of energy scales ω . These ω then parameterise the RG flows of URG, compared to the single RG flow of PMS. Since SWT is formally the same as PMS, these is also a comparison between SWT and URG. Both PMS and SWT trivialize the quantum fluctuation scales of URG by replacing it with the bare energy values.

CUT-RG is philosophically different from the other transformations. Its goal is to gradually reduce the contributions of the off-diagonal terms by making them decay along a certain scale l . Off-diagonal terms that connect states with large energy differences decay faster. In this sense, there is no sequential dropping out of off-diagonal terms; all off-diagonal terms disappear at $l = \infty$. In this sense, it is like a continuous version of SWT. While SWT strives to remove an entire off-diagonal term in one-shot, CUT RG does this gradually by introducing a scale l . This separation of scales is absent in SWT. It does exist in URG and PMS, albeit in a different fashion. There, the separation comes in when we decouple single electron states starting from the Brillouin zone boundary Λ_N and come down to the Fermi surface Λ_0 . Each Λ provides a natural energy scale for separating the high and low energy physics.

If one integrates the continuum generator η over all the scales, one should recover something analogous to the SWT generator. This generator is however necessarily perturbative in the off-diagonal term, since by definition η will only be of first order in \mathcal{H}_X . This is in contrast to the non-perturbative generators in URG and, at least in principle, PMS. This non-perturbative form is encapsulated in the presence of a second completely different set of energy scales ω (or E in PMS). This second energy scale is absent in CUT RG because it takes care of at most the second order term.

Another point to note is that since SWT keeps the entire off-diagonal piece in the generator, new terms will

almost certainly be generated at every step, and they have to be truncated. This is not the case with URG or PMS, because in those methods, we decouple just a single-electron at each step, and so those electrons become integrals of motion at that step, leading to their removal from the off-diagonal piece, and very often the Hamiltonian retains the same form as the bare model. This makes the philosophy of URG and PMS easier to work with. Tied to this is the fact that CUT RG often takes a certain type of interaction in the generator part, and not the entire off-diagonal piece. Hence, at the limit of the flow parameter going to ∞ , the chosen off-diagonal piece goes to zero but the remaining off-diagonal pieces still remain. As a result, the Hamiltonian is almost block diagonal at this stage. On the other hand, URG progressively decouples single electrons, meaning all scattering terms corresponding to that electron vanish at each step.

One last thing to note is that URG, being unitarily implemented with a well-defined generator, does not accommodate for spontaneous symmetry breaking (SSB). In order to see SSB, the symmetry-breaking term has to be added to the bare model explicitly; if this term grows under the RG, then the ground state will be symmetry-broken. CUT RG, however, does allow for SSB through the idea that the generator is not uniquely defined. If the generator commutes with a particular symmetry, then the family of Hamiltonians will also have the symmetry [30]. However, if the generator is replaced by something that is normal ordered w.r.t a particular expectation value, then the CUT RG flow will usually be towards either the symmetry-preserved state or the symmetry-broken state, depending on whichever is stable [32].

Figure 4.3: Comparison of the various unitary transformations, depicting how each of them are related to one another.

Chapter 5

URG of the SIAM and its Spin and Charge Generalizations

5.1 URG of the SIAM

5.1.1 Setting up the various terms in the URG

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

$$\mathcal{H} = \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{k\sigma} \left(V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right) + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \quad (5.1.1)$$

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

$$\mathcal{H} = \sum_{k\sigma} \epsilon_k \tau_{k\sigma} + \sum_{k\sigma} \left(V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right) + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \quad (5.1.2)$$

The renormalization is

$$c_{q\beta}^\dagger T\eta + T^\dagger c_{q\beta} \eta_0^\dagger \quad (5.1.3)$$

We will be decoing an electron $q\beta$ at the energy shell ϵ_q . The diagonal part (that comes down in the denominator) is

$$\mathcal{H}_d = \epsilon_q \tau_{q\beta} + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \quad (5.1.4)$$

Since this is the first step of the RG, the shell being decoupled is the highest one, which we call Λ_N .

5.1.2 Calculation of renormalization

The η is

$$\begin{aligned} \eta &= \frac{1}{\hat{\omega} - \mathcal{H}_d} T^\dagger c_{q\beta} = \frac{1}{\hat{\omega} - \epsilon_q \tau_{q\beta} - \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} - U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow}} V_q^* c_{d\beta}^\dagger c_{q\beta} \\ &= \frac{1}{\hat{\omega} + \frac{1}{2}\epsilon_q - \epsilon_d - (\epsilon_d + U) \hat{n}_{d\overline{\beta}}} V_q^* c_{d\beta}^\dagger c_{q\beta} \end{aligned} \quad (5.1.5)$$

We substituted $\tau_{q\beta} = -\frac{1}{2}$ and $\hat{n}_{d\beta} = 1$ because of the off-diagonal terms in the numerator. The renormalization in the particle sector ($\hat{n}_{q\beta} = \hat{n}_{q\overline{\beta}} = 1$), at an energy $-\epsilon_q$ is

$$\Delta\mathcal{H} = c_{q\beta}^\dagger T\eta = \frac{|V_q|^2}{\hat{\omega} - \frac{1}{2}\epsilon_q - \epsilon_d - (\epsilon_d + U) \hat{n}_{d\overline{\beta}}} \left(1 - \hat{n}_{d\beta} \right) \hat{n}_{q\beta} \quad (5.1.6)$$

Similarly, the renormalization in the hole sector ($\hat{n}_{q\beta} = \hat{n}_{q\bar{\beta}} = 0$), at an energy ϵ_q is:

$$\Delta\mathcal{H} = T^\dagger c\eta_0^\dagger = \frac{|V_q|^2}{\hat{\omega} - \frac{1}{2}\epsilon_q - \epsilon_d \hat{n}_{d\bar{\beta}}} \left(1 - \hat{n}_{q\beta}\right) \hat{n}_{d\beta} \quad (5.1.7)$$

Therefore, the total renormalization obtained from decoupling a particle state ($\hat{n}_{q\beta} = 1$) at $-\epsilon_q$ and a hole state ($\hat{n}_{q\beta} = 0$) at ϵ_q is

$$\begin{aligned} \Delta\mathcal{H} &= \frac{|V_q|^2 \left(1 - \hat{n}_{d\beta}\right)}{\hat{\omega} - \frac{1}{2}\epsilon_q - \epsilon_d - (\epsilon_d + U) \hat{n}_{d\bar{\beta}}} + \frac{|V_q|^2 \hat{n}_{d\beta}}{\hat{\omega} - \frac{1}{2}\epsilon_q - \epsilon_d \hat{n}_{d\bar{\beta}}} \\ &= |V_q|^2 \left[\frac{\left(1 - \hat{n}_{d\beta}\right) \hat{n}_{d\bar{\beta}}}{\omega_1 - \frac{1}{2}\epsilon_q - 2\epsilon_d - U} + \frac{\left(1 - \hat{n}_{d\beta}\right) \left(1 - \hat{n}_{d\bar{\beta}}\right)}{\omega_2 - \frac{1}{2}\epsilon_q - \epsilon_d} + \frac{\hat{n}_{d\beta} \hat{n}_{d\bar{\beta}}}{\omega_3 - \frac{1}{2}\epsilon_q - \epsilon_d} + \frac{\hat{n}_{d\beta} \left(1 - \hat{n}_{d\bar{\beta}}\right)}{\omega_4 - \frac{1}{2}\epsilon_q} \right] \end{aligned} \quad (5.1.8)$$

To relate the ω_i , we look at the their values obtained by substituting the energies of the initial states:

$$\begin{aligned} \omega_1 &= \omega_4 = -\frac{1}{2}\epsilon_q + \epsilon_d \\ \omega_2 &= -\frac{1}{2}\epsilon_q \\ \omega_3 &= -\frac{1}{2}\epsilon_q + 2\epsilon_d + U \end{aligned} \quad (5.1.9)$$

Defining $\omega \equiv \omega_2$ (because ω_2 has the simplest form), we can write

$$\begin{aligned} \omega_1 &= \omega_4 = \omega + \epsilon_d \\ \omega_2 &= \omega \\ \omega_3 &= \omega + 2\epsilon_d + U \end{aligned} \quad (5.1.10)$$

The renormalization then becomes

$$\Delta\mathcal{H} = |V_q|^2 \left[\frac{\left(1 - \hat{n}_{d\beta}\right) \hat{n}_{d\bar{\beta}}}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d - U} + \frac{\left(1 - \hat{n}_{d\beta}\right) \left(1 - \hat{n}_{d\bar{\beta}}\right)}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d} + \frac{\hat{n}_{d\beta} \hat{n}_{d\bar{\beta}}}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d + U} + \frac{\hat{n}_{d\beta} \left(1 - \hat{n}_{d\bar{\beta}}\right)}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d} \right] \quad (5.1.11)$$

5.1.3 Scaling equations

Once we have the renormalization for decoupling one electronic or hole state, we can just sum over the spins and momenta to get the total renormalization upon decoupling the entire shells $\pm\epsilon_q$. From the structure of $\Delta\mathcal{H}$ in eq. 5.1.11, we can see that there are renormalizations to all three configuration energies of the impurity: the doublon energy E_2 corresponding to the state $\hat{n}_{d\beta} \hat{n}_{d\bar{\beta}}$, the single energy E_1 corresponding to $(\hat{n}_{d\beta}(1 - \hat{n}_{d\bar{\beta}}) + \hat{n}_{d\bar{\beta}}(1 - \hat{n}_{d\beta}))$, and the holon energy E_0 corresponding to $(1 - \hat{n}_{d\beta})(1 - \hat{n}_{d\bar{\beta}}) + \hat{n}_{d\bar{\beta}}(1 - \hat{n}_{d\beta})$.

$$\begin{aligned} \Delta E_2 &= +2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d + U} \\ \Delta E_1 &= + \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d} + \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d - U} \\ \Delta E_0 &= +2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d} \end{aligned} \quad (5.1.12)$$

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

$$\begin{aligned} \Delta\epsilon_d &= + \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d} + \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d - U} - 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d} \\ \Delta U &= \sum_q \frac{2|V_q|^2}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d + U} + \sum_q \frac{2|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d} - \sum_q \frac{2|V_q|^2}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d} - \sum_q \frac{2|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d - U} \end{aligned} \quad (5.1.13)$$

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5.1.4 Connection to Poor Man's scaling

To obtain the results of Poor Man's scaling [26][33], we can look at various regimes. First we look at the case when both ϵ_d and U are small such that both the singly-occupied and doubly-occupied subspaces of the impurity are comfortably inside the bandwidth, $U, \epsilon_d \ll \epsilon_q$. We can then ignore the ϵ_d and U in the denominator compared to the ϵ_q .

$$\begin{aligned}\Delta\epsilon_d &= \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} + \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} - 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} \\ \Delta U &= 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} + 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} - 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} - 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q}\end{aligned}\quad (5.1.14)$$

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

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

$$\begin{aligned}\Delta\epsilon_d &= \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} - 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} \\ \Delta U &= 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} - 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q}\end{aligned}\quad (5.1.15)$$

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

$$\begin{aligned}\Delta U &= 0 \\ \delta\epsilon_d &= -\frac{\Delta}{\pi} \frac{1}{\omega - \frac{1}{2}D}\end{aligned}\quad (5.1.16)$$

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

$$\delta\epsilon_d = \frac{\Delta}{\pi} \frac{\delta D}{D} \quad (5.1.17)$$

This is the one-loop scaling equation.

5.1.5 Particle-Hole symmetry

The Anderson model Hamiltonian, eq. 5.2.7, has an impurity particle-hole symmetry for a certain condition of the couplings. To see this, we apply the particle-hole transformation $c_k \rightarrow c_k^\dagger, c_d \rightarrow -c_d^\dagger$ to the Hamiltonian. Since we are looking at the impurity symmetry, we will only look at the terms involving the impurity. The particle-hole symmetry of the conduction bath is a separate thing and that requires a specific lattice. Hence we will not consider kinetic energy term in this discussion. The rest of the terms transform as

$$\epsilon_d \sum_\sigma \hat{n}_{d\sigma} \rightarrow 2\epsilon_d - \epsilon_d \sum_\sigma \hat{n}_{d\sigma} \quad (5.1.18)$$

$$U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \rightarrow U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} - U \sum_\sigma \hat{n}_{d\sigma} + U \quad (5.1.19)$$

$$\sum_{k\sigma} V(k) c_{k\sigma}^\dagger c_{d\sigma} + hc \rightarrow \sum_{k\sigma} -V(k) c_{k\sigma} c_{d\sigma}^\dagger + hc = \sum_{k\sigma} V^*(k) c_{k\sigma}^\dagger c_{d\sigma} + hc \quad (5.1.20)$$

$$S^z \sum_{kq} s_{kq}^z \rightarrow (-S^z) \sum_{kq} (-s_{kq}^z) = S^z \sum_{kq} s_{kq}^z \quad (5.1.21)$$

$$S^\pm \sum_{kq} s_{kq}^\mp \rightarrow (-S^\pm) \sum_{kq} (-s_{kq}^\mp) = S^\pm \sum_{kq} s_{kq}^\mp \quad (5.1.22)$$

The transformation of the spin terms, eqs. 5.1.21 and 5.1.22, can be understood from the fact that since a spin degree of freedom can be written in terms of the number operator as $\hat{S} = \hat{n} - \frac{1}{2}$, it must transform by flipping its sign: $\hat{S} = \hat{n} - \frac{1}{2} \rightarrow \frac{1}{2} - \hat{n} = -\hat{S}$. The spin terms are thus invariant under the particle-hole transformation. The impurity-bath hopping term can be made symmetric by making $V(k)$ real; then we would have, from eq. 5.1.20,

$$\text{87} \quad V(k) \left(c_{k\sigma}^\dagger c_{d\sigma} + c_{d\sigma}^\dagger c_{k\sigma} \right) \rightarrow V(k) \left(c_{d\sigma}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger c_{d\sigma} \right) \quad (5.1.23)$$

The impurity diagonal terms, ϵ_d and U , require a specific condition. Combining eqs. 5.1.18 and 5.1.19,

$$\epsilon_d \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \rightarrow (-\epsilon_d - U) \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \quad (5.1.24)$$

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

$$\epsilon_d = -\epsilon_d - U \implies \epsilon_d + \frac{1}{2}U = 0 \quad (5.1.25)$$

This same condition can be obtained in a more physical way. If we consider the singly-occupied state of the impurity as the reference state, the doubly-occupied state is the particle-excitation and the vacant state is the hole excitation. The energy of this particle state is $E_2 = 2\epsilon_d + U$ and that of the hole state is $E_0 = 0$. Particle-hole symmetry then requires the particle and hole levels to be degenerate, which means $E_2 = E_0$, and we recover the condition eq. 5.1.25.

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

$$\Delta \left(\epsilon_d + \frac{1}{2}U \right) = 0 \quad (5.1.26)$$

The quantity $\gamma = \epsilon_d + \frac{1}{2}U$ is thus an RG-invariant for the particle-hole symmetric model; it does not change under the RG flow. It is often referred to as the asymmetry parameter; it quantifies the asymmetry in the model. We need to check if our equations satisfy this. Looking at the RG equations for ϵ_d and U , we can find the RG equation for the asymmetry parameter. The slightly easier way is to just note that the renormalization in E_2 should be equal to the renormalization in E_0 , in order for p-h symmetry to hold.

$$\Delta E_2 = 2 \frac{\Delta}{\pi} \frac{1}{\omega - D + \epsilon_d + U}, \Delta E_0 = 2 \frac{\Delta}{\pi} \frac{1}{\omega - D - \epsilon_d} \quad (5.1.27)$$

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

5.1.6 Numerical analysis of symmetric SIAM

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

$$\Delta \epsilon_d = -4|V|^2 \frac{\epsilon_d}{\left(\omega - \frac{1}{2}D\right)^2 - \epsilon_d^2} \quad (5.1.28)$$

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

$$\Delta |\epsilon_d| = -4|V|^2 \frac{|\epsilon_d|}{\left(\omega - \frac{1}{2}D\right)^2 - \epsilon_d^2} \quad (5.1.29)$$

Figure 5.2: Left: Irrelevant flow towards $|\epsilon_d| = 0$, at low ω . Right: Relevant flow towards large $|\epsilon_d|$, at large ω . The former can be thought of as the projection of the strong-coupling flow on to the $\epsilon_d - D$ plane. The latter is the flow towards the local moment fixed point, if we start from a negative ϵ_d .

Depending on the signature of the denominator, the flows will be either relevant or irrelevant. For the flow to the local moment fixed point, the fixed point value of $|\epsilon_d|$ grows as we increase the bandwidth. This implies that for a thermodynamically large system, the local moment fixed point will be at $-\epsilon_d \rightarrow \infty$. This behavior is shown in fig. 5.3.

Figure 5.3: Change in fixed point value of $|\epsilon_d|$ with system size.

5.2 Anderson-Kondo (spin) model URG

In order to obtain a renormalization in V , we will introduce a spin-spin interaction between the impurity and the mobile electrons. Such terms are generated when one does a Schrieffer-Wolff transformation on the SIAM, but we will find it prudent to keep these terms in the bare model itself. 10

5.2.1 Spin-spin interaction

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

$$\mathcal{H}_I = \sum_{k,k',\sigma_i} u c_{d\sigma_2}^\dagger c_{d\sigma_4} c_{k'\sigma_3} c_{k\sigma_1}^\dagger \delta_{(\sigma_1+\sigma_2=\sigma_3+\sigma_4)} \quad (5.2.1)$$

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

$$\mathcal{H}_I = \underbrace{\sum_{k,k',\sigma,\sigma'} u_1 \hat{n}_{d\sigma'} c_{k\sigma}^\dagger c_{k'\sigma}}_{\text{spin-preserving scattering}} + \underbrace{\sum_{k,k',\sigma} u_2 c_{d\sigma}^\dagger c_{d\sigma} c_{k\sigma}^\dagger c_{k'\overline{\sigma}}}_{\text{spin-flip scattering}} \quad (5.2.2)$$

At this point, we drop the dependence of u on the momenta and assume it depends only on the spin transfer. The first term (attached with u_1) involves no spin-flip between the scattering momenta or the scattering impurity electrons ($k\sigma \rightarrow k'\sigma, d\sigma' \rightarrow d\sigma'$). We label this coupling as u_P . The other coupling involves a spin-flip scattering, so we label that as u_A . 27

$$\mathcal{H}_{I,N} = \sum_{k,k',\sigma,\sigma'} u_P \hat{n}_{d\sigma'} c_{k\sigma}^\dagger c_{k'\sigma} + \sum_{k,k',\sigma} u_A c_{d\sigma}^\dagger c_{d\sigma} c_{k\sigma}^\dagger c_{k'\overline{\sigma}} \quad (5.2.3)$$

where the N in the denominator means the sum is over all momenta up to $|k| = \Lambda_N$. The parallel scattering has two components, when expanded, is of the form 28

$$u_{\uparrow\uparrow} \hat{n}_{d\uparrow} c_{k\uparrow}^\dagger c_{k'\uparrow} + u_{\downarrow\downarrow} \hat{n}_{d\downarrow} c_{k\downarrow}^\dagger c_{k'\downarrow} + u_{\uparrow\downarrow} \hat{n}_{d\uparrow} c_{k\downarrow}^\dagger c_{k'\uparrow} + u_{\downarrow\uparrow} \hat{n}_{d\downarrow} c_{k\uparrow}^\dagger c_{k'\downarrow} \quad (5.2.4)$$

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

$$\begin{aligned} \mathcal{H}_I &= J_z \frac{\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow}}{2} \sum_{kk'} \left(\underbrace{c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow}}_3 \right) + J_t \sum_{kk'} \left[c_{d\uparrow}^\dagger c_{d\downarrow} c_{k\downarrow}^\dagger c_{k'\uparrow} + c_{d\downarrow}^\dagger c_{d\uparrow} c_{k\uparrow}^\dagger c_{k'\downarrow} \right] \\ &= 2J_z S_d^z s^z + J_t (S_d^+ s^- + S_d^- s^+) \end{aligned} \quad (5.2.5)$$

The spin-like operators are defined as

$$\begin{aligned} S_d^z &\equiv \frac{1}{2} \left(\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow} \right) & S_d^+ &\equiv c_{d\uparrow}^\dagger c_{d\downarrow} & S_d^- &\equiv c_{d\downarrow}^\dagger c_{d\uparrow} \\ s_{kk'}^z &\equiv \frac{1}{2} \left(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow} \right) & s_{kk'}^+ &\equiv c_{k\uparrow}^\dagger c_{k'\downarrow} & s_{kk'}^- &\equiv c_{k\downarrow}^\dagger c_{k'\uparrow} \\ s^a &\equiv \sum_{kk'} s_{kk'}^a \end{aligned} \quad (5.2.6)$$

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

$$\mathcal{H} = \sum_{k\sigma} \left(\epsilon_k \hat{n}_{k\sigma} + V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right) + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + 2J_z S_d^z s^z + J_t \left(S_d^+ s^- + S_d^- s^+ \right) \quad (5.2.7)$$

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

$$\mathcal{H}_I = J \left[S_d^z s^z + \frac{1}{2} \left(S_d^+ s^- + S_d^- s^+ \right) \right] = J \mathbf{S}_d \cdot \mathbf{s} \quad (5.2.8)$$

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

$$\begin{aligned} \mathcal{H}_N &= H_{N-1} + H_{imp} + \epsilon_q \hat{n}_{q\beta} + 2J_z S_d^z s_q^z + V_q c_{q\beta}^\dagger c_{d\beta} + h.c. + \\ &\quad \sum_{k < \Lambda_N} \left[J_z S_d^z \beta \left(c_{k\beta}^\dagger c_{q\beta} + c_{q\beta}^\dagger c_{k\beta} \right) + J_t \left(c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} + c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\bar{\beta}} \right) \right] \\ &\quad + J_t \left(c_{d\beta}^\dagger c_{d\bar{\beta}} c_{q\bar{\beta}}^\dagger c_{q\beta} + c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{q\bar{\beta}} \right) \end{aligned} \quad (5.2.9)$$

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

$$H_{N-1} = \sum_{k < \Lambda_N, \sigma} \left[\left(\epsilon_k + \sigma J_z S_d^z \right) \hat{n}_{k\sigma} + V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right] + H_{I,N-1} \quad (5.2.10)$$

The diagonal (number-preserving) part is

$$\mathcal{H}_D = H_{N-1}^D + \epsilon_q \left(\hat{n}_{q\beta} + \hat{n}_{q\bar{\beta}} \right) + 2J_z S_d^z s_q^z + H_{imp} \quad (5.2.11)$$

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

$$\mathcal{H}_D = \epsilon_q \hat{n}_{q\beta} + 2J_z S_d^z s_q^z + H_{imp} \quad (5.2.12)$$

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

$$\sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} = \sum_{k\sigma} \epsilon_k \hat{\tau}_{k\sigma} + \mathcal{C} \quad (5.2.13)$$

where $\tau \equiv \hat{n} - \frac{1}{2}$ and \mathcal{C} is non-dynamic and will hence be dropped. This transforms the diagonal part \mathcal{H}^D . Eq. 5.2.12 becomes

$$\mathcal{H}_D = \epsilon_q \tau_{q\beta} + 2J_z S_d^z s_q^z + H_{imp} \quad (5.2.14)$$

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

$$\begin{aligned} \mathcal{H}_X = & \underbrace{V_1^* c_{d\beta}^\dagger c_{q\beta} \hat{n}_{d\bar{\beta}}}_{T_1^\dagger c_{q\beta}} + \overbrace{V_0^* c_{d\beta}^\dagger c_{q\beta} (1 - \hat{n}_{d\bar{\beta}})}^{T_2^\dagger c_{q\beta}} + \underbrace{\sum_{k < \Lambda_N} J_0^z \hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}}) c_{k\beta}^\dagger c_{q\beta}}_{T_3^\dagger c_{q\beta}} \\ & - \underbrace{\sum_{k < \Lambda_N} J_1^z \hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta}) c_{k\beta}^\dagger c_{q\beta}}_{T_4^\dagger c_{q\beta}} + \underbrace{\sum_{k < \Lambda_N} J^t c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta}}_{T_5^\dagger c_{q\beta}} + \underbrace{J^t c_{d\beta}^\dagger c_{d\bar{\beta}} c_{q\bar{\beta}}^\dagger c_{q\beta}}_{T_6^\dagger c_{q\beta}} + \text{h.c.} \end{aligned} \quad (5.2.15)$$

The various parts of the off-diagonal piece are

$$\begin{aligned} T_1 &= V_1 c_{d\beta} \hat{n}_{d\bar{\beta}} \\ T_2 &= V_0 c_{d\beta} (1 - \hat{n}_{d\bar{\beta}}) \\ T_3 &= \sum_{k < \Lambda_N} J_0^z \hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}}) c_{k\beta} \\ T_4 &= - \sum_{k < \Lambda_N} J_1^z \hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta}) c_{k\beta} \\ T_5 &= \sum_{k < \Lambda_N} J^t c_{d\bar{\beta}}^\dagger c_{d\beta} c_{k\bar{\beta}} \end{aligned} \quad (5.2.16)$$

5.2.2 Calculation of renormalization in particle sector

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

$$c_{q\beta}^\dagger T \eta \quad (5.2.17)$$

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

$$\eta = \sum_{i=1}^5 \frac{1}{\omega_i - E_i^0} T_i^\dagger c_{q\beta} \quad (5.2.18)$$

We need to compute a quantity of the form

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

The diagonal parts E_i^0 are

$$\begin{aligned} E_1^0 &= \frac{\epsilon_q}{2} + 2\epsilon_d + U \\ E_2^0 = E_5^0 = E_4^0 &= \frac{\epsilon_q}{2} + \epsilon_d - \frac{J_z}{2} \\ E_3^0 &= \frac{\epsilon_q}{2} + \epsilon_d + \frac{J_z}{2} \end{aligned} \quad (5.2.19)$$

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

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

$$\begin{aligned} & \sum_{ij} \left(\frac{1}{\omega_i - E_i^0} + \frac{1}{\omega_j - E_j^0} \right) T_i T_j^\dagger \\ &= \frac{|V_1|^2}{\xi_1} \left(1 - \hat{n}_{d\beta}\right) \hat{n}_{d\bar{\beta}} + \frac{|V_0|^2}{\xi_2} \left(1 - \hat{n}_{d\beta}\right) \left(1 - \hat{n}_{d\bar{\beta}}\right) \\ &+ \frac{1}{4} \left[J_0^z \frac{\hat{n}_{d\beta} \left(1 - \hat{n}_{d\bar{\beta}}\right)}{\xi_3} + J_1^z \frac{\hat{n}_{d\bar{\beta}} \left(1 - \hat{n}_{d\beta}\right)}{\xi_4} \right] c_{k'\beta} c_{k\beta}^\dagger + \frac{1}{\xi_5} J_t^2 \left(1 - \hat{n}_{d\beta}\right) \hat{n}_{d\bar{\beta}} c_{k'\bar{\beta}} c_{k\bar{\beta}}^\dagger \\ &- \frac{1}{2} \left(\frac{1}{\xi_2} + \frac{1}{\xi_5} \right) J_t \left(1 - \hat{n}_{d\beta}\right) \left(V_0 c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} + \text{h.c.}\right) - \frac{1}{2} \left(\frac{1}{\xi_2} + \frac{1}{\xi_3} \right) \frac{J_0^z}{2} \left(1 - \hat{n}_{d\bar{\beta}}\right) \left(V_0 c_{k\beta}^\dagger c_{d\beta} + \text{h.c.}\right) \\ &- \frac{1}{2} \left(\frac{1}{\xi_3} + \frac{1}{\xi_5} \right) \frac{J_t J_0^z}{2} \left(c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{k'\beta} + \text{h.c.}\right) \end{aligned} \quad (5.2.20)$$

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

5.2.3 Calculation of renormalization in hole sector

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

$$T_{q\beta}^\dagger c \eta_0^\dagger \quad (5.2.21)$$

where η_0^\dagger is of the form

$$\eta_0^\dagger = \sum_{i=1}^5 \frac{1}{\omega'_i - E_i^1} c_{q\beta}^\dagger T_i \quad (5.2.22)$$

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

$$\begin{aligned} E_1^1 = E_4^1 = E_5^1 &= \frac{\epsilon_q}{2} + \epsilon_d - \frac{J_z}{2} \\ E_2^1 &= \frac{\epsilon_q}{2} \\ E_3^1 &= \frac{\epsilon_q}{2} + \epsilon_d + \frac{J_z}{2} \end{aligned} \quad (5.2.23)$$

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

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

$$\begin{aligned}
 & -\frac{1}{2} \left(\frac{1}{\xi'_4} + \frac{1}{\xi'_1} \right) \frac{J_1^z}{2} \hat{n}_{d\bar{\beta}} \left(V_1 c_{k\beta}^\dagger c_{d\beta} + \text{h.c.} \right) - \frac{1}{2} \left(\frac{1}{\xi'_1} + \frac{1}{\xi'_5} \right) J_t \hat{n}_{d\beta} \left(V_1 c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} + \text{h.c.} \right) \\
 & - \frac{1}{2} \left(\frac{1}{\xi'_4} + \frac{1}{\xi'_5} \right) \frac{J_t J_1^z}{2} \left(c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{k'\beta} + \text{h.c.} \right)
 \end{aligned}$$

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

5.2.4 Relating the ω_i and ω'_i

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

$$\begin{aligned}
 \omega_1 &= -\frac{1}{2}\epsilon_q + \epsilon_d \\
 \omega_2 &= -\frac{1}{2}\epsilon_q \\
 \omega_3 &= -\frac{1}{2}\epsilon_q + \epsilon_d + \frac{J_z}{2} \\
 \omega_5 &= \omega_4 = -\frac{1}{2}\epsilon_q + \epsilon_d - \frac{J_z}{2}
 \end{aligned} \tag{5.2.24}$$

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

$$\begin{aligned}
 \omega_1 &= \omega + \frac{J_z}{2} + \epsilon_d \\
 \omega_2 &= \omega + \frac{J_z}{2} \\
 \omega_3 &= \omega + J_z + \epsilon_d \\
 \omega_5 &= \omega_4 = \omega + \epsilon_d
 \end{aligned} \tag{5.2.25}$$

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

$$\begin{aligned}
 \xi_1 &= \omega - \frac{\epsilon_q}{2} - \epsilon_d - U + \frac{J_z}{2} \\
 \xi_2 &= \omega - \frac{\epsilon_q}{2} - \epsilon_d + J_z \\
 \xi_3 = \xi_4 = \xi_5 &= \omega - \frac{\epsilon_q}{2} + \frac{J_z}{2}
 \end{aligned} \tag{5.2.26}$$

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

$$\begin{aligned}
 \omega'_1 &= -\frac{1}{2}\epsilon_q + 2\epsilon_d + U \\
 \omega'_2 &= -\frac{1}{2}\epsilon_q + \epsilon_d \\
 \omega'_3 &= -\frac{1}{2}\epsilon_q + \epsilon_d + \frac{J_z}{2} \\
 \omega'_4 = \omega'_5 &= -\frac{1}{2}\epsilon_q + \epsilon_d - \frac{J_z}{2}
 \end{aligned} \tag{5.2.27}$$

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

$$\begin{aligned}
 \omega'_1 &= \omega + U + \frac{J_z}{2} \\
 \omega'_2 &= \omega + \epsilon_d + \frac{J_z}{2} \\
 \omega'_3 &= \omega + \epsilon_d + J_z \\
 \omega'_4 = \omega'_5 &= \omega + \epsilon_d
 \end{aligned} \tag{5.2.28}$$

The denominators are therefore

$$\begin{aligned}\xi'_1 &= \omega - \frac{\epsilon_q}{2} + \epsilon_d + U + J_z \\ \xi'_2 &= \omega - \frac{\epsilon_q}{2} + \epsilon_d + \frac{J_z}{2} \\ \xi'_3 = \xi'_4 = \xi'_5 &= \omega - \frac{\epsilon_q}{2} + \frac{J_z}{2} = \xi_3 = \xi_4 = \xi_5\end{aligned}\tag{5.2.29}$$

5.2.5 Making sense of the various terms

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

$$\frac{|V_1|^2}{\xi_1} (1 - \hat{n}_{d\beta}) \hat{n}_{d\bar{\beta}} + \frac{|V_0|^2}{\xi_2} (1 - \hat{n}_{d\beta}) (1 - \hat{n}_{d\bar{\beta}}) + \frac{|V_1|^2}{\xi'_1} \hat{n}_{d\bar{\beta}} \hat{n}_{d\beta} + \frac{|V_0|^2}{\xi'_2} \hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}})\tag{5.2.30}$$

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

$$\Delta E_2 = \frac{|V_1|^2}{\xi'_1}, \quad \Delta E_1 = \frac{|V_1|^2}{2\xi_1} + \frac{|V_0|^2}{2\xi'_2}, \quad \Delta E_0 = \frac{|V_0|^2}{\xi'_2}\tag{5.2.31}$$

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

$$\begin{aligned}\Delta \epsilon_d &= \frac{|V_1|^2}{2\xi_1} + \frac{|V_0|^2}{2\xi'_2} - \frac{|V_0|^2}{\xi_2} \\ \Delta U &= \frac{|V_1|^2}{\xi'_1} + \frac{|V_0|^2}{\xi_2} - \frac{|V_1|^2}{\xi_1} - \frac{|V_0|^2}{\xi'_2}\end{aligned}\tag{5.2.32}$$

The J_z^2 terms, together, give

$$\frac{J_z^2}{4} \left[\frac{\hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}})}{\xi_3} + \frac{\hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta})}{\xi_4} \right] c_{k'\beta} c_{k\beta}^\dagger + \frac{1}{4} \left[\frac{\hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}})}{\xi'_3} + \frac{\hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta})}{\xi'_4} \right] c_{k\beta}^\dagger c_{k'\beta}\tag{5.2.33}$$

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

$$\frac{J_z^2}{4\xi_3} \left[\hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}}) + \hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta}) \right] (c_{k'\beta} c_{k\beta}^\dagger + c_{k\beta}^\dagger c_{k'\beta}) = \frac{J_z^2}{4\xi_3} [\hat{n}_d - 2\hat{n}_{d\beta} \hat{n}_{d\bar{\beta}}] \delta_{kk'}\tag{5.2.34}$$

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

$$\begin{aligned}\Delta \epsilon_d &= \frac{J_z^2}{4\xi_3} \delta_{kk'} \\ \Delta U &= -2 \frac{J_z^2}{4\xi_3} \delta_{kk'}\end{aligned}\tag{5.2.35}$$

We next look at the $J_z V$ terms:

$$-\frac{J_z}{4} \left[\left(\frac{1}{\xi_2} + \frac{1}{\xi_3} \right) (1 - \hat{n}_{d\bar{\beta}}) V_0 c_{k\beta}^\dagger c_{d\beta} + \left(\frac{1}{\xi'_4} + \frac{1}{\xi'_1} \right) \hat{n}_{d\bar{\beta}} V_1 c_{k\beta}^\dagger c_{d\beta} \right] + \text{h.c.}\tag{5.2.36}$$

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

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

$$\begin{aligned}\Delta V_0 &= -\frac{1}{2} \frac{J_z}{2} V_0 \left(\frac{1}{\xi_2} + \frac{1}{\xi_3} \right) \\ \Delta V_1 &= -\frac{1}{2} \frac{J_z}{2} V_1 \left(\frac{1}{\xi'_1} + \frac{1}{\xi_3} \right)\end{aligned}\tag{5.2.37}$$

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

$$\begin{aligned}\Delta V_0 &= -\left(\frac{J_z}{4} V_0 + J_t V_0 \right) \left(\frac{1}{\xi_2} + \frac{1}{\xi_3} \right) \\ \Delta V_1 &= -\left(\frac{J_z}{4} V_1 + J_t V_1 \right) \left(\frac{1}{\xi'_1} + \frac{1}{\xi_3} \right)\end{aligned}\tag{5.2.38}$$

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

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

$$\begin{aligned}&\frac{1}{\xi_5} J_t^2 \left(1 - \hat{n}_{d\beta} \right) \hat{n}_{d\bar{\beta}} c_{k'\bar{\beta}} c_{k\bar{\beta}}^\dagger + \frac{1}{\xi'_5} J_t^2 \left(1 - \hat{n}_{d\bar{\beta}} \right) \hat{n}_{d\beta} c_{k\bar{\beta}}^\dagger c_{k'\bar{\beta}} \\ &= \frac{1}{\xi_3} J_t^2 c_{k\bar{\beta}}^\dagger c_{k'\bar{\beta}} \left[\left(1 - \hat{n}_{d\bar{\beta}} \right) \hat{n}_{d\beta} - \left(1 - \hat{n}_{d\beta} \right) \hat{n}_{d\bar{\beta}} \right] + \delta_{kk'} \frac{1}{\xi_3} J_t^2 \left(1 - \hat{n}_{d\beta} \right) \hat{n}_{d\bar{\beta}} \\ &= -\frac{1}{\xi_3} 2 J_t^2 c_{k\bar{\beta}}^\dagger c_{k'\bar{\beta}} \frac{\hat{n}_{d\bar{\beta}} - \hat{n}_{d\beta}}{2} + \delta_{kk'} \frac{1}{\xi_3} J_t^2 \left(1 - \hat{n}_{d\beta} \right) \hat{n}_{d\bar{\beta}}\end{aligned}\tag{5.2.39}$$

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

$$\Delta J_z = -\frac{1}{2\xi_3} 2 J_t^2\tag{5.2.40}$$

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

$$\begin{aligned}\Delta \epsilon_d &= \frac{1}{2\xi_3} J_t^2 \delta_{kk'} \\ \Delta U &= -\frac{1}{\xi_3} J_t^2 \delta_{kk'}\end{aligned}\tag{5.2.41}$$

The remaining terms are those with $J_z J_t$:

$$\left[-\frac{1}{2} \left(\frac{1}{\xi_3} + \frac{1}{\xi_5} \right) \frac{J_t J_0^z}{2} c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{k'\beta} - \frac{1}{2} \left(\frac{1}{\xi'_4} + \frac{1}{\xi'_5} \right) \frac{J_t J_1^z}{2} c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{k'\beta} \right] + \text{h.c.}\tag{5.2.42}$$

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

$$\Delta J_t = -\frac{1}{\xi_3} J_t J_0^z\tag{5.2.43}$$

5.2.6 Scaling equations

Looking at eqs. 5.2.32, 5.2.35, 5.2.41, 5.2.38, 5.2.40 and 5.2.43, and summing over β , we can write down the scaling equations for the Anderson-Kondo model.

$$\begin{aligned}
 \Delta\epsilon_d &= \frac{|V_1|^2}{\xi'_1} + \frac{|V_0|^2}{\xi'_2} - \frac{2|V_0|^2}{\xi_2} + \sum_k \frac{1}{\xi_3} \left(J_t^2 + \frac{1}{2} J_z^2 \right) \\
 \Delta U &= \frac{2|V_1|^2}{\xi'_1} + \frac{2|V_0|^2}{\xi'_2} - \frac{2|V_1|^2}{\xi_1} - \frac{2|V_0|^2}{\xi'_2} - \sum_k \frac{1}{\xi_3} \left(2J_t^2 + J_z^2 \right) \\
 \Delta V_0 &= -V_0 \left(\frac{J_z}{2} + J_t \right) \left(\frac{1}{\xi_2} + \frac{1}{\xi_3} \right) \\
 \Delta V_1 &= -V_1 \left(\frac{J_z}{2} + J_t \right) \left(\frac{1}{\xi'_1} + \frac{1}{\xi_3} \right) \\
 \Delta J_z &= -\frac{2}{\xi_3} J_t^2 \\
 \Delta J_t &= -\frac{2}{\xi_3} J_t J_z^2
 \end{aligned} \tag{5.2.44}
 \quad \left| \begin{aligned}
 \xi_1 &= \omega - \frac{\epsilon_q}{2} - \epsilon_d - U + \frac{J_z}{2} \\
 \xi_2 &= \omega - \frac{\epsilon_q}{2} - \epsilon_d + J_z \\
 \xi'_1 &= \omega - \frac{\epsilon_q}{2} + \epsilon_d + U + J_z \\
 \xi'_2 &= \omega - \frac{\epsilon_q}{2} + \epsilon_d + \frac{J_z}{2} \\
 \xi'_3 &= \xi'_4 = \xi'_5 \\
 &= \omega - \frac{\epsilon_q}{2} + \frac{J_z}{2} \\
 &= \xi_3 = \xi_4 = \xi_5
 \end{aligned} \right.$$

5.2.7 Particle-Hole symmetry

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

$$\begin{aligned}
 &\epsilon_d \hat{n}_d + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + J_z (\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow}) (\hat{n}_{q\uparrow} - \hat{n}_{q\downarrow}) \\
 &\rightarrow 2\epsilon_d + U - (\epsilon_d + U) \hat{n}_d + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + J_z (\hat{n}_{d\downarrow} - \hat{n}_{d\uparrow}) (\hat{n}_{q\downarrow} - \hat{n}_{q\uparrow})
 \end{aligned} \tag{5.2.45}$$

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

$$\Delta (2\epsilon_d + U) = \frac{|V_1|^2}{\xi'_1} - \frac{|V_1|^2}{\xi_2} \tag{5.2.46}$$

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

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

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

$$\begin{aligned}
 \frac{1}{\xi_1} &= \frac{1}{\xi'_1} \approx 0 \\
 \xi_2 &= \xi'_2 \approx \omega - \frac{\epsilon_q}{2}
 \end{aligned} \tag{5.2.47}$$

These give

$$\begin{aligned}
 \Delta U &\approx 0 \\
 \Delta\epsilon_d &\approx -\frac{|V_0|^2}{\xi_2} \approx -\frac{|V_0|^2}{\omega - \frac{\epsilon_q}{2}}
 \end{aligned} \tag{5.2.48}$$

This is the same form that we had in the pure SIAM, and we can again repeat what we did in subsection 5.1.4.

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

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

$$\Delta J = -\frac{1}{\xi_3} J^2 = -J^2 \frac{1}{\omega - \frac{\epsilon_q}{2} + \frac{J_z}{2}} \tag{5.2.49}$$

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

$$\Delta J = -J^2 \frac{1}{-\epsilon_q + \frac{1}{4}J} \quad (5.2.50)$$

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

$$\Delta J = J^2 \frac{1}{\epsilon_q} \quad (5.2.51)$$

This is the Kondo model one-loop form.

5.3 Anderson-Kondo (charge) model URG

Performing the Schrieffer-Wolff transformation on the SIAM generates four types of terms. The simplest terms are ones that renormalize the impurity scales ϵ_d and U . The next are the potential scattering terms that describe interactions between mobile electrons with the impurity simply acting as a stationary potential. The third term is the familiar Kondo model interaction terms that involve a Heisenberg-like interaction between the impurity spin $S_d^z = \frac{1}{2}(\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow})$ and the global spin of the mobile electrons $\frac{1}{2} \sum_{kk'\alpha\beta} c_{k\alpha}^\dagger \vec{\sigma}_{\alpha\beta} c_{k'\beta}$. The fourth term is the interactions that modify the charge of either entity by 2, $c_{k\alpha}^\dagger c_{k'\bar{\alpha}}^\dagger c_{d\alpha} c_{d\bar{\alpha}}$. We will be considering the last kind of terms in this section. For that, we define the Nambu spinor [34, 35].

$$\psi^k = \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow}^\dagger \end{pmatrix} \quad (5.3.1)$$

and the charge isospin [36] for the mobile conduction electrons

$$\vec{C} = \sum_{kk'} \psi^{k\dagger} \vec{S} \psi^{k'} = \frac{1}{2} \sum_{kk'\alpha\beta} \psi_\alpha^{k\dagger} \vec{\sigma}_{\alpha\beta} \psi_\beta^{k'} \quad (5.3.2)$$

The various components of the isospin are

$$\begin{aligned} C^z &= \sum_{kk'\sigma} \frac{1}{2} \psi_\sigma^{k\dagger} \sigma_{\sigma\sigma}^z \psi_\sigma^{k'} = \frac{1}{2} \sum_{kk'} \left(\text{70} c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k'\downarrow} c_{k\downarrow}^\dagger \right) \equiv \frac{1}{2} \sum_{kk'} \left(c_{k\uparrow}^\dagger c_{k'\uparrow} + c_{k\downarrow}^\dagger c_{k'\downarrow} - \delta_{kk'} \right) \\ &= \frac{1}{2} \sum_{kk'\sigma} \left(c_{k\sigma}^\dagger c_{k'\sigma} - \frac{1}{2} \delta_{kk'} \right) \\ C^x &= \sum_{kk'\sigma} \frac{1}{2} \psi_\sigma^{k\dagger} \sigma_{\sigma\bar{\sigma}}^x \psi_\sigma^{k'} = \frac{1}{2} \sum_{kk'} \left(\text{27} c_{k\uparrow}^\dagger c_{k'\downarrow}^\dagger + c_{k\downarrow} c_{k'\uparrow} \right) = \sum_{kk'\sigma} \frac{\sigma}{4} \left(\text{3} c_{k\sigma}^\dagger c_{k'\bar{\sigma}}^\dagger + \text{h.c.} \right) \\ C^y &= \sum_{kk'\sigma} \frac{1}{2} \psi_\sigma^{k\dagger} \sigma_{\sigma\bar{\sigma}}^y \psi_\sigma^{k'} = -\frac{i}{2} \sum_{kk'} \left(c_{k\uparrow}^\dagger c_{k'\downarrow}^\dagger - c_{k\downarrow} c_{k'\uparrow} \right) = \sum_{kk'\sigma} -\frac{i\sigma}{4} \left(\text{14} c_{k\sigma}^\dagger c_{k'\bar{\sigma}}^\dagger - \text{h.c.} \right) \end{aligned} \quad (5.3.3)$$

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

$$[A, B^\dagger] = \frac{1}{4} \sum_{kk', qq'} \left[\text{3} c_{k\uparrow}^\dagger c_{k'\downarrow}^\dagger, i c_{q'\downarrow} c_{q\uparrow} \right] = \frac{i}{4} \sum_{kq} \left(c_{k\uparrow}^\dagger c_{q\uparrow} - c_{k\downarrow} c_{q\downarrow}^\dagger \right) \quad (5.3.4)$$

and therefore

$$\Rightarrow [C^x, C^y] = \frac{i}{2} \sum_{kq} \left(c_{k\uparrow}^\dagger c_{q\uparrow} - c_{k\downarrow} c_{q\downarrow}^\dagger \right) = i C^z \quad (5.3.5)$$

There are similar operators for the impurity electron:

$$\begin{aligned}\psi_d &= \begin{pmatrix} c_{d\uparrow} \\ c_{d\downarrow}^\dagger \end{pmatrix} \\ C_d^z &= \frac{1}{2} (c_{d\uparrow}^\dagger c_{d\uparrow} + c_{d\downarrow}^\dagger c_{d\downarrow} - 1) = \frac{1}{2} (\hat{n}_d - 1) \\ C_d^x &= \frac{1}{2} (c_{d\uparrow}^\dagger c_{d\downarrow}^\dagger + c_{d\downarrow} c_{d\uparrow}) = \sum_{\sigma} \frac{\sigma}{4} (c_{d\sigma}^\dagger c_{d\sigma}^\dagger + \text{h.c.}) \\ C_d^y &= -i \frac{1}{2} (c_{d\uparrow}^\dagger c_{d\downarrow}^\dagger - c_{d\downarrow} c_{d\uparrow}) = -i \sum_{\sigma} \frac{\sigma}{4} (c_{d\sigma}^\dagger c_{d\sigma}^\dagger - \text{h.c.})\end{aligned}\tag{5.3.6}$$

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

$$4K_z C_d^z C^z + K_t (C_d^+ C^- + C_d^- C^+) \tag{5.3.7}$$

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

$$C^+ = \sum_{kk'} \overset{4}{c}_{k\uparrow}^\dagger c_{k'\downarrow}^\dagger, \quad C^- = \sum_{kk'} c_{k'\downarrow} c_{k\uparrow} \tag{5.3.8}$$

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

$$KC_d^z C^z + \frac{1}{2} K (C_d^+ C^- + C_d^- C^+) = K \vec{C}_d \cdot \vec{C} \tag{5.3.9}$$

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

$$\begin{aligned}\mathcal{H}_d &= \epsilon_q \tau_{q\beta} + H_{imp} + K_z (\hat{n}_d - 1) \tau_{q\beta} \\ \mathcal{H}_X &= V_q c_{q\beta}^\dagger c_{d\beta} + \text{h.c.} + K_z (\hat{n}_d - 1) \sum_k (c_{q\beta}^\dagger c_{k\beta} + \text{h.c.}) + K_t \sum_k (c_{d\beta}^\dagger c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}} c_{q\beta} + \text{h.c.})\end{aligned}\tag{5.3.10}$$

As usual, we have considered only one mobile electron on the shell we are decoupling, and we keep only the energy of that electron and the impurity in the diagonal part which comes down in the denominator. Note that the factors of half in C^z are cancelled by the factor of 4 in $4K_z$. The last term in \mathcal{H}_d is obtained by setting $k = k' = q$ and $\sigma = \beta$ in eq. 5.3.3, and then recognizing that $\hat{n}_{q\beta} - \frac{1}{2} = \tau_{q\beta}$. The K_z part of \mathcal{H}_X is obtained by noting:

$$\begin{aligned}C_{q \neq k}^z &= \frac{1}{2} (c_{q\uparrow}^\dagger c_{k\uparrow} + c_{k\uparrow}^\dagger c_{q\uparrow} - c_{k\downarrow}^\dagger c_{q\downarrow} - c_{q\downarrow}^\dagger c_{k\downarrow}) \\ &= \frac{1}{2} (c_{q\uparrow}^\dagger c_{k\uparrow} + c_{k\uparrow}^\dagger c_{q\uparrow} + c_{q\downarrow}^\dagger c_{k\downarrow} + c_{k\downarrow}^\dagger c_{q\downarrow}) \\ &= \frac{1}{2} \sum_{\sigma} (c_{q\sigma}^\dagger c_{k\sigma} + \text{h.c.})\end{aligned}\tag{5.3.11}$$

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

$$\begin{aligned}T_1 &= V_1 c_{d\beta} \hat{n}_{d\bar{\beta}} \\ T_2 &= V_0 c_{d\beta} (1 - \hat{n}_{d\bar{\beta}}) \\ T_3 &= K_z^1 \hat{n}_{d\beta} \hat{n}_{d\bar{\beta}} c_{k\beta} \\ T_4 &= -K_z^0 (1 - \hat{n}_{d\beta}) (1 - \hat{n}_{d\bar{\beta}}) c_{k\beta} \\ T_5 &= K_t c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} c_{d\beta}\end{aligned}\tag{5.3.12}$$

5.3.1 Calculation of renormalization in particle sector

The renormalization in this sector is

$$c_{q\beta}^\dagger T \eta \quad (5.3.13)$$

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

$$\begin{aligned} & \left(1 - \hat{n}_{d\beta}\right) \left[\hat{n}_{d\bar{\beta}} \frac{|V_1|^2}{\xi_1} + \left(1 - \hat{n}_{d\bar{\beta}}\right) \frac{|V_0|^2}{\xi_2} \right] + \left[\frac{K_z^{12}}{\xi_3} \hat{n}_{d\beta} \hat{n}_{d\bar{\beta}} + \frac{K_z^{02}}{\xi_4} \left(1 - \hat{n}_{d\beta}\right) \left(1 - \hat{n}_{d\bar{\beta}}\right) \right] c_{k'\beta} c_{k\beta}^\dagger \\ & + \frac{K_t^2}{\xi_5} \left(1 - \hat{n}_{d\beta}\right) \left(1 - \hat{n}_{d\bar{\beta}}\right) c_{k\bar{\beta}}^\dagger c_{k'\bar{\beta}} - \frac{1}{2} \left(\frac{1}{\xi_1} + \frac{1}{\xi_3} \right) V_1 K_z^1 \hat{n}_{d\bar{\beta}} \left(c_{k\beta}^\dagger c_{d\beta} + \text{h.c.} \right) \\ & + \frac{1}{2} \left(\frac{1}{\xi_1} + \frac{1}{\xi_5} \right) V_1 K_t \left(1 - \hat{n}_{d\beta}\right) \left(c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} + \text{h.c.} \right) - \frac{1}{2} \left(\frac{1}{\xi_3} + \frac{1}{\xi_5} \right) K_z^1 K_t \left(c_{d\beta}^\dagger c_{d\bar{\beta}}^\dagger c_{k'\bar{\beta}} c_{k\beta} + \text{h.c.} \right) \end{aligned} \quad (5.3.14)$$

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

The intermediate energies, E_i^0 , are

$$\begin{aligned} E_1^0 &= E_3^0 = \frac{\epsilon_q}{2} + 2\epsilon_d + U \\ E_2^0 &= \frac{\epsilon_q}{2} + \epsilon_d \\ E_4^0 &= \frac{\epsilon_q}{2} \\ E_5^0 &= \frac{\epsilon_q}{2} + 2\epsilon_d + U - K_z \end{aligned} \quad (5.3.15)$$

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

5.3.2 Calculation of renormalization in hole sector

The renormalization in the hole sector is given by

$$T^\dagger c_{q\beta} \eta_0^\dagger \quad (5.3.16)$$

at energy ϵ_q . That comes out to be

$$\begin{aligned} & \frac{|V_1|^2}{\xi'_1} \hat{n}_{d\beta} \hat{n}_{d\bar{\beta}} + \frac{|V_0|^2}{\xi'_2} \hat{n}_{d\beta} \left(1 - \hat{n}_{d\bar{\beta}}\right) + \left[\frac{K_z^{12}}{\xi'_3} \hat{n}_{d\beta} \hat{n}_{d\bar{\beta}} + \frac{K_z^{02}}{\xi'_4} \left(1 - \hat{n}_{d\beta}\right) \left(1 - \hat{n}_{d\bar{\beta}}\right) \right] c_{k\beta}^\dagger c_{k'\beta} \\ & + \frac{K_t^2}{\xi'_5} \hat{n}_{d\beta} \hat{n}_{d\bar{\beta}} c_{k'\bar{\beta}} c_{k\bar{\beta}}^\dagger - \frac{1}{2} \left(\frac{1}{\xi'_2} + \frac{1}{\xi'_4} \right) V_0 K_z^0 \left(1 - \hat{n}_{d\bar{\beta}}\right) \left(c_{k\beta}^\dagger c_{d\beta} + \text{h.c.} \right) \\ & + \frac{1}{2} \left(\frac{1}{\xi'_2} + \frac{1}{\xi'_5} \right) V_0 K_t \hat{n}_{d\beta} \left(c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} + \text{h.c.} \right) - \frac{1}{2} \left(\frac{1}{\xi'_4} + \frac{1}{\xi'_5} \right) K_z^0 K_t \left(c_{d\beta}^\dagger c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}} c_{k'\beta} + \text{h.c.} \right) \end{aligned} \quad (5.3.17)$$

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

$$\begin{aligned} E_1^1 &= \frac{\epsilon_q}{2} + \epsilon_d \\ E_2^1 &= E_4^1 = \frac{\epsilon_q}{2} \\ E_3^1 &= \frac{\epsilon_q}{2} + 2\epsilon_d + U \\ E_5^1 &= \frac{\epsilon_q}{2} - K_z \end{aligned} \quad (5.3.18)$$

5.3.3 Relating the ω

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

First the particle sector ω_i :

$$\begin{aligned}\omega_1 &= -\frac{\epsilon_q}{2} + \epsilon_d \\ \omega_2 = \omega_5 &= -\frac{\epsilon_q}{2} - K_z \\ \omega_3 &= -\frac{\epsilon_q}{2} + 2\epsilon_d + U \\ \omega_4 &= -\frac{\epsilon_q}{2}\end{aligned}\tag{5.3.19}$$

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

$$\begin{aligned}\omega_1 &= \omega + \epsilon_d + K_z \\ \omega_2 = \omega_5 &= \omega \\ \omega_3 &= \omega + 2\epsilon_d + U + K_z \\ \omega_4 &= \omega + K_z\end{aligned}\tag{5.3.20}$$

For the hole sector, we get

$$\begin{aligned}\omega'_1 = \omega'_5 &= -\frac{\epsilon_q}{2} + 2\epsilon_d + U - K_z \\ \omega'_2 &= -\frac{\epsilon_q}{2} + \epsilon_d \\ \omega'_3 &= -\frac{\epsilon_q}{2} + 2\epsilon_d + U \\ \omega'_4 &= -\frac{\epsilon_q}{2}\end{aligned}\tag{5.3.21}$$

and, in terms of ω ,

$$\begin{aligned}\omega'_1 = \omega'_5 &= \omega + 2\epsilon_d + U \\ \omega'_2 &= \omega + \epsilon_d + K_z \\ \omega'_3 &= \omega + 2\epsilon_d + U + K_z \\ \omega'_4 &= \omega + K_z\end{aligned}\tag{5.3.22}$$

The denominators can thus be written as

$$\begin{aligned}\xi_1 &= \omega - \frac{\epsilon_q}{2} - \epsilon_d - U + K_z, & \xi'_1 &= \omega - \frac{\epsilon_q}{2} + \epsilon_d + U \\ \xi_2 &= \omega - \frac{\epsilon_q}{2} - \epsilon_d, & \xi'_2 &= \omega - \frac{\epsilon_q}{2} + \epsilon_d + K_z \\ \xi_3 = \xi_4 &= \omega - \frac{\epsilon_q}{2} + K_z, & \xi'_3 = \xi'_4 &= \omega - \frac{\epsilon_q}{2} + K_z \\ \xi_5 &= \omega - \frac{\epsilon_q}{2} - 2\epsilon_d - U + K_z, & \xi'_5 &= \omega - \frac{\epsilon_q}{2} + 2\epsilon_d + U + K_z\end{aligned}\tag{5.3.23}$$

5.3.4 Scaling Equations

$$\begin{aligned}
 \Delta\epsilon_d &= \frac{|V_1|^2}{\xi'_1} + \frac{|V_0|^2}{\xi'_2} - \frac{2|V_0|^2}{\xi_2} - \sum_k \left(2\frac{K_z^2}{\xi_3} + \frac{K_t^2}{\xi_5} \right) \\
 \Delta U &= \frac{2|V_1|^2}{\xi'_1} + \frac{2|V_0|^2}{\xi_2} - \frac{2|V_1|^2}{\xi_1} - \frac{2|V_0|^2}{\xi'_2} + 2 \sum_k \left(2\frac{K_z^2}{\xi_3} + \frac{K_t^2}{\xi_5} \right) \\
 \Delta V_1 &= -\frac{1}{4} \left[V_1 K_z \left(\frac{1}{\xi_1} + \frac{1}{\xi_3} \right) - V_0 K_t \left(\frac{1}{\xi'_2} + \frac{1}{\xi'_5} \right) \right] \\
 \Delta V_0 &= -\frac{1}{4} \left[V_0 K_z \left(\frac{1}{\xi'_2} + \frac{1}{\xi'_4} \right) - V_1 K_t \left(\frac{1}{\xi_1} + \frac{1}{\xi_5} \right) \right] \\
 \Delta K_z &= -K_t^2 \frac{1}{\xi_5} \\
 \Delta K_t &= -K_z K_t \left(\frac{1}{\xi_3} + \frac{1}{\xi_5} + \frac{1}{\xi'_4} + \frac{1}{\xi'_5} \right)
 \end{aligned} \tag{5.3.24}$$

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

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

$$\epsilon_d \hat{n}_d + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + K_z (\hat{n}_d - 1) \left(c_{k'\uparrow}^\dagger c_{k'\uparrow} - c_{k'\downarrow}^\dagger c_{k'\downarrow} \right) + \frac{K_t}{2} \left(c_{d\beta}^\dagger c_{d\bar{\beta}}^\dagger c_{k\beta} c_{k'\bar{\beta}} + \text{h.c.} \right) \tag{5.3.25}$$

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

$$\epsilon_d = -\epsilon_d - U, \quad V_1 = V_0, \quad 2K_z = K_t = \frac{K}{2} \tag{5.3.26}$$

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

$$\begin{aligned}
 \Delta\epsilon_d &= -\frac{1}{2} \Delta U \\
 \Delta V_1 &= \Delta V_0 = \frac{V_1 K}{8} \left(\frac{1}{\xi_1} + \frac{1}{\xi_6} \right) \\
 \Delta K &= K^2 \frac{1}{\xi_5}
 \end{aligned} \tag{5.3.27}$$

Chapter 6

URG of Full Generalized SIAM

6.1 The spin-charge-SIAM Hamiltonian

In this section, we will consider the SIAM with both spin and charge fluctuations. This will be a combination of the last two sections. The total Hamiltonian will be

$$\begin{aligned} \mathcal{H} = & \sum_{k\sigma} \tau_{k\sigma} + \epsilon_d \hat{n}_d + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \sum_{k\sigma} \left(V_k c_{k\sigma}^\dagger c_{d\sigma} + \text{h.c.} \right) + J_z S_d^z \sum_{kk'} \left(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow} \right) \\ & + J_t \sum_{kk'\sigma} c_{d\sigma}^\dagger c_{d\sigma} c_{k\sigma}^\dagger c_{k'\sigma}^{\text{1}} + K_z C_d^z \sum_{kk'} \left(c_{k\sigma}^\dagger c_{k'\sigma} - \frac{1}{2} \delta_{kk'} \right) + K_t \sum_{kk'\sigma} \left(c_{d\sigma}^\dagger c_{d\sigma}^\dagger c_{k\sigma} c_{k'\sigma} + \text{h.c.} \right) \end{aligned} \quad (6.1.1)$$

There are eight different type of scattering terms:

Figure 6.1: Schematic diagram of the generalized SIAM model.

$$\begin{aligned} c_{q\beta}^\dagger T_1 &= V_1 c_{q\beta}^\dagger c_{d\beta} \hat{n}_{d\bar{\beta}}, & c_{q\beta}^\dagger T_2 &= V_0 c_{q\beta}^\dagger c_{d\beta} \left(1 - \hat{n}_{d\bar{\beta}} \right) \\ c_{q\beta}^\dagger T_3 &= \sum_{k < \Lambda_N} J_0^z \hat{n}_{d\beta} \left(1 - \hat{n}_{d\bar{\beta}} \right) c_{q\beta}^\dagger c_{k\beta}, & c_{q\beta}^\dagger T_4 &= - \sum_{k < \Lambda_N} J_1^z \hat{n}_{d\bar{\beta}} \left(1 - \hat{n}_{d\beta} \right) c_{q\beta}^\dagger c_{k\beta} \\ c_{q\beta}^\dagger T_5 &= \sum_{k < \Lambda_N} J^t c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\bar{\beta}}, & c_{q\beta}^\dagger T_6 &= K_z^1 \sum_{k < \Lambda_N} \hat{n}_{d\beta} \hat{n}_{d\bar{\beta}} c_{q\beta}^\dagger c_{k\beta} \\ c_{q\beta}^\dagger T_7 &= -K_z^0 \sum_{k < \Lambda_N} \left(1 - \hat{n}_{d\beta} \right) \left(1 - \hat{n}_{d\bar{\beta}} \right) c_{q\beta}^\dagger c_{k\beta}, & c_{q\beta}^\dagger T_8 &= K_t \sum_{k < \Lambda_N} c_{q\beta}^\dagger c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} c_{d\beta} \end{aligned} \quad (6.1.2)$$

6.2 Obtaining the RG equations

6.2.1 Particle Sector

Renormalization is

$$c_{q\beta}^\dagger T \eta = c_{q\beta}^\dagger \sum_{ij} T_i \eta_j \quad (6.2.1)$$

The terms that survive are

$$\begin{aligned}
 c_{q\beta}^\dagger T \eta &= \sum_{i=1}^8 \frac{1}{\omega_i - E_i} \hat{n}_{q\beta} T_i T_i^\dagger + \left(\frac{1}{\omega_2 - E_2} + \frac{1}{\omega_5 - E_5} \right) \hat{n}_{q\beta} (T_2 T_5^\dagger + T_5 T_2^\dagger) \\
 &+ \left(\frac{1}{\omega_2 - E_2} + \frac{1}{\omega_3 - E_3} \right) \hat{n}_{q\beta} (T_2 T_3^\dagger + T_3 T_2^\dagger) + \left(\frac{1}{\omega_3 - E_3} + \frac{1}{\omega_5 - E_5} \right) \hat{n}_{q\beta} (T_3 T_5^\dagger + T_5 T_3^\dagger) \\
 &+ \left(\frac{1}{\omega_1 - E_1} + \frac{1}{\omega_6 - E_6} \right) \hat{n}_{q\beta} (T_1 T_6^\dagger + T_6 T_1^\dagger) + \left(\frac{1}{\omega_1 - E_1} + \frac{1}{\omega_8 - E_8} \right) \hat{n}_{q\beta} (T_1 T_8^\dagger + T_8 T_1^\dagger) \\
 &+ \left(\frac{1}{\omega_6 - E_6} + \frac{1}{\omega_8 - E_8} \right) \hat{n}_{q\beta} (T_6 T_8^\dagger + T_8 T_6^\dagger) \\
 &= \frac{|V_1|^2}{\xi_1} (1 - \hat{n}_{d\beta}) \hat{n}_{d\bar{\beta}} + \frac{|V_0|^2}{\xi_2} (1 - \hat{n}_{d\beta}) (1 - \hat{n}_{d\bar{\beta}}) + \frac{1}{\xi_5} J_t^2 (1 - \hat{n}_{d\beta}) \hat{n}_{d\bar{\beta}} c_{k'\bar{\beta}} c_{k\bar{\beta}}^\dagger \\
 &+ \frac{1}{4} \left[J_0^z \frac{\hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}})}{\xi_3} + J_1^z \frac{\hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta})}{\xi_4} \right] c_{k'\beta} c_{k\beta}^\dagger - \frac{1}{2} \left(\frac{1}{\xi_2} + \frac{1}{\xi_5} \right) J_t (1 - \hat{n}_{d\beta}) (V_0 c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} + \text{h.c.}) \quad (6.2.2) \\
 &- \frac{1}{2} \left(\frac{1}{\xi_2} + \frac{1}{\xi_3} \right) \frac{J_0^z}{2} (1 - \hat{n}_{d\bar{\beta}}) (V_0 c_{k\beta}^\dagger c_{d\beta} + \text{h.c.}) - \frac{1}{2} \left(\frac{1}{\xi_3} + \frac{1}{\xi_5} \right) \frac{J_t J_0^z}{2} (c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{k'\beta} + \text{h.c.}) \\
 &+ \left[\frac{K_z^{12}}{\xi_6} \hat{n}_{d\beta} \hat{n}_{d\bar{\beta}} + \frac{K_z^{02}}{\xi_7} (1 - \hat{n}_{d\beta}) (1 - \hat{n}_{d\bar{\beta}}) \right] c_{k'\beta} c_{k\beta}^\dagger + \frac{K_t^2}{\xi_8} (1 - \hat{n}_{d\beta}) (1 - \hat{n}_{d\bar{\beta}}) c_{k\bar{\beta}}^\dagger c_{k'\bar{\beta}} \\
 &- \frac{1}{2} \left(\frac{1}{\xi_1} + \frac{1}{\xi_6} \right) V_1 K_z^1 \hat{n}_{d\bar{\beta}} (c_{k\beta}^\dagger c_{d\beta} + \text{h.c.}) + \frac{1}{2} \left(\frac{1}{\xi_1} + \frac{1}{\xi_8} \right) V_1 K_t (1 - \hat{n}_{d\beta}) (c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} + \text{h.c.}) \\
 &- \frac{1}{2} \left(\frac{1}{\xi_6} + \frac{1}{\xi_8} \right) K_z^1 K_t (c_{d\beta}^\dagger c_{d\bar{\beta}}^\dagger c_{k'\bar{\beta}} c_{k\beta} + \text{h.c.})
 \end{aligned}$$

where $\xi_i = \omega_i - E_i$ and we substituted $\hat{n}_{q\beta} = 1$. The energies in the denominators are

$$\begin{aligned}
 E_1 = E_8 &= \frac{\epsilon_q}{2} + 2\epsilon_d + U - \frac{1}{2} K_z, & E_2 = E_4 = E_5 &= \frac{\epsilon_q}{2} + \epsilon_d - \frac{1}{2} J_z \\
 E_3 &= \frac{\epsilon_q}{2} + \epsilon_d + \frac{1}{2} J_z, & E_6 &= \frac{\epsilon_q}{2} + 2\epsilon_d + U + \frac{1}{2} K_z \quad (6.2.3) \\
 E_7 &= \frac{\epsilon_q}{2} - \frac{1}{2} K_z, & E_8 &= \frac{\epsilon_q}{2} + 2\epsilon_d + U - \frac{1}{2} K_z
 \end{aligned}$$

The quantum fluctuation scales are

$$\begin{aligned}
 \omega_1 &= \omega + \epsilon_d + \frac{1}{2} K_z, & \omega_3 &= \omega + \epsilon_d + \frac{1}{2} K_z + J_z \\
 \omega_2 &= \omega_8 = \omega + \frac{1}{2} J_z, & \omega_4 &= \omega_5 = \omega + \epsilon_d + \frac{1}{2} K_z \\
 \omega_6 &= \omega + 2\epsilon_d + U + \frac{1}{2} J_z + K_z, & \omega_7 &= \omega + \frac{1}{2} J_z \quad (6.2.4)
 \end{aligned}$$

6.2.2 Hole sector

Renormalization is

$$\begin{aligned}
 \eta c_{q\beta}^\dagger T &= \left(1 - \hat{n}_{q\beta}\right) \left[\sum_{i=1}^8 \frac{1}{\omega'_i - E'_i} T_i T_i^\dagger + \left(\frac{1}{\omega'_1 - E'_1} + \frac{1}{\omega'_4 - E'_4} \right) (T_1 T_4^\dagger + T_4 T_1^\dagger) \right. \\
 &\quad + \left(\frac{1}{\omega'_1 - E'_1} + \frac{1}{\omega'_5 - E'_5} \right) (T_1 T_5^\dagger + T_5 T_1^\dagger) + \left(\frac{1}{\omega'_2 - E'_2} + \frac{1}{\omega'_7 - E'_7} \right) (T_2 T_7^\dagger + T_7 T_2^\dagger) \\
 &\quad + \left(\frac{1}{\omega'_2 - E'_2} + \frac{2}{\omega'_8 - E'_8} \right) (T_2 T_8^\dagger + T_8 T_2^\dagger) + \left(\frac{1}{\omega'_4 - E'_4} + \frac{1}{\omega'_5 - E'_5} \right) (T_4 T_5^\dagger + T_5 T_4^\dagger) \\
 &\quad \left. + \left(\frac{1}{\omega'_7 - E'_7} + \frac{1}{\omega'_8 - E'_8} \right) \hat{n}_{q\beta} (T_7 T_8^\dagger + T_8 T_7^\dagger) \right] \\
 &= \frac{|V_1|^2}{\xi'_1} \hat{n}_{d\bar{\beta}} \hat{n}_{d\beta} + \frac{|V_0|^2}{\xi'_2} \hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}}) + \frac{1}{4} \left[J_0^{z^2} \frac{\hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}})}{\xi'_3} + J_1^{z^2} \frac{\hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta})}{\xi'_4} \right] c_{k\beta}^\dagger c_{k'\beta} \\
 &\quad + \frac{1}{\xi'_5} J_t^2 (1 - \hat{n}_{d\bar{\beta}}) \hat{n}_{d\beta} c_{k\bar{\beta}}^\dagger c_{k'\bar{\beta}} - \frac{1}{2} \left(\frac{1}{\xi'_4} + \frac{1}{\xi'_1} \right) \frac{J_1^z}{2} \hat{n}_{d\bar{\beta}} (V_1 c_{k\beta}^\dagger c_{d\beta} + \text{h.c.}) \\
 &\quad - \frac{1}{2} \left(\frac{1}{\xi'_1} + \frac{1}{\xi'_5} \right) J_t \hat{n}_{d\beta} (V_1 c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} + \text{h.c.}) - \frac{1}{2} \left(\frac{1}{\xi'_4} + \frac{1}{\xi'_5} \right) \frac{J_t J_1^z}{2} (c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{k'\beta} + \text{h.c.}) \\
 &\quad + \left[\frac{K_z^{1^2}}{\xi'_6} \hat{n}_{d\beta} \hat{n}_{d\bar{\beta}} + \frac{K_z^{0^2}}{\xi'_7} (1 - \hat{n}_{d\beta}) (1 - \hat{n}_{d\bar{\beta}}) \right] c_{k\beta}^\dagger c_{k'\beta} + \frac{K_t^2}{\xi'_8} \hat{n}_{d\beta} \hat{n}_{d\bar{\beta}} c_{k'\bar{\beta}}^\dagger c_{k\bar{\beta}} \\
 &\quad - \frac{1}{2} \left(\frac{1}{\xi'_2} + \frac{1}{\xi'_7} \right) V_0 K_z^0 (1 - \hat{n}_{d\bar{\beta}}) (c_{k\beta}^\dagger c_{d\beta} + \text{h.c.}) + \frac{1}{2} \left(\frac{1}{\xi'_2} + \frac{1}{\xi'_8} \right) V_0 K_t \hat{n}_{d\beta} (c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} + \text{h.c.}) \\
 &\quad - \frac{1}{2} \left(\frac{1}{\xi'_7} + \frac{1}{\xi'_8} \right) K_z^0 K_t (c_{d\beta}^\dagger c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}} c_{k'\beta} + \text{h.c.})
 \end{aligned} \tag{6.2.5}$$

The denominator energies are

$$\begin{aligned}
 E'_1 = E'_3 = E'_5 &= \frac{\epsilon_q}{2} + \epsilon_d - \frac{1}{2} J_z, & E'_4 &= \frac{\epsilon_q}{2} + \epsilon_d + \frac{1}{2} J_z \\
 E'_2 &= \frac{\epsilon_q}{2} - \frac{1}{2} K_z, & E'_7 &= \frac{\epsilon_q}{2} + \frac{1}{2} K_z \\
 E'_6 &= \frac{\epsilon_q}{2} + 2\epsilon_d + U - \frac{1}{2} K_z, & E'_8 &= \frac{\epsilon_q}{2} + \epsilon_d - \frac{1}{2} K_z
 \end{aligned} \tag{6.2.6}$$

The quantum fluctuation scales are

$$\begin{aligned}
 \omega'_1 &= \omega + 2\epsilon_d + U + \frac{1}{2}J_z \\
 \omega'_2 &= \omega + \epsilon_d + \frac{1}{2}K_z \\
 \omega'_3 &= \omega'_5 = \omega + \epsilon_d + \frac{1}{2}K_z \\
 \omega'_4 &= \omega + \epsilon_d + \frac{1}{2}K_z + J_z \\
 \omega'_6 &= \omega + 2\epsilon_d + U + \frac{1}{2}J_z \\
 \omega'_7 &= \omega + \frac{1}{2}J_z + K_z \\
 \omega'_8 &= \omega + \epsilon_d + \frac{1}{2}J_z
 \end{aligned} \tag{6.2.7}$$

6.2.3 Scaling equations

The denominators ξ_i, ξ'_i are

$$\begin{aligned}
 \xi_1 &= \omega - \frac{\epsilon_q}{2} - \epsilon_d - U + K_z \\
 \xi_2 &= \omega - \frac{\epsilon_q}{2} - \epsilon_d + J_z \\
 \xi_3 &= \xi_4 = \xi_5 = \xi_6 = \xi_7 = \omega - \frac{\epsilon_q}{2} + \frac{1}{2}J_z + \frac{1}{2}K_z \\
 \xi_8 &= \omega - \frac{\epsilon_q}{2} - 2\epsilon_d - U + \frac{1}{2}J_z + \frac{1}{2}K_z \\
 \xi'_1 &= \omega - \frac{\epsilon_q}{2} + \epsilon_d + U + J_z \\
 \xi'_2 &= \omega - \frac{\epsilon_q}{2} + \epsilon_d + K_z \\
 \xi'_3 &= \xi'_4 = \xi'_5 = \xi'_6 = \xi'_7 = \omega - \frac{\epsilon_q}{2} + \frac{1}{2}J_z + \frac{1}{2}K_z \\
 \xi'_8 &= \omega - \frac{\epsilon_q}{2} + 2\epsilon_d + U + \frac{1}{2}J_z + \frac{1}{2}K_z
 \end{aligned} \tag{6.2.8}$$

The RG equations are

$$\begin{aligned}
 \Delta\epsilon_d &= \frac{|V_1|^2}{\xi_1} + \frac{|V_0|^2}{\xi'_2} - 2\frac{|V_0|^2}{\xi_2} - \sum_k \left(\frac{K_z^2}{2\xi_6} + \frac{K_t^2}{\xi_8} - \frac{J_z^2}{2\xi_3} - \frac{J_t^2}{\xi_3} \right) \\
 \Delta U &= \frac{2|V_1|^2}{\xi'_1} + \frac{2|V_0|^2}{\xi_2} - \frac{2|V_1|^2}{\xi_1} - \frac{2|V_0|^2}{\xi'_2} + 2 \sum_k \left(\frac{K_z^2}{2\xi_6} + \frac{K_t^2}{\xi_8} - \frac{J_z^2}{2\xi_3} - \frac{J_t^2}{\xi_3} \right) \\
 \Delta V_1 &= -\frac{1}{4} \left[V_1 \frac{K_z}{2} \left(\frac{1}{\xi_1} + \frac{1}{\xi_6} \right) - V_0 K_t \left(\frac{1}{\xi'_2} + \frac{1}{\xi'_8} \right) \right] - V_1 \left(\frac{J_z}{2} + J_t \right) \left(\frac{1}{\xi'_1} + \frac{1}{\xi_3} \right) \\
 \Delta V_0 &= -\frac{1}{4} \left[V_0 \frac{K_z}{2} \left(\frac{1}{\xi'_2} + \frac{1}{\xi'_7} \right) - V_1 K_t \left(\frac{1}{\xi_1} + \frac{1}{\xi_8} \right) \right] - V_0 \left(\frac{J_z}{2} + J_t \right) \left(\frac{1}{\xi_2} + \frac{1}{\xi_3} \right) \\
 \Delta J_z &= -2 \frac{J_t^2}{\xi_3} \\
 \Delta J_t &= -2 \frac{J_z J_t}{\xi_3} \\
 \Delta K_z &= -2 \frac{K_t^2}{\xi_8} \\
 \Delta K_t &= -\frac{K_z K_t}{2} \left(\frac{1}{\xi_6} + \frac{1}{\xi_8} + \frac{1}{\xi'_7} + \frac{1}{\xi'_8} \right)
 \end{aligned} \tag{6.2.9}$$

Note that these are the renormalizations are for each momentum state q on the isoenergetic shell - the total renormalization is obtained by summing over the q .

6.3 Numerical and analytical analysis of the symmetric model

6.3.1 Nature of RG flows for the symmetric model at $V = 0$

With the conditions $\epsilon_d = -\epsilon_d - U, J_z = J_t = \frac{1}{2}J, V_0 = V_1, K_z = K_t = \frac{1}{2}K$,

$$\begin{aligned}
 \Delta U &= \sum_k \frac{3}{4} \frac{K^2 - J^2}{\omega - \frac{\epsilon_q}{2} + \frac{1}{4}J + \frac{1}{4}K} \\
 \Delta J &= -\frac{J^2}{\omega - \frac{\epsilon_q}{2} + \frac{1}{4}J + \frac{1}{4}K} \\
 \Delta K &= -\frac{K^2}{\omega - \frac{\epsilon_q}{2} + \frac{1}{4}J + \frac{1}{4}K}
 \end{aligned} \tag{6.3.1}$$

For $\omega - \frac{\epsilon_q}{2} + \frac{1}{4}J + \frac{1}{4}K > 0$, the flow is towards a weak coupling theory, but ¹⁷ these are not URG fixed points. Such flows are shown in fig. 6.2. For the rest of the values of ω , we get RG flows towards a strong-coupling fixed point, with large value of J and K , fig. 6.3. For sufficiently small values of $\frac{J}{K}$, the flow is towards zero U . All such flows characterise a resonant-level strong coupling fixed point, where the four atomic impurity levels are degenerate and located exactly at the Fermi surface. For larger values of $\frac{J}{K}$, there exist flows towards a large positive U . Such fixed points energetically favour an impurity occupation of 1. Both these classes of flows of U are depicted in fig. 6.4.

Figure 6.2: $\omega > 0$. Left: Decay of J towards zero under RG. Right: Flow of U under the same RG. Titles of plots show bare values.

From the RG equations for J and K , we can write down an RG-invariant.

$$\frac{\Delta J}{\Delta K} = \frac{J^2}{K^2} \implies \frac{1}{J} - \frac{1}{K} = \mathcal{C} = \frac{1}{J_0} - \frac{1}{K_0} \tag{6.3.2}$$

Figure 6.3: $\omega < 0$. Flow of J and K to large values, signaling a strong-coupling fixed point.

 Figure 6.4: Left: Flow of U to zero, implying ²a four-fold degenerate impurity. Right: Flow of U to large value, making the impurity singly-occupied, leading to the formation of a local moment.

where \mathcal{C} is a constant. For the case of $J_0 = K_0$ (J_0 is the bare value of J), we must have $J = K$. The RG flows in the K vs J plane are shown in fig. 6.5.

For the case when $\omega + \frac{J}{4} \gg \frac{1}{2}\epsilon_q - \frac{K}{4}$, we can integrate the equation for J :

$$\Delta J \approx -\rho(0)J^2 \frac{1}{\omega + \frac{J}{4}} \Rightarrow -\frac{dJ}{d \ln \frac{D}{D_0}} \approx -\rho(0)J^2 \frac{1}{\omega + \frac{J}{4}} \Rightarrow dJ \left(\frac{\omega}{J^2} + \frac{1}{4J} \right) \approx -\rho(0)d \ln \frac{D}{D_0} \quad (6.3.3)$$

We replaced the density of states by that at the Fermi surface. Integrating this equation from J_0 to J^* on the left hand side and from D_0 to D^* on the right hand side gives

$$\omega \left(\frac{1}{J^*} - \frac{1}{J_0} \right) + \frac{1}{4} \ln \frac{J_0}{J^*} = \rho(0) \ln \frac{D^*}{D_0} \Rightarrow D^* \approx \left(\frac{J_0}{J^*} \right)^{\frac{1}{4\rho(0)}} \exp \left\{ -\frac{1}{\rho(0)} \left(\frac{1}{4} + \frac{\omega}{J_0} \right) \right\} \quad (6.3.4)$$

This gives an estimate of the bandwidth of the emergent window:

 Figure 6.5: RG flows in K vs J plane. Legend indicates relations of bare values.

6.3.2 Eigenstates of symmetrical model at $V = 0$

For the case of $V = 0$, the RG equations simplify considerably.

$$\begin{aligned} \Delta U &= 2 \sum_k \frac{3}{8} \frac{K^2 - J^2}{\omega - \frac{\epsilon_q}{2} + \frac{1}{4}J + \frac{1}{4}K} \\ \Delta J &= -\frac{J^2}{\omega - \frac{\epsilon_q}{2} + \frac{1}{4}J + \frac{1}{4}K} \\ \Delta K &= -\frac{K^2}{\omega - \frac{\epsilon_q}{2} + \frac{1}{4}J + \frac{1}{4}K} \end{aligned} \quad (6.3.5)$$

The strong-coupling fixed points is reached for $\omega - \frac{\epsilon_q}{2} + \frac{1}{4}J + \frac{1}{4}K < 0$. Since the denominator is thus negative, we will have

$$\Delta U \begin{cases} > 0, & J > K \\ < 0, & J < K \end{cases} \quad (6.3.6)$$

This implies that for $J > K$, the flow is towards an impurity which is singly-occupied, while $J < K$ will mean the impurity will be four-fold degenerate with all four levels at the Fermi surface.

The effective Hamiltonian is

$$\mathcal{H}^* = \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} - 2U^* (S_d^z)^2 + \sum_{kk' < \Lambda^*} [J^* \vec{S}_d \cdot \vec{s}_{kk'} + K^* \vec{C}_d \cdot \vec{C}_{kk'}] + \sum_{q > \Lambda^*} [J_q S_d^z s_q^z + K_q C_d^z C_q^z] \quad (6.3.7)$$

where $S_d^z = \frac{1}{2} (\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow})$. Since the interaction terms do not couple the $\hat{n}_d = 1$ and $\hat{n}_d = 0, 2$ subspaces, we can diagonalize the Hamiltonian separately in these subspaces.

In the singly-occupied subspace, the Hamiltonian is

$$\mathcal{H}_1^* = \sum_k \epsilon_k \hat{n}_{k\sigma} - \frac{1}{2} U^* + \sum_{kk' < \Lambda^*} J^* \vec{S}_d \cdot \vec{s}_{kk'} + \sum_{q > \Lambda^*} J^{**} S_d^z s_q^z \quad (6.3.8)$$

The ground state in this subspace is

$$|\Psi\rangle_1^* = \frac{1}{N} \sum_{\substack{kk' < \Lambda^* \\ q > \Lambda^*}} \left[|S_d^z = \frac{1}{2}\rangle |s_{kk'}^z = -\frac{1}{2}\rangle |s_q^z = -\frac{1}{2}\rangle - |S_d^z = -\frac{1}{2}\rangle |s_{kk'}^z = \frac{1}{2}\rangle |s_q^z = \frac{1}{2}\rangle \right] \quad (6.3.9)$$

with an eigenvalue (besides the energy of the bath)

$$E_1 = -\frac{U^*}{2} - \frac{3}{4} J^* - \frac{1}{4} J^{**} \quad (6.3.10)$$

In the complementary subspace, the Hamiltonian is

$$\mathcal{H}_{0,2}^* = \sum_k \epsilon_k \hat{n}_{k\sigma} + \sum_{kk' < \Lambda^*} K^* \vec{C}_d \cdot \vec{C}_{kk'} + \sum_{q > \Lambda^*} K^{**} C_d^z C_q^z \quad (6.3.11)$$

The ground state in this subspace is

$$|\Psi\rangle_{0,2}^* = \frac{1}{N} \sum_{\substack{kk' < \Lambda^* \\ q > \Lambda^*}} \left[|C_d^z = \frac{1}{2}\rangle |C_{kk'}^z = -\frac{1}{2}\rangle |C_q^z = -\frac{1}{2}\rangle - |C_d^z = -\frac{1}{2}\rangle |C_{kk'}^z = \frac{1}{2}\rangle |C_q^z = \frac{1}{2}\rangle \right] \quad (6.3.12)$$

with an eigenvalue (besides the energy of the bath)

$$E_{0,2} = -\frac{3}{4} K^* - \frac{1}{4} K^{**} \quad (6.3.13)$$

Depending on the bare values of J, K and U , we can have the following fixed point situations:

U	J, K	U^*	J^*, K^*	class	ground state	ground state energy
> 0	$J > K$	$\gg 0$	$J^* > K^*$	screened spin	spin singlet	$-\frac{U^*}{2} - \frac{3}{4} J^* - \frac{1}{4} J^{**}$
> 0	$J < K$	0	$J^* < K^*$	screened charge	charge singlet	$-\frac{3}{4} K^* - \frac{1}{4} K^{**}$
< 0	$J > K$	0	$J^* > K^*$	screened spin	spin singlet	$-\frac{3}{4} J^* - \frac{1}{4} J^{**}$
< 0	$J < K$	$\ll 0$	$J^* < K^*$	screened charge	charge singlet	$-\frac{3}{4} K^* - \frac{1}{4} K^{**}$

Table 6.1: Classification of fixed points for various bare values, at $V = 0$

Figure 6.6: Fixed point phases in the plane of bare couplings, at $V = 0$.

6.3.3 Effect of non-zero V on the RG flows

The introduction of V into the RG equations make them analytically intractable, and we have to solve them numerically. The general observation is that we now get both zero and non-zero values of U^* in all the phases. The low quantum fluctuation scale behaviour in the first quadrant is shown in fig. 6.7. It is very similar to that obtained from NRG, as was shown in fig. 2.5.

Figure 6.7: $U - J$ multiple RG flows in first quadrant.

 Figure 6.8: Flows of the couplings for bare values in the first quadrant: $J - K, U > 0$.

First quadrant The first quadrant shows the flow from a free orbital fixed point near $V = U = J = 0$ to an intermediate local moment phase with large U with a final crossover to a stable fixed point at $J^* \gg J_0, U^* = 0$. The initial free orbital fixed point involves four degenerate impurity states at the impurity, and hence no local moment. The intermediate phase involves a local moment because of the large U . The final stable phase involves an impurity which is strongly-coupled to the impurity because of the large V and J . This crossover is depicted in fig. 6.9.

 Figure 6.9: $U - J$ and $U - V$ RG flows.

We have also checked that the fixed point values of J and V go on increasing as we increase the system size.

Third quadrant In the third quadrant ($U_0 < 0, K_0 > J_0$), we see the flow to large negative value of U , leading to a large contribution of the holon-doublon sectors of the impurity subspace, and a large value of K^* which means that the impurity charge sector couples very strongly with the bath charge sector. This is essentially the charge analogue of the Kondo effect; the relevant transformation is

$$|\uparrow\rangle \rightarrow |2\rangle, |\downarrow\rangle \rightarrow |0\rangle, J \rightarrow K, U \rightarrow -U \quad (6.3.14)$$

The ground state in this sector will be a charge singlet, as shown in the next section. This was also reported by Taraphder and Coleman in [37].

6.3.4 Phase diagram for $V > 0$

We can now summarize the various fixed point phases. The physically relevant ones are the first and third quadrants. The first quadrant features a large spin-exchange coupling J and a positive U in the bare model, and the stable flows are towards a large J^* and a very small (≈ 0) U^* . The fixed point state will be mostly a spin singlet, in which the impurity polarization gets quenched by the spin-flip scattering of the conduction electrons. The third quadrant is the regime of the charge-Kondo effect, and involves a negative U at the bare level which physically motivates a large charge-Kondo coupling K . The fixed point again involves flow to a large K^* , but the U flows to large negative here, implying a state where the charge sectors dominate heavily and the ground state is primarily a charge-singlet in which the destruction or annihilation of the Cooper-pair like states becomes prohibited.

These results are summarized in the table below.

6.4 Effective Hamiltonian and ground state for the $V \neq 0$ symmetric problem

The fixed point Hamiltonian can be written in general, as

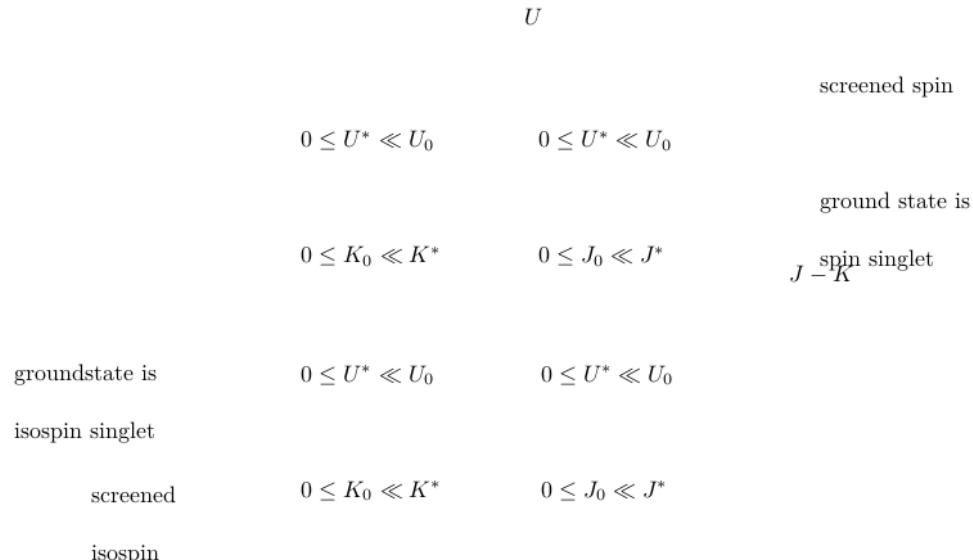
$$\mathcal{H}^* = \sum_{\sigma, k} \epsilon_k \tau_{k\sigma} - \frac{U^*}{2} \hat{n}_d + U^* \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \sum_{\sigma, k < \Lambda^*} \left(V^* c_{k\sigma}^\dagger c_{d\sigma} + \text{h.c.} \right) + J^* \vec{S}_d \cdot \vec{s} + K^* \vec{C}_d \cdot \vec{C} + \sum_{q > \Lambda^*} \left(J_q^z S_d^z s_q^z + K_q^z C_d^z C_q^z \right) \quad (6.4.1)$$

The first term is the kinetic energy of all the electrons. The next two terms are the impurity-diagonal pieces, featuring the renormalised interaction U^* . The next three terms are the residual interactions between the impurity

Figure 6.10: Increase in the fixed point values of J and V with system size.

 Figure 6.11: Flow of U to large negative value and K to large positive value in the third quadrant.

U	J, K	U^*	J^*, K^*	class	ground state
> 0	$J > K$	$\gtrsim 0$	$J^* > K^*$	screened spin	spin singlet + charge triplet
> 0	$J < K$	$\gtrsim 0$	$J^* < K^*$	screened charge	charge singlet
< 0	$J > K$	$\gtrsim 0$	$J^* > K^*$	screened spin	spin singlet + charge triplet
< 0	$J < K$	$\ll 0$	$J^* < K^*$	screened charge	charge singlet

 Table 6.2: Classification of fixed points for various bare values, at $V > 0$

 Figure 6.12: Low ω fixed point phases for the SIAM with $V > 0$.

and the metal, with the renormalised couplings V^* , J^* and K^* . The summations in these terms extend from the fixed point momentum cutoff Λ^* to 0. This is the region of momentum space which the URG was unable to decouple. The operators \vec{s} and \vec{C} represent the macroscopic magnetic and charge spins formed by the remaining electrons that are lying inside the window $[0, \Lambda^*]$:

$$\vec{s} = \sum_{\substack{kk' < \Lambda^* \\ \alpha\beta}} c_{k\alpha}^\dagger \vec{\sigma}_{\alpha\beta} c_{k'\beta} \quad (6.4.2)$$

The final two terms represent the diagonal pieces of the RG steps that have been completed. These survive because the URG removes only the number-off-diagonal terms; terms like $S_z^d s_z$ and $C_z^d C_z$ conserve the number of particles and hence survive. These will also be renormalised, and hence the subscript q on J_q^z signifies that it is has been renormalised up to a certain momentum.

1 Our goal here is to write down the ground state wavefunction for the low-energy Hamiltonian

$$\mathcal{H}_{IR} = \sum_{\sigma, k < \Lambda^*} \epsilon_k \tau_{k\sigma} - \frac{U^*}{2} \hat{n}_d + U^* \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \sum_{\sigma, k < \Lambda^*} (V^* c_{k\sigma}^\dagger c_{d\sigma} + \text{h.c.}) + J^* \vec{S}_d \cdot \vec{s} + K^* \vec{C}_d \cdot \vec{C} \quad (6.4.3)$$

To make progress with the ground state, we will simplify the effective Hamiltonian by mapping it onto a two-site problem. One site is of course the impurity site. The other site will be formed by the centre of mass degree of freedom of the conduction electrons, which we define as

$$c_{2\sigma} \equiv \frac{1}{\sqrt{N^*}} \sum_k c_{k\sigma} = c_\sigma (\vec{r} = 0) \quad (6.4.4)$$

25 where N^* is the number of electrons inside the window $[-\Lambda^*, \Lambda^*]$. This operator essentially creates a conduction electron at the origin. It is easy to prove that this operator is Fermionic:

$$\begin{aligned} \{c_{2\sigma}, c_{2\sigma}^\dagger\} &= \frac{1}{N^*} \sum_{kk'} \{c_{k\sigma}, c_{k'\sigma}^\dagger\} = \frac{1}{N^*} \sum_{kk'} \delta_{kk'} = 1 \\ \{c_{2\sigma}, c_{2\sigma}\} &= \frac{1}{N^*} \sum_{kk'} \{c_{k\sigma}, c_{k'\sigma}\} = 0 \end{aligned} \quad (6.4.5)$$

The number operator corresponding to this degree of freedom is

$$\hat{n}_{2\sigma} = c_{2\sigma}^\dagger c_{2\sigma} = \frac{1}{N^*} \sum_{kk'} c_{k\sigma}^\dagger c_{k'\sigma} \quad (6.4.6)$$

Because of the anticommutation algebra in eq. 6.4.5, this operator behaves essentially like a Fermion: $\hat{n}_{2\sigma}^2 = \hat{n}_{2\sigma}$. For our two-site problem, we will imagine this to be the annihilation operator for the site 2, for the spin sigma. The corresponding operator for the first site is of course just the impurity electron annihilation operator:

$$c_{1\sigma} \equiv c_{d\sigma} \quad (6.4.7)$$

The various terms of the Hamiltonian can now be written in terms of these operators. We write the Fourier decomposition of the dispersion of the conduction bath.

$$\epsilon_{\vec{k}} = \frac{1}{N^*} \sum_{\vec{r}} e^{i\vec{k} \cdot \vec{r}} \epsilon(\vec{r}) \quad (6.4.8)$$

The inverse transformation is

$$\epsilon(\vec{r}) = \sum_{|\vec{k}| < \Lambda^*} e^{-i\vec{k} \cdot \vec{r}} \epsilon_{\vec{k}} \quad (6.4.9)$$

We now make a simplifying assumption: Guided by the observation that the important degree of freedom at the fixed point is the COM operator $c_{2\sigma}$, we keep only the $\vec{r} = 0$ mode of the decomposition:

$$\epsilon_{\vec{k}} \approx \frac{1}{N^*} \epsilon(\vec{r} = 0) = \frac{1}{N^*} \sum_{k < \Lambda^*} \epsilon_k = \frac{1}{N^*} \sum_{\epsilon_k \in [\epsilon_F - D^*, \epsilon_F + D^*]} \epsilon_k = \epsilon_F \quad (6.4.10)$$

ϵ_F is the Fermi energy, which we henceforth set to 0. The energy term for the second site is thus simply zero. The impurity diagonal part of \mathcal{H}_{IR} will survive only when $\hat{n}_d = \hat{n}_1 = 1$. So we write it as

$$-\frac{U^*}{2}\hat{n}_d + U^*\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} = -\frac{U^*}{2}\left(\hat{n}_{d\uparrow} + \hat{n}_{d\downarrow} - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right) = -\frac{U^*}{2}\left(\hat{n}_{1\uparrow} - \hat{n}_{1\downarrow}\right)^2 \equiv \epsilon_d\left(\hat{n}_{1\uparrow} - \hat{n}_{1\downarrow}\right)^2 \quad (6.4.11)$$

where $\epsilon_d = -\frac{U^*}{2}$. The off-diagonal terms can also be similarly transformed into a two-site problem. The bath spin can be written as

$$\begin{aligned} \vec{S}_d &\equiv \vec{S}_1 \\ J^*\vec{s} &= J^*\frac{1}{2}\sum_{\substack{kk' \\ \alpha\beta}} c_{k\alpha}^\dagger \vec{\sigma}_{\alpha\beta} c_{k'\beta} \\ &= J^*\frac{1}{2}\sum_{\alpha\beta} c_{2\alpha}^\dagger \vec{\sigma}_{\alpha\beta} c_{2\beta} \\ &= J^*N^*\frac{1}{2}\left[\hat{z}\left(c_{2\uparrow}^\dagger c_{2\uparrow} - c_{2\downarrow}^\dagger c_{2\downarrow}\right) + \hat{x}\left(c_{2\uparrow}^\dagger c_{2\downarrow} + c_{2\downarrow}^\dagger c_{2\uparrow}\right) - i\hat{y}\left(c_{2\uparrow}^\dagger c_{2\downarrow} - c_{2\downarrow}^\dagger c_{2\uparrow}\right)\right] \\ &\equiv J^*N^*\vec{S}_2 \\ &\equiv j\vec{S}_2 \end{aligned} \quad (6.4.12)$$

where $j \equiv J^*N^*$ and

$$\vec{S}_2 = \frac{1}{2N^*}\sum_{\substack{kk' \\ \alpha\beta}} c_{k\alpha}^\dagger \vec{\sigma}_{\alpha\beta} c_{k'\beta} \quad (6.4.13)$$

The charge isospins can also be rewritten similarly. From eq. 5.3.3,

$$\begin{aligned} K^*C^z &= K^*\frac{1}{2}\sum_{kk'}\left(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k'\downarrow}^\dagger c_{k\downarrow}\right) = \frac{1}{2}N^*K^*\left(c_{2\uparrow}^\dagger c_{2\uparrow} - c_{2\downarrow}^\dagger c_{2\downarrow}\right) = kC_2^z \\ K^*C^x &= K^*\frac{1}{2}\sum_{kk'}\left(c_{k\uparrow}^\dagger c_{k'\downarrow}^\dagger + c_{k\downarrow}^\dagger c_{k'\uparrow}^\dagger\right) = \frac{1}{2}N^*K^*\left(c_{2\uparrow}^\dagger c_{2\downarrow} + c_{2\downarrow}^\dagger c_{2\uparrow}\right) = kC_2^x \end{aligned} \quad (6.4.14)$$

and similarly for C^y . We defined $k \equiv K^*N^*$. The diagonal component C^z can also be written as

$$C^z = \frac{1}{2}N^*\sum_\sigma\left(c_{2\sigma}^\dagger c_{2\sigma} - \frac{1}{2}\right) = \frac{1}{2}N^*\tau_2 \quad (6.4.15)$$

where $\tau_2 = \sum_\sigma \tau_{2\sigma} = \sum_\sigma \left(\hat{n}_{2\sigma} - \frac{1}{2}\right)$. The hybridisation term can be written as

$$V\sum_k c_{k\sigma}^\dagger = V\sqrt{N^*}c_{2\sigma}^\dagger = vc_{2\sigma}^\dagger \quad (6.4.16)$$

where $v \equiv V\sqrt{N^*}$. The charge isospins can be written down similarly. Combining these, the interaction part can be written as

$$v\sum_\sigma\left(c_{1\sigma}^\dagger c_{2\sigma} + \text{h.c.}\right) + j\vec{S}_1 \cdot \vec{S}_2 + k\vec{C}_1 \cdot \vec{C}_2 \quad (6.4.17)$$

with $k = K^*N^*$. The total Hamiltonian for the two-site problem is

$$\mathcal{H}_{IR} = \epsilon_d m_1^2 + v\sum_\sigma\left(c_{1\sigma}^\dagger c_{2\sigma} + \text{h.c.}\right) + j\vec{S}_1 \cdot \vec{S}_2 + k\vec{C}_1 \cdot \vec{C}_2 \quad (6.4.18)$$

where we have dropped the * on the couplings for brevity and $\hat{n}_{1\uparrow} - \hat{n}_{1\downarrow} = m_1$ is the magnetization on the first site. We will use the following notation to represent kets of this two-site system: $|n_{1\uparrow}n_{1\downarrow}n_{2\uparrow}n_{2\downarrow}\rangle$. For example, a state $|1001\rangle$ represents a ket with an up electron on site 1 and a down electron on site 2. This Hamiltonian conserves

Figure 6.13: Two-site effective problem of fixed point Hamiltonian

the total number operator $\hat{n} \equiv \hat{n}_1 + \hat{n}_2$, so we can analyse the various subspaces corresponding to particular values of \hat{n} separately.

We will adopt the following notation to represent the states in this Hilbert space. A general state will be represented in the Fock space basis as $|n_{1\uparrow} n_{1\downarrow} n_{2\uparrow} n_{2\downarrow}\rangle$. For example,

$$|1101\rangle = c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger |-\rangle \quad (6.4.19)$$

$|-\rangle$ is the vacuum state.

First lets get the trivial cases of $\hat{n} = 0, 4$ out of the way. The only possible states are $|0000\rangle$ and $|1111\rangle$ respectively. Both these states are eigenstates because the first one has no electron to scatter, and the second one has no vacant state to scatter into. These states have energy eigenvalues $\frac{1}{4}k$

The subspaces $\hat{n} = 1, 3$ are each four-dimensional. More precisely speaking, the $\hat{n} = 1$ subspace can have the following basis

$$|\uparrow, 0\rangle, |0, \uparrow\rangle, |\downarrow, 0\rangle, |0, \downarrow\rangle \quad (6.4.20)$$

However, since the Hamiltonian conserves the total spin (both magnetic and charge), we can divide this Hilbert subspace into two smaller subspaces which do not talk to each other - one having the states $|\uparrow, 0\rangle, |0, \uparrow\rangle$ and hence a total spin magnetization of $+\frac{1}{2}$, and the other having the remaining states and a total spin magnetization of $-\frac{1}{2}$. The action of the Hamiltonian on this subspace is

$$\begin{aligned} \mathcal{H}_{IR} |1000\rangle &= [\epsilon_d m_1^2 + v c_{2\uparrow}^\dagger c_{1\uparrow}] c_{1\uparrow}^\dagger |-\rangle = \epsilon_d |1000\rangle + v |0010\rangle \\ \mathcal{H}_{IR} |0010\rangle &= [\epsilon_d m_1^2 + v c_{1\uparrow}^\dagger c_{2\uparrow}] c_{2\uparrow}^\dagger |-\rangle = v |1000\rangle \end{aligned} \quad (6.4.21)$$

The Hamiltonian in first subspace can be represented by the matrix

$$\begin{pmatrix} |\uparrow, 0\rangle & |0, \uparrow\rangle \\ \epsilon_d & v \\ v & 0 \end{pmatrix} \quad (6.4.22)$$

The eigenstates (un-normalised) are

$$-4v |\uparrow, 0\rangle + 2 [\epsilon_d \mp \Delta(\epsilon_d, v)] |0, \uparrow\rangle, \quad E_\pm^1 = \frac{1}{2} \epsilon_d \pm \frac{1}{2} \Delta(\epsilon_d, v) \quad (6.4.23)$$

where $\Delta(\epsilon_d, v) = \sqrt{\epsilon_d^2 + 4v^2}$. The other two eigenstates (corresponding to magnetization $-\frac{1}{2}$) need not be calculated separately; since the Hamiltonian is invariant under the transformation $\uparrow \leftrightarrow \downarrow$, we can do a similar transformation on the eigenkets to get the eigenkets for the other subspace.

$$-4v |\downarrow, 0\rangle + 2 [\epsilon_d \mp \Delta(\epsilon_d, v)] |0, \downarrow\rangle \quad (6.4.24)$$

with exactly the same eigenvalue.

The $\hat{n} = 3$ subspace is very similar. We can obtain the basis directly from the $\hat{n} = 1$ case by substituting the holes with doubles:

$$|\uparrow, \uparrow\downarrow\rangle, |\uparrow\downarrow, \uparrow\rangle, |\downarrow, \uparrow\downarrow\rangle, |\uparrow\downarrow, \downarrow\rangle \quad (6.4.25)$$

Since a double impurity has the same energy as a vacant impurity (because of p-h symmetry, both are zero), the diagonal part corresponding to the first site will not change. We can then write down the eigenstates and

eigenvalues directly from those of $\hat{n} = 1$, simply by making the transformation $|0\rangle \rightarrow |\uparrow\downarrow\rangle$.

$$\left. \begin{aligned} -4v|\uparrow,\uparrow\downarrow\rangle + 2[\epsilon_d \mp \Delta(\epsilon_d, v)]|\uparrow\downarrow,\uparrow\rangle \\ -4v|\downarrow,\uparrow\downarrow\rangle + 2[\epsilon_d \mp \Delta(\epsilon_d, v)]|\uparrow\downarrow,\downarrow\rangle \end{aligned} \right\} E = \frac{1}{2}\epsilon_d \pm \frac{1}{2}\Delta(\epsilon_d, v) \quad (6.4.26)$$

The most interesting subspace is $\hat{n} = 2$. This is six dimensional. Since the Hamiltonian conserves both the total spins S^2 and C^2 as well the z-components $S^z = S_1^z + S_2^z$ and $C^z = C_1^z + C_2^z$, it would be prudent to choose our basis with this in mind. The action of the hybridisation term on the various states are

$$\begin{aligned} v \left(\text{55} c_{2\downarrow} + \text{39} c_{2\uparrow} c_{1\uparrow} \right) c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger |-\rangle &= v \left(c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger c_{2\downarrow} c_{2\uparrow}^\dagger + c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger c_{1\uparrow} c_{1\downarrow}^\dagger \right) |-\rangle = v |\uparrow\downarrow, 0\rangle + v |\downarrow, \uparrow\downarrow\rangle \\ v \left(c_{1\uparrow}^\dagger c_{2\uparrow} + c_{2\downarrow}^\dagger c_{1\downarrow} \right) c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger |-\rangle &= v \left(-c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger c_{2\uparrow} c_{2\downarrow}^\dagger - c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger c_{1\uparrow} c_{1\downarrow}^\dagger \right) |-\rangle = -v |\uparrow\downarrow, 0\rangle - v |\downarrow, \uparrow\downarrow\rangle \\ v \left(c_{2\uparrow}^\dagger c_{1\uparrow} + c_{2\downarrow}^\dagger c_{1\downarrow} \right) c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger |-\rangle &= v \left(-c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger c_{1\uparrow} c_{1\downarrow}^\dagger + c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger c_{1\downarrow} c_{1\uparrow}^\dagger \right) |-\rangle = -v |\downarrow, \uparrow\rangle + v |\uparrow, \downarrow\rangle \\ v \left(c_{1\uparrow}^\dagger c_{2\uparrow} + c_{1\downarrow}^\dagger c_{2\downarrow} \right) c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger |-\rangle &= v \left(c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger c_{2\uparrow} c_{2\downarrow}^\dagger - c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger c_{2\downarrow} c_{2\uparrow}^\dagger \right) |-\rangle = v |\uparrow, \downarrow\rangle - v |\downarrow, \uparrow\rangle \end{aligned} \quad (6.4.27)$$

$$\mathcal{H}_{IR} |\uparrow, \uparrow\rangle = \left(\epsilon_d + \frac{1}{4}j \right) |\uparrow, \uparrow\rangle \quad (6.4.28)$$

$$\mathcal{H}_{IR} |\downarrow, \downarrow\rangle = \left(\epsilon_d + \frac{1}{4}j \right) |\downarrow, \downarrow\rangle \quad (6.4.29)$$

$$\mathcal{H}_{IR} \frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle) \mapsto \left(\epsilon_d + \frac{1}{4}j \right) \frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle) \quad (6.4.30)$$

$$\mathcal{H}_{IR} \frac{1}{\sqrt{2}} (|\uparrow\downarrow, 0\rangle - |0, \uparrow\downarrow\rangle) = -\frac{3}{4}k \frac{1}{\sqrt{2}} (|\uparrow\downarrow, 0\rangle - |0, \uparrow\downarrow\rangle) \quad (6.4.31)$$

$$\mathcal{H}_{IR} \frac{1}{\sqrt{2}} (|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle) = \frac{1}{4}k \frac{1}{\sqrt{2}} (|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle) + 2v \frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) \quad (6.4.32)$$

$$\mathcal{H}_{IR} \frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) = \left(\epsilon_d - \frac{3}{4}j \right) \frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + 2v \frac{1}{\sqrt{2}} (|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle) \quad (6.4.33)$$

The first four states are eigenstates. The last two are not, but they form a two-dimensional subspace which can be easily diagonalized. The eigenstates of this subspace are

$$\begin{aligned} |\pm\rangle &= c_\pm^s \frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + c_\pm^c \frac{1}{\sqrt{2}} (|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle) \\ E_\pm^2 &= v \left[\gamma \pm \sqrt{\gamma^2 + 4} \right] + \epsilon_d - \frac{3}{4}j \end{aligned} \quad (6.4.34)$$

The symbol γ stands for the quantity

$$\gamma = \frac{1}{2v} \left[\frac{1}{4} (3j + k) - \epsilon_d \right] \quad (6.4.35)$$

and the coefficients $c_\pm^{s,c}$ for the spin and charge singlets (the superscripts s, c designate which singlet the coefficient sticks to) are

$$c_\pm^s = \frac{1}{\sqrt{2\sqrt{\gamma^2 + 4}}} \sqrt{\sqrt{\gamma^2 + 4} \mp \gamma} = \mp c_\mp^c \quad (6.4.36)$$

The ground state is of course E_-^2 .

$$E_-^2 = v \left[\gamma - \sqrt{\gamma^2 + 4} \right] + \epsilon_d - \frac{3}{4}j \quad (6.4.37)$$

The probabilities for the spin and charge sectors for the ground state look simpler:

$$\begin{aligned} \left(c_-^s\right)^2 &= \frac{1}{2\sqrt{\gamma^2+4}} \left(\sqrt{\gamma^2+4} + \gamma\right) \\ \left(c_-^c\right)^2 &= \frac{1}{2\sqrt{\gamma^2+4}} \left(\sqrt{\gamma^2+4} - \gamma\right) \end{aligned} \quad (6.4.38)$$

In the first quadrant, we will have $J^* > K^*$. As we increase the system size, J^* increases, which implies $j - k$ will increase. In the limit of very large $j - k$, we can write

$$\gamma \rightarrow \infty \implies \left(c_-^s\right)^2 \rightarrow 1 \text{ and } \left(c_-^c\right)^2 \rightarrow 0 \quad (6.4.39)$$

The spin singlet becomes the all-important piece in this situation. This change is shown in fig. 6.14. We have the variation of the probabilities and of γ for the first quadrant. γ increases with system size, and so does the spin probability $\left(c_s^s\right)^2$. The ground state in such a limit becomes purely a singlet:

$$\begin{aligned} |\Psi\rangle_{\text{gs}} &\approx \frac{1}{\sqrt{2}} (|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle) \\ E_{\text{gs}} &\approx \epsilon_d - \frac{3j}{4} \end{aligned} \quad (6.4.40)$$

Figure 6.14: *Left:* Variation of the probabilities $(c_s^s)^2$ and $(c_s^c)^2$ with system size. *Right:* Variation of γ with system size.

The full list of eigenstates is

\hat{n}	S^z	eigenstate	eigenvalue
0	0	$ 0,0\rangle$	$\frac{1}{4}k$
4	0	$ 2,2\rangle$	$\frac{1}{4}k$
1	$\frac{1}{2}$	$-4v \uparrow,0\rangle + 2[\epsilon_d \mp \Delta(\epsilon_d, v)] 0,\uparrow\rangle$	$\frac{1}{2}\epsilon_d \pm \frac{1}{2}\Delta(\epsilon_d, v)$
	$-\frac{1}{2}$	$-4v \downarrow,0\rangle + 2[\epsilon_d \mp \Delta(\epsilon_d, v)] 0,\downarrow\rangle$	
3	$\frac{1}{2}$	$-4v \uparrow,2\rangle + 2[\epsilon_d \mp \Delta(\epsilon_d, v)] 2,\uparrow\rangle$	$\epsilon_d + \frac{1}{4}j$
	$-\frac{1}{2}$	$-4v \downarrow,2\rangle + 2[\epsilon_d \mp \Delta(\epsilon_d, v)] 2,\downarrow\rangle$	
1,-1		$ \uparrow,\uparrow\rangle, \downarrow,\downarrow\rangle$	$\epsilon_d + \frac{1}{4}j$
		$ \uparrow,\downarrow\rangle + \downarrow,\uparrow\rangle$	
2	0	$ 2,0\rangle - 0,2\rangle$	$-\frac{3}{4}k$
		$c_{\pm}^s \frac{1}{\sqrt{2}} (\uparrow,\downarrow\rangle - \downarrow,\uparrow\rangle) + c_{\pm}^c \frac{1}{\sqrt{2}} (\uparrow,\downarrow\rangle + \downarrow,\uparrow\rangle)$	$v[\gamma \pm \sqrt{\gamma^2+4}] + \epsilon_d - \frac{3}{4}j$

Table 6.3: Eigenstates for effective two-site Hamiltonian

Although E_-^2 is the ground state of this two-dimensional subspace, we haven't yet checked what is the true ground state of the full Hilbert space. The eigenstates eq. 6.4.28 through 6.4.30 are obviously higher than E_-^2 , because of the presence of the singlet $-\frac{3}{4}j$ and the negative γ contribution in E_-^2 compared to the positive triplet contribution $\frac{1}{4}j$ in those equations. The only other competitors are the one [9] eq. 6.4.31 which we call E_c^2 , and the low energy eigenstate in eq. 6.4.23, which we call E_-^1 . We first show that $E_-^1 > E_-^2$. The difference between E_-^2 and E_-^1 is

$$E_-^2 - E_-^1 = -\frac{3}{4}(j+k) - \sqrt{4v^2 + \frac{\epsilon_d^2}{4} + \frac{9}{64}(j-k)^2} - \frac{3}{8}\epsilon_d(j-k) + \sqrt{\frac{1}{4}\epsilon_d^2 + v^2} \quad (6.4.41)$$

From the nature of the fixed point phases, we know that

$$J^* > K^* \stackrel{4}{\implies} \epsilon_d^* \leq 0 \quad (6.4.42)$$

and

$$J^* < K^* \stackrel{4}{\implies} \epsilon_d^* \geq 0 \quad (6.4.43)$$

such that

$$\epsilon_d(j-k) \leq 0 \quad (6.4.44)$$

This result then very easily implies that

$$4v^2 + \frac{\epsilon_d^2}{4} + \frac{9}{64}(j-k)^2 - \frac{3}{8}\epsilon_d(j-k) > \frac{1}{4}\epsilon_d^2 + v^2 \quad (6.4.45)$$

and we can apply this inequality to the difference between E_-^2 and E_-^1 to see that E_-^2 is greater than E_-^1 .

We now compare E_-^2 and E_c^2 :

$$\Delta E_g \equiv E_-^2 - E_c^2 = \frac{1}{2}\epsilon_d - \frac{3j+k}{8} + k - \sqrt{4v^2 + \left(\frac{3j+k}{8} - \frac{1}{2}\epsilon_d\right)^2} \quad (6.4.46)$$

Because of the presence of the large v in the first quadrant, this will necessarily be negative there. So, the true ground state in the first quadrant is E_-^2 . In the third quadrant, the large value of k will make the difference positive and the true ground state will be the charge singlet.

These conclusions have been checked numerically and shown in fig. 6.15, where we have plotted the sign of ΔE_g as a function of $K_0 - J_0$. For positive values of $K_0 - J_0$, we are in the third quadrant, and the sign of ΔE_g being +1 implies that $E_-^2 > E_c^2$, and so the third quadrant ground state is the charge singlet (E_c^2). On the other hand, as $K_0 - J_0$ becomes negative, we move into the first quadrant, and the sign of ΔE_g also flips, implying that we have a transition from the charge singlet to the (mostly) spin-singlet ground state.

One of the most striking conclusions of this chapter is that the normalized ground state of the SIAM in the Kondo regime is purely a singlet. The holon-doublon contributions of the ground state die out in the limit of large system size, and we are left purely with spin-sector contributions.

Figure 6.15: Shift in the ground state in going from the first to third quadrant, depicted via the switch in sign of ΔE_g .

Chapter 7

Results and Features of the Low-Energy Theory

7.1 Effective Kondo temperature

We now define an energy scale for the low energy fluctuations:

$$T_K \equiv \frac{2N^*}{\pi} (D^* - 2\omega) \quad (7.1.1)$$

The term in brackets, $D^* - 2\omega$, is the fluctuation energy at the fixed point. The factor of $2N^*$ is inserted to make the Kondo temperature intensive (we see below that the N^* allows it to be written in terms of parameters of the two-site Hamiltonian) - $2N^*$ is the total number of momentum states in the fixed point theory. The factor of $\frac{1}{\pi}$ is for aesthetic reasons. From the fixed-point condition $\omega - \frac{D}{2} + \frac{J+K}{4} = 0$, the Kondo temperature can be written as

$$T_K = \frac{2N^*}{\pi} \frac{1}{2} (J^* + K^*) = \frac{1}{\pi} (j + k) \quad (7.1.2)$$

7.2 Magnetic susceptibility

The thermal susceptibility is defined as

$$\chi(\beta) = \beta \left(\left\langle (S_d^z)^2 \right\rangle - \left\langle S_d^z \right\rangle^2 \right) \quad (7.2.1)$$

There is an alternate way of calculating this. We insert a fictitious magnetic field that couples only to the impurity site. The Hamiltonian in the presence of this field is

$$\mathcal{H}'(B) = \mathcal{H} + BS_d^z \quad (7.2.2)$$

The susceptibility is then given by

$$\chi(\beta) = \lim_{B \rightarrow 0} \frac{1}{\beta} \left[\frac{1}{Z(B)} \frac{\partial^2 Z(B)}{\partial B^2} - \frac{1}{Z(B)^2} \left(\frac{\partial Z(B)}{\partial B} \right)^2 \right] \quad (7.2.3)$$

where $Z(B)$ is the partition function of the Hamiltonian $\mathcal{H}'(B)$. The following is to prove that the RHS of eqs. 7.2.1 and 7.2.3 are the same. We start with 7.2.3. The first derivative can be written as

$$\frac{\partial Z(B)}{\partial B} = \text{Trace} \left[\frac{\partial}{\partial B} \exp \left\{ -\beta (\mathcal{H} + BS_d^z) \right\} \right] = \text{Trace} \left[-\beta S_d^z \exp \left\{ -\beta (\mathcal{H} + BS_d^z) \right\} \right] \quad (7.2.4)$$

which means the first term becomes

$$\lim_{B \rightarrow 0} -\frac{1}{Z(B)^2} \left(\frac{\partial Z(B)}{\partial B} \right)^2 = - \left(\beta \frac{1}{\text{Trace} [\exp \{-\beta \mathcal{H}\}]} \text{Trace} [S_d^z \exp \{-\beta \mathcal{H}\}] \right)^2 = -\beta^2 \langle S_d^z \rangle^2 \quad (7.2.5)$$

The second derivative is

$$\frac{\partial^2 Z(B)}{\partial B^2} = \text{Trace} \left[-\beta S_d^z \frac{\partial}{\partial B} \exp \left\{ -\beta (\mathcal{H} + BS_d^z) \right\} \right] = \text{Trace} \left[\beta^2 (S_d^z)^2 \exp \left\{ -\beta (\mathcal{H} + BS_d^z) \right\} \right] \quad (7.2.6)$$

so the second term becomes

$$\lim_{B \rightarrow 0} \frac{1}{Z(B)} \frac{\partial^2 Z(B)}{\partial B^2} = \beta^2 \frac{1}{\text{Trace} [\exp \{-\beta \mathcal{H}\}]} \text{Trace} \left[(S_d^z)^2 \exp \{-\beta \mathcal{H}\} \right] = \beta^2 \langle (S_d^z)^2 \rangle \quad (7.2.7)$$

The full thing becomes

$$\begin{aligned} \lim_{B \rightarrow 0} \frac{1}{\beta} \left[\frac{1}{Z(B)} \frac{\partial^2 Z(B)}{\partial B^2} - \frac{1}{Z(B)^2} \left(\frac{\partial Z(B)}{\partial B} \right)^2 \right] &= \frac{1}{\beta} \left(-\beta^2 \langle S_d^z \rangle^2 + \beta^2 \langle (S_d^z)^2 \rangle \right) \\ &= \beta \left(\langle (S_d^z)^2 \rangle - \langle S_d^z \rangle^2 \right) \end{aligned} \quad (7.2.8)$$

This completes the proof.

7.2.1 For $v = 0$

In the presence of a magnetic field coupling term BS_1^z , the eigenvalues become (setting $v = 0$)

$$\begin{aligned} \hat{n} = 0, 4 \rightarrow E^0 &= \frac{1}{4}k \\ \hat{n} = 1, 3 \rightarrow &\begin{cases} E_{\pm,\uparrow}^1 = \frac{1}{2} \left(\epsilon_d + \frac{1}{2}B \right) \pm \frac{1}{2}\Delta \left(\epsilon_d + \frac{1}{2}B, v \right) = \epsilon_d + \frac{1}{2}B, 0 \\ E_{\pm,\downarrow}^1 = \frac{1}{2} \left(\epsilon_d - \frac{1}{2}B \right) \pm \frac{1}{2}\Delta \left(\epsilon_d - \frac{1}{2}B, v \right) = \epsilon_d - \frac{1}{2}B, 0 \end{cases} \\ \hat{n} = 2 \rightarrow &\begin{cases} \epsilon_d + \frac{1}{4}j + \frac{1}{2}B \\ \epsilon_d + \frac{1}{4}j - \frac{1}{2}B \\ \frac{1}{4}k \\ -\frac{3}{4}k \\ \epsilon_d - \frac{1}{4}j \pm \frac{1}{2}\Gamma \end{cases} \end{aligned} \quad (7.2.9)$$

where we defined $\Gamma = \sqrt{B^2 + j^2}$. The eigenvalues in $\hat{n} = 2$ can be elaborated upon. The action of the total Hamiltonian \mathcal{H}' (with $v = 0$) is

$$|\uparrow, \uparrow\rangle \mapsto \left(\epsilon_d + \frac{1}{4}j + \frac{1}{2}B \right) |\uparrow, \uparrow\rangle \quad (7.2.10)$$

$$|\downarrow, \downarrow\rangle \mapsto \left(\epsilon_d + \frac{1}{4}j - \frac{1}{2}B \right) |\downarrow, \downarrow\rangle \quad (7.2.11)$$

$$\frac{1}{\sqrt{2}} (|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle) \mapsto \frac{1}{4}k \frac{1}{\sqrt{2}} (|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle) \quad (7.2.12)$$

$$\frac{1}{\sqrt{2}} (|\uparrow\downarrow, 0\rangle - |0, \uparrow\downarrow\rangle) \mapsto -\frac{3}{4}k \frac{1}{\sqrt{2}} (|\uparrow\downarrow, 0\rangle - |0, \uparrow\downarrow\rangle) \quad (7.2.13)$$

$$\frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle) \mapsto \left(\epsilon_d + \frac{1}{4}j \right) \frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle) + \frac{1}{2}B \frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) \quad (7.2.14)$$

$$\frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) \mapsto \left(\epsilon_d - \frac{3}{4}j \right) \frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + \frac{1}{2}B \frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle) \quad (7.2.15)$$

(7.2.16)

The first four states directly give the first four eigenvalues in $\hat{n} = 2$. The remaining two states form the matrix

$$\begin{pmatrix} \epsilon_d + \frac{1}{4}j & \frac{1}{2}B \\ \frac{1}{2}B & \epsilon_d - \frac{3}{4}j \end{pmatrix} \quad (7.2.17)$$

The eigenvalues satisfy the equation

$$0 = \left(E - \epsilon_d + \frac{3}{4}j \right) \left(E - \epsilon_d - \frac{1}{4}j \right) - \frac{1}{4}B^2 = \left(E - \epsilon_d - \frac{1}{4}j \right)^2 + j \left(E - \epsilon_d - \frac{1}{4}j \right) - \frac{1}{4}B^2 \quad (7.2.18)$$

The solutions are

$$E = \epsilon_d + \frac{1}{4}j + \frac{-j \pm \sqrt{j^2 + B^2}}{2} = \epsilon_d - \frac{1}{4}j \pm \frac{1}{2}\Gamma \quad (7.2.19)$$

which are the final two eigenvalues.

The partition function is

$$\begin{aligned} Z(B) &= 2 \exp \left\{ -\beta \frac{k}{4} \right\} + 2 \left(\exp \left\{ -\beta \left(\epsilon_d + \frac{1}{2}B \right) \right\} + e^0 \right) + 2 \left(\exp \left\{ -\beta \left(\epsilon_d - \frac{1}{2}B \right) \right\} + e^0 \right) \\ &\quad + \exp \left\{ -\beta \left(\epsilon_d + \frac{1}{4}j + \frac{1}{2}B \right) \right\} + \exp \left\{ -\beta \left(\epsilon_d + \frac{1}{4}j - \frac{1}{2}B \right) \right\} \\ &\quad + \exp \left\{ -\beta \frac{k}{4} \right\} + \exp \left\{ \beta \frac{3k}{4} \right\} + \exp \left\{ -\beta \left(\epsilon_d - \frac{1}{4}j + \frac{1}{2}\Gamma \right) \right\} + \exp \left\{ -\beta \left(\epsilon_d - \frac{1}{4}j - \frac{1}{2}\Gamma \right) \right\} \\ &= 4 + 3 \exp \left\{ -\beta \frac{k}{4} \right\} + \exp \left\{ \beta \frac{3k}{4} \right\} + 4e^{-\beta \epsilon_d} \cosh \beta \frac{B}{2} + 2e^{-\beta(\epsilon_d + \frac{j}{4})} \cosh \beta \frac{B}{2} \\ &\quad + 2e^{-\beta(\epsilon_d - \frac{j}{4})} \cosh \beta \frac{1}{2}\Gamma \\ &= 4 + 3 \exp \left\{ -\beta \frac{k}{4} \right\} + \exp \left\{ \beta \frac{3k}{4} \right\} + \left[4e^{-\beta \epsilon_d} + 2e^{-\beta(\epsilon_d + \frac{j}{4})} \right] \cosh \left(\beta \frac{B}{2} \right) \\ &\quad + 2e^{-\beta(\epsilon_d - \frac{j}{4})} \cosh \left(\beta \frac{1}{2}\Gamma \right) \end{aligned} \quad (7.2.20)$$

We can now compute the derivatives.

$$\begin{aligned}
 Z' &\equiv \frac{\partial Z}{\partial B} = \left[4e^{-\beta\epsilon_d} + 2e^{-\beta(\epsilon_d+\frac{j}{4})} \right] \frac{\beta}{2} \sinh\left(\beta\frac{B}{2}\right) + 2e^{-\beta(\epsilon_d-\frac{j}{4})} \frac{1}{2} \beta \sinh\left(\frac{1}{2}\beta\Gamma\right) \frac{\partial\Gamma}{\partial B} \\
 &= \left[4e^{-\beta\epsilon_d} + 2e^{-\beta(\epsilon_d+\frac{j}{4})} \right] \frac{\beta}{2} \sinh\left(\beta\frac{B}{2}\right) + e^{-\beta(\epsilon_d-\frac{j}{4})} \beta \sinh\left(\frac{1}{2}\beta\Gamma\right) \frac{B}{\Gamma} \\
 Z'' &\equiv \frac{\partial^2 Z}{\partial B^2} = \left[4e^{-\beta\epsilon_d} + 2e^{-\beta(\epsilon_d+\frac{j}{4})} \right] \left(\frac{\beta}{2} \right)^2 \cosh\left(\beta\frac{B}{2}\right) \\
 &\quad + e^{-\beta(\epsilon_d-\frac{j}{4})} \beta \left[\cosh\left(\frac{1}{2}\beta\Gamma\right) \times \frac{1}{2} \beta \left(\frac{B}{\Gamma} \right)^2 + \sinh\left(\frac{1}{2}\beta\Gamma\right) \left(-\frac{B}{\Gamma^2} \times \frac{B}{\Gamma} + \frac{1}{\Gamma} \right) \right]
 \end{aligned} \tag{7.2.21}$$

Taking the limit of $B \rightarrow 0$ gives

$$\begin{aligned}
 Z|_{B=0} &= 4 + 3 \exp\left\{-\beta\frac{k}{4}\right\} + \exp\left\{\beta\frac{3k}{4}\right\} + 4e^{-\beta\epsilon_d} + 2e^{-\beta(\epsilon_d+\frac{j}{4})} + 2e^{-\beta(\epsilon_d-\frac{j}{4})} \cosh\left(\beta\frac{j}{2}\right) \\
 Z'|_{B=0} &= 0 \\
 Z''|_{B=0} &= \left[4e^{-\beta\epsilon_d} + 2e^{-\beta(\epsilon_d+\frac{j}{4})} \right] \left(\frac{\beta}{2} \right)^2 + e^{-\beta(\epsilon_d-\frac{j}{4})} \beta \sinh\left(\beta\frac{j}{2}\right) \frac{1}{j}
 \end{aligned} \tag{7.2.22}$$

The susceptibility is thus

$$\begin{aligned}
 \chi(\beta) &= \frac{1}{\beta} \frac{\left[4e^{-\beta\epsilon_d} + 2e^{-\beta(\epsilon_d+\frac{j}{4})} \right] \left(\frac{\beta}{2} \right)^2 + e^{-\beta(\epsilon_d-\frac{j}{4})} \beta \sinh\left(\beta\frac{j}{2}\right) \frac{1}{j}}{4 + 3 \exp\left\{-\beta\frac{k}{4}\right\} + \exp\left\{\beta\frac{3k}{4}\right\} + 4e^{-\beta\epsilon_d} + 2e^{-\beta(\epsilon_d+\frac{j}{4})} + 2e^{-\beta(\epsilon_d-\frac{j}{4})} \cosh\left(\beta\frac{j}{2}\right)} \\
 &= \frac{\left[2e^{-\beta\epsilon_d} + e^{-\beta(\epsilon_d+\frac{j}{4})} \right] \frac{1}{2} \beta + e^{-\beta(\epsilon_d-\frac{j}{4})} \sinh\left(\beta\frac{j}{2}\right) \frac{1}{j}}{4 + 3 \exp\left\{-\beta\frac{k}{4}\right\} + \exp\left\{\beta\frac{3k}{4}\right\} + 4e^{-\beta\epsilon_d} + 2e^{-\beta(\epsilon_d+\frac{j}{4})} + 2e^{-\beta(\epsilon_d-\frac{j}{4})} \cosh\left(\beta\frac{j}{2}\right)}
 \end{aligned} \tag{7.2.23}$$

At high temperatures, we can write

$$\frac{\chi}{\beta}|_{\beta \rightarrow 0} = \frac{[4+2]\frac{1}{4} + \frac{1}{2} \lim_{\beta \rightarrow 0} \sinh\left(\beta\frac{j}{2}\right) \frac{2}{\beta j}}{4+3+1+[4+2]+2} = \frac{\frac{3}{2} + \frac{1}{2}}{16} = \frac{1}{8} \quad \left[\lim_{x \rightarrow 0} \frac{\sinh x}{x} = 1 \right] \tag{7.2.24}$$

At low temperatures,

$$\chi|_{\beta \rightarrow \infty} = \lim_{\beta \rightarrow \infty} \frac{e^{-\beta(\epsilon_d-\frac{j}{4})} \sinh\left(\beta\frac{j}{2}\right) \frac{1}{j}}{\exp\left\{\beta\frac{3k}{4}\right\} + 2e^{-\beta(\epsilon_d-\frac{j}{4})} \cosh\left(\beta\frac{j}{2}\right)} = \frac{1}{2j} \lim_{\beta \rightarrow \infty} \frac{1}{\exp\left\{\beta\left(\frac{3k}{4} + \epsilon_d - \frac{3j}{4}\right)\right\} + 1} \tag{7.2.25}$$

There we used $\sinh x \approx \cosh x \approx \frac{1}{2}e^x$ for $x \rightarrow \infty$. The exponential will take the following limiting values:

$$\exp\left\{\beta\left(\frac{3k}{4} + \epsilon_d - \frac{3j}{4}\right)\right\} \rightarrow \begin{cases} \infty, & \text{if } \frac{3k}{4} + \epsilon_d - \frac{3j}{4} > 0 \\ 1, & \text{if } \frac{3k}{4} + \epsilon_d - \frac{3j}{4} = 0 \\ 0, & \text{if } \frac{3k}{4} + \epsilon_d - \frac{3j}{4} < 0 \end{cases} \tag{7.2.26}$$

which means

$$\left[\exp \left\{ \beta \left(\frac{3k}{4} + \epsilon_d - \frac{3j}{4} \right) \right\} + 1 \right]^{-1} \rightarrow \begin{cases} 0, & \text{if } \frac{3k}{4} + \epsilon_d - \frac{3j}{4} > 0 \\ \frac{1}{2}, & \text{if } \frac{3k}{4} + \epsilon_d - \frac{3j}{4} = 0 \\ 1, & \text{if } \frac{3k}{4} + \epsilon_d - \frac{3j}{4} < 0 \end{cases} = \Theta \left(\frac{3j}{4} - \frac{3k}{4} - \epsilon_d \right) \quad (7.2.27)$$

where the theta function (Heaviside function) is defined as

$$\Theta(x) = \begin{cases} 1, & \text{if } x > 0 \\ \frac{1}{2}, & \text{if } x = 0 \\ 0, & \text{if } x < 0 \end{cases} \quad (7.2.28)$$

The thermal susceptibility at high temperatures is thus

$$\chi|_{\beta \rightarrow \infty} = \frac{1}{2j} \Theta \left(\frac{3j}{4} - \frac{3k}{4} - \epsilon_d \right) \quad (7.2.29)$$

If we are in the first quadrant, then the fixed point values are such that $\frac{3k}{4} + \epsilon_d - \frac{3j}{4} < 0$, so the theta function will evaluate to 1, and we can write

$$\chi|_{\beta \rightarrow \infty} = \frac{1}{2j} \quad (7.2.30)$$

For sufficiently large values of j compared to k , we can also approximate the Kondo temperature T_K as $T_K \approx \frac{j}{\pi}$. Then, the zero temperature value of χ deep in the first quadrant is

$$\chi(T=0) \approx (2\pi T_K)^{-1} \quad (7.2.31)$$

This is in accordance with the results obtained from Bethe ansatz in [38].

On the other hand, in the third quadrant, we have $\frac{3k}{4} + \epsilon_d - \frac{3j}{4} > 0$, and Θ gives

$$\chi|_{\beta \rightarrow \infty} = 0 \quad (7.2.32)$$

Figure 7.1: Variation of $\chi \times T$ over six decades of temperature. The low temperature behaviour is characteristic of a local Fermi liquid paramagnetic susceptibility, while at high temperatures we see the Curie-Weiss susceptibility resulting from the local moment.

Figure 7.2: Variation of $(T_k \times \chi)^{-1}$ with temperature.

Figure 7.3: Variation of χ against temperature. It saturates to a value close to $(2\pi T_K)^{-1}$

7.3 Charge Susceptibility

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We can also calculate the impurity contribution to the charge susceptibility of the system in a very similar fashion. We insert a magnetic field that couples to the impurity charge isospin:

$$\mathcal{H}'(B) = \mathcal{H} + BC_d^z \quad (7.3.1)$$

We again work in the simpler case of $v = 0$. The energy eigenvalues for this Hamiltonian are

$$\begin{aligned}\hat{n} = 0 &\rightarrow \frac{1}{4}k - \frac{B}{2} \\ \hat{n} = 4 &\rightarrow \frac{1}{4}k + \frac{B}{2} \\ \hat{n} = 1, 3 &\rightarrow \begin{cases} \epsilon_d - \frac{1}{2}B, 0 \\ \epsilon_d + \frac{1}{2}B, 0 \end{cases} \\ \hat{n} = 2 &\rightarrow \begin{cases} \epsilon_d + \frac{1}{4}j \\ \epsilon_d - \frac{3}{4}j \\ \epsilon_d - \frac{1}{4}k \pm \frac{1}{2}\Gamma \end{cases} \times 3\end{aligned}\quad (7.3.2)$$

where $\Gamma \equiv \sqrt{k^2 + B^2}$. We will again use eq. 7.2.3 to calculate the susceptibility. The partition function and its derivatives are

$$\begin{aligned}\lim_{B \rightarrow 0} Z &= 2e^{-\beta \frac{k}{4}} + 4 + 4e^{-\beta \epsilon_d} + 3e^{-\beta(\epsilon_d + \frac{j}{4})} + e^{\beta(3\frac{j}{4} - \epsilon_d)} + 2e^{\beta(\frac{k}{4} - \epsilon_d)} \cosh \beta \frac{k}{2} \\ \lim_{B \rightarrow 0} \frac{\partial Z}{\partial B} &= 0 \\ \lim_{B \rightarrow 0} \frac{\partial^2 Z}{\partial B^2} &= \frac{\beta^2}{2} \left[e^{-\beta \frac{k}{4}} + 2e^{-\beta \epsilon_d} \right] + \frac{\beta}{k} e^{\beta(\frac{k}{4} - \epsilon_d)} \sinh \beta \frac{k}{2}\end{aligned}\quad (7.3.3)$$

The charge susceptibility is thus

$$\chi_c = \frac{1}{\beta} \frac{\frac{\beta^2}{2} \left[e^{-\beta \frac{k}{4}} + 2e^{-\beta \epsilon_d} \right] + \frac{\beta}{k} e^{\beta(\frac{k}{4} - \epsilon_d)} \sinh \beta \frac{k}{2}}{2e^{-\beta \frac{k}{4}} + 4 + 4e^{-\beta \epsilon_d} + 3e^{-\beta(\epsilon_d + \frac{j}{4})} + e^{\beta(3\frac{j}{4} - \epsilon_d)} + 2e^{\beta(\frac{k}{4} - \epsilon_d)} \cosh \beta \frac{k}{2}}\quad (7.3.4)$$

An important result that we will use later is the value at $T = 0$.

$$\chi_c(T = 0) = \frac{1}{2k} \lim_{\beta \rightarrow \infty} \frac{1}{1 + e^{\frac{3\beta}{4}(j-k)}}\quad (7.3.5)$$

There we used the observation that near the fixed point, ϵ_d is either close to zero or large positive such that $e^{-\beta \epsilon_d}$ does not affect the value of χ_c at $T = 0$. In the Kondo regime of the SIAM ($j \gg k$), the denominator diverges and the charge susceptibility vanishes at $T = 0$.

$$\chi_c(T = 0) \Big|_{j \gg k} = 0\quad (7.3.6)$$

The charge susceptibility at large temperatures becomes

$$(\chi_c \times T)(T \rightarrow \infty) = \frac{1}{8}\quad (7.3.7)$$

Figure 7.4: Flow of charge susceptibility to 0 at low temperatures for the spin-Kondo regime ($J > K$).

7.4 Specific heat

The specific heat is calculated by diagonalizing the fixed point Hamiltonian, numerically. The obtained spectrum is denoted by $\{\mathcal{E}_i\}$. The total average energy of the impurity+cloud at temperature T is then

$$\langle \mathcal{E} \rangle = \frac{1}{Z} \sum_i \mathcal{E}_i e^{-\beta \mathcal{E}_i}\quad (7.4.1)$$

Figure 7.5: Behavior of $\chi_c \times T$ for the charge-Kondo regime. It is qualitatively very similar to the behavior of the magnetic susceptibility in the spin-Kondo regime.

where $Z = \sum_i e^{-\beta E_i}$ is the partition function. The specific heat of this system is thus

$$\begin{aligned} C_v &= \frac{\partial \langle \mathcal{E} \rangle}{\partial T} \\ &= -\frac{1}{k_B T^2} \frac{\partial \langle \mathcal{E} \rangle}{\partial \beta} \\ &= \frac{1}{k_B T^2} \left[\frac{1}{Z} \sum_i \mathcal{E}_i^2 e^{-\beta \mathcal{E}_i} - \left(\frac{1}{Z} \sum_i \mathcal{E}_i e^{-\beta \mathcal{E}_i} \right)^2 \right] \end{aligned} \quad (7.4.2)$$

In the absence of impurity, the eigenvalues of the Hamiltonian are $\{\mathcal{E}_i^0\}$ with a partition function $Z^0 = \sum_i e^{-\beta E_i^0}$, so the bath specific heat is

$$C_v^0 = \frac{1}{k_B T^2} \left[\frac{1}{Z_0} \sum_i \mathcal{E}_i^2 e^{-\beta \mathcal{E}_i^0} - \left(\frac{1}{Z_0} \sum_i \mathcal{E}_i^0 e^{-\beta \mathcal{E}_i^0} \right)^2 \right] \quad (7.4.3)$$

The impurity specific heat is the difference.

$$C_v^{\text{imp}} = C_v - C_v^0 \quad (7.4.4)$$

These values were calculated numerically and plotted against temperature in fig. 7.6.

Figure 7.6: Impurity specific heat

7.5 Impurity Spectral function

In this section we will obtain the impurity spectral function, which is defined in terms of the impurity Green's function as

$$\mathcal{A}(\omega) = -\frac{1}{\pi} \text{Im} [G_{dd}^\sigma(\omega)] \quad (7.5.1)$$

The impurity retarded Green's function (assuming the Hamiltonian to be time-independent, which it is) is defined as

$$G_{dd}^\sigma(t) = -i\theta(t) \left\langle \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger \right\} \right\rangle \quad (7.5.2)$$

where the average $\langle \rangle$ is over a canonical ensemble at temperature T . What follows is a standard calculation where we write the Green's function in the Lehmann representation. We will write the ensemble average in terms of the exact eigenstates of the fixed point Hamiltonian:

$$\begin{aligned} H^* |n\rangle &= E_n^* |n\rangle \\ \langle \hat{O} \rangle &\equiv \frac{1}{Z} \sum_n \langle n | \hat{O} | n \rangle e^{-\beta E_n^*} \end{aligned} \quad (7.5.3)$$

where $Z = \sum_n e^{-\beta E_n^*}$ is the fixed point partition function and $\{|n\rangle\}$ is the set of eigenfunctions of the fixed point Hamiltonian. We can therefore write

$$\begin{aligned}
 & \left\langle \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger \right\} \right\rangle \\
 &= \sum_m e^{-\beta E_m} \langle m | \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger \right\} | m \rangle \\
 &= \sum_{m,n} e^{-\beta E_m} \langle m | \left(c_{d\sigma}(t) | n \rangle \langle n | c_{d\sigma}^\dagger + c_{d\sigma}^\dagger | n \rangle \langle n | c_{d\sigma}(t) \right) | m \rangle \quad [9] \\
 &= \sum_{m,n} e^{-\beta E_m} \langle m | \left(e^{iH^* t} c_{d\sigma} e^{-iH^* t} | n \rangle \langle n | c_{d\sigma}^\dagger + c_{d\sigma}^\dagger | n \rangle \langle n | e^{iH^* t} c_{d\sigma} e^{-iH^* t} \right) | m \rangle \\
 &= \sum_{m,n} e^{-\beta E_m} \left(e^{i(E_m - E_n)t} \langle m | c_{d\sigma} | n \rangle \langle n | c_{d\sigma}^\dagger | m \rangle + e^{i(E_n - E_m)t} \langle m | c_{d\sigma}^\dagger | n \rangle \langle n | c_{d\sigma} | m \rangle \right) \\
 &= \sum_{m,n} e^{i(E_m - E_n)t} \| \langle m | c_{d\sigma} | n \rangle \|^2 \left(e^{-\beta E_m} + e^{-\beta E_n} \right)
 \end{aligned} \tag{7.5.4}$$

The time-domain impurity [5] Green's function can thus be written as (this) is the so-called Lehmann representation)

$$G_{dd}^\sigma = -i\theta(t) \sum_{m,n} e^{i(E_m - E_n)t} \| \langle m | c_{d\sigma} | n \rangle \|^2 \left(e^{-\beta E_m} + e^{-\beta E_n} \right) \tag{7.5.5}$$

We are interested in the frequency domain form.

$$\begin{aligned}
 G_{dd}^\sigma(\omega) &= \int_{-\infty}^{\infty} dt e^{i\omega t} G_{dd}^\sigma(t) \\
 &= \sum_{m,n} \| \langle m | c_{d\sigma} | n \rangle \|^2 \left(e^{-\beta E_m} + e^{-\beta E_n} \right) (-i) \int_{-\infty}^{\infty} dt \theta(t) e^{i(\omega + E_m - E_n)t}
 \end{aligned} \tag{7.5.6}$$

To evaluate the time-integral, we will use the integral representation of the Heaviside function:

$$\theta(t) = \frac{1}{2\pi i} \lim_{\eta \rightarrow 0^+} \int_{-\infty}^{\infty} \frac{1}{x - i\eta} e^{ixt} dx \tag{7.5.7}$$

With this definition, the integral in $G_{dd}^\sigma(\omega)$ becomes

$$\begin{aligned}
 (-i) \int_{-\infty}^{\infty} dt \theta(t) e^{i(\omega + E_m - E_n)t} &= (-i) \frac{1}{2\pi i} \lim_{\eta \rightarrow 0^+} \int_{-\infty}^{\infty} dx \frac{1}{x - i\eta} \int_{-\infty}^{\infty} dt e^{i(\omega + E_m - E_n + x)t} \\
 &= (-i) \frac{1}{2\pi i} \lim_{\eta \rightarrow 0^+} \int_{-\infty}^{\infty} dx \frac{1}{x - i\eta} 2\pi\delta(\omega + E_m - E_n + x) \\
 &= (-i) \frac{1}{i} \lim_{\eta \rightarrow 0^+} \frac{-1}{\omega + E_m - E_n - i\eta} \\
 &= \frac{1}{\omega + E_m - E_n}
 \end{aligned} \tag{7.5.8}$$

The frequency-domain Green's function is thus

$$G_{dd}^\sigma(\omega) = \sum_{m,n} \| \langle m | c_{d\sigma} | n \rangle \|^2 \left(e^{-\beta E_m} + e^{-\beta E_n} \right) \frac{1}{\omega + E_m - E_n} \tag{7.5.9}$$

The zero temperature Green's function is obtained by taking the limit of $\beta \rightarrow \infty$:

$$\begin{aligned}
 G_{dd}^\sigma(\omega, \beta \rightarrow \infty) &= \sum_{m,n} \| \langle m | c_{d\sigma} | n \rangle \|^2 (\delta(E_m) + \delta(E_n)) \frac{1}{\omega + E_m - E_n} \\
 &= \sum_{m,0} \left[\| \langle 0 | c_{d\sigma} | n \rangle \|^2 \frac{1}{\omega - E_n} + \| \langle m | c_{d\sigma} | 0 \rangle \|^2 \frac{1}{\omega + E_m} \right]
 \end{aligned} \tag{7.5.10}$$

The label 0 sums over all states with zero energy eigenvalue. The spectral function is the imaginary part of this Green's function. To extract the imaginary part, we insert an infinitesimal imaginary part in the denominator:

$$G_{dd}^\sigma(\omega, T = 0, \eta) = \lim_{\eta \rightarrow 0^+} \sum_{m,0} \left[\|\langle 0 | c_{d\sigma} | n \rangle\|^2 \frac{1}{\omega - E_n + i\eta} + \|\langle m | c_{d\sigma} | 0 \rangle\|^2 \frac{1}{\omega + E_m + i\eta} \right] \quad (7.5.11)$$

The spectral function can then be written as

$$\begin{aligned} \mathcal{A}(\omega) &= -\frac{1}{\pi} \text{Im} [G_{dd}^\sigma(\omega)] \\ &= -\frac{1}{\pi} \text{Im} \left[\lim_{\eta \rightarrow 0^+} \sum_{m,0} \left(\|\langle 0 | c_{d\sigma} | n \rangle\|^2 \frac{-i\eta}{(\omega - E_n)^2 + \eta^2} + \|\langle m | c_{d\sigma} | 0 \rangle\|^2 \frac{-i\eta}{(\omega + E_m)^2 + \eta^2} \right) \right] \\ &= \frac{1}{\pi} \sum_{m,0} \left[\|\langle 0 | c_{d\sigma} | n \rangle\|^2 \pi \delta(\omega - E_n) + \|\langle m | c_{d\sigma} | 0 \rangle\|^2 \pi \delta(\omega + E_m) \right] \\ &= \sum_{m,0} \left[\|\langle 0 | c_{d\sigma} | n \rangle\|^2 \delta(\omega - E_n) + \|\langle m | c_{d\sigma} | 0 \rangle\|^2 \delta(\omega + E_m) \right] \end{aligned} \quad (7.5.12)$$

Since this is in terms of the exact eigenstates, it is a discrete sum of delta-functions. In practice, we get a continuous distribution. To compare with experiment, we need to convert the discrete sum into a continuous function. Following [39], we replace the delta-functions by Gaussian functions:

$$\delta(\omega - E_n) \rightarrow \frac{1}{w\sqrt{\pi}} e^{-\frac{1}{w}(\omega - E_n)^2} \quad (7.5.13)$$

where the width w will be set to the fixed-point bandwidth: $w = D^*$. So the function that we will numerically compute and plot is

$$\mathcal{A}(\omega) = \sum_{m,0} \left[\|\langle 0 | c_{d\sigma} | n \rangle\|^2 \frac{1}{w\sqrt{\pi}} e^{-\frac{1}{w}(\omega - E_n)^2} + \|\langle m | c_{d\sigma} | 0 \rangle\|^2 \frac{1}{w\sqrt{\pi}} e^{-\frac{1}{w}(\omega + E_m)^2} \right] \quad (7.5.14)$$

The fixed-point Hamiltonian H^* is diagonalized numerically to obtain $\{E_m, |m\rangle\}$. The spectral function is plotted for three sets of bare values in fig. 7.7. For low values of U , the profile is that of a single peak at zero frequency. As U increases, shoulder-like structures appear on either side of the peak, which finally, at larger U , develop into two side-peaks.

The physics of the three peaks can now be looked into. Since the central peak is at zero energy, it has to do with excitations that do not cost any energy. There are two such excitations: excitations within the spin sector and within the charge sector.

$$\begin{array}{ccc} JS_d^- & & KC_d^- \\ |\uparrow\rangle \xleftrightarrow{JS_d^-} |\downarrow\rangle, & & |\uparrow\rangle \xleftrightarrow{KC_d^-} |\Downarrow\rangle \\ JS_d^+ & & KC_d^+ \end{array} \quad (7.5.15)$$

The thick arrow \uparrow represents the charge isospin. At particle-hole symmetry, both the spin configurations have energy of ϵ_d , while the charge configurations have energy of $2\epsilon_d + U = 0$ and 0. Hence, no energy is required for these excitations, which is why see a macroscopic number of cloud electrons resonating with the impurity at the Fermi surface. Also note that if \hat{S}_i and \hat{C}_j are two operators of the spin and charge sector ($i, j \in \{x, y, z\}$), then

$$\hat{S}_i \hat{C}_j = \hat{C}_j \hat{S}_i = 0 \quad (7.5.16)$$

We can see this by applying that operator on a basis state. Since the set of four states

$$|\hat{S}_i = \pm \frac{1}{2}, \hat{C}_j = 0\rangle, |\hat{S}_i = 0, \hat{C}_j = \pm \frac{1}{2}\rangle \quad (7.5.17)$$

are all independent, they form a basis. If we apply the operator on these states:

$$\begin{aligned}\hat{S}_i \hat{C}_j |\hat{S}_i\rangle &= 0, & \hat{C}_j \hat{S}_i |S_i\rangle &= S_i \hat{C}_j |S_i\rangle = 0 \\ \hat{C}_j \hat{S}_i |C_j\rangle &= 0, & \hat{S}_i \hat{C}_j |\hat{C}_j\rangle &= C_j \hat{S}_i |\hat{C}_j\rangle = 0\end{aligned}\quad (7.5.18)$$

This shows that each operator acts only on its own subspace. S_i does not act on the charge sector, and vice-versa. There is no single-particle excitation here.

The physics of the side-peaks is that of single number fluctuations on the impurity. These are brought about by the term $Vc_{0\sigma}^\dagger c_{d\sigma} + h.c.$

$$(\epsilon_d) |\sigma\rangle \xrightleftharpoons[Vc_{d\sigma}/Vc_{d\sigma}^\dagger]{Vc_{d\sigma}^\dagger/Vc_{d\sigma}} |n_d = 2, 0\rangle (0)\quad (7.5.19)$$

These transitions involve energy transfer of the order of ϵ_d . This is why, at very small U , they remain absorbed inside the central peak. These transitions do not involve any spin or charge-flip, rather they take the impurity between the spin and charge sectors.

Figure 7.7: Impurity spectral function for three sets of bare values. The increase in value of U is accompanied by the appearance of the side-peaks. For all the plots, $V = 0.001$ and $D = 1$.

7.6 Renormalization of impurity spectral function

Another interesting study that we conducted is the change in the spectral function under reverse-RG. Doing the actual reverse RG would require diagonalizing a huge matrix. Instead, we mimic the reverse journey by starting from the fixed point and then increasing the U (it was irrelevant in the forward RG) and decreasing J (it was relevant in the forward RG). The spectral function is then calculated at these points. The result is shown in fig. 7.8. At the

Figure 7.8: Variation of the spectral function as we move away from the strong-coupling fixed point (top) towards the local moment fixed point (bottom).

1 8 strong-coupling fixed-point, we have a screened-local moment which only has a zero-energy excitation at the Fermi energy. As we move away from the fixed-point, the resonance at the Fermi surface disappears, and is replaced by two side peaks which are indicative of the two orientations of a local moment.

7.7 Effective Hamiltonian for excitations of the Kondo cloud

To find an effective Hamiltonian for the excitations of the Kondo cloud, we will integrate out the impurity part of the wavefunction. The Schrodinger equation for the $J > K$ ground state is

$$\begin{aligned}E_g &\left[c_-^s (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + c_-^c (|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle) \right] \\ &= \mathcal{H} \left[c_-^s (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + c_-^c (|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle) \right] \\ &= \mathcal{H}_0^* \left[c_-^s (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + c_-^c (|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle) \right] \\ &+ V \sum_{\beta} \left[c_{2\beta}^\dagger c_{1\beta} - c_{2\beta} c_{1\beta}^\dagger \right] \left[c_-^s (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + c_-^c (|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle) \right] \\ &+ J \vec{S}_d \cdot \vec{s} \left[c_-^s (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + c_-^c (|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle) \right] \\ &+ K \vec{C}_d \cdot \vec{c} \left[c_-^s (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + c_-^c (|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle) \right]\end{aligned}\quad (7.7.1)$$

The last two lines gives

$$\frac{1}{2} J c_-^s \left[s^z (|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle) + s^+ |\downarrow, \downarrow\rangle - s^- |\uparrow, \uparrow\rangle \right] + \frac{1}{2} K c_-^c \left[c^z (|\uparrow\downarrow, 0\rangle - |0, \uparrow\downarrow\rangle) + c^+ |0, 0\rangle + c^- |2, 2\rangle \right] \quad (7.7.2)$$

The second line gives

$$V c_{2\uparrow}^\dagger \left[c_-^s (|0, \downarrow\rangle) + c_-^c (|\downarrow, 0\rangle) \right] + V c_{2\downarrow}^\dagger \left[c_-^s (-|0, \uparrow\rangle) + c_-^c (|\uparrow, 0\rangle) \right] \\ - V c_{2\uparrow} \left[c_-^s (-|\uparrow\downarrow, \uparrow\rangle) + c_-^c (|\uparrow, \uparrow\downarrow\rangle) \right] - V c_{2\downarrow} \left[c_-^s (-|\uparrow\downarrow, \downarrow\rangle) + c_-^c (|\downarrow, \uparrow\downarrow\rangle) \right] \quad (7.7.3)$$

We will now write down four equations by comparing the coefficients of $|\uparrow\rangle, |\downarrow\rangle, |0\rangle$ and $|2\rangle$ of the impurity sector:

$$\begin{aligned} (E_g - H_0^*) c_-^s |\downarrow\rangle &= V c_-^c \left(c_{2\downarrow}^\dagger |0\rangle - c_{2\uparrow} |2\rangle \right) + \frac{1}{2} J c_-^s \left(s^z |\downarrow\rangle - s^- |\uparrow\rangle \right) && [\text{eq. from } |\uparrow\rangle] \\ (-E_g + H_0^*) c_-^s |\uparrow\rangle &= V c_-^c \left(c_{2\uparrow}^\dagger |0\rangle - c_{2\downarrow}^\dagger |2\rangle \right) + \frac{1}{2} J c_-^s \left(s^z |\uparrow\rangle + s^+ |\downarrow\rangle \right) && [\text{eq. from } |\downarrow\rangle] \\ (E_g - H_0^*) c_-^c |\mathbf{2}\rangle &= V c_-^s \left(c_{2\uparrow}^\dagger |\downarrow\rangle - c_{2\downarrow}^\dagger |\uparrow\rangle \right) + \frac{1}{2} K c_-^c \left(-c^z |2\rangle + c^+ |0\rangle \right) && [\text{eq. from } |0\rangle] \\ (E_g - H_0^*) c_-^c |0\rangle &= V c_-^s \left(c_{2\uparrow}^\dagger |\uparrow\rangle + c_{2\downarrow}^\dagger |\downarrow\rangle \right) + \frac{1}{2} K c_-^c \left(c^z |0\rangle + c^- |2\rangle \right) && [\text{eq. from } |2\rangle] \end{aligned} \quad (7.7.4)$$

These can be rearranged into

$$\begin{aligned} \left(E_g - H_0^* - \frac{1}{2} J s^z \right) |\downarrow\rangle &= V \lambda^{-1} \left(c_{2\downarrow}^\dagger |0\rangle - c_{2\uparrow} |2\rangle \right) - \frac{1}{2} J s^- |\uparrow\rangle \\ \left(E_g - H_0^* + \frac{1}{2} J s^z \right) |\uparrow\rangle &= V \lambda^{-1} \left(c_{2\downarrow} |2\rangle - c_{2\uparrow}^\dagger |0\rangle \right) - \frac{1}{2} J s^+ |\downarrow\rangle \\ \left(E_g - H_0^* + \frac{1}{2} K c^z \right) |2\rangle &= V \lambda \left(c_{2\uparrow}^\dagger |\downarrow\rangle - c_{2\downarrow}^\dagger |\uparrow\rangle \right) + \frac{1}{2} K c^+ |0\rangle \\ \left(E_g - H_0^* - \frac{1}{2} K c^z \right) |0\rangle &= V \lambda \left(c_{2\uparrow}^\dagger |\uparrow\rangle + c_{2\downarrow}^\dagger |\downarrow\rangle \right) + \frac{1}{2} K c^- |2\rangle \end{aligned} \quad (7.7.5)$$

where $\lambda = \frac{c_-^s}{c_-^c}$. We want to find the effective Hamiltonian in the subspace of $|\downarrow\rangle$. We first eliminate the charge sector from these equations:

$$\begin{aligned} |0\rangle &= V \lambda \left[\frac{1}{A_-^K} c_{2\uparrow} + \frac{K}{2} \frac{1}{A_-^K} c^- - \frac{1}{A_+^K - \left(\frac{K}{2}\right)^2 c^+ \frac{1}{A_-^K} c^-} \left(\frac{K}{2} c^+ \frac{1}{A_-^K} c_{2\uparrow} - c_{2\downarrow}^\dagger \right) \right] |\uparrow\rangle \\ &\quad + V \lambda \left[\frac{1}{A_-^K} c_{2\downarrow} + \frac{K}{2} \frac{1}{A_-^K} c^- - \frac{1}{A_+^K - \left(\frac{K}{2}\right)^2 c^+ \frac{1}{A_-^K} c^-} \left(c_{2\uparrow}^\dagger + \frac{K}{2} c^+ \frac{1}{A_-^K} c_{2\downarrow} \right) \right] |\downarrow\rangle \quad (7.7.6) \\ |\mathbf{2}\rangle &= \frac{V \lambda}{A_+^K - \left(\frac{K}{2}\right)^2 c^+ \frac{1}{A_-^K} c^-} \left[\left(c_{2\uparrow}^\dagger + \frac{K}{2} c^+ \frac{1}{A_-^K} c_{2\downarrow} \right) |\downarrow\rangle + \left(\frac{K}{2} c^+ \frac{1}{A_-^K} c_{2\uparrow} - c_{2\downarrow}^\dagger \right) |\uparrow\rangle \right] \end{aligned}$$

where

$$A_\pm^K = E_g - H_0^* \pm \frac{1}{2} K c^z \quad (7.7.7)$$

For ease of labeling, we will think of these equations as

$$|0\rangle = a_0^\uparrow |\uparrow\rangle + a_0^\downarrow |\downarrow\rangle, |2\rangle = a_2^\uparrow |\uparrow\rangle + a_2^\downarrow |\downarrow\rangle \quad (7.7.8)$$

The remaining two equations can then be written as

$$\begin{aligned} A_-^J |\downarrow\rangle &= \frac{V}{\lambda} \left[c_{2\downarrow}^\dagger (a_0^\uparrow |\uparrow\rangle + a_0^\downarrow |\downarrow\rangle) - c_{2\uparrow} (a_2^\uparrow |\uparrow\rangle + a_2^\downarrow |\downarrow\rangle) \right] - \frac{J}{2} s^- |\uparrow\rangle \\ A_+^J |\uparrow\rangle &= \frac{V}{\lambda} \left[c_{2\downarrow} (a_2^\uparrow |\uparrow\rangle + a_2^\downarrow |\downarrow\rangle) - c_{2\uparrow}^\dagger (a_0^\uparrow |\uparrow\rangle + a_0^\downarrow |\downarrow\rangle) \right] - \frac{J}{2} s^+ |\downarrow\rangle \end{aligned} \quad (7.7.9)$$

where

$$A_\pm^J = E_g - H_0^* \pm \frac{1}{2} J s^z \quad (7.7.10)$$

Eliminating $|\downarrow\rangle$ and solving for $|\uparrow\rangle$ gives

$$\begin{aligned} A_+^J |\uparrow\rangle &= \frac{V}{\lambda} \left(c_{2\downarrow} a_2^\uparrow - c_{2\uparrow} a_0^\uparrow \right) |\uparrow\rangle + \left(\frac{V}{\lambda} c_{2\downarrow} a_2^\downarrow - \frac{V}{\lambda} c_{2\uparrow} a_0^\downarrow - \frac{J}{2} s^+ \right) |\downarrow\rangle \\ &= \frac{V}{\lambda} \left(c_{2\downarrow} a_2^\uparrow - c_{2\uparrow} a_0^\uparrow \right) |\uparrow\rangle \\ &\quad + \left[\frac{V}{\lambda} \left(c_{2\downarrow} a_2^\downarrow - c_{2\uparrow} a_0^\downarrow \right) - \frac{J}{2} s^+ \right] \frac{1}{A_-^J - \frac{V}{\lambda} \left(c_{2\downarrow}^\dagger a_0^\downarrow - c_{2\uparrow}^\dagger a_2^\downarrow \right)} \left[\frac{V}{\lambda} \left(c_{2\downarrow}^\dagger a_0^\uparrow - c_{2\uparrow} a_2^\uparrow \right) - \frac{J}{2} s^- \right] |\uparrow\rangle \end{aligned} \quad (7.7.11)$$

The effective Hamiltonian for the $|\uparrow\rangle$ state is

$$\begin{aligned} H_0^* - \frac{J}{2} s^z + \frac{V}{\lambda} \left(c_{2\downarrow} a_2^\uparrow - c_{2\uparrow} a_0^\uparrow \right) + \left[\frac{V}{\lambda} \left(c_{2\downarrow} a_2^\downarrow - c_{2\uparrow} a_0^\downarrow \right) - \frac{J}{2} s^+ \right] \frac{1}{A_-^J - \frac{V}{\lambda} \left(c_{2\downarrow}^\dagger a_0^\downarrow - c_{2\uparrow}^\dagger a_2^\downarrow \right)} \\ \times \left[\frac{V}{\lambda} \left(c_{2\downarrow}^\dagger a_0^\uparrow - c_{2\uparrow} a_2^\uparrow \right) - \frac{J}{2} s^- \right] \end{aligned} \quad (7.7.12)$$

To get a clearer picture of this effective Hamiltonian, we will keep up to two-particle interactions. We first write down the full forms of $a_{0,2}^\sigma$:

$$\begin{aligned} a_0^\sigma &= V\lambda \left[\frac{\frac{1}{A_-^K} c_{2\sigma}}{\frac{1}{A_-^K} c_{2\sigma} + \frac{K}{2} \frac{1}{A_-^K} c^-} \frac{\frac{1}{A_+^K} c^+}{\frac{1}{A_+^K} c^+ - \left(\frac{K}{2} \right)^2 c^+ \frac{1}{A_-^K} c^-} \left(\frac{K}{2} c^+ \frac{1}{A_-^K} c_{2\sigma} - \sigma c_{2\sigma}^\dagger \right) \right] \\ a_2^\sigma &= \frac{V\lambda}{A_+^K - \left(\frac{K}{2} \right)^2 c^+ \frac{1}{A_-^K} c^-} \left(-\sigma c_{2-\sigma}^\dagger + \frac{K}{2} c^+ \frac{1}{A_-^K} c_{2\sigma} \right) \end{aligned} \quad (7.7.13)$$

We will first look at the special case of $K = 0$. There, the above expressions simplify to

$$\begin{aligned} a_0^\sigma &= V\lambda \frac{1}{A_-^K} c_{2\sigma} = \frac{V\lambda}{E_g} \left[1 + \frac{1}{E_g} (H_0^*) + \frac{1}{E_g^2} (H_0^*)^2 \right] c_{2\sigma} + \mathcal{O}(H_0^{*3}) \\ a_2^\sigma &= -\sigma V\lambda \frac{1}{A_+^K} c_{2-\sigma}^\dagger = -\sigma \frac{V\lambda}{E_g} \left[1 + \frac{1}{E_g} (H_0^*) + \frac{1}{E_g^2} (H_0^*)^2 \right] c_{2-\sigma}^\dagger + \mathcal{O}(H_0^{*3}) \end{aligned} \quad (7.7.14)$$

We will make use of the following commutators:

$$\begin{aligned} \left[(H_0^*)^m, c_{2\sigma} \right] &= - \sum_k \frac{\epsilon_k^m}{\sqrt{N^*}} c_{k\sigma}, & \left[(H_0^*)^m, c_{2\sigma}^\dagger \right] &= \sum_k \frac{\epsilon_k^m}{\sqrt{N^*}} c_{k\sigma}^\dagger, \quad m = 1, 2 \\ \left[(H_0^*)^m, s^+ \right] &= \sum_{kk'} (\epsilon_k^m - \epsilon_{k'}^m) c_{k\beta}^\dagger c_{k'\bar{\beta}}, & m &= 1, 2 \\ \left[(s^z)^m, c_{2\sigma} \right] &= - \left(\frac{\sigma}{2} \right)^m c_{2\sigma}, & \left[(s^z)^m, c_{2\sigma}^\dagger \right] &= \left(\frac{\sigma}{2} \right)^m c_{2\sigma}^\dagger, \quad m = 1, 2 \\ \left[(c^z)^m, c_{2\sigma} \right] &= - \left(\frac{1}{2} \right)^m c_{2\sigma}, & \left[(c^z)^m, c_{2\sigma}^\dagger \right] &= \left(\frac{1}{2} \right)^m c_{2\sigma}^\dagger, \quad m = 1, 2 \end{aligned} \quad (7.7.15)$$

Now we evaluate the various terms in the effective Hamiltonian.

$$\begin{aligned}
 \mathbf{c}_{2\downarrow} \mathbf{a}_2^\uparrow &= -\frac{V\lambda}{E_g} c_{2\downarrow} \left[1 + \frac{1}{E_g} (H_0^*) + \frac{1}{E_g^2} (H_0^*)^2 \right] c_{2\downarrow}^\dagger \\
 &= -\frac{V\lambda}{E_g} \left[c_{2\downarrow} + \frac{1}{E_g} (H_0^*) c_{2\downarrow} + \sum_k \frac{\epsilon_k}{E_g \sqrt{N^*}} c_{k\downarrow} + \frac{1}{E_g^2} (H_0^*)^2 c_{2\downarrow} + \sum_k \frac{\epsilon_k^2}{E_g^2 \sqrt{N^*}} c_{k\downarrow} \right] c_{2\downarrow}^\dagger \\
 &= -\frac{V\lambda}{E_g} \left[1 + \frac{H_0^*}{E_g} + \left(\frac{H_0^*}{E_g} \right)^2 \right] c_{2\downarrow} c_{2\downarrow}^\dagger - \frac{V\lambda}{E_g N^*} \sum_{kk'} \left(\frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2} \right) c_{k\downarrow} c_{k'\downarrow}^\dagger \\
 \mathbf{c}_{2\uparrow} \mathbf{a}_2^\downarrow &= -\frac{V\lambda}{E_g} \left[1 + \frac{H_0^*}{E_g} + \left(\frac{H_0^*}{E_g} \right)^2 \right] c_{2\uparrow} c_{2\uparrow}^\dagger - \frac{V\lambda}{E_g N^*} \sum_{kk'} \left(\frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2} \right) c_{k\uparrow} c_{k'\uparrow}^\dagger \\
 \mathbf{c}_{2\uparrow}^\dagger \mathbf{a}_0^\uparrow &= c_{2\uparrow}^\dagger \frac{V\lambda}{E_g} \left[1 + \frac{1}{E_g} (H_0^*) + \frac{1}{E_g^2} (H_0^*)^2 \right] c_{2\uparrow} \\
 &= \frac{V\lambda}{E_g} \left[1 + \frac{H_0^*}{E_g} + \left(\frac{H_0^*}{E_g} \right)^2 \right] c_{2\uparrow}^\dagger c_{2\uparrow} - \frac{V\lambda}{E_g N^*} \sum_{kk'} \left(\frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2} \right) c_{k\uparrow}^\dagger c_{k'\uparrow} \\
 \mathbf{c}_{2\downarrow}^\dagger \mathbf{a}_0^\downarrow &= \frac{V\lambda}{E_g} \left[1 + \frac{H_0^*}{E_g} + \left(\frac{H_0^*}{E_g} \right)^2 \right] c_{2\downarrow}^\dagger c_{2\downarrow} - \frac{V\lambda}{E_g N^*} \sum_{kk'} \left(\frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2} \right) c_{k\downarrow}^\dagger c_{k'\downarrow} \\
 \mathbf{c}_{2\downarrow} \mathbf{a}_2^\downarrow &= \frac{V\lambda}{E_g} c_{2\downarrow} \left[1 + \frac{1}{E_g} (H_0^*) + \frac{1}{E_g^2} (H_0^*)^2 \right] c_{2\downarrow}^\dagger \\
 &= \frac{V\lambda}{E_g} \left[1 + \frac{H_0^*}{E_g} \right] c_{2\downarrow} c_{2\downarrow}^\dagger + \frac{V\lambda}{E_g N^*} \sum_{kk'} \left(\frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2} \right) c_{k\downarrow} c_{k'\uparrow}^\dagger \\
 \mathbf{c}_{2\uparrow} \mathbf{a}_2^\uparrow &= -\frac{V\lambda}{E_g} \left[1 + \frac{1}{E_g} (H_0^*) \right] c_{2\uparrow} c_{2\downarrow}^\dagger - \frac{V\lambda}{E_g N^*} \sum_{kk'} \left(\frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2} \right) c_{k\uparrow} c_{k'\downarrow}^\dagger \\
 \mathbf{c}_{2\uparrow}^\dagger \mathbf{a}_0^\downarrow &= \frac{V\lambda}{E_g} \left[1 + \frac{H_0^*}{E_g} \right] c_{2\uparrow}^\dagger c_{2\downarrow} - \frac{V\lambda}{E_g N^*} \sum_{kk'} \left(\frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2} \right) c_{k\uparrow}^\dagger c_{k'\downarrow} \\
 \mathbf{c}_{2\downarrow}^\dagger \mathbf{a}_0^\uparrow &= \frac{V\lambda}{E_g} \left[1 + \frac{H_0^*}{E_g} \right] c_{2\downarrow}^\dagger c_{2\uparrow} - \frac{V\lambda}{E_g N^*} \sum_{kk'} \left(\frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2} \right) c_{k\downarrow}^\dagger c_{k'\uparrow} \\
 \mathbf{c}_{2\downarrow} \mathbf{a}_2^\uparrow - \mathbf{c}_{2\uparrow} \mathbf{a}_0^\uparrow &= -\frac{V\lambda}{E_g} \left[1 + \frac{H_0^*}{E_g} + \left(\frac{H_0^*}{E_g} \right)^2 \right] \times 2 + \frac{V\lambda}{E_g N^*} \sum_{kk'} \left(\frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2} \right) \left(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow} c_{k'\downarrow}^\dagger \right) \\
 \mathbf{c}_{2\downarrow} \mathbf{a}_2^\downarrow - \mathbf{c}_{2\uparrow}^\dagger \mathbf{a}_0^\downarrow &= \frac{V\lambda}{E_g} \left[1 + \frac{1}{E_g} (H_0^*) \right] c_{2\downarrow} c_{2\downarrow}^\dagger \times 2 + \frac{V\lambda}{E_g N^*} \sum_{kk'} \left(\frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2} \right) \left(c_{k\downarrow} c_{k'\uparrow}^\dagger + c_{k\uparrow}^\dagger c_{k'\downarrow} \right) \\
 \mathbf{c}_{2\downarrow}^\dagger \mathbf{a}_0^\downarrow - \mathbf{c}_{2\uparrow} \mathbf{a}_2^\downarrow &= \frac{V\lambda}{E_g N^*} \sum_{kk'} \left(\frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2} \right) \left(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow} \right) \\
 \mathbf{c}_{2\downarrow}^\dagger \mathbf{a}_0^\uparrow - \mathbf{c}_{2\uparrow} \mathbf{a}_2^\uparrow &= \frac{V\lambda}{E_g N^*} \sum_{kk'} \left(\frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2} \right) \left(c_{k\uparrow} c_{k'\downarrow}^\dagger - c_{k\downarrow}^\dagger c_{k'\uparrow} \right)
 \end{aligned}$$

In all the expressions, we have dropped terms that have more than 4 operators in product. Also, in the last four equations, we have substituted $\hat{n}_{2\uparrow} - \hat{n}_{2\downarrow} = 1$, because this is the effective Hamiltonian for the state with $s^z = \frac{1}{2}$. We now substitute these expressions into the effective Hamiltonian:

$$\begin{aligned}
 H_0^* - \frac{J}{2}s^z - \frac{2V^2}{E_g} & \left[1 + \frac{H_0^*}{E_g} + \left(\frac{H_0^*}{E_g} \right)^2 \right] + \frac{V^2}{E_g N^*} \sum_{kk'} \xi_k \left(\overset{\text{1}}{c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow} c_{k'\downarrow}^\dagger} \right) \\
 & + \left[\frac{V}{\lambda} \left(c_{2\downarrow} a_2^\dagger - c_{2\uparrow}^\dagger a_0^\dagger \right) \right] \frac{1}{A_-^J - \frac{V^2}{E_g N^*} \sum_{kk'} \xi_k \left(\overset{\text{1}}{c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow}} \right)} \left[\frac{V}{\lambda} \left(\overset{\text{1}}{c_{2\downarrow}^\dagger a_0^\dagger - c_{2\uparrow} a_2^\dagger} \right) \right] \\
 & + \left[\frac{V}{\lambda} \left(c_{2\downarrow} a_2^\dagger - c_{2\uparrow}^\dagger a_0^\dagger \right) \right] \frac{1}{A_-^J - \frac{V^2}{E_g N^*} \sum_{kk'} \xi_k \left(\overset{\text{1}}{c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow}} \right)} \left[-\frac{J}{2}s^- \right] \\
 & + \left[-\frac{J}{2}s^+ \right] \frac{1}{A_-^J - \frac{V^2}{E_g N^*} \sum_{kk'} \xi_k \left(\overset{\text{1}}{c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow}} \right)} \left[\frac{V}{\lambda} \left(\overset{\text{1}}{c_{2\downarrow}^\dagger a_0^\dagger - c_{2\uparrow} a_2^\dagger} \right) \right] \\
 & + \frac{J^2}{4} \left[s^+ \right] \frac{1}{A_-^J - \frac{V^2}{E_g N^*} \sum_{kk'} \xi_k \left(\overset{\text{1}}{c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow}} \right)} \left[s^- \right]
 \end{aligned} \tag{7.7.16}$$

where $\xi_k = \frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2}$. We first consider only zeroth order terms of the central propagator.

$$\begin{aligned}
 H_0^* - \frac{J}{2} \underbrace{s^z}_{\frac{1}{2}} - \frac{2V^2}{E_g} & \left[1 + \frac{H_0^*}{E_g} + \left(\frac{H_0^*}{E_g} \right)^2 \right] + \frac{V^2}{E_g N^*} \sum_{kk'} \left(\overset{\text{1}}{\xi_k} \right) \left(\overset{\text{1}}{c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow} c_{k'\downarrow}^\dagger} \right) \\
 & + \frac{V^4}{E_g^2 N^{*2} \left(E_g + \frac{J}{4} \right)} \sum_{kk'} \left(\xi_{k'} + 2 - \overset{\text{1}}{\xi_k} \right) \overset{\text{1}}{c_{k\uparrow}^\dagger c_{k'\downarrow}} \sum_{kk'} \left(\xi_k + \xi_{k'} \right) \overset{\text{1}}{c_{k\downarrow}^\dagger c_{k'\uparrow}} \\
 & + \frac{V^2 J}{2E_g \left(E_g + \frac{J}{4} \right) N^*} \sum_{kk'} \left(\xi_{k'} + 2 - \overset{\text{1}}{\xi_k} \right) \overset{\text{1}}{c_{k\uparrow}^\dagger c_{k'\downarrow}} \sum_{kk'} \overset{\text{1}}{c_{k\downarrow}^\dagger c_{k'\uparrow}} \\
 & + \frac{JV^2}{2E_g \left(E_g + \frac{J}{4} \right) N^*} \sum_{kk'} \overset{\text{1}}{c_{k\uparrow}^\dagger c_{k'\downarrow}} \sum_{kk'} \left(\xi_k + \xi_{k'} \right) \overset{\text{1}}{c_{k\downarrow}^\dagger c_{k'\uparrow}} \\
 & + \frac{J^2}{4 \left(E_g + \frac{J}{4} \right)} \underbrace{s^+ s^-}_{s^z + \frac{1}{2} = 1}
 \end{aligned} \tag{7.7.17}$$

We have set $s^z = -\frac{1}{2}$ in the denominator, hence the $E_g = \frac{J}{4}$. If we also consider the first and second order terms from the central propagator, note that they will produce terms of more than quartic interactions in the first three terms. For the last term, we get

$$\frac{J^2}{4 \left(E_g + \frac{J}{4} \right)} s^+ \left[\frac{H_0^*}{E_g + \frac{J}{4}} + \left(\frac{H_0^*}{E_g + \frac{J}{4}} \right)^2 \right] s^- \tag{7.7.18}$$

Using the commutator of H_0^* with s^+ to bring H_0^* to the left, and using $s^+ s^- = s^z + \frac{1}{2} = 1$, we get

$$\frac{J^2}{4 \left(E_g + \frac{J}{4} \right)} \left[\frac{H_0^*}{E_g + \frac{J}{4}} + \left(\frac{H_0^*}{E_g + \frac{J}{4}} \right)^2 - \sum_{kk'qq'} \left(\xi_k^J - \xi_{k'}^J \right) \overset{\text{1}}{c_{k\uparrow}^\dagger c_{k'\downarrow} c_{q\downarrow}^\dagger c_{q'\uparrow}} \right] \tag{7.7.19}$$

where $\xi_k^J = \frac{\epsilon_k}{E_g + \frac{J}{4}} + \frac{\epsilon_k^2}{\left(E_g + \frac{J}{4}\right)^2}$. The full effective Hamiltonian, for $K = 0$, up to quartic interactions, is

$$H_0^* + \frac{J}{4} \left(\frac{J}{E_g + \frac{J}{4}} - 1 \right) - \frac{2V^2}{E_g} + \frac{V^2}{E_g N^*} \sum_{kk'} (\xi_k) \left(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow} c_{k'\downarrow}^\dagger \right) - \frac{2V^2}{E_g} \left[\frac{H_0^*}{E_g} + \left(\frac{H_0^*}{E_g} \right)^2 \right] \\ + \frac{J^2}{4 \left(E_g + \frac{J}{4} \right)} \left[\frac{H_0^*}{E_g + \frac{J}{4}} + \left(\frac{H_0^*}{E_g + \frac{J}{4}} \right)^2 \right] + \sum_{kk'qq'} F_{kk'qq'} c_{k\uparrow}^\dagger c_{k'\downarrow} c_{q\downarrow}^\dagger c_{q'\uparrow} \quad (7.7.20)$$

The coefficient $F_{kk'qq'}$ is

$$F_{kk'qq'} = \frac{V^2}{E_g N^* \left(E_g + \frac{J}{4} \right)} \left[\frac{V^2}{E_g N^*} (\xi_{k'} + 2 - \xi_k) (\xi_q + \xi_{q'}) + \frac{J}{2} (\xi_{k'} + 2 - \xi_k + \xi_q + \xi_{q'}) \right] \\ + \frac{J^2}{4 \left(E_g + \frac{J}{4} \right)} (\xi_{k'}^J - \xi_k^J) \quad (7.7.21)$$

There are two main types of interactions that gets generated upon integrating out the impurity. One is the Fermi liquid type interactions arising from the H_0^{*2} terms. The Fermi liquid part of the Hamiltonian is

$$\left[\frac{J^2}{4 \left(E_g + \frac{J}{4} \right)^2} - \frac{2V^2}{E_g^2} \right] H_0^* + \left[\frac{J^2}{4 \left(E_g + \frac{J}{4} \right)^2} - \frac{2V^2}{E_g^3} \right] H_0^{*2} \\ = \left[\frac{J^2}{4 \left(E_g + \frac{J}{4} \right)^2} - \frac{2V^2}{E_g^2} \right] \left[H_0^* + \sum_{kk'\sigma\sigma'} f_{kk'} \hat{n}_{k\sigma} \hat{n}_{k'\sigma'} \right] \quad (7.7.22)$$

where the Landau parameter is given by

$$f_{kk'} = \left[\frac{J^2}{4 \left(E_g + \frac{J}{4} \right)^2} - \frac{2V^2}{E_g^2} \right]^{-1} \left[\frac{J^2}{4 \left(E_g + \frac{J}{4} \right)^3} - \frac{2V^2}{E_g^3} \right] \epsilon_k \epsilon_{k'} \quad (7.7.23)$$

The more interesting interaction is the off-diagonal term

$$\sum_{kk'qq'} F_{kk'qq'} c_{k\uparrow}^\dagger c_{k'\downarrow} c_{q\downarrow}^\dagger c_{q'\uparrow} \quad (7.7.24)$$

This interaction arises from the enhanced entanglement between the impurity and the conduction electrons; removing the impurity from the singlet and the triplet generates these off-diagonal scatterings. As such, this is an indicator of the macroscopic entanglement of the singlet formed at the IR fixed point, and plotted in fig. 7.13.

It is also very enlightening [10] note that this scattering is a signature of the change in Luttinger's count in going from the free orbital or local moment fixed point to the strong-coupling fixed point, as shown in eq. 7.9.28. Both this off-diagonal scattering as well as the change in Luttinger's count are a direct consequence of the non-number conserving term $V c_k^\dagger c_d$ in the full Hamiltonian. The topological change of Luttinger's count is concomitant with the presence of the off-diagonal scattering term in the effective Hamiltonian. Just the Fermi liquid piece in eq. 7.7.23 will give neither the enhanced mutual information nor the change in Luttinger's count.

We have shown the enhancement of this off-diagonal scattering during the flow towards the IR fixed point by computing it during the reverse RG program, in fig. 7.9. It is clear from this plot that the growth of this non-Fermi-liquid type interaction happens simultaneously with the formation of the singlet.

Figure 7.9: Variation of the coefficient of the two-particle off-diagonal scattering in the effective Hamiltonian, eq. 7.7.21 along the RG flow.

7.8 Calculation of Wilson ratio from effective local Fermi liquid

In this section, we will calculate the zero temperature Wilson ratio of the impurity in the Kondo regime of the SIAM. Since this is a low energy property, our starting point will be the fixed point Hamiltonian of eq. 6.4.3, after substituting $U^* = K^* = 0$ (because we are in the first quadrant):

$$\mathcal{H}^* = \sum_{\sigma, k} \epsilon_k \tau_{k\sigma} + \sum_{\sigma, k < \Lambda^*} \left(V^* c_{k\sigma}^\dagger c_{d\sigma} + \text{h.c.} \right) + J^* \vec{S}_d \cdot \vec{s} \quad (7.8.1)$$

We also convert τ to \hat{n} , ignoring the constant part, and write the kinetic energy part as a nearest-neighbor hopping problem:

$$\mathcal{H}^* = t \sum_{\sigma \langle i, j \rangle} \left(c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.} \right) + \sum_{\sigma} \left(V^* c_{k\sigma}^\dagger c_{d\sigma} + \text{h.c.} \right) + J^* \vec{S}_d \cdot \vec{s} \quad (7.8.2)$$

We know that the ground state for the interacting part is predominantly the spin-singlet (it was shown while calculating the ground states of the effective zero-mode Hamiltonian that the ground state is a mixture of singlet and triplet, and the triplet part dies out at large system sizes, see eq. 6.4.40), so we will take that as our reference state and treat the hopping part that connects the origin to the first site,

$$V = t \sum_{\vec{r}_1, \sigma} c_{0\sigma}^\dagger c_{\vec{r}_1, \sigma} + \text{h.c.} \quad (7.8.3)$$

as a weak perturbation. \vec{r}_1 here spans over the sites that are nearest to the origin. Once that is taken care of, we will have a decoupled singlet formed by the impurity and the zeroth site, and the rest of the lattice formed by $N - 1$ sites along with the interaction induced by the perturbation. The goal here is to see whether the effect of the perturbation is to lower the energy of the singly-occupied state $|\hat{n}_1 = 1\rangle$ compared to the doubly-occupied state $|\hat{n}_1 = 2\rangle$ or to raise it. If the perturbation shifts the energy of the singly-occupied state below the doubly-occupied state, then we can conclude that the effect of the perturbation is to raise the energy of the doubly-occupied state, which can then be modeled by a repulsive term $|U|\hat{n}_{1\uparrow}\hat{n}_{1\downarrow}$. If, on the other hand, the effect is to raise the energy of the singly-occupied state with respect to the $\hat{n}_1 = 2$ state, then that effect is equivalent to an attractive term $-|U|\hat{n}_{1\uparrow}\hat{n}_{1\downarrow}$.

To be precise, we will compare the energy shifts corresponding to the two states

$$\begin{aligned} |\phi_1^{(0)}\rangle &= \underbrace{|\uparrow\rangle}_{\text{site 1}} \otimes \frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) \\ |\phi_2^{(0)}\rangle &= \underbrace{|\uparrow, \downarrow\rangle}_{\text{site 1}} \otimes \frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) \end{aligned} \quad (7.8.4)$$

In the singlet part, the first entry is the configuration of the zeroth site while the second entry is the configuration of the impurity site. Choosing the \uparrow configuration for the site 1 is not a problem because both the non-perturbative and the perturbative interactions are SU(2)-symmetric. To demonstrate this, note that all energy shifts will depend on the unperturbed states $|\phi^{(0)}\rangle$ in two ways: through the energies in the denominator and through the matrix element in the numerator. The unperturbed energy goes not depend on the configuration of the \vec{r}_1 site, because the energy is dominated by the singlet. The matrix element is also independent of the sigma:

$$\begin{aligned} V |\sigma\rangle \otimes \frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) &= \left(t \sum_{\vec{r}_1, \sigma} c_{0\sigma}^\dagger c_{\vec{r}_1, \sigma} + \text{h.c.} \right) |\sigma\rangle \otimes \frac{1}{\sqrt{2}} \sum_{\alpha} \alpha |\alpha, \bar{\alpha}\rangle \\ &= t \frac{1}{\sqrt{2}} (|2\rangle |0, \bar{\sigma}\rangle - |0\rangle |2, \sigma\rangle) \end{aligned} \quad (7.8.5)$$

The first order correction will be zero as we will see shortly, but the short version is that $V|\phi^{(0)}\rangle$ is obviously orthogonal to $|\phi^{(0)}\rangle$. All higher energy shifts can be represented as

$$\langle \phi^{(0)} | V X V | \phi^{(0)} \rangle \quad (7.8.6)$$

where X , for example, is

$$\sum_{m^{(0)}} \frac{|\langle m^{(0)} | |\phi^{(0)}\rangle|^2}{E_\phi^{(0)} - E_m^{(0)}} \quad (7.8.7)$$

for the ¹⁸ second order shift, and does not operate on the impurity. Since X does not operate on the impurity, the shift can be written as

$$\begin{aligned} \langle \phi^{(0)} | V X V | \phi^{(0)} \rangle &= \frac{t^2}{2} (\langle 2 | \langle 0, \bar{\sigma} | - \langle 0 | \langle 2, \sigma |) X (\langle 2 | \langle 0, \bar{\sigma} | - \langle 0 | \langle 2, \sigma |) \\ &= \frac{t^2}{2} \langle 2 | \langle 0, \bar{\sigma} | X | 2 \rangle \langle 0, \bar{\sigma} | + \frac{t^2}{2} \langle 0 | \langle 2, \sigma | X | 0 \rangle \langle 2, \sigma | \\ &= \frac{t^2}{2} \langle 2 | \langle 0 | X | 2 \rangle \langle 0 | \langle \bar{\sigma} | \bar{\sigma} \rangle + \frac{t^2}{2} \langle 0 | \langle 2 | X | 0 \rangle \langle 2 | \langle \sigma | \sigma \rangle \\ &= \frac{t^2}{2} \langle 2 | \langle 0 | X | 2 \rangle \langle 0 | + \frac{t^2}{2} \langle 0 | \langle 2 | X | 0 \rangle \langle 2 | \end{aligned} \quad (7.8.8)$$

This proves that the shift is independent of σ . The reason we could shift the bra $\langle \sigma |$ across the X without any sign change is that X will have even number of operators in product, because it operates on 0 and 1.

The energy corresponding to this singlet state (for both $\hat{n}_1 = 1$ and $\hat{n}_1 = 2$) is

$$E_1^{(0)} = E_2^{(0)} = -\frac{3J^*}{4} \quad (7.8.9)$$

The full list of unperturbed eigenstates are

$$\{|\hat{n}_1 = 0\rangle, |\hat{n}_1 = 1\rangle, |\hat{n}_1 = 2\rangle\} \otimes \{|S = 0\rangle, |S = 1, S^z = -1, 0, 1\rangle, |S_0^z \times S_d^z = 0\rangle\} \quad (7.8.10)$$

Since V takes $|\phi_{1,2}^{(0)}\rangle$ to completely orthogonal states, the first order corrections are 0:

$$\begin{aligned} E_1^{(1)} &= \langle \phi_1^{(0)} | V | \phi_1^{(0)} \rangle = \langle \phi_1^{(0)} | \frac{t}{\sqrt{2}} (-|0, 2, \uparrow\rangle - |2, 0, \uparrow\rangle) = 0 \\ E_2^{(1)} &= \langle \phi_2^{(0)} | V | \phi_2^{(0)} \rangle = \langle \phi_2^{(0)} | \frac{t}{\sqrt{2}} (|\downarrow, 2, \uparrow\rangle - |\uparrow, 2, \downarrow\rangle) = 0 \end{aligned} \quad (7.8.11)$$

The second order correction for a general unperturbed state $|\phi^{(0)}\rangle$ is given by the formula

$$E^{(2)} = \sum_{m^{(0)} \neq \phi^{(0)}} \frac{|\langle m^{(0)} | V | \phi^{(0)} \rangle|^2}{E_\phi^{(0)} - E_m^{(0)}} \quad (7.8.12)$$

The index m sums over all unperturbed eigenstates not equal to $|\phi^{(0)}\rangle$, and $E_\phi^{(0)}, E_m^{(0)}$ are the unperturbed energies for the states $|\phi^{(0)}\rangle$ and $|m^{(0)}\rangle$. If we look at the forms of $V|\phi_{1,2}^{(0)}\rangle$ that we calculated above, the only eigenstates $|m^{(0)}\rangle$ that give non-zero numerators are

$$\{ |m^{(0)}\rangle \} = \begin{cases} |0, 2, \uparrow\rangle, |2, 0, \uparrow\rangle & \text{if } |\phi^{(0)}\rangle = |\phi_1^{(0)}\rangle \\ |\downarrow, 2, \uparrow\rangle, |\uparrow, 2, \downarrow\rangle & \text{if } |\phi^{(0)}\rangle = |\phi_2^{(0)}\rangle \end{cases} \quad (7.8.13)$$

which then means that the only non-zero value of the numerator is

$$\left(\pm \frac{t}{\sqrt{2}} \right)^2 = \frac{t^2}{2} \quad (7.8.14)$$

7.8. CALCULATION OF WILSON RATIO FROM EFFECTIVE LOCAL FERMI LIQUID

Also, because all the states in $\{|m^{(0)}\rangle\}$ involve $S_0^z = 0$, those states will have zero energy, so all the denominators will have the value

$$E_{\phi_{1,2}}^{(0)} - E_m^{(0)} = E_{\phi_{1,2}}^{(0)} = -\frac{3J^*}{4} \quad (7.8.15)$$

The upshot of all this is that the second order shift will be same for both the single and doubly-occupied states, so we will ignore that correction as it can be absorbed into the zero-point energy.

The third order correction is given by

$$E^{(3)} = \sum_{i^{(0)}, j^{(0)} \neq \phi} \frac{\langle \phi^{(0)} | V | j^{(0)} \rangle \langle j^{(0)} | V | i^{(0)} \rangle \langle i^{(0)} | V | \phi^{(0)} \rangle}{(E_\phi^{(0)} - E_i^{(0)}) (E_\phi^{(0)} - E_j^{(0)})} - E_\phi^{(1)} \sum_{m^{(0)} \neq \phi} \frac{|\langle m^{(0)} | V | \phi^{(0)} \rangle|^2}{(E_\phi^{(0)} - E_m^{(0)})^2} \quad (7.8.16)$$

This correction can also be argued to be zero, as follows. The second term is of course trivially zero because $E_\phi^{(1)}$ itself is 0. For the first term, note that $|i^{(0)}\rangle$ must have $\hat{n}_0 = 0, 2$ in order to give non-zero inner product with $V|\phi^{(0)}\rangle$. If we continue this, $V|i^{(0)}\rangle$ will have $\hat{n}_0 = 1$, so $|j^{(0)}\rangle$ must also have the same. Then, $V|j^{(0)}\rangle$ will have $\hat{n}_0 = 0, 2$ and hence the inner product $\langle \phi^{(0)} | V | j^{(0)} \rangle$ will be 0. The third order corrections for both the single and doubly occupied states are thus 0.

We move on to the fourth order correction. The general formula is quite formidable, so we only write down the terms that aren't outright zero for this problem:

$$E^{(4)} = \sum_{i^{(0)}, j^{(0)}, k^{(0)} \neq \phi} \frac{\langle \phi^{(0)} | V | k^{(0)} \rangle \langle k^{(0)} | V | j^{(0)} \rangle \langle j^{(0)} | V | i^{(0)} \rangle \langle i^{(0)} | V | \phi^{(0)} \rangle}{(E_\phi^{(0)} - E_k^{(0)}) (E_\phi^{(0)} - E_j^{(0)}) (E_\phi^{(0)} - E_i^{(0)})} - E_\phi^{(2)} \sum_{m^{(0)} \neq \phi} \frac{|\langle m^{(0)} | V | \phi^{(0)} \rangle|^2}{(E_\phi^{(0)} - E_m^{(0)})^2} \quad (7.8.17)$$

For the singly-occupied state, the calculation pans out as follows:

$$\begin{aligned} \{|i^{(0)}\rangle\} &= \begin{cases} |0, 2, \uparrow\rangle \implies \{|j^{(0)}\rangle\} = \begin{cases} |\uparrow\rangle \otimes |S = 1, S^z = 0\rangle \implies \{|k^{(0)}\rangle\} = \begin{cases} |0, 2, \uparrow\rangle \\ |2, 0, \uparrow\rangle \end{cases} \\ |\downarrow\rangle \otimes |\uparrow, \uparrow\rangle \implies \{|k^{(0)}\rangle\} = |0, 2, \uparrow\rangle \end{cases} \\ |2, 0, \uparrow\rangle \implies \{|j^{(0)}\rangle\} &= \begin{cases} |\uparrow\rangle \otimes |S = 1, S^z = 0\rangle \implies \{|k^{(0)}\rangle\} = \begin{cases} |0, 2, \uparrow\rangle \\ |2, 0, \uparrow\rangle \end{cases} \\ |\downarrow\rangle \otimes |\uparrow, \uparrow\rangle \implies \{|k^{(0)}\rangle\} = |0, 2, \uparrow\rangle \end{cases} \end{cases} \end{aligned} \quad (7.8.18)$$

The inner products in the numerators can be calculated from these states. The energies of the intermediate states are

$$E_i^{(0)} = 0, \quad E_j^{(0)} = \frac{J^*}{4}, \quad E_k^{(0)} = 0 \quad (7.8.19)$$

which allow calculating the denominators. The total fourth order change for the singly-occupied state is

$$E_1^{(4)} = -\frac{16t^4}{3J^{*3}} \quad (7.8.20)$$

Carrying out a similar calculation for the doubly-occupied state gives

$$E_2^{(4)} = -\frac{16t^4}{9J^{*3}} \quad (7.8.21)$$

The last two equations together mean that the effect of the perturbation is to raise the energy of the doubly-occupied state by an amount

$$u \sim \frac{t^4}{J^{*3}} \quad (7.8.22)$$

and we can replace the perturbative term V by an effective repulsive term on the first site (a.k.a, the "local Fermi liquid", [8]):

$$u\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} \quad (7.8.23)$$

The total system now consists of two decoupled parts - the singlet composed of the impurity and the zeroth site, and the remaining lattice composed of N-1 sites with a tight-binding dispersion and a local interaction at the 1-th site. The effective Hamiltonian for the remaining lattice is

$$\sum_{i=1}^{\infty} t \left(c_{i\sigma}^\dagger c_{i+1\sigma} + c_{i+1\sigma}^\dagger c_{i\sigma} \right) + u\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} \quad (7.8.24)$$

We will now invoke the mean-field approximation in simplifying this term. We will be dealing with thermodynamic

Figure 7.10: *Left:* The nearest-neighbor hopping described by the effective Hamiltonian. The red circle at the center is the impurity at the origin. The black cloud at the center demarcates the collection of electrons at the origin of the lattice (which couple to the impurity). The green circles represent lattice sites that are nearest to the origin. The blue circles represent next-nearest sites. *Right:* After treating the hopping between origin and its nearest neighbors as perturbation, we get a system consisting of two decoupled parts: one part is the impurity+cloud singlet, the other part is the rest of the lattice sites. The effect of the hopping between the origin and the green sites is a repulsion term on the green sites.

quantities soon, so the operators will be replaced by their thermodynamic values, that is, the values that minimize the free energy functional.

$$\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} \rightarrow \langle \hat{n}_{1\uparrow}\hat{n}_{1\downarrow} \rangle = \langle \delta n_{1\uparrow} \delta n_{1\downarrow} \rangle + \langle n_{1\uparrow} \rangle \langle n_{1\downarrow} \rangle \quad (7.8.25)$$

where $\delta n_{1\sigma} \equiv n_{1\sigma} - \langle n_{1\sigma} \rangle$ is the fluctuation of the particle number above the ground state. The mean-field approximation then involves dropping the first term which is a quadratic fluctuation - since we are interested in values of quantities at $T \rightarrow 0$, this quadratic fluctuation is very small. The interaction we are left with is

$$u\langle n_{1\uparrow} \rangle \langle n_{1\downarrow} \rangle = \sum_{kq\sigma} f_{kq} \langle n_{k\sigma} \rangle \langle n_{q\bar{\sigma}} \rangle \quad (7.8.26)$$

This interaction converts the problem to that of a Landau Fermi liquid, with the quasiparticle energy functional being given by

$$\epsilon_{k\sigma} = \epsilon_k + \sum_q f_{kq} \langle \hat{n}_{q\bar{\sigma}} \rangle \quad (7.8.27)$$

From the form of the quasiparticle energy functional, we can see that there is no spin-parallel term, so we can write

$$f_{kk'\sigma\sigma} = 0, f_{kk'\sigma\bar{\sigma}} = f_{kk'} \quad (7.8.28)$$

We will now use this Fermi liquid form to extract the Wilson ratio. We will make use of the following definitions/results:

$$\begin{aligned} dn_{k\sigma} &= \frac{\partial n}{\partial \epsilon_{k\sigma}} (d\epsilon_{k\sigma} - d\mu) && [\text{follows from differentiating FD distribution}] \\ C_v &= \frac{d\epsilon}{dT} \\ \chi^{s,c} &= \frac{d}{d(B, \mu)} (n_\uparrow \mp n_\downarrow) \\ 2f_0^{s,a} &= \sum_k (f_{kk'\uparrow\uparrow} \pm f_{kk'\uparrow\downarrow}) \\ F_0^{s,a} &= \rho(0) f_0^{s,a} \end{aligned} \quad (7.8.29)$$

7.8.1 Low- T Specific heat

$$\begin{aligned}
 C &= \frac{d}{dT} \sum_{k\sigma} \epsilon_{k\sigma} n_{k\sigma} \\
 &\approx \sum_{k\sigma} \epsilon_{k\sigma}^0 \frac{dn_{k\sigma}}{dT} \quad [\text{no quasiparticles at ground state}] \\
 &\approx \sum_{k\sigma} \epsilon_{k\sigma}^0 \frac{dn_{k\sigma}}{dT} \quad [\text{same expression as Fermi gas but with modified distribution function}] \\
 &= \rho(0)T
 \end{aligned} \tag{7.8.30}$$

where ρ is the total quasiparticle DOS with contributions from conduction bath and impurity.

$$\rho \sim \text{Im Trace}[G] = \text{Im} \sum_{d\sigma} G_{dd}^\sigma + \text{Im} \sum_{k\sigma} G_{kk}^\sigma = \rho_0 + \rho_{\text{imp}} \tag{7.8.31}$$

which gives

$$C_{\text{imp}} \equiv C - C_0 = \rho_{\text{imp}}(0)T \tag{7.8.32}$$

7.8.2 Low- T Charge Susceptibility

$$\chi^c = \frac{dN}{d\mu} \tag{7.8.33}$$

Due to change in chemical potential, $\delta\epsilon_{k\sigma}$ is isotropic and SU(2)-symmetric. Hence

$$\begin{aligned}
 d\epsilon_{k\sigma} &= \sum_{k'\sigma'} f_{kk'\sigma\sigma'} dn_{k'\sigma'} \\
 &= dn \sum_{k'} (f_{kk'\uparrow\uparrow} + f_{kk'\uparrow\downarrow}) \quad [dn = dn_{k'\uparrow} = dn_{k'\downarrow}] \\
 &= 2dnf_0^s
 \end{aligned} \tag{7.8.34}$$

Therefore,

$$\begin{aligned}
 dN &= \sum_{k\sigma} dn_{k\sigma} \\
 &= \sum_{k\sigma} \frac{\partial n}{\partial \epsilon_{k\sigma}} (d\epsilon_{k\sigma} - d\mu) \\
 &= \sum_{k\sigma} -\frac{1}{2}\rho (2dnf_0^s - d\mu) \\
 &= -\rho(0)dNf_0^s + d\mu\rho(0) \\
 &\approx d\mu\rho(0) - \rho(0)f_0^s d\mu\rho(0) \quad [\text{substitute } dN \text{ back into itself}] \\
 \xrightarrow{86} \frac{dN}{d\mu} &= \rho(0) (1 - \rho(0)f_0^s) \\
 \xrightarrow{86} \chi_{\text{imp}}^c &= \rho(0)_{\text{imp}} - \rho(0)f_0^s
 \end{aligned} \tag{7.8.35}$$

At an intermediate state, we substituted dN back into itself and kept only the leading order term. This is justified because $f_{kk'}$ goes as $\frac{1}{NJ}$. At the fixed point and for a thermodynamically large system, both J and N are very large, so keeping only the leading order suffices.

From a previous calculation, we know that the charge susceptibility at $T = 0$ is zero, so we can write down the following relation:

$$f_0^s = \frac{\rho(0)_{\text{imp}}}{\rho(0)} \tag{7.8.36}$$

7.8.3 Low- T Spin Susceptibility

$$\chi^s = \frac{dm}{d\mu} \quad (7.8.37)$$

Due to change in magnetic field, change in $\epsilon_{k\sigma}$ should be isotropic and SU(2)-antisymmetric. Hence

$$\begin{aligned} d\epsilon_{k\sigma} &= -\frac{1}{2}dB\sigma + \sum_{k'\sigma'} f_{kk'\sigma\sigma'} dn_{k'\sigma'} \\ &= -\frac{1}{2}dB\sigma + dn_\sigma \sum_{k'} (f_{kk'\uparrow\uparrow} - f_{kk'\uparrow\downarrow}) \quad [dn_{k'\uparrow} = -dn_{k'\downarrow}] \\ &= -\frac{1}{2}dB\sigma + 2dn_\sigma f_0^a \end{aligned} \quad (7.8.38)$$

Since the total number remains constant, $\mu = 0$. Therefore,

$$\begin{aligned} dm &= \sum_k (dn_{k\uparrow} - dn_{k\downarrow}) \\ &= -\frac{1}{2} \sum_k \rho (d\epsilon_{k\uparrow} - d\epsilon_{k\downarrow}) \\ &= -\frac{1}{2} \sum_k \rho (-dB + 2f_0^a (dn_{k\uparrow} - dn_{k\downarrow})) \\ &= dB\rho(0) - dm\rho(0)f_0^a \\ &\approx dB\rho(0) - \rho(0)f_0^a B\rho(0) \quad [\text{substitute } dm \text{ back into itself}] \\ \implies \frac{dm}{dB} &= \rho(0) (1 - \rho(0)f_0^a) \\ \implies \chi_{imp}^s &= \rho(0)_{imp} - \rho(0)f_0^a \end{aligned} \quad (7.8.39)$$

7.8.4 Wilson ratio

The Wilson ratio for the impurity is defined as

$$R = \frac{\chi_{imp}^s}{\frac{C_{imp}}{T}} \quad (7.8.40)$$

From eq. 7.8.28, we have $f_0^s = -f_0^a$, which, when combined with eq. 7.8.36, gives

$$\chi_{imp}^s = 2\rho(0)_{imp} \quad (7.8.41)$$

The Wilson ratio becomes

$$R = \frac{2\rho(0)_{imp}}{\rho(0)_{imp}} = 2 \quad (7.8.42)$$

7.9 Luttinger's and Friedel's sum rules

The subsequent discussions are for the first quadrant where $U^* = 0$ and $J^* > K^*$. At high temperatures, we see that the impurity susceptibility attains the value of

$$\frac{1}{8k_B T} \quad (7.9.1)$$

which implies that the impurity behaves as a free orbital in this limit, having no coupling with the bath. We can write down the following effective Hamiltonian for such a limit:

$$\mathcal{H}_{\text{high-T}} = \tilde{\epsilon}_d \hat{n}_d + \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} \quad (7.9.2)$$

Since the impurity is decoupled from the bath, we can immediately write down the Hamiltonian just for the impurity:

$$\mathcal{H}_{\text{high-T, imp}} = \tilde{\epsilon}_d \hat{n}_d \quad (7.9.3)$$

We consider the resonant-level model:

$$\mathcal{H}_{\text{res}} = \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \epsilon_d n_d + \sum_{k\sigma} (V_k c_{k\sigma}^\dagger c_{d\sigma} + \text{h.c.}) \quad (7.9.4)$$

The total Green's function is

$$G(z) = \frac{1}{z - \mathcal{H}_{\text{res}}} \quad (7.9.5)$$

The impurity diagonal Green's function is

$$G_{dd}(z) = \frac{1}{z - \epsilon_d - \Sigma_d(z)}, \quad G_d(z) = G_{dd} |d\rangle \langle d| \quad (7.9.6)$$

where $\Sigma_d(z)$ is in general complex and is zero at the free orbital fixed point. The conduction electron Green's function is

$$G_{kk}(z) = G_k^0(z) + [G_k^0(z) V_k]^2 G_{dd}(z), \quad G_c(z) \equiv \sum_k |k\rangle \langle k| G_{kk}(z), \quad G_{c0}(z) \equiv \sum_k G_{kk}^0(z) |k\rangle \langle k| \quad (7.9.7)$$

The total Green's function can be written as

$$\begin{aligned} G(z) &= \left(\sum_k |k\rangle \langle k| + |d\rangle \langle d| \right) G \left(\sum_k |k\rangle \langle k| + |d\rangle \langle d| \right) \\ &= \sum_k |k\rangle \langle k| G_{kk}(z) + G_{dd}(z) |d\rangle \langle d| + \text{off-diagonal terms} \\ &= G_c(z) + G_d(z) + \text{off-diagonal terms} \end{aligned} \quad (7.9.8)$$

The total number of electrons is given by

$$\begin{aligned} N &= \oint \frac{dz}{2\pi i} n_F(z) \text{Tr} [G(z)] \\ &= \oint \frac{dz}{2\pi i} n_F(z) \text{Tr} [G_d(z) + G_c(z)] \end{aligned} \quad (7.9.9)$$

The contour Γ counts all the singularities of $\text{Tr}G(z)$, and thus encloses only the real axis of the complex plane (since $G(z)$ comes from a Hermitian matrix \mathcal{H}_{res} , all its singularities are real). At this point, we can use an identity:

$$\begin{aligned} \text{Tr} [G_d(z)] &= \text{Tr} \left[\frac{|d\rangle \langle d|}{z - \epsilon_d - \Sigma_d(z)} \right] \\ &= \text{Tr} \left[\frac{|d\rangle \langle d|}{z - \epsilon_d - \Sigma_d(z)} \frac{\partial(z - \epsilon_d)}{\partial z} \right] \\ &= \text{Tr} \left[|d\rangle \langle d| G_{dd} \frac{\partial \{G_{dd}^{-1}(z) + \Sigma_d(z)\}}{\partial z} \right] \\ &= \text{Tr} \left[G_d(z) \frac{\partial G_d^{-1}(z)}{\partial z} \right] + \text{Tr} \left[G_d(z) \frac{\partial \Sigma_d(z)}{\partial z} \right] \\ &\equiv \frac{\partial}{\partial z} \left[\ln \text{Det} G_d^{-1}(z) \right] + \text{Tr} \left[G_d(z) \frac{\partial \Sigma_d(z)}{\partial z} \right] \end{aligned} \quad (7.9.10)$$

In the last step, we converted the trace to a determinant using

$$\text{Tr} \left[A \frac{\partial A^{-1}}{\partial z} \right] = \frac{\partial}{\partial z} \text{Tr} \ln A^{-1} = \frac{\partial}{\partial z} \sum_i \ln \lambda_i = \frac{\partial}{\partial z} \ln \prod_i \lambda_i = \frac{\partial}{\partial z} \ln \text{Det} A^{-1} \quad (7.9.11)$$

where λ_i are the eigenvalues of A^{-1} . Substituting $\text{Tr} [G_d(z)]$ into the total number of particles gives

$$N = \oint \frac{dz}{2\pi i} n_F(z) \left[\frac{\partial}{\partial z} \ln \text{Det} \left\{ G_d^{-1}(z) \right\} + \text{Tr} \left(G_d(z) \frac{\partial}{\partial z} \Sigma_d(z) \right) + \text{Tr} G_c(z) \right] \quad (7.9.12)$$

The conduction electron part can also be simplified:

$$\begin{aligned} \text{Tr} G_c(z) &= \text{Tr} \left[G_{c0}(z) + \sum_k \left\{ G_k^0(z) V_k \right\}^2 G_{dd}(z) |k\rangle \langle k| \right] \\ &= \text{Tr} [G_{c0}(z)] + \sum_k \left[G_k^0(z) V_k \right]^2 G_{dd}(z) \end{aligned} \quad (7.9.13)$$

Since $G_{c0}^{-1}(z) = z - \sum_k \epsilon_k \hat{n}_k$, we can write $\text{Tr} [G_{c0}(z)] = \text{Tr} \left[G_{c0}(z) \frac{\partial}{\partial z} G_{c0}^{-1} \right]$ and hence

$$\text{Tr} G_c(z) = \frac{\partial}{\partial z} \left[\ln \text{Det} G_{c0}^{-1}(z) \right] + \sum_k \left[G_k^0(z) V_k \right]^2 G_{dd}(z) \quad (7.9.14)$$

Updating the total particles with this leads to

$$\begin{aligned} N &= \oint \frac{dz}{2\pi i} n_F(z) \left[\frac{\partial}{\partial z} \ln \text{Det} \left\{ G_d^{-1}(z) \right\} + \frac{\partial}{\partial z} \ln \text{Det} \left\{ G_{c0}^{-1}(z) \right\} + \text{Tr} \left(G_d(z) \frac{\partial}{\partial z} \Sigma_d(z) \right) \right. \\ &\quad \left. + \sum_k \left(V_k G_k^0 \right)^2 G_{dd}(z) \right] \end{aligned} \quad (7.9.15)$$

For the resonant-level model, we have

$$\Sigma_d = \sum_k V_k^2 G_k^0 = \sum_k \frac{V_k^2}{z - \epsilon_k} \quad (7.9.16)$$

such that

$$\text{Tr} \left(G_d(z) \frac{\partial}{\partial z} \Sigma_d(z) \right) = -G_{dd}(z) \sum_k \left(V_k G_k^0 \right)^2 \quad (7.9.17)$$

which allows us to write

$$N = \oint \frac{dz}{2\pi i} n_F(z) \left[\frac{\partial}{\partial z} \ln \text{Det} \left\{ G_d^{-1}(z) \right\} + \frac{\partial}{\partial z} \ln \text{Det} \left\{ G_{c0}^{-1}(z) \right\} \right] \quad (7.9.18)$$

At $T = 0$, n_F is defined as 1 below the FS, $\frac{1}{2}$ at the FS and 0 above it.

$$N = \left[\oint_{\Gamma_<} + \frac{1}{2} \oint_{\Gamma_0} \right] \frac{dz}{2\pi i} \left[\frac{\partial}{\partial z} \ln \text{Det} \left\{ G_d^{-1}(z) \right\} + \frac{\partial}{\partial z} \ln \text{Det} \left\{ G_{c0}^{-1}(z) \right\} \right] \quad (7.9.19)$$

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Following Seki and Yunoki, we can define a winding number for a Green's function $G(z)$:

$$n_{\text{Det} G^{-1}}(C) = \oint_C \frac{dz}{2\pi i} \frac{\partial \ln \text{Det} G^{-1}(z)}{\partial z} = \oint_{\text{Det} G^{-1}(C)} \frac{d \text{Det} G^{-1}}{\text{Det} G^{-1}} \quad (7.9.20)$$

Since $n_{\text{Det } G^{-1}(C)}$ counts the number of times the curve $\text{Det } G^{-1}(C)$ winds around the origin, it is integer-valued and topological. Seki and Yunoki also show that this number is given by

$$n_{\text{Det } G^{-1}(C)} = P_{\text{Det } G}(C) - Z_{\text{Det } G}(C) \quad (7.9.21)$$

where $P_{f(z)}(C)$ is the number of poles of $f(z)$ enclosed by the contour C , and Z is the corresponding number of zeros. The total number of particles in the resonant level model can thus be written as

$$\begin{aligned} N &= P_{\text{Det } G_d}(\Gamma_<) - Z_{\text{Det } G_d}(\Gamma_<) + \frac{1}{2} [P_{\text{Det } G_d}(\Gamma_0) - Z_{\text{Det } G_d}(\Gamma_0)] \\ &\quad + P_{\text{Det } G_{c0}}(\Gamma_<) - Z_{\text{Det } G_{c0}}(\Gamma_<) + \frac{1}{2} [P_{\text{Det } G_{c0}}(\Gamma_0) - Z_{\text{Det } G_{c0}}(\Gamma_0)] \end{aligned} \quad (7.9.22)$$

The average number of particles can thus be expressed purely in terms of the number of poles and zeros of the impurity and the conduction electron Green's functions. As shown by Seki and Yunoki, the second line gives the Luttinger volume V_L :

$$N = P_{\text{Det } G_d}(\Gamma_<) - Z_{\text{Det } G_d}(\Gamma_<) + \frac{1}{2} [P_{\text{Det } G_d}(\Gamma_0) - Z_{\text{Det } G_d}(\Gamma_0)] + V_L \quad (7.9.23)$$

If we start from a non-interacting model ($V_k = 0$), we can write

$$N = \mathcal{N}_{imp}^0 + V_L^0 \quad (7.9.24)$$

where \mathcal{N}_{imp}^0 is simply the number of singularities of G_d on the real axis, for the non-interacting case. We now turn up the interaction V_k , keeping the total number of particles conserved at N . With a non-zero V_k , the impurity self-energy can be written (assuming a constant density of states) as

$$\Sigma_d(z) = \Sigma_d^{\text{real}}(z) - i\Delta \quad (7.9.25)$$

so that the impurity Greens function becomes

$$G_d(z) = \frac{1}{z - \epsilon_d - \Sigma_d^{\text{real}}(z) + i\Delta} \quad (7.9.26)$$

We can see that the presence of an imaginary part lifts the pole of $G_d(z)$ off the real axis, and since the contour Γ_0 encloses only the real axis, this will count as a loss in the number of poles of $G_d(z)$. Also, if we specialize to the case where the renormalized impurity site energy $\epsilon_d^* = \epsilon_d + \Sigma_d^{\text{real}} = 0$, this loss will happen at the Fermi surface, and will hence be multiplied by a factor of half. We can therefore write

$$\begin{aligned} N &= \mathcal{N}_{imp} + V_L = \mathcal{N}_{imp}^0 - \frac{1}{2} + V_L \\ \implies V_L &= V_L^0 + \frac{1}{2} \end{aligned} \quad (7.9.27)$$

If we take into account the spin-degeneracy and redefine V_L to mean the Luttinger volume for both momentum and spin degrees of freedom, we get

$$V_L = V_L^0 + 1 \quad (7.9.28)$$

This is a specific case of the more general result for Kondo lattices obtained by Oshikawa using flux-insertion arguments in [40]. One can now ask what happens to this result once we also incorporate the spin-exchange interaction $J\vec{S}_d \cdot \vec{s}$; we can expect that it will complicate the self-energy of the impurity. It cannot, however, preclude the loss of the real pole, nor can it create a new singularity - to do so would require the self-energy to diverge, and we are working with finite systems here. This suggests that the eq. 7.9.28 would still hold.

We have also not accounted for the RG flow from the local moment fixed point to the strong-coupling fixed point. The local moment fixed point is characterized by a decoupled quantum top:

$$\mathcal{H}_{LM} = \epsilon_d \hat{n}_d + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \quad (7.9.29)$$

⁷⁸ It can be shown that the single-particle Green's function for this effective Hamiltonian is similar to the one at the free-orbital fixed point. We will use the equation of motion technique to solve for the Green's function. The time-domain retarded Green's function is defined as

$$G_{d\sigma}(t, t') = -i\theta(t - t') \left\langle \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger(t') \right\} \right\rangle \quad (7.9.30)$$

Since the Hamiltonian is time-translation invariant, we can drop one of the instants:

$$G_{d\sigma}(t, 0) = -i\theta(t) \left\langle \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle \quad (7.9.31)$$

The time derivative is

$$\begin{aligned} \partial_t G_{d\sigma} &= -i \left[\partial_t \theta(t) \left\langle \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle + \theta(t) \partial_t \left\langle \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle \right] \\ &= -i \left[\delta(t) \left\langle \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle + \theta(t) \left\langle \left\{ \partial_t c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle \right] \\ &= -i\delta(t) - i\theta(t) \left\langle \left\{ \partial_t c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle \end{aligned} \quad (7.9.32)$$

From the Heisenberg equations of motion, we get

$$i\partial_t c_{d\sigma}(t) = [c_{d\sigma}(t), \mathcal{H}_{LM}(t)] = [\epsilon_d + U \hat{n}_{d\bar{\sigma}}(t)] c_{d\sigma}(t) \quad (7.9.33)$$

Substituting this into the time-derivative gives

$$\begin{aligned} \partial_t G_{d\sigma} &= -i\delta(t) - i\theta(t) \left\langle \left\{ -i[\epsilon_d + U \hat{n}_{d\bar{\sigma}}(t)] c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle \\ &= -i\delta(t) - i\epsilon_d G_{d\sigma} - U\theta(t) \left\langle \hat{n}_{d\bar{\sigma}}(t) \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle \end{aligned} \quad (7.9.34)$$

We define another Greens function

$$G' = -i\theta(t) \left\langle \hat{n}_{d\bar{\sigma}}(t) \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle \quad (7.9.35)$$

¹ which satisfies the equation of motion

$$\partial_t G' = -i\delta(t) - i\theta(t) \left\langle \left\{ \partial_t \hat{n}_{d\bar{\sigma}}(t) c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle - i\theta(t) \left\langle \left\{ \hat{n}_{d\bar{\sigma}}(t) \partial_t c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle \quad (7.9.36)$$

The second term vanishes because $[\hat{n}_{d\bar{\sigma}}, \mathcal{H}_{LM}] = 0$ and hence $\partial_t \hat{n}_{d\bar{\sigma}} = 0$. Also,

$$\hat{n}_{d\bar{\sigma}}(t) \partial_t c_{d\sigma}(t) = -i\hat{n}_{d\bar{\sigma}}(t) [\epsilon_d + U \hat{n}_{d\bar{\sigma}}(t)] c_{d\sigma}(t) = -i[\epsilon_d + U] \hat{n}_{d\bar{\sigma}}(t) c_{d\sigma}(t) \quad (7.9.37)$$

Therefore,

$$\partial_t G' = -i\delta(t) \langle \hat{n}_{d\bar{\sigma}}(0) \rangle - [\epsilon_d + U] \theta(t) \left\langle \left\{ \hat{n}_{d\bar{\sigma}}(t) c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle = -i\delta(t) - i(\epsilon_d + U) G' \quad (7.9.38)$$

Changing all quantities to frequency-domain:

$$\begin{aligned} G'(t) &= \int_{-\infty}^{\infty} d\omega e^{-i\omega t} G'(\omega) \\ \partial_t G'(t) &= - \int_{-\infty}^{\infty} d\omega i\omega e^{-i\omega t} G'(\omega) \\ \delta(t) &= \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \end{aligned} \quad (7.9.39)$$

Substituting these forms in the equation and comparing the coefficients of $e^{i\omega t}$ gives

$$\omega G'(\omega) = \langle \hat{n}_{d\bar{\sigma}}(0) \rangle + (\epsilon_d + U) G'(\omega) \implies G'(\omega) = \frac{\langle \hat{n}_{d\bar{\sigma}}(0) \rangle}{\omega - \epsilon_d - U} \quad (7.9.40)$$

The equation of motion $G_{d\sigma}$ can now be solved

$$\begin{aligned} \partial_t G_{d\sigma}(t) &= -i\delta(t) - i\epsilon_d G_{d\sigma}(t) - iUG'_{d\sigma}(t) \\ \implies \omega G_{d\sigma}(\omega) &= 1 + \epsilon_d G_{d\sigma}(\omega) + U \frac{\langle \hat{n}_{d\bar{\sigma}}(0) \rangle}{\omega - \epsilon_d - U} \\ \implies G_{d\sigma}(\omega) &= \frac{1}{\omega - \epsilon_d} + \frac{U \langle \hat{n}_{d\bar{\sigma}}(0) \rangle}{(\omega - \epsilon_d)(\omega - \epsilon_d - U)} \end{aligned} \quad (7.9.41)$$

For a particle-hole symmetric system, we can substitute $\epsilon_d = -|\epsilon_d|$ and $\epsilon_d + U = |\epsilon_d|$.

$$G_{d\sigma}(\omega) = \frac{1}{\omega + |\epsilon_d|} + \frac{U \langle \hat{n}_{d\bar{\sigma}}(0) \rangle}{(\omega + |\epsilon_d|)(\omega - |\epsilon_d|)} \quad (7.9.42)$$

which reveals two poles at $\pm|\epsilon_d|$, one above and one below the Fermi surface. Since the RHS of eq. 7.9.23 counts the number of poles on or below the FS, we will still count one pole for $G_{d\sigma}$. Thus, this Green's function is topological similar to the free-orbital one at $T = 0$.

⁴ The scattering phase shift suffered by the conduction electrons at the Fermi surface, off the impurity, can be calculated from the impurity occupancy, using the Friedel sum rule. From the ground state wavefunction, we can calculate the average number of particles on the impurity:

$$\langle n_d \rangle = \langle GS | \sum_{\sigma} \hat{n}_{d\sigma} | GS \rangle \quad (7.9.43)$$

$|GS\rangle$ is the lower energy state in eq. 6.4.34. Performing the inner product gives

$$\langle n_d \rangle = \left(c_s^- \right)^2 + \left(c_c^- \right)^2 = 1 \quad (7.9.44)$$

The phase shift is thus

$$\frac{1}{\pi} \sum_{\sigma} \delta_{\sigma}(0) = \langle n_d \rangle \implies \delta_{\sigma}(0) = \frac{\pi}{2} \quad (7.9.45)$$

There we used $\delta_{\uparrow} = \delta_{\downarrow}$ because the model is SU(2)-symmetric. This line of arguments was first presented for the Kondo model in [24].

The change in Luttinger's number also allows us to calculate the Wilson ratio of the system, from eq. 2.7.7.

$$R = 1 + \sin^2 \left(\frac{\pi}{2} \Delta N_L \right) = 1 + \sin^2 \frac{\pi}{2} = 2 \quad (7.9.46)$$

7.10 Reverse RG analysis

The goal here is to chart the journey starting from the IR fixed point towards the UV regime, by following one particular wavefunction. We will start with a very simple IR ground state wavefunction, and then go back towards the UV ground state by applying the inverse unitary operator U^\dagger :

$$\begin{aligned} U : \underbrace{|1, 2, \dots, N\rangle}_{\text{UV ground state}} &\rightarrow |1, 2, \dots, N-1\rangle |N\rangle \rightarrow \dots \rightarrow \underbrace{|1, 2, \dots, N^*\rangle |N^*+1\rangle \dots |N\rangle}_{\text{IR ground state}} \\ U^\dagger : \underbrace{|1, 2, \dots, N^*\rangle |N^*+1\rangle \dots |N\rangle}_{\text{IR ground state}} &\rightarrow |1, 2, \dots, N^*+1\rangle |N^*+2\rangle \dots |N\rangle \rightarrow \dots \rightarrow \underbrace{|1, 2, \dots, N\rangle}_{\text{UV ground state}} \end{aligned}$$

Figure 7.11: Algorithm of reverse RG. We start with a Hamiltonian with an impurity site (red) coupled with two conduction electrons (dark green), with four other decoupled electrons (bright green). The dotted rectangle represents the emergent window $(-\Lambda_j, \Lambda_j)$ at each step; the electrons inside that rectangle are still entangled with the impurity, while the ones inside have been decoupled. The next step of reverse RG involves applying the inverse transformation on the Hamiltonian, which will couple two more electrons from the IOMS (hence four dark green circles in the second step), leading to an enlargement of the emergent window. The unitary varies for each step, hence the notation U_j .

Figure 7.12: Increase in the number of coupled elements under reverse RG. We start with the impurity coupled with two electrons, which increases at each step of the reverse RG. The weight of the bonds changes at each step, and is described by the running couplings V_j, J_j, K_j . The onsite energy of the impurity itself also varies at each step, which is essentially the renormalization in ϵ_d and U .

The first process is the forward RG which we used to obtain the scaling equations. The second process is the reverse RG which we will undertake now. *The IR ground state we will start with will consist of four momenta states, $k_{-2,-1,1,2}$. $k_{1,2}$ will be the states above the Fermi surface while $k_{-1,-2}$ will be the ones below it.* The algorithm of reverse RG is shown in fig. 7.11.

For the purpose of illustrating how we will construct the many-body ground state however, we will work with just two momenta states instead of four, one above and one below.

$$|\text{cloud}\rangle = c_-^s (|\uparrow^d, \downarrow\rangle - |\downarrow^d, \uparrow\rangle) + c_-^c (|\uparrow_c^d, \downarrow_c\rangle + |\downarrow_c^d, \uparrow_c\rangle) \quad (7.10.1)$$

where \uparrow_c represents a state with $C^z = \frac{1}{2}$ and the d in the superscript indicates it is for the impurity. Cloud refers to the system of the still-entangled electrons and the impurity. To construct the states $|\uparrow\rangle, |\downarrow\rangle, |\uparrow_c\rangle$ and $|\downarrow_c\rangle$, we will look at the two-site spin and charge operators. The impurity states are easy to construct. \uparrow and \downarrow consist of singly occupied impurities with the respective spins, while the charge versions involve double-occupied and vacant impurities respectively.

For the conduction electrons, we have

$$S_2^z = \frac{1}{2N^*} \sum_{kk'} \left(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow} \right) \quad (7.10.2)$$

The eigenstate for this operator, with an eigenvalue of $+\frac{1}{2}$, is

$$|\uparrow\rangle \equiv \frac{1}{N^*} \sum_{k \in [-\Lambda^*, \Lambda^*]} |k\uparrow\rangle = \frac{1}{N^*} \sum_{k \in [-\Lambda^*, \Lambda^*]} |\hat{n}_{k\uparrow} = 1, \hat{n}_{q\sigma \neq k\uparrow} = 0\rangle \quad (7.10.3)$$

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The state $|k\uparrow\rangle$ is formally $c_{k\uparrow}^\dagger |0\rangle$, $|0\rangle$ being the state with no particles. In other words, the state $|\uparrow\rangle$ is simply the equal superposition of all states with a single up electron.

To show that this is indeed the eigenstate of S_2^z , we compute the action of S_2^z on this state:

$$S_2^z |\uparrow\rangle = \frac{1}{2N^{*2}} \sum_{kk'q} \left(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow} \right) |q\uparrow\rangle \quad (7.10.4)$$

We have dropped the regime of the summation because it is understood that all momenta are summed inside the

fixed point window. We can drop the second part $c_{k\downarrow}^\dagger c_{k'\downarrow}$ because there is no down spin electron to annihilate.

$$\begin{aligned}
 S_2^z |\uparrow\rangle &= \frac{1}{2N^{*2}} \sum_{kk'q} c_{k\uparrow}^\dagger c_{k'\uparrow} |q\uparrow\rangle \\
 &= \frac{1}{2N^{*2}} \sum_{kk'q} c_{k\uparrow}^\dagger c_{k'\uparrow} \delta_{k'q} |q\uparrow\rangle \\
 &\stackrel{3}{=} \frac{1}{2N^{*2}} \sum_{kk'} c_{k\uparrow}^\dagger |0\rangle \\
 &= \frac{1}{2N^*} \sum_k c_{k\uparrow}^\dagger |0\rangle \quad \left[\sum_{k'} = N^* \right] \\
 &= \frac{1}{2} |\uparrow\rangle
 \end{aligned} \tag{7.10.5}$$

We can find the other eigenstate by applying on this state with S_2^- :

$$\begin{aligned}
 S_2^- |\uparrow\rangle &= \frac{1}{N^{*2}} \sum_{kk'q} c_{k\downarrow}^\dagger c_{k'\uparrow} |q\uparrow\rangle \\
 &\equiv \frac{1}{N^*} \sum_k c_{k\downarrow}^\dagger |0\rangle \\
 &= \frac{1}{N^*} \sum_k |k\downarrow\rangle
 \end{aligned} \tag{7.10.6}$$

Thus, the eigenstate for $S_2^z = -\frac{1}{2}$ is

$$|\downarrow\rangle = \frac{1}{N^*} \sum_k |k\downarrow\rangle \tag{7.10.7}$$

Now we turn to the eigenstates of C_2^z . That operator is defined as

$$C_2^z = \frac{1}{2N^*} \sum_{kk'} (c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k'\downarrow}^\dagger c_{k\downarrow}) \tag{7.10.8}$$

The eigenstate for $C_2^z = +\frac{1}{2}$ will be

$$|\uparrow_c\rangle \equiv \frac{1}{N^{*2}} \sum_{kk'} |k\uparrow, k'\downarrow\rangle \tag{7.10.9}$$

which means you consider all pairs of momenta and place an up electron on one of them and a down on the other. The action of C_2^z on this state is

$$\begin{aligned}
 C_2^z |\uparrow_c\rangle &= \frac{1}{2N^{*3}} \sum_{kk'qq'} \left(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k'\downarrow}^\dagger c_{k\downarrow} \right) |q\uparrow, q'\downarrow\rangle \\
 &= \frac{1}{2N^{*3}} \sum_{kk'qq'} \left[c_{k\uparrow}^\dagger c_{k'\uparrow} |q\uparrow, q'\downarrow\rangle - (\delta_{k'k} - c_{k\downarrow}^\dagger c_{k'\downarrow}) |q\uparrow, q'\downarrow\rangle \right] \\
 &= \frac{1}{2N^{*3}} \sum_{kk'qq'} \left[\delta_{k'q} |k\uparrow, q'\downarrow\rangle - \delta_{k'k} |q\uparrow, q'\downarrow\rangle + \delta_{k'q'} |q\uparrow, k\downarrow\rangle \right]
 \end{aligned} \tag{7.10.10}$$

Since all the momenta labels are dummy indices, we exchange the labels k and q' in the third term. The second and third terms then cancel out, and we are left with

$$\begin{aligned}
 C_2^z |\uparrow_c\rangle &= \frac{1}{2N^{*2}} \sum_{kk'qq'} |k\uparrow, q'\downarrow\rangle \\
 &= \frac{1}{2} |\uparrow_c\rangle
 \end{aligned} \tag{7.10.11}$$

The down eigenstate is

$$\begin{aligned} C_2^- |\uparrow_c\rangle &= \frac{1}{N^{*3}} \sum_{kk'qq'} c_{k\downarrow} c_{k'\uparrow} |q\uparrow, q'\downarrow\rangle \\ &= |0\rangle \end{aligned} \quad (7.10.12)$$

which is the state with all states empty. We can thus write down the still-entangled of the ground state wavefunction:

$$|\text{cloud}\rangle = c_-^s \left[|\uparrow^d\rangle \frac{1}{\sqrt{2}} (|k_1\downarrow\rangle + |k_{-1}\downarrow\rangle) - |\downarrow^d\rangle \frac{1}{\sqrt{2}} (|k_1\uparrow\rangle + |k_{-1}\uparrow\rangle) \right] + c_-^c \left[|2^d\rangle |0\rangle \right. \\ \left. + |0^d\rangle \frac{1}{N^*} \sum_{kk'} |k\uparrow, k'\downarrow\rangle \right] \quad (7.10.13)$$

This state will of course be in direct product with the disentangled electronic states (integrals of motions, IOMS) outside the emergent window. If we assume there are two such momenta (hence four momenta+spin) states on either side of the emergent window (which we label as $k_{\pm 2}\sigma, k_{\pm 3}\sigma$), and if we recall that we had used the configuration $\hat{n} = 0$ for the IOMS above the FS and $\hat{n} = 1$ for the ones below, the total state becomes

$$|\text{IR}\rangle \equiv |\Psi_0\rangle = |\hat{n}_{k-2} = \hat{n}_{k-3} = 2\rangle \otimes |\text{cloud}\rangle \otimes |\hat{n}_{k_2} = \hat{n}_{k_3} = 0\rangle \quad (7.10.14)$$

In order to allow a numerical implementation of the reverse RG, we need to write this wavefunction completely as sums of Fock states. We will use the following notation:

$$|\underbrace{n_{k_3\uparrow}n_{k_3\downarrow}n_{k_2\uparrow}n_{k_2\downarrow}}_{\text{unoccupied IOMS}}, \underbrace{n_{k_1\uparrow}n_{k_1\downarrow}}_{\text{cloud above FS}}, \underbrace{n_{d\uparrow}n_{d\downarrow}}_{\text{impurity}}, \underbrace{n_{k_{-1}\uparrow}n_{k_{-1}\downarrow}}_{\text{cloud below FS}}, \underbrace{n_{k_{-2}\uparrow}n_{k_{-2}\downarrow}n_{k_{-3}\uparrow}n_{k_{-3}\downarrow}}_{\text{occupied IOMS}}\rangle \quad (7.10.15)$$

$$|\Psi_0\rangle = \frac{c_-^s}{\sqrt{2}} |0000\rangle \otimes |\uparrow^d\rangle |k_1\downarrow, k_{-1}\downarrow\rangle \otimes |1111\rangle - \frac{c_-^s}{\sqrt{2}} |0000\rangle \otimes |\downarrow^d\rangle |k_1\uparrow, k_{-1}\uparrow\rangle \otimes |1111\rangle \\ \frac{c_-^c}{\sqrt{2}} |0000\rangle \otimes |2^d\rangle |0\rangle \otimes |1111\rangle + \frac{c_-^c}{\sqrt{2}} |0000\rangle \otimes |0^d\rangle |k_1\uparrow, k_1\downarrow, k_{-1}\uparrow, k_{-1}\downarrow\rangle \otimes |1111\rangle \\ = |0000\rangle \otimes \left[\frac{c_-^s}{\sqrt{2}} |01\rangle \underbrace{|10\rangle |01\rangle}_{\text{imp}} - \frac{c_-^s}{\sqrt{2}} |10\rangle \underbrace{|01\rangle |10\rangle}_{\text{imp}} + \frac{c_-^c}{\sqrt{2}} |00\rangle \underbrace{|11\rangle |00\rangle}_{\text{imp}} \right. \\ \left. + \frac{c_-^c}{\sqrt{2}} |11\rangle \underbrace{|00\rangle |11\rangle}_{\text{imp}} \right] \otimes |1111\rangle \quad (7.10.16)$$

The next step is to write down the unitaries that will take us from the IR ground state to the UV ground state. In the forward RG, we used the following unitaries for decoupling an electron $q\beta$:

$$\begin{aligned} U_{0\beta} &= \frac{1}{\sqrt{2}} [1 - \eta_{0\beta}^\dagger + \eta_{0\beta}] \\ U_{1\beta} &= \frac{1}{\sqrt{2}} [1 + \eta_{1\beta}^\dagger - \eta_{1\beta}] \end{aligned} \quad (7.10.17)$$

where the subscripts 0 and 1 indicate it decouples an electron above and below the Fermi surface respectively, and the subscript β indicates the spin of that electron. The total unitary is

$$U = \frac{1}{4} [1 + \eta_{1\uparrow}^\dagger + \eta_{0\uparrow} + \eta_{1\downarrow}^\dagger + \eta_{0\downarrow}] \quad (7.10.18)$$

The inverse transformation for re-entangling $q\beta$ is

$$U^\dagger = \frac{1}{2} [1 + \eta_{1\uparrow} + \eta_{0\uparrow}^\dagger + \eta_{1\downarrow} + \eta_{0\downarrow}^\dagger] \quad (7.10.19)$$

Here, $U_{0\beta}^\dagger$ re-couples an electron $q\beta$ above the Fermi surface. The η -s are

$$\begin{aligned}\eta_{0\beta}^\dagger = V \left[\lambda_2 \hat{n}_{d\bar{\beta}} + \lambda_1 (1 - \hat{n}_{d\bar{\beta}}) \right] c_{q\beta}^\dagger c_{d\beta} + \lambda_3 \sum_k \left\{ \frac{J}{2} \left(S_d^z \beta c_{q\beta}^\dagger c_{k\beta} + c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\bar{\beta}} \right) \right. \\ \left. + \frac{K}{2} \left(C_d^z c_{q\beta}^\dagger c_{k\beta} + c_{q\beta}^\dagger c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} c_{d\beta} \right) \right\}\end{aligned}\quad (7.10.20)$$

$$\begin{aligned}\eta_{1\beta} = V^* \left[\lambda_1 \hat{n}_{d\bar{\beta}} + \lambda_2 (1 - \hat{n}_{d\bar{\beta}}) \right] c_{d\beta}^\dagger c_{q\beta} + \lambda_3 \sum_k \left\{ \frac{J}{2} \left(S_d^z \beta c_{k\beta}^\dagger c_{q\beta} + c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \right) \right. \\ \left. + \frac{K}{2} \left(C_d^z c_{k\beta}^\dagger c_{q\beta} + c_{d\beta}^\dagger c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}} c_{q\beta} \right) \right\}\end{aligned}\quad (7.10.21)$$

with

$$\lambda_1 = \frac{1}{\omega - \frac{1}{2}D + \epsilon_d + \frac{1}{2}K}, \quad \lambda_2 = \frac{1}{\omega - \frac{1}{2}D - \epsilon_d + \frac{1}{2}J}, \quad \lambda_3 = \frac{1}{\omega - \frac{1}{2}D + \frac{1}{4}(J+K)} \quad (7.10.22)$$

The wavefunction after reversing one step of the RG will thus be

$$|\Psi_1\rangle = U_{0\uparrow}^\dagger U_{0\downarrow}^\dagger U_{1\uparrow}^\dagger U_{1\downarrow}^\dagger |\Psi_0\rangle \quad (7.10.23)$$

The results of the reverse RG study [4] are depicted in the following plots. We have used two types of quantities in the process - mutual information and correlation functions. The mutual information between two subsystems **A** and **B** in a wavefunction with many subsystems is defined as

$$I(A : B) = S_A + S_B - S_{AB} \quad (7.10.24)$$

where $S_{ij..q}$ is the von-Neumann entropy of the reduced density matrix obtained after tracing out all degrees of freedom except those in the subscript of S .

The mutual information between two electrons inside the entangled cloud increases as we go towards the IR fixed point. This can be understood in the following manner; as the wavefunction flows towards a smaller sized emergent cloud, the entanglement between those electrons gets distilled out.

We have also computed some correlation functions. All of them increase towards the IR fixed point. The increase in the correlation function $\langle \hat{n}_{k_1\uparrow} \hat{n}_{k_2\downarrow} \rangle$ arises from the crystallization of the spin singlet at the fixed point. The increase in the correlation function $\langle \hat{n}_{k\uparrow} \hat{n}_{k\downarrow} \rangle$ arises from the charge triplet content of the wavefunction, showing the increase of the charge contribution on the momenta. The increase in the off-diagonal correlation function $\langle c_{k\uparrow}^\dagger c_{k'\downarrow} c_{q\downarrow}^\dagger c_{q'\uparrow} \rangle$ shows that there is a large and non-trivial interaction between the electrons of the cloud that is being mediated by the impurity electron. This interaction is not of the Fermi liquid type, but instead was obtained in the effective Hamiltonian for the Kondo cloud.

Figure 7.13: *Left:* Mutual information between two conduction electrons inside the cloud. *Right:* Mutual information between a conduction electron inside the cloud and an impurity electron.

Figure 7.14: Diagonal correlation functions between cloud electrons

Figure 7.15: off-diagonal correlation function

Chapter 8

Conclusions and Future Directions

In this work, we have seen that the fate of the SIAM at low temperatures is a growth in the spin, charge and hybridisation couplings J, K and V . This confirms the NRG and Bethe ansatz result that the low energy behavior is that of a screened impurity. We stress that the spin or the charge exchange coupling, J or K , is necessary to screen the corresponding degree of freedom on the impurity. The ground state wavefunction for the low energy theory is primarily a spin-singlet with some charge-triplet content in the spin-Kondo regime. In the charge-Kondo regime, we find a charge-singlet instead. The susceptibility is seen to increase as we go to lower temperatures, signaling increased spin-flip scattering and providing a justification for the increase in resistivity after the Kondo temperature T_K . At high temperatures the susceptibility saturates to $\frac{1}{8}$, mimicking a four-fold degenerate object because at high temperatures, the impurity energy scales become blurred.

We also obtain a Hamiltonian for the Kondo cloud (the set of electrons which screen the impurity) - it has a Fermi liquid number⁷⁵ diagonal term as well as an off-diagonal non-Fermi liquid piece. It is this off-diagonal piece that is responsible for the strong entanglement between the impurity and the conduction electrons. This contribution is found to increase as we move towards the infrared fixed point. Higher order scattering processes will give more complicated terms in the effective Hamiltonian. We also calculate information-theoretic quantities like mutual information between impurity and conduction electrons. They show that the conduction electrons become more strongly-entangled as we move towards the infrared fixed point. They also reveal an increase in off-diagonal correlations between conduction electrons which is indicative of an increase in the off-diagonal scattering content in the effective Hamiltonian of the Kondo cloud. We also find the value of the zero-temperature Wilson ratio to be 2 in the Kondo regime. Closely related to this is the result that the Luttinger's volume at the fixed point accommodates the impurity site into the Fermi volume such that Luttinger's count increases by 1 compared to the value at the free-orbital or local moment fixed points. The renormalization of the impurity spectral across the RG shows the emergence of the central resonance at the strong-coupling fixed point.

This work still leaves some problems untouched. Some new questions and interesting prospects have also emerged. We discuss them now.

- Can we obtain an analytical expression for the finite temperature Wilson ratio? The zero temperature value was obtained using low temperature approximations, so a finite temperature calculation would need to be non-perturbative. In other words, the full effect of the conduction bath will most probably come into play.
- The spectral function of the impurity is another interesting quantity to explore. It is not yet completely certain which parts of the effective Hamiltonian for the cloud lead to which features of the spectral function. It would be interesting to check whether the Fermi liquid part gives the central peak and the non-Fermi liquid the side humps, or something else altogether. We also intend to explore the bath spectral function and its variation under the RG.
- In Chapter 4, we find that the URG renormalization in Hamiltonian has a form similar to that of URG - a generalized double-bracket form. This suggests that URG might have uses in linear algebra as well. It is well-known that transformations of the double-bracket form are unitary and can be used in minimization and

sorting problems [10]. It has also been shown that the unitary flows correspond to motion along a geodesic if a suitable manifold is defined. This suggests that we can look for a quantity which is minimized by URG in the journey towards the fixed point and see if it can be used to provide a faster and more robust algorithm for optimization problems.

- One can also look into the lattice versions of these models - the Kondo lattice and the Anderson lattice problems which involve two interacting bands - one for the impurity and the other for the conduction electrons [41]. Since there is a macroscopic number of impurity electrons, such a model shows phase transitions. One big project for the future can be to look into such models, map the phase diagram and search for superconducting phases or non-Fermi liquid phases.
- We have seen that the zero-mode of the low-energy effective Hamiltonian is essentially a two-site Anderson model(a.k.a Anderson dimer), which can be solved exactly. An interesting endeavor in this context could be to see if there is a unitary transformation that converts the Anderson dimer to a two-site Hubbard model (Hubbard dimer). The point of this exercise would be to shed some light on the inner workings of DMFT. The imposition of the self-consistency requirement in DMFT introduces a translational invariance into the Anderson model and converts it into the Hubbard model. If we could figure out a transformation that does the same (albeit, between dimers and not the full-fledged models), it might lead to new insights into DMFT). This might allow us to see a metal-insulator phase transition, specially because of the impurity spectral function morphing that we saw from the effective Hamiltonian, shown again in fig. 8.1.

Figure 8.1: Change in the spectral function from single peak to double peak structure under increase of U . A similar change happens under DMFT for the bath spectral function of the Hubbard model.

- It is known from DMFT calculations that the spectral function of the bath changes under a change of U , leading to a metal-insulator transition. An interesting project could be to redo the URG of the SIAM with more complicated baths (by inserting non-trivial self-energies into the bath), and see if the phase-diagram changes. As it stands now, there is no provision for a phase transition in the SIAM because there is only one stable phase. If the inclusion of a non-trivial bath brings about a phase-transition in the impurity phase diagram, that is essentially a mirror of the phase transition happening in the Hubbard model. The importance of this potential discovery is that the self-energies that we wish to insert into the bath have been obtained from a URG treatment of the Hubbard model, and the appearance of the phase transition would then show that URG can be used to do much of the work that DMFT does, and it provides an avenue of improving/remodeling DMFT.

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