

Unitary Renormalization Group Approach to Single-Impurity Anderson Model

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1 Introduction

The single-impurity Anderson model (SIAM) is one of the most well-studied models in condensed matter physics and is the prototypical model for magnetism. It shows how strong correlations between electrons give rise to a residual local moment. a 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 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 reveals a criterion for the formation of local moments; this criterion is similar to the Stoner criterion for ferromagnetism. This mean-field analysis is of course only valid at high temperatures where electron-correlations are not so important. At low temperatures, it was found that the resistivity of the material reaches a minimum at some temperature, and then increases as $\ln T$ as we further reduce the temperature. This is in contrast to the previews results. And that was not all; at a sufficiently low temperature, it was found that the $\ln T$ -dependence disappears and the susceptibility became constant, implying the formation of a singlet state.

The fact that this logarithmic dependence vanishes once the singlet is formed suggests that it arises from the local moment on the impurity; once the local moment disappears (singlet), the log dependence vanishes as well. This led people to design a model in which the impurity interacted with the conduction bath through a Heisenberg-like spin-spin interaction. This model can be related to the SIAM through a canonical transformation followed by a projection to the low energy subspace. In 1964, Jun Kondo[3] found that a perturbative calculation of the transition probability of electrons from scattering via the impurity, up to second order in the exchange coupling J , revealed a logarithmic dependence of the resistivity on temperature. The crucial scattering process was that in which the spin of the incoming electron flipped (the S^+s^- and S^-s^+ terms). This explained the mystery of the resistivity minimum and the logarithmic dependence. But the mystery of the singlet state at very low temperatures still remained. The perturbative analysis would break down at low temperatures, so it was unreliable. The log term showed that the physics of the singlet involved all energy scales; one could not hope to capture it simply by taking the first few terms of a perturbative expansion. This problem came to be known as the Kondo problem.

In 1970, Anderson attacked this problem by a renormalization group approach to account for all energy scales. In his "Poor Man's Scaling" approach, he progressively reduced the bandwidth while taking account of the eliminated states into the couplings via second order perturbation theory. This showed how the couplings would flow as we went to low temperatures, but it still could not remove the divergence as it was perturbative. Anderson found that the exchange coupling increased as we go to lower temperatures, so he surmised that the low energy theory was one where $J = \infty$. In 1975, Kenneth Wilson solved the problem by using his numerical renormalization group method in which he iteratively

diagonalized chains of increasing length to go to the low energy physics. He proved that Anderson's guess was right and the low energy Hamiltonian was the same as that with $J = \infty$. Later calculations with Bethe ansatz in 1980 by Andrei and Weigmann [4],[5] corroborated Wilson's findings.

A similar sequence of events also happened in the context of the Anderson model. In 1977 and 1978, Jefferson and Haldane independently calculated the "Poor Man's" scaling equations for the asymmetric SIAM, in the limit of infinitely large onsite repulsion. They were unable to access the strong-coupling fixed point (analogous to the $J = \infty$ fixed point in Kondo model), but their equations revealed which were the important regimes to consider. Later, in 1975, Krishnamurthy, Wilkins and Wilson applied the NRG method to the symmetric Anderson model and obtained the non-perturbative fixed points and susceptibility. Their calculations were again supported by later Bethe ansatz calculations by Weigman and Tsvelick[6].

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 mobile electron at low temperatures resulting in the screening of the local moment via spin-flip scatterings with the mobile electrons 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.

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.
- *Can we get Hamiltonians and wavefunctions in the **crossover region** ($T \sim T_K$)?* NRG does give us some Hamiltonians, but those are valid very close to the fixed points. The harder challenge is to get Hamiltonians for all energy scales, possibly in the form of some running couplings. That would also show us exactly how the wavefunctions morph as we reduce the bandwidth. T_K is the temperature at which the crossover occurs, so that is the most interesting regime.
- *What is the nature of the strong-coupling fixed point for a **finite system** ($J \neq \infty$)? Will the results change if we introduce a **non-uniform density of states**?* NRG and Bethe ansatz work very well for continuum systems where the bandwidth is essentially infinite. As a result, they get an infinite J strong-coupling fixed point. For a finite lattice, things are different. It would be interesting to know how the finite J fixed point looks like and whether the conclusions of NRG break down.

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- Can we get **better estimates of thermodynamic quantities** in the crossover region? Calculation of thermodynamic quantities like magnetic susceptibility and specific heat require not just the ground state but the excited states as well. Since NRG projects out most of the states above the ground state, it is difficult to get very accurate estimates of such quantities far away from the fixed point. Bethe ansatz calculations also typically employ approximations like $T \gg T_K$. Moreover, Bethe ansatz equations have to be solved numerically so they lack the transparency of analytical solutions.
 - Is it possible to show the **transfer of spectral weight** along the flow, possibly by tracking the bath spectral function or the many-particle entanglement? Such an exercise will require the entire spectrum to be preserved along the flow. NRG, being projective will not work here. If the entire spectrum is available, computing the many-particle entanglement of the spectral function along the flow should indicate how the spectral weight is being distributed between the impurity and the conduction bath.
 - 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.

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.

The work is organized as follows. Section 2 goes over the available work on the Anderson and Kondo model. Section 3 lays out the URG formalism and prescription. Section 5 solves the Kondo model using the URG method. Section 6 contains the URG analysis of the SIAM.

2 Preliminaries

2.1 T-matrix and S-matrix

T -matrix is defined as[7]

$$V\psi = T\phi \quad (2.1)$$

where ψ is the total scattered wavefunction and ϕ is the incoming wavefunction. They satisfy the Schrodinger equations

$$H_0\phi = E\phi \quad (2.2)$$

$$(H_0 + V)\psi = E\psi \quad (2.3)$$

Since we are assuming elastic scattering, both have the same energy. The Schrodinger equation for ψ can be rearranged into

$$\psi = \phi + G_0V\psi \quad (2.4)$$

where $G_0^{-1} = E - H_0$. This is also called the Lippmann-Schwinger equation. Using the definition of T gives

$$\begin{aligned} \psi &= \phi + G_0T\phi \\ \implies \psi &= (1 + G_0T)\phi \end{aligned} \quad (2.5)$$

Eq. 2.4 can also be written as

$$\psi = (1 - G_0V)^{-1}\phi \quad (2.6)$$

Comparing the last two equations gives

$$\begin{aligned} 1 &= (1 - G_0V)(1 + G_0T) \\ \implies T &= V + VG_0T \end{aligned} \quad (2.7)$$

The last equation allows us to perturbatively expand the T - matrix.

$$T = V + VG_0V + VG_0VG_0V + \dots \quad (2.8)$$

From scattering theory, we can write

$$\psi = (2\pi)^{-\frac{3}{2}} \left[e^{ikx} + f \frac{e^{ikr}}{r} \right] \quad (2.9)$$

where the wave amplitude $f(k', k) \sim \langle k' | V | \psi \rangle$. Using the definition of T , we get

$$f(k', k) \sim \langle k' | T | k \rangle \quad (2.10)$$

By definition, the S -matrix is

$$S(\omega) = e^{2i\pi\delta(\omega)} \quad (2.11)$$

Also,

$$S = 1 - 2i\pi\rho T \quad (2.12)$$

Therefore,

$$T = \frac{1}{2i\pi\rho} (1 - e^{2i\pi\delta(\omega)}) = -\frac{e^{i\delta} \sin \delta}{\pi\rho} \quad (2.13)$$

2.2 An identity

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

$$HA = A(\lambda + H) \quad (2.14)$$

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

$$(E - H)A = AE - A(\lambda + H) = A(E - \lambda - H) \quad (2.15)$$

$$\implies A(E - \lambda - H)^{-1} = (E - H)^{-1}A \quad (2.16)$$

2.3 Landau's theory of Fermi liquid

This section is adapted from ref. [8]. 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,

$$n_{k\sigma} = \begin{cases} 1 & k \leq k_F \\ 0 & k > k_F \end{cases} \quad (2.17)$$

Excitations involve adding an electron above k_F or deleting 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.

$$\Psi^* \xrightarrow{\text{turn interactions off}} \Phi \quad (2.18)$$

$$\Phi^* \xrightarrow{\text{turn interactions off}} \Psi \quad (2.19)$$

If some state Γ^* , instead of flowing into an ideal excited state, gets lost while the interactions are being turned off, then we aren't considering that system. All excited states must flow into some ideal state and vice-versa. This means that the interacting excited states

can be labelled 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 + quasip 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,

$$|IGS\rangle \otimes |k_+\rangle \xrightarrow{\text{turn interactions on}} |RGS\rangle \otimes |k_+\rangle^* \quad (2.20)$$

$$|IGS\rangle \otimes |k_-\rangle \xrightarrow{\text{turn interactions on}} |RGS\rangle \otimes |k_-\rangle^* \quad (2.21)$$

$$(2.22)$$

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

$$c_{k_+}^\dagger |IGS\rangle \xrightarrow{\text{turn interactions on}} \eta_{k_+}^\dagger |RGS\rangle \quad (2.23)$$

$$c_{k_-} |IGS\rangle \xrightarrow{\text{turn interactions on}} \eta_{k_-} |RGS\rangle \quad (2.24)$$

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

$$\delta n_k = n_k - n_k^0 \quad (2.25)$$

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.

$$\mathcal{E}^0[n_k] = \sum_k n_k \epsilon_k \quad (2.26)$$

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

$$\mathcal{E}[n_k] = \mathcal{E}[n_k^0] + \sum_k \frac{\partial \mathcal{E}}{\partial n_k} \delta n_k \quad (2.27)$$

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

$$\delta \mathcal{E} \equiv \mathcal{E}[n_k] - \mathcal{E}[n_k^0] = \sum_k \xi_k \delta n_k \quad (2.28)$$

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

$$n_k^2 - n_k^1 = \begin{cases} 0 & k \neq q \\ 1 & k = q \end{cases} \quad (2.29)$$

Then, up to first order,

$$\mathcal{E}[n_k^2] - \mathcal{E}[n_k^1] = \sum_k \xi_k (n_k^2 - n_k^1) = \xi_q \quad (2.30)$$

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 upto first order.

$$\xi_k = \xi_k^0 + \sum_q \frac{\partial \xi_k}{\partial n_q} \delta n_q \quad (2.31)$$

Eq. 2.28 then becomes

$$\delta \mathcal{E} = \sum_k \xi_k^0 \delta n_k + \sum_{k,q} f(k,q) \delta n_k \delta n_q \quad (2.32)$$

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 ,

$$f(\xi) = [e^{(\xi-\mu)\beta} + 1]^{-1} \quad (2.33)$$

where $\mu = \mathcal{E}_i(N+1) - \mathcal{E}_i(N) = \frac{\partial \mathcal{E}_0}{\partial N}$ 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

$$F[\delta n_k] = \delta \mathcal{E}[\delta n_k] - TS[\delta n_k] \quad (2.34)$$

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

$$\xi_k(T) = \xi_k^0 + \sum_q f(k,q) \langle \delta n_q \rangle \quad (2.35)$$

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

$$\left. \frac{dF}{d\delta n_q} \right|_{\delta n_q = \langle \delta n_q \rangle} = 0 \quad (2.36)$$

2.4 The model

$$H = \epsilon_d \hat{n}_d + \sum_k \epsilon_k \hat{n}_k + \sum_{k\sigma} t \left(c_{k\sigma}^\dagger c_{d\sigma} + c_{d\sigma}^\dagger c_{k\sigma} \right) + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \quad (2.37)$$

Energy scales:

- ϵ_d
- U
- $\frac{2\Delta}{\hbar} = \tau^{-1} = \frac{2\pi}{\hbar} t^2 \sum_k \rho(\epsilon_k) \rightarrow$ extent of hybridisation (rate of transition) between conduction band and impurity site

Situations:

- $U \gg \epsilon_d \gg \Delta$: 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.

2.5 Atomic limit - no hopping:

$$H_{\text{atomic}} = E_d + E_{CB} + U n_{d\uparrow} n_{d\downarrow} \quad (2.38)$$

Since we are not interested in the Fermi sea, the E_{CB} is dropped:

$$H_{\text{atomic}} = \epsilon_d n_d + U n_{d\uparrow} n_{d\downarrow} \quad (2.39)$$

For a magnetic solution, we need

$$(\epsilon_\uparrow = \epsilon_\downarrow) \epsilon_d < (\epsilon_0, \epsilon_{\uparrow\downarrow}) 0, 2\epsilon_d + U \quad (2.40)$$

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

$$\epsilon_d > -U \quad (2.41)$$

2.6 Non-interacting limit - no onsite repulsion:

$$H_{\text{non-int}} = \epsilon_d n_d + \sum_k \epsilon_k n_k + \sum_{k\sigma} t \left(c_{k\sigma}^\dagger c_{d\sigma} + c_{d\sigma}^\dagger c_{k\sigma} \right) \quad (2.42)$$

2.6.1 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

$$G_d^0(E) = \frac{1}{E - \epsilon_d} \quad (2.43)$$

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

$$G_d^0 \Sigma_c G_d^0, \text{ where } \Sigma_c = t \left(\sum_k G_k^0 \right) t = \sum_k \frac{t^2}{E - \epsilon_k} \quad (2.44)$$

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

$$\begin{aligned} G_d(E) &= G_d^0 + G_d^0 \Sigma_c G_d^0 + G_d^0 \Sigma_c G_d^0 \Sigma_c G_d^0 + G_d^0 \Sigma_c G_d^0 \Sigma_c G_d^0 \Sigma_c G_d^0 + \dots \\ &= G_d^0 \left[1 + (\Sigma_c G_d^0)^2 + \dots \right] = G_d^0 \frac{1}{1 - \Sigma_c G_d^0} = \frac{1}{E - \epsilon_d - \Sigma_c(E)} \end{aligned} \quad (2.45)$$

Now,

$$\frac{1}{t^2} \Sigma_c(E) = \sum_k \frac{1}{E - \epsilon_k} = \lim_{\eta \rightarrow 0} \int_{-W}^W d\epsilon \rho(\epsilon) \frac{1}{E - \epsilon + i\eta} \quad (2.46)$$

$$\Rightarrow \frac{1}{t^2} \text{Re} [\Sigma_c(E)] = \int_{-W}^W d\epsilon \rho(\epsilon) \frac{1}{E - \epsilon}, \text{ and} \quad (2.47)$$

$$\frac{1}{t^2} \text{Im} [\Sigma_c(E)] = \int_{-W}^W d\epsilon \rho(\epsilon) (-i\pi) \delta(E - \epsilon) \quad (2.48)$$

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

$$\Sigma_c(E) = \text{Im} [\Sigma_c(E)] = -i\pi t^2 \rho(E) = -i\Delta \quad (2.49)$$

Therefore,

$$G_d(E) = \frac{1}{E - \epsilon_d + i\Delta} \quad (2.50)$$

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

$$\rho_d^0(E) = -\frac{1}{\pi} \text{Im} [G_d^0] = -\frac{1}{\pi} \lim_{\eta \rightarrow 0} \frac{1}{E - \epsilon_d + i\eta} = \delta(E - \epsilon_d) \quad (2.51)$$

$$\rho_d(E) = -\frac{1}{\pi} \text{Im} [G_d] = -\frac{1}{\pi} \lim_{\eta \rightarrow 0} \frac{1}{E - \epsilon_d + i(\eta + \Delta)} = \frac{1}{\pi} \frac{\Delta}{(E - \epsilon_d)^2 + \Delta^2} \quad (2.52)$$

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:

$$\langle n_d \rangle = 2 \int d\epsilon \rho_d(\epsilon) = \frac{2\Delta}{\pi} \int \frac{d\epsilon}{(\epsilon - \epsilon_d)^2 + \Delta^2} = \frac{2}{\pi} \cot^{-1} \left(\frac{\epsilon_d}{\Delta} \right) \quad (2.53)$$

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

T -matrix is defined by

$$T = V + VGT \quad (2.54)$$

We also have

$$\begin{aligned} G &= G_0 + G_0VG = G_0 + G_0T \frac{1}{1 + GT} G \\ &= G_0 + G_0T(1 - GT + \dots)(G_0 + G_0VG_0 + \dots) \\ &= G_0 + G_0TG_0 \end{aligned} \quad (2.55)$$

The conduction electron Green's function can be calculated as

$$\begin{aligned} G_c(k, k', E) &= \delta_{k,k'} G_c^0(k, E) + G_c^0(k) t G_d^0 t G_c^0(k') + \\ &G_c^0(k) t G_d^0 t \sum_q G_c^0(q) t G_d^0 t G_c^0(k') + \dots \end{aligned} \quad (2.56)$$

Noting that

$$t \sum_q G_c^0(q) t = \Sigma_c, \quad (2.57)$$

we have

$$G_c(k, k', E) = \delta_{k,k'} G_c^0(k, E) + G_c^0(k) t^2 G_d(E) G_c^0(k') \quad (2.58)$$

Comparing with the final form of G in eq. 2.55, we can write

$$T(k, k', E) = t^2 G_d(E) = \frac{t^2}{E - \epsilon_d + i\Delta} = -\frac{t^2}{\Delta} \frac{1}{\frac{\epsilon_d - E}{\Delta} - i} \quad (2.59)$$

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

$$\text{Im}[T] = -\frac{t^2 \Delta}{(E - \epsilon_d)^2 + \Delta^2} = -\pi t^2 \rho_d \quad (2.60)$$

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

$$\rho_d = -\frac{1}{\pi} \text{Im}[G_d] = -\frac{1}{\pi t^2} \text{Im}[t^2 G_d] = -\frac{1}{\pi t^2} \text{Im}[T] \quad (2.61)$$

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

$$T = e^{2i\delta} - 1 = e^{i\delta} (e^{i\delta} - e^{-i\delta}) \sim \frac{1}{\cot \delta - i} \quad (2.62)$$

Comparing with eq. 2.59, we can write

$$\delta(E) = \cot^{-1} \left(\frac{\epsilon_d - E}{\Delta} \right) \quad (2.63)$$

When $E = \epsilon_d$, the phase shift is π , and the scattering is head on (the conduction electron is reflected back). Comparing with eq. 2.53,

$$\frac{2}{\pi} \delta(0) = \langle n_d \rangle \quad (2.64)$$

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

2.6.3 Coulomb blockade

This section follows the discussion in reference [9]. A quantum dot is a set of electrons that are localised in a sufficiently small region so that their spectrum is quantised. The localization means that double occupation will come at a cost of U .

$$H_{\text{dot}} = \sum_{m\sigma} \epsilon_m n_{m\sigma} + U \frac{N(N+1)}{2} \quad (2.65)$$

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.

$$H_{\text{dot}} = \sum_{m\sigma} (\epsilon_m - eV) n_{m\sigma} + U \frac{N(N+1)}{2} \quad (2.66)$$

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

$$\Delta E = UN + \epsilon_N - eV \quad (2.67)$$

Tuning the voltage can make these two levels degenerate.

$$eV^* = UN + \epsilon_N \quad (2.68)$$

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,

$$G(V) = G_0 \rho(0) = \frac{2e^2}{h} \frac{\Delta^2}{(\epsilon_m - eV)^2 + \Delta^2} \quad (2.69)$$

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

2.7 Total Hamiltonian: Mean field treatment

$$n_{d\uparrow}n_{d\downarrow} \approx n_{d\uparrow}\langle n_{d\downarrow} \rangle + n_{d\downarrow}\langle n_{d\uparrow} \rangle + \text{constant} \quad (2.70)$$

$$H \approx \sum_k \epsilon_k n_k + \sum_\sigma [\epsilon_d + U\langle n_{d\bar{\sigma}} \rangle] n_{d\sigma} + t \sum_{k\sigma} \left(c_{k\sigma}^\dagger c_{d\sigma} + c_{d\sigma}^\dagger c_{k\sigma} \right) \quad (2.71)$$

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

$$\rho_{d\sigma} = \frac{1}{\pi} \frac{\Delta}{(E - \epsilon_{d\sigma})^2 + \Delta^2} \implies \langle n_{d\sigma} \rangle = \int \rho_{d\sigma} = \frac{1}{\pi} \cot^{-1} \left(\frac{\epsilon_{d\sigma}}{\Delta} \right) \quad (2.72)$$

An alternative way of writing that is

$$\frac{\epsilon_{d\sigma}}{\Delta} = \frac{\epsilon_d + U\langle n_{d\bar{\sigma}} \rangle}{\Delta} = \cot(\pi\langle n_{d\bar{\sigma}} \rangle) \implies \langle n_{d\sigma} \rangle = \frac{\Delta}{U} \left[\cot(\pi\langle n_{d\bar{\sigma}} \rangle) - \frac{\epsilon_d}{\Delta} \right] \quad (2.73)$$

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

$$\begin{aligned} \langle n_{d\uparrow} - n_{d\downarrow} \rangle &\equiv m = \frac{\Delta}{U} [\cot(\pi\langle n_{d\downarrow} \rangle) - \cot(\pi\langle n_{d\uparrow} \rangle)] \\ &= \frac{\Delta}{U} \left[\cot \frac{\pi}{2} (n_d - m) - \cot \frac{\pi}{2} (n_d + m) \right] \end{aligned} \quad (2.74)$$

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

$$\cot(a+x) \approx \cot a - x(\sin a)^{-2} \implies \cot(a-x) - \cot(a+x) \approx 2x(\sin a)^{-2} \quad (2.75)$$

we get

$$m = \frac{\Delta}{U} \left[-\pi \frac{m}{\sin^2 \frac{\pi}{2} n_d} \right] \implies 1 = \lim_{m \rightarrow 0} \frac{U}{\pi \Delta} \frac{1}{1 + \cot^2 \frac{\pi n_d}{2}} \quad (2.76)$$

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. 2.76,

$$1 = \frac{U_c}{\pi} \frac{\Delta}{\Delta^2 + \left(\frac{U_c n_d}{2} + \epsilon_d \right)^2} \quad (2.77)$$

Magnetism will prevail for $U \geq U_c$. Comparing with eq. 2.73,

$$1 = U_c \rho_d(E=0) \quad (2.78)$$

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

$$U_c = \pi \Delta \quad (2.79)$$

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

$$\langle n_{d\uparrow} \rangle = \frac{1+m}{2} \quad (2.80)$$

$$\langle n_{d\downarrow} \rangle = \frac{1-m}{2} \quad (2.81)$$

$$\epsilon_{d\sigma} = \epsilon_d + U\langle n_{d\bar{\sigma}} \rangle = \epsilon_d + \frac{U}{2} \pm \frac{U}{2} m = \pm \frac{U}{2} m \quad (2.82)$$

$$\rho_d = \rho_{d\uparrow} + \rho_{d\downarrow} = \frac{\Delta}{\pi} \left[\frac{1}{\Delta^2 + \left(E - \frac{Um}{2} \right)^2} + \frac{1}{\Delta^2 + \left(E + \frac{Um}{2} \right)^2} \right] \quad (2.83)$$

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

2.8 Some points:

- The mean field solution predicts that local moments are sustained in the limit of large U and small $|\epsilon_d|$.
- 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 behaviour stops at some very low temperature T_K .
- The temperature T_K is also that at which the magnetisation vanishes, and the susceptibility becomes constant, suggesting that the impurity spin has condensed into a singlet.
- Since the disappearance of the $\ln T$ behaviour is coincident with the condensation of the spin degree of freedom, it is natural to hope that the resistivity minimum is a result of the interaction between the impurity and the conduction spins.
- To describe such an interaction, the way to proceed is to strip the model of the charge excitations (via a *Schrieffer-Wolff transformation*). The resultant Hamiltonian consists of an antiferromagnetic interaction between the itinerant spins and the impurity spin, and is called the Kondo model.
- Calculating the scattering rate up to second order using the Kondo model produces a logarithmic term, which explains the log-dependence.
- Since this perturbative treatment will fail at small temperatures (where the log term diverges), we need some other technique to find out the fate of the model at low temperatures.
- Anderson's poor man's scaling wraps the effects of high energy scatterings into the low energy model, showing that the antiferromagnetic 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 $T \rightarrow 0$.

2.9 Derivation of the Kondo Hamiltonian

Deriving the Kondo Hamiltonian involves separating the impurity spinon subspace ($\hat{n}_{d\uparrow} \neq \hat{n}_{d\downarrow}$) from the doublon and holon subspaces ($\hat{n}_{d\uparrow} = \hat{n}_{d\downarrow}$). The canonical (pun intended) way of doing this is via a Schrieffer-Wolff transformation [10]. 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 [9]. An alternate derivation via a projector operator method due to [11] is shown in 9.3.

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

$$\text{low energy (L)} \rightarrow \begin{cases} |\uparrow\rangle \\ |\downarrow\rangle \end{cases} \quad (2.84)$$

$$\text{high energy (H)} \rightarrow \begin{cases} | \rangle \\ |\uparrow\downarrow\rangle \end{cases}$$

$$H = H_0 + V = \begin{array}{cc} & \begin{matrix} \text{low} & \text{high} \end{matrix} \\ \begin{matrix} \text{low} \\ \text{high} \end{matrix} & \begin{pmatrix} H^L & v^\dagger \\ v & H^H \end{pmatrix} \end{array} \quad (2.85)$$

$$H_0 = \sum_k \epsilon_k n_k + \epsilon_d n_d + U n_{d\uparrow} n_{d\downarrow}, V = \sum_{k\sigma} \left(V_k c_{k\sigma}^\dagger c_{d\sigma} + V_k^* c_{d\sigma}^\dagger c_{k\sigma} \right) \quad (2.86)$$

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

$$\bar{H} = e^{-S} H e^S = H_0 + (V + [H_0, S]) + \frac{1}{2} ([V, S] + [[H_0, S], S]) \quad (2.87)$$

Defining S such that the first order term vanishes,

$$V = [S, H_0] \quad (2.88)$$

$$\bar{H} = H_0 + \frac{1}{2} [V, S] \quad (2.89)$$

Take $S = \begin{pmatrix} 0 & -s^\dagger \\ s & 0 \end{pmatrix}$. From eq. 2.88,

$$\begin{aligned} V &= \begin{pmatrix} 0 & -s^\dagger \\ s & 0 \end{pmatrix} \begin{pmatrix} H^L & 0 \\ 0 & H^H \end{pmatrix} - \begin{pmatrix} H^L & 0 \\ 0 & H^H \end{pmatrix} \begin{pmatrix} 0 & -s^\dagger \\ s & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & -s^\dagger H^H + H^L s^\dagger \\ s H^L - H^H s & 0 \end{pmatrix} \end{aligned} \quad (2.90)$$

Comparing with the definition of V , we can write

$$v_{ij}^\dagger = s_{ij}^\dagger (E_i^L - E_j^H), v_{ij} = s_{ij} (E_j^L - E_i^H) \quad (2.91)$$

$$\implies s_{ij}^\dagger = \frac{v_{ij}^\dagger}{E_i^L - E_j^H}, s_{ij} = \frac{v_{ij}}{E_j^L - E_i^H} \quad (2.92)$$

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

$$[V, S] = \begin{pmatrix} 0 & v^\dagger \\ v & 0 \end{pmatrix} \begin{pmatrix} 0 & -s^\dagger \\ s & 0 \end{pmatrix} - \begin{pmatrix} 0 & -s^\dagger \\ s & 0 \end{pmatrix} \begin{pmatrix} 0 & v^\dagger \\ v & 0 \end{pmatrix} = \begin{pmatrix} v^\dagger s + s^\dagger v & 0 \\ 0 & -v s^\dagger - s v^\dagger \end{pmatrix} \quad (2.93)$$

Hence,

$$\bar{H} = H_0 + \frac{[V, S]}{2} = \begin{pmatrix} H^L + \frac{1}{2} (v^\dagger s + s^\dagger v) & 0 \\ 0 & H^H - v s^\dagger - s v^\dagger \end{pmatrix} \quad (2.94)$$

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

$$\mathcal{H} = \langle L | \bar{H} | L \rangle = H^L + \frac{1}{2} (v^\dagger s + s^\dagger v) \quad (2.95)$$

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

$$\begin{aligned} \Delta H &= \frac{1}{2} (v^\dagger s + s^\dagger v) = \frac{1}{2} \left(v^\dagger \sum_{HL} s_{HL} |H\rangle \langle L| + \text{h.c.} \right) \\ &= \frac{1}{2} \sum_{HL} \left[v^\dagger |H\rangle \langle L| \frac{v_{HL}}{E_L - E_H} + |L\rangle \langle H| \frac{v_{LH}^\dagger}{E_L - E_H} v \right] \end{aligned} \quad (2.96)$$

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

$$\Delta H_{ll'} = \langle l | \Delta H | l' \rangle = \frac{1}{2} \sum_H v_{lH}^\dagger v_{Hl'} \left(\frac{1}{E_{l'} - E_H} + \frac{1}{E_l - E_H} \right) \quad (2.97)$$

This can also be written as

$$\Delta H_{ll'} = \frac{1}{2} [T_{ll'}(E_l) + T_{ll'}(E_{l'})] \quad (2.98)$$

where

$$T_{ll'}(E) = \sum_H \frac{v_{lH}^\dagger v_{Hl'}}{E - E_H} = \sum_H \frac{V_{lH}^\dagger V_{Hl'}}{E - E_H} \quad (2.99)$$

$T(E)$, here, is the second order contribution of the T -matrix due to scattering off the interaction V . The $|H\rangle$ act as the intermediate states during the second order scatterings. This is a slight generalization from second order perturbation theory. In second order perturbation, we only consider the scattering amplitude between the same states, but here we consider the scattering between two potentially different states $|l\rangle, |l'\rangle$. The total amplitude is an average of these two amplitudes.

If we assume the high energy subspace is very far away from the low energy one ($E_H \gg E_L$), we can assume $E_l \approx E_{l'} = E_L$, we can write

$$\begin{aligned} \Delta H_{ll'} &= \sum_H v_{lH}^\dagger v_{Hl'} \frac{1}{E_L - E_H} \\ \Rightarrow \Delta H &= V \left(\sum_H \frac{1}{\Delta_{LH}} |H\rangle \langle H| \right) V \end{aligned} \quad (2.100)$$

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,

$$\Delta_{LH_1} = \epsilon_d - 0 = \epsilon_d, \Delta_{LH_2} = \epsilon_d - (2\epsilon_d + U) = -\epsilon_d - U \quad (2.101)$$

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

$$\begin{aligned} \Delta H &= V \frac{|0\rangle \langle 0|}{\epsilon_d} V - V \frac{|\uparrow\downarrow\rangle \langle \uparrow\downarrow|}{\epsilon_d + U} V \\ &= \sum_{k_1, k_2, \sigma_1, \sigma_2} V(k_1) V^*(k_2) \left[\frac{c_{d\sigma_2}^\dagger c_{k_2\sigma_2} |0\rangle \langle 0| c_{k_1\sigma_1}^\dagger c_{d\sigma_1}}{\epsilon_d} - \frac{c_{k_1\sigma_1}^\dagger c_{d\sigma_1} |\uparrow\downarrow\rangle \langle \uparrow\downarrow| c_{d\sigma_2}^\dagger c_{k_2\sigma_2}}{\epsilon_d + U} \right] \\ &= \sum_{k_1, k_2, \sigma_1, \sigma_2} V(k_1) V^*(k_2) \frac{c_{d\sigma_2}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_1} |d\sigma_1, h_{k_1\sigma_1}\rangle \langle d\sigma_1, h_{k_1\sigma_1}|}{\epsilon_d} \\ &\quad - \sum_{k_1, k_2, \sigma_1, \sigma_2} V(k_1) V^*(k_2) \frac{c_{k_1\sigma_1}^\dagger c_{d\sigma_1} c_{d\sigma_2}^\dagger c_{k_2\sigma_2} |d\sigma_2, e_{k_2\sigma_2}\rangle \langle d\sigma_2, e_{k_2\sigma_2}|}{\epsilon_d + U} \\ &= \sum_{k_1, k_2, \sigma_1, \sigma_2} V(k_1) V^*(k_2) \left[\frac{c_{d\sigma_2}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_1}}{\epsilon_d} - \frac{c_{k_1\sigma_1}^\dagger c_{d\sigma_1} c_{d\sigma_2}^\dagger c_{k_2\sigma_2}}{\epsilon_d + U} \right] P_{n_d=1} \end{aligned} \quad (2.102)$$

Using 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

$$\begin{aligned} c_{d\sigma_2}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_1} &= \sum_{\sigma_3, \sigma_4} c_{d\sigma_3}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_4} \delta_{\sigma_1\sigma_3} \delta_{\sigma_4\sigma_2} \\ &= \frac{1}{2} \sum_{\sigma_3, \sigma_4} c_{d\sigma_3}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_4} (\delta_{\sigma_1\sigma_2} \delta_{\sigma_3\sigma_4} + \vec{\sigma}_{\sigma_1\sigma_2} \cdot \vec{\sigma}_{\sigma_3\sigma_4}) \\ &= \frac{1}{2} c_{k_2\sigma_1} c_{k_1\sigma_1}^\dagger n_d + c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} \cdot \sum_{\sigma_3, \sigma_4} c_{d\sigma_3}^\dagger \frac{\vec{\sigma}_{\sigma_3\sigma_4}}{2} c_{d\sigma_4} \end{aligned} \quad (2.103)$$

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

$$c_{d\sigma_2}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_1} = -\frac{1}{2} c_{k_1\sigma_1}^\dagger c_{k_2\sigma_1} - c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2} \cdot \sum_{\sigma_3, \sigma_4} c_{d\sigma_3}^\dagger \frac{\vec{\sigma}_{\sigma_3\sigma_4}}{2} c_{d\sigma_4} \quad (2.104)$$

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

$$c_{d\sigma_2}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_1} = -\frac{1}{2} c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2} \cdot \vec{\sigma}_d \quad (2.105)$$

Similarly,

$$c_{k_1\sigma_1}^\dagger c_{d\sigma_1} c_{d\sigma_2}^\dagger c_{k_2\sigma_2} = -\frac{1}{2} c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2} \cdot \vec{\sigma}_d \quad (2.106)$$

Finally, putting all this together,

$$\begin{aligned} \Delta H &= \frac{1}{2} \sum_{k_1, k_2, \sigma_1, \sigma_2} V(k_1) V^*(k_2) \left[\frac{1}{\epsilon_d + U} - \frac{1}{\epsilon_d} \right] c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2} \cdot \vec{\sigma}_d \\ &= \frac{1}{2} \sum_{k_1, k_2, \sigma_1, \sigma_2} J(k_1, k_2) c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2} \cdot \vec{\sigma}_d \end{aligned} \quad (2.107)$$

where

$$J(k_1, k_2) = V(k_1) V^*(k_2) \left[\frac{1}{\epsilon_d + U} - \frac{1}{\epsilon_d} \right] \quad (2.108)$$

Assuming $V(k) \equiv t$,

$$H_K = \sum_k \epsilon_k n_k + \frac{J}{2} \vec{\sigma}_e \cdot \vec{\sigma}_d \quad (2.109)$$

where

$$\vec{\sigma}_e = \sum_{k_1, k_2, \sigma_1, \sigma_2} c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2} = \sum_{\sigma_1, \sigma_2} c_{\sigma_1}^\dagger (\vec{r}=0) \vec{\sigma}_{\sigma_1\sigma_2} c_{\sigma_2} (\vec{r}=0) \quad (2.110)$$

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

2.10 Obtaining the resistivity minimum and log-dependence

The next few sections follow the approach in [12]. The model we are working with is

$$H_K = H_0 + V = \sum_k \epsilon_k n_k + \frac{J}{2} \sum_{k_1, k_2, \sigma_1, \sigma_2} c_{k_1\sigma_1}^\dagger \vec{\sigma}_d \cdot \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2} \quad (2.111)$$

$$\begin{aligned} \sum_{\sigma_1, \sigma_2} c_{k_1\sigma_1}^\dagger \vec{\sigma}_d \cdot \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2} &= \sigma_d^z \left(c_{k_1\uparrow}^\dagger c_{k_2\uparrow} - c_{k_1\downarrow}^\dagger c_{k_2\downarrow} \right) + \sigma_d^x \left(c_{k_1\downarrow}^\dagger c_{k_2\uparrow} + c_{k_1\uparrow}^\dagger c_{k_2\downarrow} \right) \\ &\quad - i\sigma_d^y \left(c_{k_1\uparrow}^\dagger c_{k_2\downarrow} - c_{k_1\downarrow}^\dagger c_{k_2\uparrow} \right) \end{aligned} \quad (2.112)$$

$$= \sigma_d^z \left(c_{k_1\uparrow}^\dagger c_{k_2\uparrow} - c_{k_1\downarrow}^\dagger c_{k_2\downarrow} \right) + c_{k_1\downarrow}^\dagger c_{k_2\uparrow} \sigma_d^+ + c_{k_1\uparrow}^\dagger c_{k_2\downarrow} \sigma_d^- \quad (2.113)$$

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

$$\begin{aligned} H_K &= \sum_k \epsilon_k n_k + \frac{J}{2} \sum_{k_1, k_2} \left[\sigma_d^z \left(c_{k_1\uparrow}^\dagger c_{k_2\uparrow} - c_{k_1\downarrow}^\dagger c_{k_2\downarrow} \right) + \sigma_d^+ c_{k_1\downarrow}^\dagger c_{k_2\uparrow} + \sigma_d^- c_{k_1\uparrow}^\dagger c_{k_2\downarrow} \right] \\ &= \sum_k \epsilon_k n_k + J \sum_{k_1, k_2} \left[S_d^z \left(c_{k_1\uparrow}^\dagger c_{k_2\uparrow} - c_{k_1\downarrow}^\dagger c_{k_2\downarrow} \right) + S_d^+ c_{k_1\downarrow}^\dagger c_{k_2\uparrow} + S_d^- c_{k_1\uparrow}^\dagger c_{k_2\downarrow} \right] \end{aligned} \quad (2.114)$$

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

$$T = V + V G_0 V \quad (2.115)$$

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

2.10.1 First order scattering

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

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

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

$$T_{\text{nonflip}}^{(1)} = T_{k_\uparrow, d_\sigma \rightarrow q_\uparrow, d_\sigma} = \langle q_\uparrow, d_\sigma | V | k_\uparrow, d_\sigma \rangle = m_d J \quad (2.116)$$

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

$$\mathcal{P}_{k_\sigma, d_{\sigma'} \rightarrow q_\sigma, d_{\sigma'}} = 2\pi \sum_{\epsilon} \rho(\epsilon) T_{k_\uparrow, d_\sigma \rightarrow q_\uparrow, d_\sigma}^2 = 2\pi \rho(0) J^2 m_d^2 \quad (2.117)$$

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

$$\mathcal{P}_1 = 2\pi \rho(0) J^2 m_d^2 \quad (2.118)$$

For spin-flip, the matrix element is

$$T_{\text{flip}}^{(1)} = T_{k_\uparrow, d_\downarrow \rightarrow q_\downarrow, d_\uparrow} = \langle q_\downarrow, d_\uparrow | V | k_\uparrow, d_\downarrow \rangle = \lambda_+ J \quad (2.119)$$

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

$$\mathcal{P}_2 = \mathcal{P}_{k_\uparrow, d_\downarrow \rightarrow q_\downarrow, d_\uparrow} = 2\pi \rho(0) J [s_d(s_d + 1) - m_d(m_d + 1)] \quad (2.120)$$

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

$$\begin{aligned} \mathcal{P}^{(1)} &= \frac{1}{2s_d + 1} \sum_{m_d = -s_d}^{s_d} (\mathcal{P}_1 + \mathcal{P}_2) = \frac{2\pi \rho(0) J^2}{(2s_d + 1)} \sum_{m_d = -s_d}^{s_d} (s_d(s_d + 1) - m_d) \\ &= 2\pi \rho(0) J^2 s_d(s_d + 1) \end{aligned} \quad (2.121)$$

2.10.2 Second order scattering

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

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

The second order transition matrix contribution is of the form

$$T_{i \rightarrow j}^{(2)} = \langle j | V G_0 V | i \rangle = \sum_l \frac{\langle j | V | l \rangle \langle l | V | i \rangle}{E_i - E_l} \quad (2.122)$$

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

$$\begin{aligned} T_{11}^{(2)} &= \sum_q \frac{\langle k'_{\uparrow} d_{\sigma} | V | q_{\uparrow} d_{\sigma} \rangle \langle q_{\uparrow} d_{\sigma} | V | k_{\uparrow} d_{\sigma} \rangle}{\epsilon_k - \epsilon_q} \\ &= (Jm_d)^2 \sum_q \frac{1 - P(q)}{\epsilon_k - \epsilon_q} = J^2 m_d^2 \sum_q \frac{1 - P(q)}{\epsilon_k - \epsilon_q} \end{aligned} \quad (2.123)$$

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,

$$T_{12}^{(2)} = \sum_q \frac{\langle q_{\uparrow} k'_{\uparrow} d_{\sigma} | V | k'_{\uparrow} k_{\uparrow} d_{\sigma} \rangle \langle k'_{\uparrow} k_{\uparrow} d_{\sigma} | V | q_{\uparrow} k_{\uparrow} d_{\sigma} \rangle}{\epsilon_q - \epsilon_{k'}} P(q) \quad (2.124)$$

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

$$T_{12}^{(2)} = -J^2 m_d^2 \sum_q \frac{P(q)}{\epsilon_q - \epsilon_k} = J^2 m_d^2 \sum_q \frac{P(q)}{\epsilon_k - \epsilon_q} \quad (2.125)$$

For the third process,

$$T_{13}^{(2)} = \sum_q \frac{\langle k'_{\uparrow} d_{\downarrow} | V | q_{\downarrow} d_{\uparrow} \rangle \langle q_{\downarrow} d_{\uparrow} | V | k_{\uparrow} d_{\downarrow} \rangle}{\epsilon_k - \epsilon_q} \quad (2.126)$$

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

$$T_{13}^{(2)} = \lambda_+^2 J^2 \sum_q \frac{1 - P(q)}{\epsilon_k - \epsilon_q} \quad (2.127)$$

For the fourth process,

$$\begin{aligned} T_{14}^{(2)} &= \sum_q \frac{\langle q_{\downarrow} k'_{\uparrow} d_{\uparrow} | V | k'_{\uparrow} k_{\uparrow} d_{\downarrow} \rangle \langle k'_{\uparrow} k_{\uparrow} d_{\downarrow} | V | q_{\downarrow} k_{\uparrow} d_{\uparrow} \rangle}{\epsilon_q - \epsilon'_k} \\ &= -\lambda_-^2 J^2 \sum_q \frac{P(q)}{\epsilon_q - \epsilon_k} \\ &= \lambda_-^2 J^2 \sum_q \frac{P(q)}{\epsilon_k - \epsilon_q} \end{aligned} \quad (2.128)$$

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

$$\begin{aligned} T_{\text{nonflip}}^{(2)} &= \sum_{i=1}^4 T_{1i}^{(2)} = J^2 \sum_q \frac{m_d^2 + \lambda_+^2 - P(q) (\lambda_+^2 - \lambda_-^2)}{\epsilon_k - \epsilon_q} \\ &= J^2 \sum_q \frac{s(s+1) - m_d + 2m_d P(q)}{\epsilon_k - \epsilon_q} \\ &= J^2 [s(s+1) - m_d] (\alpha + \gamma) + 2J^2 m_d \gamma \end{aligned} \quad (2.129)$$

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.

$$\begin{aligned} T_{\text{nonflip}}^{(2)} &= 2J^2 m_d \gamma \\ &= 2J^2 m_d \int d\epsilon N(\epsilon) \frac{P(\epsilon)}{\epsilon_k - \epsilon} = \frac{\sqrt{2} J^2 m_d m^{\frac{3}{2}}}{\pi^2 \hbar^3} \int d\epsilon \frac{\sqrt{\epsilon} P(\epsilon)}{\epsilon_k - \epsilon} \end{aligned} \quad (2.130)$$

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

$$\begin{aligned} T_{\text{nonflip}}^{(2)} &= \frac{\sqrt{2} J^2 m_d m^{\frac{3}{2}}}{\pi^2 \hbar^3} \sqrt{\epsilon_k} \ln \left| \frac{\sqrt{\epsilon_k} + \sqrt{\epsilon_F}}{\sqrt{\epsilon_k} - \sqrt{\epsilon_F}} \right| \\ &= \frac{\sqrt{2} J^2 m_d m^{\frac{3}{2}}}{\pi^2 \hbar^3} \sqrt{\epsilon_k} \ln \left| \frac{\epsilon_k + \epsilon_F + 2\sqrt{\epsilon_k \epsilon_F}}{\epsilon_k - \epsilon_F} \right| \end{aligned} \quad (2.131)$$

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 $\epsilon_k = \epsilon_F$.

$$T_{\text{nonflip}}^{(2)} = \frac{\sqrt{2} J^2 m_d m^{\frac{3}{2}}}{\pi^2 \hbar^3} \sqrt{\epsilon_F} \ln \left| \frac{4T_F}{T} \right| \quad (2.132)$$

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

$$T_{\text{nonflip}}^{(2)} = 2J^2 m_d N(\epsilon_F) \ln \left| \frac{T_F}{T} \right| \quad (2.133)$$

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

$$T_{\text{nonflip}} = J m_d \left[1 + 2N(\epsilon_F) J \ln \frac{T_F}{T} \right] \quad (2.134)$$

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),

$$\begin{aligned} T_{21}^{(2)} &= -J^2 (m_d + 1) \lambda_+ \sum_q \frac{1 - P_q}{\epsilon_k - \epsilon_q} \\ T_{23}^{(2)} &= J^2 m_d \lambda_+ \sum_q \frac{1 - P_q}{\epsilon_k - \epsilon_q} \\ T_{22}^{(2)} &= J^2 (m_d + 1) \lambda_+ \sum_q \frac{P(q)}{\epsilon_k - \epsilon_q} \\ T_{24}^{(2)} &= -\lambda_+ m_d J^2 \sum_q \frac{P(q)}{\epsilon_k - \epsilon_q} \end{aligned} \quad (2.135)$$

$$T_{\text{flip}}^{(2)} = -J^2 \lambda_+ (\alpha - \gamma) \quad (2.136)$$

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

$$\begin{aligned} T_{\text{flip}}^{(2)} &= 2J^2 \lambda_+ \sum_q \frac{P(q)}{\epsilon_k - \epsilon_q} \\ &= 2J^2 \lambda_+ N(\epsilon_F) \ln \left| \frac{T_F}{T} \right| \end{aligned} \quad (2.137)$$

Adding the first order contribution,

$$T_{\text{flip}} = \lambda_+ J \left[1 + 2N(\epsilon_F) J \ln \frac{T}{T_F} \right] \quad (2.138)$$

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 $2JN(\epsilon_F) \ln \frac{T_F}{T}$.

$$\mathcal{P} = \mathcal{P}^{(2)} \left[1 + 2JN(\epsilon_F) \ln \frac{T_F}{T} \right] \quad (2.139)$$

2.11 The Kondo resonance

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

$$T_{a \rightarrow b} = \sum_{s, m_s} |\langle s, m_s | a \rangle|^2 T_s \quad (2.140)$$

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

$$T_{|k \uparrow, d_\uparrow\rangle \rightarrow |k' \uparrow, d_\uparrow\rangle} = T_1 \quad (2.141)$$

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

$$T_{|k \uparrow, d_\downarrow\rangle \rightarrow |k' \uparrow, d_\downarrow\rangle} = \frac{T_1 + T_0}{2} \quad (2.142)$$

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

$$T_{|k \uparrow, d_\downarrow\rangle \rightarrow |k' \downarrow, d_\uparrow\rangle} = \frac{T_1 - T_0}{2} \quad (2.143)$$

Therefore,

$$\begin{aligned} T_1 &= T_{|k \uparrow, d_\downarrow\rangle \rightarrow |k' \uparrow, d_\downarrow\rangle} + T_{|k \uparrow, d_\downarrow\rangle \rightarrow |k' \downarrow, d_\uparrow\rangle} = T_{\text{nonflip}} + T_{\text{flip}} \\ T_0 &= T_{|k \uparrow, d_\downarrow\rangle \rightarrow |k' \uparrow, d_\downarrow\rangle} - T_{|k \uparrow, d_\downarrow\rangle \rightarrow |k' \downarrow, d_\uparrow\rangle} = T_{\text{nonflip}} - T_{\text{flip}} \end{aligned} \quad (2.144)$$

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

$$T_{\text{nonflip}} = J \left[m_d + \frac{J}{4} \{3(\alpha + \gamma) + 4m_d(\gamma - \alpha)\} \right] \quad (2.145)$$

$$T_{\text{flip}} = J [1 + J(\gamma - \alpha)] \quad (2.146)$$

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

$$\begin{aligned} T_1 &= \frac{J}{2} \left[1 + \frac{J}{2} (\alpha + 5\gamma) \right] \\ T_0 &= -\frac{3J}{2} \left[1 - \frac{3J}{2} \left(\alpha - \frac{\gamma}{3} \right) \right] \end{aligned} \quad (2.147)$$

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

$$J \vec{S}_d \cdot \vec{\sigma}_e = 2J \vec{S}_d \cdot \vec{S}_e = J (S^2 - S_d^2 - S_e^2) = J \left(s(s+1) - \frac{3}{2} \right) = \begin{cases} -\frac{3J}{2} & \text{(singlet)} \\ \frac{J}{2} & \text{(triplet)} \end{cases} \quad (2.148)$$

Hence, the pre-factors are just the bare values of the interaction Hamiltonian, V . Hence, the equations 2.147 can be written as

$$T = V(1 + TG) \quad (2.149)$$

For the singlet and triplet T -matrices, it becomes

$$\begin{aligned} T_1 &= \frac{J}{2} [1 + T_1 (\alpha + 5\gamma)] \implies T_1 = \frac{J/2}{1 - \frac{J}{2}(\alpha + 5\gamma)} \\ T_0 &= -\frac{3J}{2} \left[1 + T_0 \left(\alpha - \frac{\gamma}{3} \right) \right] \implies T_0 = \frac{-3J/2}{1 + \frac{3J}{2}(\alpha - \gamma/3)} \end{aligned} \quad (2.150)$$

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

$$T_1 = \frac{1}{2/J - 5\gamma - \alpha} \quad (2.151)$$

$$T_0 = \frac{1}{-2/3J + \gamma/2 - \alpha} \quad (2.152)$$

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

$$T_s = \frac{1}{\text{real part} + i\pi N(0)} \quad (2.153)$$

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

$$|T_s| \leq \frac{1}{\pi N_0} \quad (2.154)$$

From eq. 2.13, we can write

$$T_s = -\frac{e^{i\delta_s} \sin \delta_s}{\pi N(0)} \quad (2.155)$$

Eq. 2.60 allows us to write

$$\rho_{d\sigma}(0) = -\frac{\text{Im}[T]}{t^2\pi} = \frac{\sin^2 \delta_s}{t^2\pi^2 N(0)} = \frac{\sin^2 \delta_s}{\pi\Delta} = \frac{1}{\pi\Delta} \sin^2 \left(\frac{\pi n_c}{2} \right) \quad (2.156)$$

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. 2.72,

$$\rho_{d\sigma}(0) = \frac{1}{\pi\Delta} \left[1 + \left(\frac{\epsilon_d + Un_c}{\Delta} \right)^2 \right]^{-1} \quad (2.157)$$

For $n_c = 1$ (half-filling), the mean field value is less than the one obtained from the spin-spin scattering. This is because the mean-field analysis does not take these scatterings into account. The large density of states at the Fermi level means that the spectral function has

three peaks in general, two of which are revealed in the mean field analysis, but a third one exists, which is of a width of the order of a very low temperature T_K , and hence is not noticed at higher temperatures.

Eq. 2.150 can be written as

$$T_1 = \frac{J/2}{1 - 2J\gamma - \frac{J}{2}(\alpha + \gamma)} \quad (2.158)$$

$$T_0 = \frac{-3J/2}{1 - 2J\gamma + \frac{3J}{2}(\alpha + \gamma)} \quad (2.159)$$

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

$$\begin{aligned} T_1 &= \frac{1}{\frac{2}{J_{\text{eff}}} - (\alpha + \gamma)} \\ T_0 &= \frac{-1}{\frac{2}{3J_{\text{eff}}} + \alpha + \gamma} \end{aligned} \quad (2.160)$$

$\alpha + \gamma$ can be calculated as

$$\begin{aligned} \alpha + \gamma &= \lim_{\eta \rightarrow 0} \int_0^\infty d\epsilon \frac{N(\epsilon)}{\epsilon_k - \epsilon + i\eta} \\ &\sim \lim_{\epsilon_{\text{up}} \rightarrow \infty} \ln \left| \frac{\sqrt{\epsilon_k} - \sqrt{\epsilon_{\text{up}}}}{\sqrt{\epsilon_k} + \sqrt{\epsilon_{\text{up}}}} \right| - i\pi N(0) \end{aligned} \quad (2.161)$$

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

$$\left| \frac{\sqrt{\epsilon_k} - \sqrt{\epsilon_{\text{up}}}}{\sqrt{\epsilon_k} + \sqrt{\epsilon_{\text{up}}}} \right| \approx \left| \frac{-\sqrt{\epsilon_{\text{up}}}}{\sqrt{\epsilon_{\text{up}}}} \right| = 1 \quad (2.162)$$

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

$$T_1 = \frac{1}{2J_{\text{eff}}^{-1} + i\pi N(0)} \sim \frac{1}{\frac{2}{\pi N(0)J_{\text{eff}}} + i} \quad (2.163)$$

Since

$$T_s \sim e^{i\delta_s} \sin \delta_s = \frac{1}{\cot \delta_s - i} \quad (2.164)$$

we can write

$$\cot \delta_1 = -\frac{2}{\pi N(0)J_{\text{eff}}} \implies \tan \delta_1 = -\frac{\pi}{2} N(0)J_{\text{eff}} \quad (2.165)$$

Similarly,

$$T_0 = \frac{-1}{\frac{2}{3J_{\text{eff}}} - i\pi N(0)} \sim \frac{-1}{\frac{2}{3J_{\text{eff}}\pi N(0)} - i} \quad (2.166)$$

giving

$$\cot \delta_0 = \frac{2}{3J_{\text{eff}}\pi N(0)} \implies \tan \delta_0 = \frac{3\pi}{2} J_{\text{eff}} N(0) \quad (2.167)$$

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

$$\psi \sim \psi_{\text{in}} - e^{2i\delta_d} \psi_{\text{out}} \quad (2.168)$$

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,

$$\psi = \frac{e^{i\delta}}{r} (e^{-i(k_F r + \delta_d)} - e^{i(k_F r + \delta_d)}) \sim \frac{e^{i\delta}}{r} \sin[k_F(r + \Delta r)] \quad (2.169)$$

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.

2.12 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 $E = 0$:

$$\Sigma(E) = \Sigma(0) + E \left. \frac{d\Sigma}{dE} \right|_{E=0} + O(E^2) \quad (2.170)$$

Defining

$$Z^{-1} \equiv 1 - \left. \frac{d\Sigma}{dE} \right|_{E=0} \quad (2.171)$$

we can write

$$\Sigma(E) = \Sigma(0) + (1 - Z^{-1}) E \quad (2.172)$$

The interacting Green's function for the impurity becomes

$$G_d(E) = \frac{1}{E - \epsilon_d - \Sigma - i\Delta} \quad (2.173)$$

where Δ is the result of the hybridisation. Substituting eq. 2.172 and gathering the terms gives

$$G_d(E) = \frac{Z}{E - Z(\epsilon_d + \Sigma(0)) - iZ\Delta} \quad (2.174)$$

Defining the renormalised parameters

$$\epsilon_d^* = Z(\epsilon_d + \Sigma(0)) \quad (2.175)$$

$$\Delta^* = Z\Delta \quad (2.176)$$

we have

$$G_d(E) = \frac{Z}{E - \epsilon_d^* - i\Delta^*} \quad (2.177)$$

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

$$Z = 1, \Sigma = 0 \implies \epsilon_d^* = \epsilon_d, \Delta^* = \Delta \quad (2.178)$$

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.2.63, and replacing the bare quantities with the renormalised versions:

$$\delta_d(0) = \cot^{-1} \frac{\epsilon_d^*}{\Delta^*} \quad (2.179)$$

Similarly, the renormalised version of eq. 2.52 is

$$\rho_d(0) = \frac{1}{\pi} \frac{\Delta^*}{\epsilon_d^{*2} + \Delta^{*2}} \quad (2.180)$$

Using eq. 2.179 gives

$$\rho_d(0) = \frac{1}{\pi} \frac{\Delta^*}{\Delta^{*2} \cot^2 \delta_d + \Delta^{*2}} = \frac{\sin^2 \delta_d}{\pi \Delta} \quad (2.181)$$

2.13 The Kondo temperature

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

$$H_K = \sum_{k>k_F} \epsilon_k n_k - \frac{3J}{2} \sum_{k,k'>k_F} c_{k'\sigma}^\dagger c_{k\sigma} \quad (2.182)$$

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

$$b_k^\dagger = \frac{1}{\sqrt{2}} (c_{k\uparrow}^\dagger c_{d\downarrow}^\dagger - c_{k\downarrow}^\dagger c_{d\uparrow}^\dagger) \quad (2.183)$$

Hence the total wavefunction of singlet+Fermi-sea is

$$|\Psi\rangle = \sum_{k>k_F} a_k b_k^\dagger |\Phi\rangle = |\Phi\rangle \otimes \sum_{k>k_F} a_k |S_k\rangle \quad (2.184)$$

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

$$a_q = \langle \Phi | \langle S_q | \sum_k a_k |S_k\rangle | \Phi \rangle = \langle \Phi | b_q | \Psi \rangle \quad (2.185)$$

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

$$\begin{aligned} E |\Psi\rangle &= H_K |\Psi\rangle = |\Phi\rangle \otimes H_k \sum_{k>k_F} a_k |S_k\rangle \\ &= |\Phi\rangle \otimes \sum_{k>k_F} a_k \left(\epsilon_k |S_k\rangle - \frac{3J}{2} \sum_{k'>k_F} |S_{k'}\rangle \right) \\ &= \sum_{k>k_F} a_k \left(\epsilon_k b_k^\dagger - \frac{3J}{2} \sum_{k'>k_F} b_{k'}^\dagger \right) |\Phi\rangle \end{aligned} \quad (2.186)$$

Multiplying b_q from left gives

$$Eb_q |\Psi\rangle = \epsilon_q a_q |\Phi\rangle - \frac{3J}{2} \sum_{k>k_F} a_k |\Phi\rangle \quad (2.187)$$

Multiplying $\langle\Phi|$ from left and looking at eq. 2.185 gives

$$\begin{aligned} E \langle\Phi| b_q |\Psi\rangle &= E a_q = a_q \epsilon_q - \frac{3J}{2} \sum_k a_k \\ \implies a_q &= \frac{3J/2}{\epsilon_q - E} \sum_k a_k \\ \implies \sum_q a_q &= \sum_q \frac{3J/2}{\epsilon_q - E} \sum_k a_k \end{aligned} \quad (2.188)$$

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

$$1 = \frac{3J}{2} \sum_{q>k_F} \frac{1}{\epsilon_q - E} \quad (2.189)$$

Converting to integral,

$$1 = \frac{3J}{2} \int_{\epsilon_F}^D d\epsilon \frac{N(\epsilon)}{\epsilon - E} \quad (2.190)$$

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

$$\begin{aligned} \frac{2}{3JN(0)} &= \ln \left| \frac{D - E}{\epsilon_F - E} \right| \approx \ln \left| \frac{D}{\epsilon_F - E} \right| \\ \implies E &= \epsilon_F - D e^{-\frac{2}{3N(0)J}} \end{aligned} \quad (2.191)$$

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

$$E_b = D e^{-\frac{2}{3N(0)J}} \quad (2.192)$$

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

$$k_B T_K \sim E_b \implies T_K = \frac{D}{k_B} e^{-\frac{2}{3N(0)J}} \quad (2.193)$$

2.14 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

$$T^{(2)} = V G_0 V \quad (2.194)$$

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

$$H' = J_z \sum_{k_1, k_2} S_d^z \left(c_{k_1\uparrow}^\dagger c_{k_2\uparrow} - c_{k_1\downarrow}^\dagger c_{k_2\downarrow} \right) + J_T \sum_{k_1, k_2} \left(S_d^+ c_{k_1\downarrow}^\dagger c_{k_2\uparrow} + S_d^- c_{k_1\uparrow}^\dagger c_{k_2\downarrow} \right) \quad (2.195)$$

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 .

2.14.1 Renormalization of J_z

First consider the process

$$k \uparrow, d \downarrow \rightarrow q \downarrow, d \uparrow \rightarrow k' \uparrow, d \downarrow \quad (2.196)$$

The T -matrix term is

$$T_1 = J_T^2 \sum_q S_d^- c_{k'\uparrow}^\dagger c_{q\downarrow} \frac{1}{E - H_0} S_d^+ c_{q\downarrow}^\dagger c_{k\uparrow} \quad (2.197)$$

Using eq. 2.16, we can write

$$(E - H_0)^{-1} c_{q\downarrow}^\dagger c_{k\uparrow} = c_{q\downarrow}^\dagger c_{k\uparrow} (E - \lambda - H_0)^{-1} \quad (2.198)$$

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,

$$T_1 = J_T^2 S_d^- S_d^+ \sum_q c_{k'\uparrow}^\dagger c_{q\downarrow} c_{q\downarrow}^\dagger c_{k\uparrow} (E - \epsilon_q + \epsilon_k - H_0)^{-1} \quad (2.199)$$

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

$$T_1 = J_T^2 S_d^- S_d^+ c_{k'\uparrow}^\dagger c_{k\uparrow} \sum_q (E - \epsilon_q + \epsilon_k - H_0)^{-1} \quad (2.200)$$

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

$$\sum_q (E - \epsilon_q + \epsilon_k - H_0)^{-1} = N |\delta D| \frac{1}{E - D + \epsilon_k} \quad (2.201)$$

N is the density of states. Also,

$$S^- S^+ = (S^x - iS^y)(S^x + iS^y) = \frac{1}{2} + i[S^x, S^y] = \frac{1}{2} - S^z \quad (2.202)$$

Putting it all together,

$$T_1 = J_T^2 \left(\frac{1}{2} - S_d^z \right) N |\delta D| c_{k'\uparrow}^\dagger c_{k\uparrow} \frac{1}{E - D + \epsilon_k} \quad (2.203)$$

For the second possible scattering,

$$q \downarrow k \uparrow d \uparrow \rightarrow k' \uparrow k \uparrow d \downarrow \rightarrow k' \uparrow q \downarrow d \uparrow \quad (2.204)$$

we get

$$T_2 = J_T^2 \sum_q S_d^+ S_d^- c_{q\downarrow}^\dagger c_{k\uparrow} \frac{1}{E - H_0} c_{k'\uparrow}^\dagger c_{q\downarrow} \quad (2.205)$$

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

$$\begin{aligned} T_2 &= J_T^2 \left(\frac{1}{2} + S_d^z \right) N |\delta D| c_{k\uparrow} c_{k'\uparrow}^\dagger \frac{1}{E - D - \epsilon_{k'}} \\ &= -J_T^2 \left(\frac{1}{2} + S_d^z \right) N |\delta D| c_{k'\uparrow}^\dagger c_{k\uparrow} \frac{1}{E - D - \epsilon_{k'}} \end{aligned} \quad (2.206)$$

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

$$k \downarrow, d \uparrow \rightarrow q \uparrow d \downarrow \rightarrow k' \downarrow d \uparrow \quad (2.207)$$

$$q \uparrow k \downarrow d \downarrow \rightarrow k' \downarrow k \downarrow d \uparrow \rightarrow k' \downarrow q \uparrow d \downarrow \quad (2.208)$$

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

$$T_3 = J_T^2 \left(\frac{1}{2} + S_d^z \right) N |\delta D| c_{k'\downarrow}^\dagger c_{k\downarrow} \frac{1}{E - D + \epsilon_k} \quad (2.209)$$

$$T_4 = -J_T^2 \left(\frac{1}{2} - S_d^z \right) N |\delta D| c_{k'\downarrow}^\dagger c_{k\downarrow} \frac{1}{E - D - \epsilon_{k'}} \quad (2.210)$$

The total second order contribution is

$$T^{(2)} = -J_T^2 S_d^z N |\delta D| \left(\frac{1}{E - D + \epsilon_k} + \frac{1}{E - D - \epsilon_{k'}} \right) (c_{k'\uparrow}^\dagger c_{k\uparrow} - c_{k'\downarrow}^\dagger c_{k\downarrow}) \quad (2.211)$$

Comparing this with the S_d^z term in the Hamiltonian

$$J_z S_d^z (c_{k'\uparrow}^\dagger c_{k\uparrow} - c_{k'\downarrow}^\dagger c_{k\downarrow}) \quad (2.212)$$

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

$$\delta J_d^z = -J_T^2 N |\delta D| \left(\frac{1}{E - D + \epsilon_k} + \frac{1}{E - D - \epsilon_{k'}} \right) \quad (2.213)$$

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

$$\frac{dJ_d^z}{dD} = -J_T^2 N \frac{2}{D} \quad (2.214)$$

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

2.14.2 Renormalization of J_T

Consider the scattering

$$k \uparrow d \downarrow \rightarrow q \downarrow d \uparrow \rightarrow k' \downarrow d \uparrow \quad (2.215)$$

$$T_1 = -J_T J_z S_d^z S_d^+ N |\delta D| c_{k'\downarrow}^\dagger c_{k\uparrow} \frac{1}{E - D + \epsilon_k} \quad (2.216)$$

The minus sign at the front comes from the term

$$-S_d^z c_{k'\downarrow}^\dagger c_{q\downarrow} \quad (2.217)$$

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

$$T_1 = -J_T J_z \frac{S_d^+}{2} N |\delta D| c_{k'\downarrow}^\dagger c_{k\uparrow} \frac{1}{E - D + \epsilon_k} \quad (2.218)$$

The second process is

$$q \uparrow k \uparrow d \downarrow \rightarrow k' \downarrow k \uparrow d \uparrow \rightarrow q \uparrow k' \downarrow d \uparrow \quad (2.219)$$

$$T_2 = -J_T J_z \frac{S_d^+}{2} N |\delta D| c_{k'\downarrow}^\dagger c_{k\uparrow} \frac{1}{E - D - \epsilon_{k'}} \quad (2.220)$$

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

$$+S_d^z c_{k'\uparrow}^\dagger c_{q\uparrow} \quad (2.221)$$

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

$$-S_d^z c_{k'\downarrow}^\dagger c_{q\downarrow} \quad (2.222)$$

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

$$T_3 = T_1 \quad (2.223)$$

$$T_4 = T_2 \quad (2.224)$$

The total contribution is

$$T^{(2)} = -J_T J_z S_d^+ N |\delta D| c_{k'\downarrow}^\dagger c_{k\uparrow} \left(\frac{1}{E - D - \epsilon_{k'}} + \frac{1}{E - D + \epsilon_k} \right) \quad (2.225)$$

Comparing with the S_d^+ term in the Hamiltonian

$$J_T S_d^+ c_{k'\downarrow}^\dagger c_{k\uparrow} \quad (2.226)$$

we can write

$$\delta J_T = -J_T J_z N |\delta D| \left(\frac{1}{E - D - \epsilon_{k'}} + \frac{1}{E - D + \epsilon_k} \right) \quad (2.227)$$

Again neglecting the terms in the denominator, we get

$$\frac{dJ_T}{dD} = -J_T J_z N \frac{2}{D} \quad (2.228)$$

This is the scaling equation for J_T .

2.14.3 Flow of the couplings

Switching to the dimensionless couplings

$$g_1 = NJ_z, g_2 = NJ_T \quad (2.229)$$

the equations become

$$\frac{dg_1}{dD} = -\frac{2g_2^2}{D} \quad (2.230)$$

$$\frac{dg_2}{dD} = -\frac{2g_1g_2}{D} \quad (2.231)$$

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

$$\frac{dg_1}{dg_2} = \frac{g_2}{g_1} \implies g_1^2 - g_2^2 = \text{constant} \quad (2.232)$$

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

$$\begin{aligned} g(D') &= \frac{g_0}{1 - 2g_0 \ln \frac{D}{D'}} \\ \implies 2g(D') &= \frac{1}{\ln \frac{D'}{T_K}} \end{aligned} \quad (2.233)$$

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. 2.193, 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.

$$g(D') = \frac{g_0}{1 - 2g_0 \ln \frac{D}{D'}} = -\frac{|g_0|}{1 + 2|g_0| \ln \frac{D}{D'}} \quad (2.234)$$

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

2.14.4 Alternate way of obtaining the scaling equations

From eq. 2.98, the interaction part can be written as

$$\Delta H_{ll'} = \frac{1}{2} [T_{ll'}(E_l) + T_{ll'}(E_{l'})] \quad (2.235)$$

where the transition matrix T is

$$T_{ll'}(E) = \sum_H \frac{V_{lH} V_{Hl'}}{E - E_H} \quad (2.236)$$

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

$$V = J \vec{S}_d \cdot \sum_{k,k',\alpha,\alpha'} c_{k\alpha}^\dagger \vec{\sigma}_{\alpha\alpha'} c_{k'\alpha'} \quad (2.237)$$

The first process is

$$k\alpha \xrightarrow{\sigma^b} q\lambda \xrightarrow{\sigma^a} k'\beta \quad (2.238)$$

$$d\sigma \xrightarrow{S_d^b} d\sigma'' \xrightarrow{S_d^a} d\sigma' \quad (2.239)$$

The transition matrix element is

$$\begin{aligned} T_1 &= \sum_{q \in \{D-\delta D\}, \lambda, \sigma''} \langle k'\beta, \sigma' | V | q\lambda, \sigma'' \rangle \langle q\lambda, \sigma'' | V | k\alpha, \sigma \rangle \frac{1}{E - E_q} \\ &= J^2 \sum_{\sigma''} (S_d^a)_{\sigma'\sigma''} (S_d^b)_{\sigma''\sigma} \sum_{\lambda} (\sigma^a)_{\beta\lambda} (\sigma^b)_{\lambda\alpha} \sum_{q \in \{D-\delta D\}} \frac{1}{E - E_q} \\ &\approx J^2 (S_d^a S_d^b)_{\sigma'\sigma} (\sigma^a \sigma^b)_{\beta\alpha} \frac{N|\delta D|}{E - D} \end{aligned} \quad (2.240)$$

The second process is

$$k\alpha \longrightarrow k\alpha \xrightarrow{\sigma^a} q\lambda \quad (2.241)$$

$$q\lambda \xrightarrow{\sigma^b} k'\beta \longrightarrow k'\beta \quad (2.242)$$

$$d\sigma \xrightarrow{S_d^b} d\sigma'' \xrightarrow{S_d^a} d\sigma' \quad (2.243)$$

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

$$\begin{aligned} T_2 &= \sum_{q \in \{D-|\delta D|\}, \lambda, \sigma''} \langle q\lambda, k'\beta, \sigma' | V | k'\beta, k\alpha, \sigma'' \rangle \langle k'\beta, k\alpha, \sigma'' | V | q\lambda, k\alpha, \sigma \rangle \frac{1}{E - (E_k + E_{k'} - E_q)} \\ &\approx -J^2 (S_d^a S_d^b)_{\sigma'\sigma} (\sigma^b \sigma^a)_{\beta\alpha} \frac{N|\delta D|}{E - D} \end{aligned} \quad (2.244)$$

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

$$\begin{aligned} T &= \frac{J^2 N |\delta D|}{D} (S_d^a S_d^b)_{\sigma'\sigma} [\sigma^b, \sigma^a]_{\beta\alpha} \\ &= \frac{J^2 N |\delta D|}{2D} [S_d^a, S_d^b]_{\sigma'\sigma} [\sigma^b, \sigma^a]_{\beta\alpha} \end{aligned} \quad (2.245)$$

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

$$\begin{aligned}
 [S_d^a, S_d^b]_{\sigma'\sigma} [\sigma^b, \sigma^a]_{\beta\alpha} &= -[S_d^a, S_d^b]_{\sigma'\sigma} [\sigma^a, \sigma^b]_{\beta\alpha} \\
 &= -i\epsilon_{abc} S_{\sigma\sigma'}^c 2i\epsilon_{abd} \sigma_{\beta\alpha}^d \\
 &= 4\delta_{cd} S_{\sigma\sigma'}^c \sigma_{\beta\alpha}^d \\
 &= 4\vec{S}_{\sigma\sigma'} \cdot \vec{\sigma}_{\beta\alpha}
 \end{aligned} \tag{2.246}$$

Therefore,

$$T = \frac{2J^2 N |\delta D|}{D} \vec{S}_{\sigma\sigma'} \cdot \vec{\sigma}_{\beta\alpha} \tag{2.247}$$

The correction to the coupling J can be read off:

$$J(D - \delta D) = J(D) - \frac{2J^2 N \delta D}{D} \tag{2.248}$$

This gives the same scaling equations we found earlier.

2.15 Universality

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

$$\frac{\partial g}{\partial \ln D} = -2g^2 + 2g^3 \tag{2.249}$$

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

$$\ln \frac{D'}{D} = - \int_{g_0}^g \frac{dg}{2g^2 - 2g^3} = - \int_{g_0}^g \frac{dg}{2g^2} (1 + g) \tag{2.250}$$

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

$$\begin{aligned}
 \ln \frac{k_B T_K}{D} &= - \int_{g_0}^1 \frac{dg}{2g^2} (1 + g) = -\frac{1}{2g_0} + \frac{1}{2} \ln g_0 + O(1) \\
 &= -\frac{1}{2g_0} + \frac{1}{2} \ln 2g_0 + O(1)
 \end{aligned} \tag{2.251}$$

This gives a better estimate of the Kondo temperature

$$T_K = \frac{D}{k_B} \sqrt{2g_0} \exp\left(-\frac{1}{2g_0}\right) \tag{2.252}$$

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

$$k_B T_K = Dy(g) \tag{2.253}$$

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

$$\frac{dT_K}{dD} = 0 \tag{2.254}$$

Substituting the form of T_K , eq. 2.253, in this equation gives

$$\begin{aligned}
 y(g) + D \frac{dy(g)}{dD} &= 0 \\
 \implies y + D \frac{dy}{dg} \frac{dg}{dD} &= 0 \\
 \implies y - 2g^2 \frac{dy}{dg} &= 0 \\
 \implies y &= e^{-\frac{1}{2g}}
 \end{aligned} \tag{2.255}$$

This gives almost the same solution as eq. 2.252:

$$T_K = \frac{D}{k_B} e^{-\frac{1}{2g}} \tag{2.256}$$

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. 2.233, up to second order, we can write

$$g(D') = g_0 \left(1 + 2g_0^2 \ln \frac{D}{D'} \right) \tag{2.257}$$

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

$$g_0 \rightarrow g = g_0 \left(1 + 2g_0 \ln \frac{T_F}{T} \right) \tag{2.258}$$

Since $g \equiv NJ$, we have recovered eq. 2.139. Since eq. 2.139 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.

2.16 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 [13]. For example,

$$S^z = \frac{\sigma^z}{2} = \sum_{ij} c_i^\dagger \frac{\sigma_{ij}^z}{2} c_j = \frac{1}{2} (c_\uparrow^\dagger c_\uparrow - c_\downarrow^\dagger c_\downarrow) \tag{2.259}$$

Similarly,

$$\begin{aligned}
 S^x &= \frac{1}{2} (c_\uparrow^\dagger c_\downarrow + c_\downarrow^\dagger c_\uparrow) \\
 S^y &= \frac{-i}{2} (c_\uparrow^\dagger c_\downarrow - c_\downarrow^\dagger c_\uparrow)
 \end{aligned} \tag{2.260}$$

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

$$|\uparrow\rangle = c_\uparrow^\dagger |0\rangle \tag{2.261}$$

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 [14]

$$\mu = -i\frac{\pi}{2}k_B T \quad (2.262)$$

The new Hamiltonian is

$$\tilde{H} = H - \mu(n_d - 1) \quad (2.263)$$

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

$$Z = \text{Tr} [\exp(-\beta H)] = \sum_{\sigma_d=\uparrow,\downarrow} \sum_k [\exp(-\beta H)] \quad (2.264)$$

The modified partition function is

$$\begin{aligned} \tilde{Z} &= \text{Tr} [\exp(-\beta (H - \mu(n_d - 1)))] \\ &= \text{Tr} \left[\exp \left(-\beta H - i\frac{\pi}{2}(n_d - 1) \right) \right] \\ &= \sum_{\sigma_d=\uparrow,\downarrow} \sum_k [\exp(-\beta H)] + \sum_k \exp \left(-\beta H + i\frac{\pi}{2} \right) + \sum_k \exp \left(-\beta H - i\frac{\pi}{2} \right) \\ &= Z \Big|_{n_d=1} + iZ \Big|_{n_d=0} - iZ \Big|_{n_d=0} \end{aligned} \quad (2.265)$$

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

$$Z \Big|_{n_d=0} = Z \Big|_{n_d=0} \quad (2.266)$$

Hence,

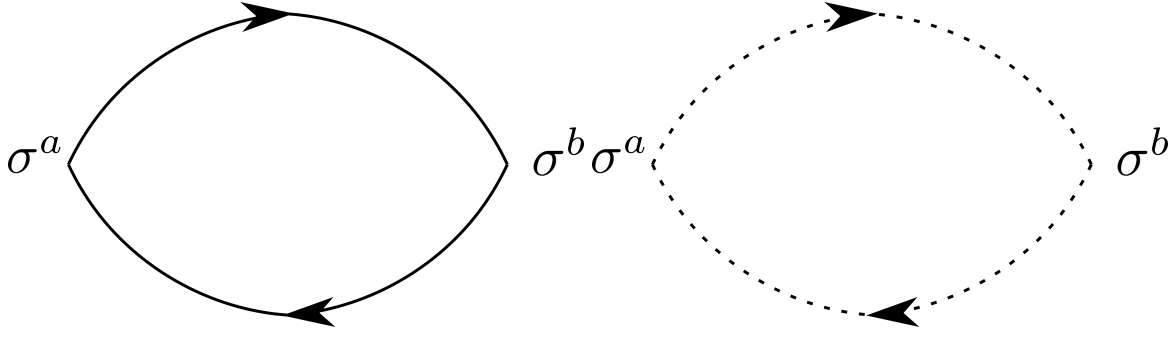
$$\tilde{Z} = Z \quad (2.267)$$

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

$$\chi_c = -k_B T \sum_{k, \omega_n, \phi_0} \langle \phi_0 | \sigma^a G(k, i\omega_n) \sigma^b G_k(i\omega_n) | \phi_0 \rangle \quad (2.268)$$



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

$$\begin{aligned}
 \chi_c &= -k_B T \sum_{k, \omega_n} \text{Tr} [\sigma^a G(k, i\omega_n) \sigma^b G(k, i\omega_n)] \\
 &= -2k_B T \sum_{k, \omega_n} G^2(k, i\omega_n) \\
 &= -2k_B T \sum_{k, \omega_n} (i\omega_n - \epsilon_k)^{-2} \\
 &= 2 \sum_k \frac{d}{d\epsilon_k} k_B T \sum_{\omega_n} (i\omega_n - \epsilon_k)^{-1}
 \end{aligned} \tag{2.269}$$

Now, it can be shown that

$$k_B T \sum_{\omega_n} (i\omega_n - \epsilon_k)^{-1} = f(\epsilon_k) - \frac{1}{2} \tag{2.270}$$

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

$$\chi_c = 2 \sum_k \frac{df(\epsilon_k)}{d\epsilon_k} = 2 \sum_k \rho(\epsilon_k) = 2N(0) \tag{2.271}$$

The second diagram gives

$$\chi_d^{(0)} = -k_B T \sum_{\omega_n} \text{Tr} [\sigma^a G_d(i\omega_n) \sigma^b G_d(i\omega_n)] \tag{2.272}$$

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

$$G_d = \frac{1}{i\omega_n - \lambda_d} \tag{2.273}$$

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

$$\chi_d^{(0)} = 2 \frac{df(\lambda_d)}{d\lambda_d} = -2\beta \frac{e^{\beta\lambda_d}}{(1 + e^{\beta\lambda_d})^2} = \beta \tag{2.274}$$

The first order diagrams are The first diagram gives

$$\chi^{(1)} = \chi_c \left(-\frac{J}{2} \right) \chi_d = -\beta J N(0) \tag{2.275}$$

The second one gives

$$\chi_d^{(1)} = \chi_d \left(-\frac{J}{2} \right) \chi_c = -\beta J N(0) \quad (2.276)$$

The total susceptibility is

$$\chi_d = \chi_d^{(0)} + \chi_d^{(1)} = \beta (1 - 2JN(0)) \quad (2.277)$$

2.17 Nozières' local Fermi liquid theory

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

$$C_V = \gamma T \quad (2.278)$$

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

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

$$E_g = J \left[2\vec{S}_e \cdot \vec{S}_d \right] = J \left[S^2 - S_d^2 - S_e^2 \right] = J \left[s(s+1) - \frac{3}{2} \right] = -\frac{3J}{2} \quad (2.279)$$

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,

$$\frac{|0_\uparrow, d_\downarrow\rangle - |0_\downarrow, d_\uparrow\rangle}{\sqrt{2}} \quad (2.280)$$

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

$$E_1 = -\frac{3}{2}J + \frac{3}{2}J = 0 \quad (2.281)$$

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 [15] 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

$$\psi \sim \frac{\sin[kr + \delta(E_k)]}{r} \quad (2.282)$$

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.

$$n = \sum_{\sigma} \frac{\delta}{\pi} \implies 1 = \frac{2\delta}{\pi} \implies \delta = \frac{\pi}{2} \quad (2.283)$$

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

$$k_F a = \delta(0) \implies \delta(0) = \frac{\pi}{2a} 2 = \frac{\pi}{2} \quad (2.284)$$

where the formula for k_F was used.

In a Fermi gas, the energy levels are separated by

$$\Delta\epsilon = \frac{\partial\epsilon}{\partial k} \Delta k \quad (2.285)$$

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

$$\Delta\epsilon = \frac{\partial\epsilon}{\partial k} \frac{\pi}{L} \quad (2.286)$$

However, this changes in the presence of the impurity. Because of eq. 2.282, the boundary condition becomes

$$k_n L + \delta(\epsilon_k) = n\pi \implies k_n = \frac{n\pi}{L} - \frac{\delta}{L} = k_n^0 - \frac{\delta(\epsilon_k)}{L} \quad (2.287)$$

The energy becomes

$$\begin{aligned} \epsilon(k) &= \epsilon(k^0) + \frac{\partial\epsilon}{\partial k} (k - k_0) \\ &= \epsilon_k - \frac{\partial\epsilon}{\partial k} \frac{\delta(\epsilon_k)}{L} \end{aligned} \quad (2.288)$$

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

$$\tilde{\epsilon}_{\sigma}(k) = \epsilon_k - \frac{\partial\epsilon}{\partial k} \frac{\delta_{\sigma}(\epsilon_k, \{n_{q,\sigma}\})}{L} \quad (2.289)$$

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 ,

$$\begin{aligned} \tilde{\epsilon}_p &= \underbrace{\epsilon_F}_{\text{Fermi gas}} + \overbrace{\frac{p_F^*}{m} (p - p_F)}^{\text{linear contribution for } p \text{ close to } p_F} \\ &+ \underbrace{\sum_{q\sigma} f(p, q) (n_q - n_q^0)}_{\text{interacting between two quasiparticles at momenta } p \text{ and } q} \end{aligned} \quad (2.290)$$

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,

$$\delta_\sigma(\tilde{\epsilon}, \{n_{q,\sigma}\}) = \delta_\sigma(\tilde{\epsilon} = \epsilon_F, n_k = n_k^0) + \alpha(\tilde{\epsilon} - \epsilon_F) + \Phi \sum_{q\sigma'} (n_{q\sigma'} - n_{q\sigma'}^0) \quad (2.291)$$

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. 2.290. Specifically, Φ represents the onsite interaction between quasiparticles of opposite spin and

$$\alpha = \frac{d\delta_\sigma}{dE} \quad (2.292)$$

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

$$\delta_\sigma(\tilde{\epsilon}, \{n_{q,\sigma}\}) = \delta_\sigma(\tilde{\epsilon} = \epsilon_F, n_k = n_k^0) + \alpha(\tilde{\epsilon} - \epsilon_F) + \Phi \sum_q \delta n_{q,-\sigma} \quad (2.293)$$

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,

$$\delta_\uparrow^0 = \frac{\pi}{2} + \Phi \sum_q \delta n_{q\downarrow}^0 \quad (2.294)$$

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

$$\delta_\uparrow^0 = \frac{\pi}{2} \quad (2.295)$$

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

$$N(\mu = 0) = N^0 \quad (2.296)$$

$$N(E' = E + \mu) = N(E' = E) + \frac{dN}{dE'}(E' - E) = N^0 + \rho\Delta\mu \quad (2.297)$$

$$\implies \sum_q \delta n_q = N - N^0 = \rho\Delta\mu \quad (2.298)$$

Hence, from eq. 2.293,

$$\begin{aligned} \delta_\uparrow &= \frac{\pi}{2} + \alpha(\epsilon'_F - \epsilon_F) + \Phi \sum_q \delta n_{q\downarrow} \\ &= \delta_\uparrow^0 + \alpha\Delta\mu + \Phi\rho\Delta\mu \end{aligned} \quad (2.299)$$

Hence the change in the phase is

$$0 = \Delta\delta_\uparrow = \Delta\mu(\alpha + \Phi\rho) \implies \alpha = -\Phi\rho \quad (2.300)$$

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

$$n_\sigma = \frac{kL}{\pi} + \frac{\delta_\sigma(E)}{\pi} = n^0 + \frac{\delta_\sigma(E)}{\pi} \quad (2.301)$$

Hence,

$$\begin{aligned} \rho &= \frac{dn_\sigma}{dE} = \rho^0 + \frac{1}{\pi} \frac{d\delta_\sigma}{dE} \\ \implies \rho &= \rho^0 + \frac{1}{\pi} \alpha \end{aligned} \quad (2.302)$$

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

$$C_v^0 = \gamma T = \frac{\pi^2 k_B^2}{3} \mathcal{N}(0) T \quad (2.303)$$

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

$$\begin{aligned} C_v &= \frac{\pi^2 k_B^2}{3} (\rho_\uparrow + \rho_\downarrow) T \\ &= \frac{2\alpha}{\pi} \frac{\pi^2 k_B^2}{3} T \end{aligned} \quad (2.304)$$

In presence of a magnetic field B , the magnetization is

$$m = \delta n \times \mu \quad (2.305)$$

where μ is the magnetic moment

$$\mu = -\frac{g}{2} \mu_B \quad (2.306)$$

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

$$\delta n = \langle n_\uparrow \rangle - \langle n_\downarrow \rangle = \frac{1}{\pi} (\delta_\uparrow - \delta_\downarrow) \quad (2.307)$$

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

$$E_\sigma^B = E - \sigma \frac{g\mu_B}{2} B \quad (2.308)$$

Hence,

$$\sum_k \delta n_{k\sigma} = N_\sigma(E_\sigma^B) - N(E) = \frac{dN}{dE^B} (E^B - E) = -\rho \frac{g\mu_B}{2} \sigma B \quad (2.309)$$

This modifies the phase shift at the Fermi surface,

$$\begin{aligned}\delta_\sigma(\epsilon_F) &= \frac{\pi}{2} + \alpha \left(\epsilon_F - \frac{g\mu_B}{2}\sigma B - \epsilon_F \right) + \Phi \sum_q \delta n_{q,-\sigma} \\ &= \frac{\pi}{2} - \sigma \frac{g\mu_B}{2} \alpha B + \Phi \rho \frac{g\mu_B}{2} \sigma B \\ &= \frac{\pi}{2} - 2\alpha \frac{g\mu_B}{2} \sigma B\end{aligned}\tag{2.310}$$

Hence,

$$\delta n = \frac{1}{\pi} (\delta_\uparrow - \delta_\downarrow) = -\frac{4\alpha B}{\pi} \frac{g\mu_B}{2}\tag{2.311}$$

The susceptibility is

$$\chi = \frac{\partial m}{\partial B} = \frac{\partial}{\partial B} \mu \delta n = \frac{4\alpha}{\pi} \left(\frac{g\mu_B}{2} \right)^2\tag{2.312}$$

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

$$\mu = -\frac{g}{2} \mu_B\tag{2.313}$$

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

$$\delta n = n_\uparrow(0) - n_\downarrow(0) = n_\uparrow(\epsilon_F - \frac{g}{2} \mu_B B) - n_\downarrow(\epsilon_F + \frac{g}{2} \mu_B B) = -\frac{1}{2} \mathcal{N}(0) g B \mu_B\tag{2.314}$$

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

$$m = \delta n \times \mu = \mathcal{N}(0) \left(\frac{g}{2} \mu_B \right)^2 B\tag{2.315}$$

The magnetic susceptibility comes out to be

$$\chi^0 = \left. \frac{\partial m}{\partial B} \right|_{B \rightarrow 0} = \mathcal{N}(0) \left(\frac{g}{2} \mu_B \right)^2\tag{2.316}$$

The Wilson ratio R can now be computed,

$$R = \frac{\chi/\chi_0}{C_v/C_v^0} = \frac{4\alpha/\pi \mathcal{N}(0)}{2\alpha/\pi \mathcal{N}(0)} = 2\tag{2.317}$$

2.18 Numerical renormalization group calculation

Wilson's idea [16] 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

$$H = \sum_k \epsilon_k n_k + J \vec{S}_d \cdot \vec{\sigma}_e\tag{2.318}$$

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 $H_c|0\rangle$,

$$|1\rangle = (\lambda_1 H_c |0\rangle + \lambda_2 |0\rangle) \quad (2.319)$$

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:

$$|1\rangle = \frac{1}{\gamma_0} (H_c |0\rangle + \lambda |0\rangle) \quad (2.320)$$

where γ_0 sets $\langle 1|1\rangle = 1$. The remaining parameter is set by requiring $\langle 1|0\rangle = 0$. That gives

$$\lambda = -\langle 0|H_c|0\rangle \quad (2.321)$$

Therefore,

$$|1\rangle = \frac{1}{\gamma_0} (H_c |0\rangle - \langle 0|H_c|0\rangle |0\rangle) \quad (2.322)$$

The general state can be shown to be

$$|n+1\rangle = \frac{1}{\gamma_n} (H_c |n\rangle - |n\rangle \langle n|H_c|n-1\rangle - |n-1\rangle \langle n-1|H_c|n\rangle) \quad (2.323)$$

From eq. 2.323, by multiplying $\langle n'|$ from left, we get

$$\delta_{n',n+1} = \frac{1}{\gamma_n} \left[(H_c)_{n',n} + (H_c)_{n,n-1} \delta_{n',n} + (H_c)_{n-1,n} \delta_{n',n-1} \right] \quad (2.324)$$

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

$$(H_c)_{n',n} = 0 \quad (2.325)$$

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

$$(H_c)_{n+1,n} = \gamma_n \quad (2.326)$$

Taking the complex conjugate of this gives

$$\gamma_n^* = (H_c^\dagger)_{n,n+1} = (H_c)_{n,n+1} \quad (2.327)$$

Defining

$$(H_c)_{n,n} = \epsilon_n \quad (2.328)$$

we can write

$$\begin{aligned} H_c &= \sum_{n_1, n_2} |n_1\rangle \langle n_1| H_c |n_2\rangle \langle n_2| \\ &= \sum_n \epsilon_n |n\rangle \langle n| + \sum_n (\gamma_n |n\rangle \langle n+1| + \gamma_n^* |n+1\rangle \langle n|) \\ &= \sum_n \epsilon_n \hat{n}_n + \sum_n \left(\gamma_n c_n^\dagger c_{n+1} + \gamma_n^* c_{n+1}^\dagger c_n \right) \end{aligned} \quad (2.329)$$

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.

2.18.1 Logarithmic discretization

First, note that up to first order

$$\epsilon_k = \epsilon_F + (k - k_F) \frac{\partial \epsilon_k}{\partial k} \quad (2.330)$$

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

$$d_n = \Lambda^{-n} (1 - \Lambda^{-1}) \quad (2.331)$$

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

$$\psi_{m,n}(k) = \frac{1}{\sqrt{d_n}} \exp\left(\frac{2\pi i m}{d_n} k\right) \quad (2.332)$$

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

$$a_{m,n}^\dagger = \sum_k \psi_m(k) c_k^\dagger \quad (2.333)$$

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

$$\phi_{m,n}(k) = \frac{1}{\sqrt{d_n}} \exp\left(-\frac{2\pi i m}{d_n} k\right) \quad (2.334)$$

$$b_{m,n}^\dagger = \sum_k \phi_m(k) c_k^\dagger \quad (2.335)$$

Then,

$$a_{m,n}^\dagger + b_{m,n}^\dagger = \frac{2}{\sqrt{d_n}} \sum_{\pm k \in \mathbb{Z}} \cos\left(\frac{2\pi m k}{d_n}\right) c_k^\dagger \quad (2.336)$$

Summing over n involves summing over all momenta.

$$\begin{aligned} \sum_n (a_{m,n}^\dagger + b_{m,n}^\dagger) &= \frac{2}{\sqrt{d_n}} \sum_k \cos\left(\frac{2\pi m k}{d_n}\right) c_k^\dagger \\ \Rightarrow \sum_n (a_{0,n}^\dagger + b_{0,n}^\dagger) &= \frac{2}{\sqrt{d_n}} \sum_k c_k^\dagger \end{aligned} \quad (2.337)$$

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

$$\sum_{k,q} c_k^\dagger c_q = \sum_k c_k^\dagger \sum_q c_q \quad (2.338)$$

Looking at eq. 2.337, 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

$$\epsilon_n = 0, \gamma = D' \Lambda^{-\frac{n}{2}} \quad (2.339)$$

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

$$H_N = D' \sum_{n=0}^{N-1} \Lambda^{-\frac{n}{2}} \left(c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n \right) + 2J \vec{S}_d \cdot \vec{S}_e \quad (2.340)$$

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

$$H_{N+1} = H_N + D' \Lambda^{-\frac{N}{2}} \left(c_N^\dagger c_{N+1} + c_{N+1}^\dagger c_N \right) \quad (2.341)$$

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. 2.340, the lowest energy scale is $\Gamma_N = D' \Lambda^{-\frac{N-1}{2}}$. Hence, the rescaled Hamiltonian is

$$\bar{H}_N = \frac{H_N}{\Gamma_N} = \frac{\Lambda^{\frac{N-1}{2}}}{D'} H_N \quad (2.342)$$

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

$$\begin{aligned} \bar{H}_{N+1} &= \frac{\Lambda^{\frac{N}{2}}}{D'} \left[H_N + \Lambda^{-\frac{N}{2}} D' \left(c_N^\dagger c_{N+1} + c_{N+1}^\dagger c_N \right) \right] \\ \Rightarrow \bar{H}_{N+1} &= \Lambda^{\frac{1}{2}} \bar{H}_N + \left(c_N^\dagger c_{N+1} + c_{N+1}^\dagger c_N \right) \end{aligned} \quad (2.343)$$

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

$$H = \lim_{N \rightarrow \infty} H_N = \lim_{N \rightarrow \infty} D' \Lambda^{\frac{1-N}{2}} \bar{H}_N \quad (2.344)$$

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

$$\bar{H}_N = \sum_m E_m |m\rangle \langle m| \quad (2.345)$$

The next Hamiltonian is then

$$\bar{H}_{N+1} = \Lambda^{\frac{1}{2}} \sum_m E_m |m\rangle \langle m| + \sum_{m,m'} (C(m, m') |m\rangle \langle m'| + \text{h.c.}) \quad (2.346)$$

This is the same equation as eq. 2.343, with \bar{H}_N expressed in its eigenbasis and the creation and annihilation operators also expressed in that basis; the $C(m, m')$ are just the matrix elements of c and c^\dagger in that basis.

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

2.19 Correspondence between the Kondo model fixed-point and a local Fermi liquid - Topological interpretation of Wilson ratio

2.19.1 Local Fermi liquid

The fixed-point Hamiltonians [17] are found to represent interacting Fermi liquids. The effective Hamiltonian can be shown to resemble the Anderson model, but with modified parameters,

$$H_{\text{eff}} = \sum_k \epsilon_k n_k + \sum_k V_k c_d^\dagger c_k + \text{h.c.} + U n_{d\uparrow} n_{d\downarrow} \quad (2.347)$$

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,

$$\begin{aligned} n_{d\uparrow} n_{d\downarrow} &\approx n_{d\uparrow} \langle n_{d\downarrow} \rangle + \langle n_{d\uparrow} \rangle n_{d\downarrow} - \langle n_{d\uparrow} \rangle \langle n_{d\downarrow} \rangle \\ \Rightarrow \langle n_{d\uparrow} n_{d\downarrow} \rangle &= \langle n_{d\uparrow} \rangle \langle n_{d\downarrow} \rangle \\ &= \sum_{k,q} \langle n_{k\sigma} \rangle \langle n_{q,-\sigma} \rangle \end{aligned} \quad (2.348)$$

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:

$$\langle n_q^> \rangle = \langle \psi^> | c_k^\dagger c_k | \psi^> \rangle = n_k^p \quad (2.349)$$

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

$$\langle n_q^< \rangle = \langle \psi^< | c_k^\dagger c_k | \psi^< \rangle = - \langle \psi^< | c_k c_k^\dagger | \psi^< \rangle = -n_k^h \quad (2.350)$$

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

$$\langle \delta n_{k,\sigma} \rangle = \begin{cases} n_k^p, & \epsilon_k > \epsilon_F \\ -n_k^h, & \epsilon_k < \epsilon_F \end{cases} \quad (2.351)$$

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

$$\epsilon_{k\sigma} = \epsilon_k + U \sum_q \langle \delta n_{q,-\sigma} \rangle \equiv \epsilon_k + U \langle \delta n_{-\sigma} \rangle \quad (2.352)$$

This is analogous to the Landau quasiparticle energy functional, eq. 2.35, 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

$$\rho_{d\sigma}(\omega) = \frac{\Delta}{\pi} \frac{1}{(\omega - \epsilon_d^*)^2 + \Delta^2} \quad (2.353)$$

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

2.19.2 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:

$$\frac{d\langle E \rangle}{dT} = \sum_{k,\sigma} \epsilon_{k\sigma} \frac{d\langle \delta n_{k\sigma} \rangle}{dT} \quad (2.354)$$

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

$$\begin{aligned} \langle \delta n_{k\sigma} \rangle(T) &= \frac{1}{e^{\beta \epsilon_{k\sigma}} + 1} \\ \Rightarrow \frac{d\langle \delta n_{k\sigma} \rangle}{dT} &= \frac{e^{\beta \epsilon_{k\sigma}}}{(e^{\beta \epsilon_{k\sigma}} + 1)^2} \left[\frac{1}{k_B T^2} \epsilon_{k\sigma} - \frac{1}{k_B T} (2\epsilon_{k\sigma} - \epsilon_k) \frac{d\langle \delta n_{k\sigma} \rangle}{dT} \right] \end{aligned} \quad (2.355)$$

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

$$\begin{aligned} \frac{d\langle E \rangle}{dT} &= \sum_{k,\sigma} \epsilon_{k\sigma} \frac{e^{\beta \epsilon_{k\sigma}}}{(e^{\beta \epsilon_{k\sigma}} + 1)^2} \frac{1}{k_B T^2} \epsilon_{k\sigma} \\ &= \frac{1}{k_B T^2} \sum_{k,\sigma} \epsilon_{k\sigma}^2 \frac{e^{\beta \epsilon_{k\sigma}}}{(e^{\beta \epsilon_{k\sigma}} + 1)^2} \\ &= \frac{1}{k_B T^2} \sum_{\sigma} \int d\epsilon_{\sigma} \rho(\epsilon_{\sigma}) \epsilon_{\sigma}^2 \frac{e^{\beta \epsilon_{k\sigma}}}{(e^{\beta \epsilon_{k\sigma}} + 1)^2} \end{aligned} \quad (2.356)$$

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

$$\begin{aligned} \frac{d\langle E \rangle}{dT} &= \frac{1}{k_B T^2} \sum_{\sigma} \rho_{\sigma}(0) \int_{-\infty}^{\infty} d\epsilon_{\sigma} \epsilon_{\sigma}^2 \frac{e^{\beta \epsilon_{k\sigma}}}{(e^{\beta \epsilon_{k\sigma}} + 1)^2} \\ &= -\frac{1}{T} \sum_{\sigma} \rho_{\sigma}(0) \int_{-\infty}^{\infty} d\epsilon_{\sigma} \epsilon_{\sigma}^2 f'(\epsilon_{\sigma}) \\ &= -\frac{1}{T} \sum_{\sigma} \rho_{\sigma}(0) \int_1^0 df \epsilon_{\sigma}^2 \end{aligned} \quad (2.357)$$

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

$$\epsilon = k_B T \ln(f^{-1} - 1) \implies \epsilon^2 = k_B^2 T^2 [\ln(f^{-1} - 1)]^2 \quad (2.358)$$

Therefore,

$$\frac{d\langle E \rangle}{dT} = -k_B^2 T \sum_{\sigma} \rho_{\sigma}(0) \int_1^0 df [\ln(f^{-1} - 1)]^2 \quad (2.359)$$

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

$$\begin{aligned}\frac{d\langle E \rangle}{dT} &= k_B^2 T \sum_{\sigma} \rho_d(0) \frac{\pi^2}{3} \\ &= 2k_B^2 T \rho_d(0) \frac{\pi^2}{3} \\ &= \gamma_{\text{imp}} T\end{aligned}\tag{2.360}$$

where

$$\gamma_{\text{imp}} \equiv \frac{C_v}{T} = \frac{2\pi^2}{3} k_B^2 \rho_d(0)\tag{2.361}$$

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

$$\frac{\gamma_{\text{imp}}}{\gamma^{(0)}} = \frac{\rho_d(0)}{\rho_d^{(0)}(0)}\tag{2.362}$$

2.19.3 Calculation of χ

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

$$\begin{aligned}m &= \frac{g\mu_B}{2} (\delta n_{\uparrow} - \delta n_{\downarrow}) \\ &= \frac{g\mu_B}{2} \sum_{\sigma} \sigma \delta n_{\sigma} \\ &= \frac{g\mu_B}{2} \sum_{k\sigma} \sigma \frac{\partial n_{\sigma}}{\partial \epsilon_{k\sigma}} \delta \epsilon_{k\sigma} \\ &= \frac{g\mu_B}{2} \sum_{k\sigma} \sigma \rho_{k\sigma} (\sigma h + U \delta n_{-\sigma}) \\ &= \frac{g\mu_B}{2} \sum_{\sigma} \sigma \rho_{\sigma} (\sigma h + U \delta n_{-\sigma})\end{aligned}\tag{2.363}$$

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

$$\delta n_{-\sigma} = \sum_q \delta n_{q,-\sigma} = \sum_q \Delta \epsilon_F \rho_{q-\sigma} = \sigma h \rho_{-\sigma}(0)\tag{2.364}$$

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

$$\begin{aligned}m &= \frac{g\mu_B}{2} h \sum_{\sigma} \sigma^2 \rho_{\sigma}(0) (1 + U \rho_{-\sigma}(0)) \\ &= \left(\frac{g\mu_B}{2} \right)^2 B \sum_{\sigma} \rho_{\sigma}(0) [1 + U \rho_{-\sigma}(0)]\end{aligned}\tag{2.365}$$

The susceptibility is

$$\begin{aligned}
 \chi_{\text{imp}} &= \lim_{h \rightarrow 0} \frac{\partial m}{\partial B} \\
 &= \left(\frac{g\mu_B}{2} \right)^2 \rho_d(0) [1 + U\rho_d(0)] \sum_{\sigma} \\
 &= \frac{(g\mu_B)^2}{2} \rho_d(0) [1 + U\rho_d(0)] \\
 &= \chi^{(0)} \frac{\rho_d(0)}{\rho_d^{(0)}(0)} [1 + U\rho_d(0)]
 \end{aligned} \tag{2.366}$$

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

$$R \equiv \frac{\chi_{\text{imp}}}{\chi^{(0)}} \frac{\gamma^{(0)}}{\gamma_{\text{imp}}} = 1 + U\rho_d(0) \tag{2.367}$$

2.19.4 Relation between the density of states and scattering phase shift

The Green's function is of the general form

$$G_d(\omega) = \frac{1}{\omega - \epsilon_d - i\Delta - \Sigma(\omega)} \tag{2.368}$$

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:

$$\begin{aligned}
 \Sigma(\omega) &= \Sigma(0, 0) + \omega\Sigma'(0) + O(i\omega^2) \\
 &\equiv \Sigma(0) + (1 - Z^{-1})\omega
 \end{aligned} \tag{2.369}$$

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

$$\begin{aligned}
 G_d(\omega) &= \frac{1}{\omega - \epsilon_d - i\Delta - \Sigma(0) - (1 - Z^{-1})\omega} \\
 &= \frac{Z}{Z\omega - Z\epsilon_d - iZ\Delta - Z\Sigma(0) - Z\omega + \omega} \\
 &= \frac{Z}{\omega - Z(\epsilon_d + \Sigma(0)) - iZ\Delta} \\
 &\equiv \frac{Z}{\omega - \epsilon_d^* - i\Delta^*}
 \end{aligned} \tag{2.370}$$

The density of states at the Fermi surface is given by

$$\begin{aligned}
 \rho_d(0) &= \frac{1}{\pi} \text{Im } G_d(\omega) \Big|_{\omega=0} \\
 &= \frac{1}{\pi} \frac{Z\Delta^*}{(\omega - \epsilon_d^*)^2 + \Delta^{*2}} \Big|_{\omega=0} \\
 &= \frac{1}{\pi} \frac{Z\Delta^*}{\epsilon_d^{*2} + \Delta^{*2}}
 \end{aligned} \tag{2.371}$$

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

$$\begin{aligned} G &= G^{(0)} + G^{(0)}VG_d^{(0)}VG^{(0)} + G^{(0)}VG_d^{(0)}VG^{(0)}VG_d^{(0)}VG^{(0)} + \dots \\ &= G^{(0)} + G^{(0)}V \left[G_d^{(0)} + G_d^{(0)}VG^{(0)}VG_d^{(0)} \right] VG^{(0)} \\ &= G^{(0)} + G^{(0)}V^2G_dG^{(0)} \end{aligned} \quad (2.372)$$

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

$$G = G_0 + G_0TG_0 \quad (2.373)$$

we can write

$$T = V^2G_d \quad (2.374)$$

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

$$\begin{aligned} e^{2i\delta(\omega)} &= 1 - 2\pi i\rho T(\omega) \\ \implies T &= V^2G_d = \frac{1}{2\pi i\rho} (1 - e^{2i\delta(\omega)}) = \frac{e^{i\delta(\omega)}}{2\pi i\rho} (-2i \sin \delta) \\ \implies G_d &= -\frac{e^{i\delta(\omega)}}{V^2\pi\rho} \sin \delta \end{aligned} \quad (2.375)$$

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

$$G_d = |G_d|e^{i\delta(\omega)} \quad (2.376)$$

From the expression for G_d in eq. 2.370, we can find the phase of G_d :

$$\begin{aligned} \delta(\omega) &= \tan^{-1} \frac{\Delta^*}{\omega - \epsilon_d^*} \\ \implies \epsilon_d^* &= -\Delta^* \cot \delta(0) \end{aligned} \quad (2.377)$$

Substituting this in the density of states expression gives

$$\rho_d(0) = \frac{Z \sin^2 \delta(0)}{\pi \Delta^*} \quad (2.378)$$

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

$$R = 1 + \frac{UZ \sin^2 \delta(0)}{\pi \Delta^*} \quad (2.379)$$

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

$$R = 1 + \frac{U}{\pi \Delta} \sin^2 \delta(0) \quad (2.380)$$

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

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

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

$$\begin{aligned}\Delta n_\uparrow &= \delta n_\uparrow(\epsilon_{k\uparrow} + \mu) - \delta n_\uparrow(\epsilon_{k\uparrow}) \\ &= \rho_d(0) (\Delta\mu + U \Delta n_\downarrow) \\ &= \rho_d(0) (\Delta\mu - U \rho_d(0) \Delta\mu) \\ &= \rho_d(0) \Delta\mu (1 - U \rho_d(0))\end{aligned}\tag{2.381}$$

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,

$$1 - U \rho_d(0) = 0 \implies U \rho_d(0) = 1\tag{2.382}$$

Substituting $\langle n_{d\sigma} \rangle = \frac{1}{2}$ and $\epsilon_d = -\frac{U}{2}$ in the density of states eq. 2.353 gives $\rho_d(0) = \frac{1}{\pi\Delta} = \frac{1}{U}$. This can be substituted in the Wilson ratio to give

$$R = 1 + \sin^2 \delta(0)\tag{2.383}$$

2.19.6 Connection to the change in Luttinger's volume

From the Friedel sum rule[18], 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:

$$\tilde{N} = \frac{1}{2\pi i} \text{Tr} \ln S(0) = \int_{\Gamma} dz \partial_z \frac{1}{2\pi i} \text{Tr} \ln S(0)\tag{2.384}$$

From the optical theorem, we can write

$$S = 1 + T G_0 = \frac{G}{G_0} \quad [\text{eq. 2.373}]\tag{2.385}$$

This allows us to write [19]

$$\tilde{N} = \int_{\Gamma} dz \partial_z \frac{1}{2\pi i} \text{Tr} \ln \frac{G}{G_0}\tag{2.386}$$

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

$$\begin{aligned}
 \tilde{N} &= \int_{\Gamma} dz \partial_z \frac{1}{2\pi i} \ln \text{Det} \frac{G}{G_0} \\
 &= - \int_{\Gamma} dz \partial_z \frac{1}{2\pi i} \ln \frac{\text{Det} G_0}{\text{Det} G} \\
 &\equiv - \int_{\Gamma} dz \partial_z \frac{1}{2\pi i} \ln D \\
 &= - \int_{\Gamma(D)} \frac{dD}{D}
 \end{aligned} \tag{2.387}$$

From the work of Seki and Yunoki [20], 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 $T = 0$.

$$\tilde{N} = - \int_{\Gamma(D)} \frac{dD}{D} = -\Delta V_L \tag{2.388}$$

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

$$\begin{aligned}
 \tilde{N} &= \frac{1}{\pi} \sum_{\sigma} \delta_{\sigma}(0) \\
 \implies \delta(0) &= \frac{\pi}{2} \tilde{N} = -\frac{\pi}{2} \Delta V_L
 \end{aligned} \tag{2.389}$$

$$\begin{aligned}
 R &= 1 + \sin^2 \left(\frac{\pi}{2} \tilde{N} \right) \\
 &= 1 + \sin^2 \left(\frac{\pi}{2} \Delta V_L \right)
 \end{aligned} \tag{2.390}$$

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 $\Delta V_L = -1 = -\tilde{N}$ [21] (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 [15].

2.20 Microscopic approach

The average occupation for the non-interacting quasiparticles can be similarly written from eq. 2.401.

$$\langle \tilde{n}_d \rangle = \frac{1}{2} - \frac{1}{\pi} \tan^{-1} \frac{\tilde{\epsilon}_d}{\tilde{\Delta}} = \frac{1}{2} - \frac{1}{\pi} \tan^{-1} \frac{\epsilon_d - \Sigma(0)}{\Delta} = \langle n_d \rangle \tag{2.391}$$

This shows that the quasiparticles are in one-one correspondence with the actual particles. For a Fermi liquid, the specific heat is given by $\tilde{C}_v = \frac{2\pi^2 k_B^2}{3} \tilde{\rho}(0) T$. Applying it to the problem at hand, we get

$$\gamma_{\text{imp}} = \frac{2\pi k_B^2}{3} \frac{\tilde{\Delta}}{\tilde{\epsilon}_d^2 + \tilde{\Delta}^2} \tag{2.392}$$

This matches with the value obtained from Nozières treatment. Luttinger also proved that, up to first order,

$$\chi_{\text{m,imp}} = \frac{g^2 \mu_B^2}{2} \alpha' \rho_d(0) \quad (2.393)$$

$$\chi_{\text{c,imp}} = 2\alpha'' \rho_d(0) \quad (2.394)$$

where

$$\alpha' = \frac{1 - \partial_h \Sigma_\sigma(\epsilon_F, 0)}{1 - \partial_E \Sigma_\sigma(\epsilon_F, 0)} \quad (2.395)$$

$$\alpha'' = \frac{1 + \partial_\mu \Sigma_\sigma(\epsilon_F, 0)}{1 - \partial_E \Sigma_\sigma(\epsilon_F, 0)} \quad (2.396)$$

2.21 Renormalized perturbation theory

This is a perturbative expansion of the Hamiltonian in terms of the renormalized interaction \tilde{U} , and the second order results obtained from this approach coincide with the phenomenological results at $T, h \rightarrow 0$. This approach is obviously more general as all terms in the original Hamiltonian are retained. This is an alternative to the full microscopic approach. In the microscopic approach, we take the exact microscopic Hamiltonian and calculate observables from it. In the renormalized perturbation, we separate the Hamiltonian into a non-interacting quasiparticle Hamiltonian which is like the low-energy free Hamiltonian, and an interacting part, and also a counter-term to prevent divergences. The original parameters of the model get replaced by renormalized parameters, and we can analyze the model perturbatively in powers of the renormalized interaction.

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

$$G_d^0 = \frac{1}{E - \epsilon_d + i\Delta} \quad (2.397)$$

Including the self energy gives

$$G_d = \frac{1}{E - \epsilon_d + i\Delta - \Sigma(E)} \quad (2.398)$$

As shown previously in section 2.12, the impurity Green's function can be shown to take the form

$$G_d = \frac{Z}{E - \tilde{\epsilon}_d + i\tilde{\Delta} - \tilde{\Sigma}(E)} \quad (2.399)$$

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

$$\begin{aligned} \tilde{\epsilon}_d &= Z(\epsilon_d + \Sigma(0)) \\ \tilde{\Delta} &= Z\Delta \\ \tilde{\Sigma} &= Z\Sigma^{\text{rem}}(E) \\ Z^{-1} &= 1 - \Sigma(0)' \\ \tilde{\Gamma}_{\sigma\sigma'}(E, E') &= z^2 \Gamma_{\sigma\sigma'}(E, E') \\ \tilde{U} &= z^2 \Gamma_{\uparrow\downarrow}(0, 0) \end{aligned} \quad (2.400)$$

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

$$\tilde{G}_d = \frac{1}{E - \tilde{\epsilon}_d + i\tilde{\Delta}} \quad (2.401)$$

The Anderson hamiltonian

$$H = \epsilon_d n_d + U n_{d\uparrow} n_{d\downarrow} + \sum_k \epsilon_k n_k + \sum_k \left(V_k c_{d\sigma}^\dagger c_{k\sigma} + V_k^* c_{k\sigma}^\dagger c_{d\sigma} \right) \quad (2.402)$$

can be written in the form

$$H = \tilde{H}_{qp} - \tilde{H}_c \quad (2.403)$$

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

$$\tilde{H}_{qp}^0 = \tilde{\epsilon}_d \tilde{n}_d + \sum_k \epsilon_k n_k + \sum_k \left(\tilde{V}_k \tilde{c}_{d\sigma}^\dagger c_{k\sigma} + \tilde{V}_k^* c_{k\sigma}^\dagger \tilde{c}_{d\sigma} \right) \quad (2.404)$$

$$\tilde{H}_{qp}^I = \tilde{U} \tilde{n}_{d\uparrow} \tilde{n}_{d\downarrow} \quad (2.405)$$

The renormalised parameters are defined in eq. 2.400. The renormalised operators are

$$\tilde{c}_d^\dagger = \sqrt{z} c_d^\dagger \quad (2.406)$$

$$\tilde{c}_d = \sqrt{z} c_d \quad (2.407)$$

The \tilde{H}_c that satisfies eq. 2.403 is

$$\tilde{H}_c = \lambda_1 \tilde{n}_d + \lambda_2 \tilde{n}_{d\uparrow} \tilde{n}_{d\downarrow} \quad (2.408)$$

where

$$\lambda_1 = z \Sigma(0, 0) \quad (2.409)$$

$$\lambda_2 = z^2 [\Gamma_{\uparrow\downarrow}(0, 0) - U] \quad (2.410)$$

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

$$\begin{aligned} \tilde{\Sigma}(0) &= 0 \\ \tilde{\Sigma}'(0) &= 0 \end{aligned} \quad (2.411)$$

Close to the Fermi surface, we also have

$$\tilde{\Gamma}_{\uparrow\downarrow}(0) = \tilde{U} \quad (2.412)$$

$$\tilde{\Gamma}_{\sigma\sigma}(0) = 0 \quad (2.413)$$

$$\implies \Gamma_{\sigma\sigma'}(0) = \tilde{U}(1 - \delta_{\sigma\sigma'}) \quad (2.414)$$

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} .

$$\lambda_i = \sum_n \lambda_i^{(n)} \tilde{U}^n \quad (2.415)$$

$$z = \sum_n z^{(n)} \tilde{U}^n \quad (2.416)$$

$$(2.417)$$

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

$$G^0 = \frac{1}{E - \tilde{\epsilon}_d + i\tilde{\Delta}} \quad (2.418)$$

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

$$\langle n_{d\sigma} \rangle = \frac{1}{2} - \frac{1}{\pi} \tan^{-1} \frac{\epsilon_d + \Sigma(0, h)}{\Delta} \quad (2.419)$$

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

$$\langle n_{d\sigma} \rangle = \frac{1}{2} - \frac{1}{\pi} \tan^{-1} \frac{\tilde{\epsilon}_d + \tilde{\Sigma}(0, h)}{\tilde{\Delta}} \quad (2.420)$$

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. 2.411. In that case, $\langle n_{d\sigma} \rangle = \langle n_{d\sigma}^0 \rangle$, that is, the quasiparticle distribution becomes the same as the free fermionic distribution.

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

$$\tilde{\Sigma}(\omega, H, T) = \tilde{U} \left(n_{d\sigma}^{(0)}(0, H, T) - n_{d\sigma}^{(0)}(0, 0, 0) \right) \quad (2.421)$$

This satisfies the constraint eq. 2.411. 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

$$m = \frac{g\mu_B}{2} \langle n_{d\uparrow} - n_{d\downarrow} \rangle \quad (2.422)$$

We can substitute the expression for the self-energy into eq. 2.420. That gives

$$\chi_d = \frac{1}{2} (g\mu_B)^2 \frac{\partial \langle n_{d\uparrow} - n_{d\downarrow} \rangle}{\partial h} = \frac{1}{2\pi} (g\mu_B)^2 \frac{\partial}{\partial h} \left(\tan^{-1} \frac{\tilde{\epsilon}_{d\downarrow}}{\tilde{\Delta}} - \tan^{-1} \frac{\tilde{\epsilon}_{d\uparrow}}{\tilde{\Delta}} \right) \quad (2.423)$$

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

$$\chi_d = \frac{1}{2\pi} (g\mu_B)^2 \frac{1}{1 + \left(\frac{\tilde{\epsilon}_d}{\tilde{\Delta}} \right)^2} \frac{1}{\tilde{\Delta}} \frac{\partial}{\partial h} [\tilde{\epsilon}_{d\downarrow} - \tilde{\epsilon}_{d\uparrow}] \quad (2.424)$$

We can recognize that

$$\frac{1}{1 + \left(\frac{\tilde{\epsilon}_d}{\tilde{\Delta}}\right)^2} \frac{1}{\pi \tilde{\Delta}} = \frac{1}{\pi} \frac{\tilde{\Delta}}{\tilde{\Delta}^2 + \tilde{\epsilon}_d^2} = \rho_d(0) \quad (2.425)$$

Therefore,

$$\chi_d = \frac{1}{2} (g\mu_B)^2 \rho_d(0) \frac{\partial}{\partial h} [\tilde{\epsilon}_{d\downarrow} - \tilde{\epsilon}_{d\uparrow}] \quad (2.426)$$

Up to first order, we can write

$$\tilde{\epsilon}_{d\downarrow} - \tilde{\epsilon}_{d\uparrow} = \epsilon_{d\downarrow} - \epsilon_{d\uparrow} + \tilde{U} \left(n_{d\downarrow}^{(0)} - n_{d\uparrow}^{(0)} \right) = 2\epsilon_d + h + \tilde{U} \left(n_{d\downarrow}^{(0)} - n_{d\uparrow}^{(0)} \right) \quad (2.427)$$

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

$$\frac{\partial}{\partial h} [\tilde{\epsilon}_{d\downarrow} - \tilde{\epsilon}_{d\uparrow}] = 1 + \tilde{U} \left(\frac{\partial n_{d\downarrow}^{(0)}}{\partial \epsilon_{d\downarrow}} \frac{\partial \epsilon_{d\downarrow}}{\partial h} - \frac{\partial n_{d\uparrow}^{(0)}}{\partial \epsilon_{d\uparrow}} \frac{\partial \epsilon_{d\uparrow}}{\partial h} \right) \quad (2.428)$$

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

$$\frac{\partial}{\partial h} [\tilde{\epsilon}_{d\downarrow} - \tilde{\epsilon}_{d\uparrow}] = 1 + \tilde{U} \rho_d(0) \quad (2.429)$$

Substituting in to the parent equation, we get

$$\chi_d = \frac{1}{2} (g\mu_B)^2 \rho_d(0) \left(1 + \tilde{U} \rho_d(0) \right) \quad (2.430)$$

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

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

$$\left(\frac{\partial}{\partial E} + \frac{\partial}{\partial \mu} \right) \Sigma(E) \Big|_{E=0} = -\rho_{d\sigma}(0) \Gamma_{\uparrow\downarrow}(0, 0) \quad (2.431)$$

$$\left(\frac{\partial}{\partial h} - \frac{\partial}{\partial E} \right) \Sigma(E) \Big|_{E=0} = -\rho_{d\sigma}(0) \Gamma_{\uparrow\downarrow}(0, 0) \quad (2.432)$$

Multiplying both equations throughout by Z , we get

$$\left(\frac{\partial}{\partial E} + \frac{\partial}{\partial \mu} \right) \tilde{\Sigma}(E) \Big|_{E=0} = -Z \rho_{d\sigma}(0) \Gamma_{\uparrow\downarrow}(0, 0) = -\frac{1}{Z} \rho_{d\sigma}(0) \tilde{U} \quad (2.433)$$

$$\left(\frac{\partial}{\partial h} - \frac{\partial}{\partial E} \right) \tilde{\Sigma}(E) \Big|_{E=0} = -Z \rho_{d\sigma}(0) \Gamma_{\uparrow\downarrow}(0, 0) = -\frac{1}{Z} \rho_{d\sigma}(0) \tilde{U} \quad (2.434)$$

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

$$\tilde{\rho}(0) \sim \frac{\tilde{\Delta}}{\tilde{\epsilon}_d^2 + \tilde{\Delta}^2} = \frac{1}{Z} \frac{\Delta}{\epsilon_d^2 + \Delta^2} = \frac{1}{Z} \rho_d(0) \quad (2.435)$$

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

$$\left. \frac{\partial \tilde{\Sigma}(E)}{\partial \mu} \right|_{E=0} = \left. \frac{\partial \tilde{\Sigma}(E)}{\partial h} \right|_{E=0} = -\tilde{\rho}_{d\sigma}(0) \tilde{U} \quad (2.436)$$

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.

$$\tilde{\gamma} \sim \tilde{\rho}_d(0) \quad (2.437)$$

The susceptibilities are given by

$$\chi_m = - \left(\frac{g\mu_B}{2} \right)^2 \tilde{\rho}_d \sum_{\sigma} \frac{\partial (\epsilon_k - h\sigma + \tilde{\Sigma})}{\partial h} = \frac{g^2 \mu_B^2}{2} \tilde{\rho}_d \left(1 - \frac{\partial \tilde{\Sigma}}{\partial h} \right) \quad (2.438)$$

Substituting from eq. 2.436,

$$\chi_m = \frac{g^2 \mu_B^2}{2} \tilde{\rho}_d \left(1 + \tilde{U} \tilde{\rho}_d(0) \right) \quad (2.439)$$

Similarly,

$$\chi_c = \frac{dn}{d\mu} = \tilde{\rho}_d(0) \sum_{\sigma} \frac{d(\epsilon_F + \tilde{\Sigma})}{d\mu} = 2\tilde{\rho}_d(0) \left(1 + \frac{\partial \tilde{\Sigma}}{\partial \mu} \right) = 2\tilde{\rho}_d(0) \left(1 - \tilde{U} \tilde{\rho}_d(0) \right) \quad (2.440)$$

2.21.1 Friedel sum rule

Looking at eq. 2.398, we can write down the density of states and hence the average occupancy of the impurity site

$$\rho_{d\sigma} = \frac{-1}{\pi} \text{Im} [G_d] \quad (2.441)$$

$$\langle n_{d\sigma} \rangle = \int_{-\infty}^0 dE \rho_{d\sigma} = -\frac{1}{\pi} \text{Im} \int_{-\infty}^0 dE G_d(E) \quad (2.442)$$

Luttinger proved that

$$\int_{-\infty}^0 \Sigma' G dE = 0 \quad (2.443)$$

In order to use this, note that

$$\begin{aligned} \ln G_d^{-1} &= \ln (E - \epsilon_d + i\Delta - \Sigma) \\ \Rightarrow \frac{d \ln G_d^{-1}}{dE} &= \frac{1}{E - \epsilon_d + i\Delta - \Sigma} (1 - \Sigma') = G_d - \Sigma' G_d \\ \Rightarrow G_d &= \Sigma' G_d - \frac{d \ln G_d}{dE} \end{aligned} \quad (2.444)$$

Substituting this expression for G_d in eq. 2.442,

$$\langle n_{d\sigma} \rangle = -\frac{1}{\pi} \text{Im} \int_{-\infty}^0 \Sigma' G dE + \frac{1}{\pi} \text{Im} \int_{-\infty}^0 \frac{d \ln G_d}{dE} dE \quad (2.445)$$

The first integral is zero, courtesy Luttinger. We get

$$\begin{aligned}
\langle n_{d\sigma} \rangle &= \frac{1}{\pi} \text{Im} \left[\ln \frac{1}{E - \epsilon_d + i\Delta - \Sigma} \right]_{-\infty}^0 \\
&= -\frac{1}{\pi} \text{Im} [\ln (E - \epsilon_d + i\Delta - \Sigma)]_{-\infty}^0 \\
&= -\frac{1}{\pi} \text{Im} [\ln e^{i\theta}]_{-\infty}^0 \quad \left[\tan \theta = \frac{\Delta}{E - \epsilon_d - \Sigma} \right] \\
&= -\frac{1}{\pi} [\theta(0) - \theta(-\infty)] \\
&= \frac{1}{\pi} \tan^{-1} \frac{\Delta}{\epsilon_d + \Sigma(0, h)} \\
&= \frac{1}{2} - \frac{1}{\pi} \tan^{-1} \frac{\epsilon_d + \Sigma(0, h)}{\Delta}
\end{aligned} \tag{2.446}$$

We can now relate the average occupancy with the density of states. From eq. 2.441,

$$\begin{aligned}
\rho_{d\sigma} &= \frac{1}{\pi} \frac{\Delta}{(\epsilon_d + \Sigma(0))^2 + \Delta^2} \\
&= \frac{1}{\pi \Delta} \left[1 + \left(\frac{\epsilon_d + \Sigma(0)}{\Delta} \right)^2 \right]^{-1} \\
&= \frac{1}{\pi \Delta} [1 + \cot^2 \pi \langle n_{d\sigma} \rangle]^{-1} \\
&= \frac{\sin^2 \pi \langle n_{d\sigma} \rangle}{\pi \Delta}
\end{aligned} \tag{2.447}$$

2.22 Scaling of Anderson model

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. 1a. 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. 1b 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 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

$$H = \sum_{k\sigma} \epsilon_{k\sigma} n_{k\sigma} + \epsilon_d \sum_{\sigma} n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow} + \sum_{k\sigma} \left(V_{kd} c_{k\sigma}^\dagger c_{d\sigma} + V_{kd}^* c_{d\sigma}^\dagger c_{k\sigma} \right) \tag{2.448}$$



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

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

$$H^{(0)} = \sum_{k < D - \delta D, \sigma} \epsilon_{k\sigma} n_{k\sigma} + \epsilon_d \sum_{\sigma} n_{d\sigma} + \sum_{k < D - \delta D, \sigma} \left(V_{kd} c_{k\sigma}^{\dagger} c_{d\sigma} + V_{kd}^* c_{d\sigma}^{\dagger} c_{k\sigma} \right) \quad (2.449)$$

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

$$H_{\sigma}^{(1,p)} = \sum_{k \in k^+} \alpha_{k\sigma} c_{d\sigma}^{\dagger} c_{k\sigma} c_{k\sigma}^{\dagger} c_{d\sigma} \quad (2.450)$$

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

$$\alpha_{k\sigma} = \frac{\langle 1_{d\sigma} | V_{kd}^* c_{d\sigma}^{\dagger} c_{k\sigma} | k\sigma \rangle \langle k\sigma | V_{kd} c_{k\sigma}^{\dagger} c_{d\sigma} | 1_{d\sigma} \rangle}{E_{1_{d\sigma}} - E_{k\sigma}} = \frac{|V_{kd}|^2}{\epsilon_d - \epsilon_k} \quad (2.451)$$

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

$$H^{(1,h)} = \sum_{k \in k^-, \sigma} \beta_{k\sigma} c_{k\sigma}^\dagger c_{d\sigma} c_{k\sigma} c_{d\sigma}^\dagger \quad (2.452)$$

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

$$\beta_{k\sigma} = \frac{\langle 0 | V_{kd}^* c_{d\sigma} c_{k\sigma}^\dagger | k\sigma \rangle \langle k\sigma | V_{kd} c_{k\sigma} c_{d\sigma}^\dagger | 0 \rangle}{E_0 - E_{k\sigma}} = \frac{|V_{kd}|^2}{\epsilon_k - \epsilon_d} \quad (2.453)$$

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

$$H^{(1)} = \sum_{k^+, \sigma} \alpha_{k\sigma} T_{k\sigma}^+ + \sum_{k^-, \sigma} \beta_{k\sigma} T_{k\sigma}^- \quad (2.454)$$

$T^{+,-}$ 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

$$\delta\epsilon_1 = \alpha_{k\sigma} = \sum_{k^+} \frac{|V_{kd}|^2}{\epsilon_d - \epsilon_k} \quad (2.455)$$

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

$$\delta\epsilon_1 = \sum_{k^+} \frac{|V_{kd}|^2}{\epsilon_d - \epsilon_k} = \int_{D-\delta D}^D dE N(E) \frac{|V(E)|^2}{\epsilon_d - E} \approx \frac{\Delta}{\pi} \frac{|\delta D|}{\epsilon_d - D} \quad (2.456)$$

The change in ϵ_0 is

$$\delta\epsilon_0 = \sum_{\sigma} \beta_{k\sigma} \approx -2 \frac{\Delta}{\pi} \frac{|\delta D|}{\epsilon_d + D} \quad (2.457)$$

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

$$\delta\epsilon_d = \delta\epsilon_1 - \delta\epsilon_0 = \frac{\Delta |\delta D|}{\pi} \left[\frac{1}{\epsilon_d - D} + \frac{2}{\epsilon_d + D} \right] = \frac{\Delta}{\pi} \frac{|\delta D|}{D} = -\frac{\Delta}{\pi} \delta \ln D \quad (2.458)$$

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

$$\frac{d\epsilon_d}{d \ln D} = -\frac{\Delta}{\pi} \quad (2.459)$$

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:

$$\frac{|V_{kd}|^2}{\epsilon_k - U - \epsilon_d} \approx \frac{|V|^2}{-D - U - \epsilon_d} \quad (2.460)$$

$-(U + \epsilon_d)$ 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

$$\delta\epsilon_d = \frac{\Delta |\delta D|}{\pi} \left(\frac{1}{\epsilon_d - D} - \frac{1}{D + U + \epsilon_d} + \frac{2}{\epsilon_d + D} \right) \quad (2.461)$$

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.

$$H^{(2)} = \sum_{k^+, q, \sigma} \alpha_{k\sigma} T_{k\sigma}^+ \gamma_{q,k,\sigma} c_{d\sigma}^\dagger c_{q\sigma} + \sum_{k^-, q, \sigma} \beta_{k\sigma} T_{k\sigma}^- \gamma_{q,k,\sigma} c_{d\sigma} c_{q\sigma}^\dagger \quad (2.462)$$

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

$$\begin{aligned} \alpha_{k\sigma} \gamma_{q,k,\sigma} &= \frac{\langle 1_{d\sigma} | V_{kd}^* c_{d\sigma}^\dagger c_{k\sigma} | k\sigma \rangle \langle k\sigma | V_{kd} c_{k\sigma}^\dagger c_{d\sigma} | 1_{d\sigma} \rangle \langle 1_{d\sigma} | V_{kd} c_{q\sigma} c_{d\sigma}^\dagger | q\sigma \rangle}{(E_{1_{d\sigma}} - E_{k\sigma})(E_q - E_k)} \\ &= \alpha_{k\sigma} \frac{V_{kd}}{\epsilon_q - \epsilon_k} \end{aligned} \quad (2.463)$$

The renormalization in V_{kd} is therefore

$$\delta V_{kd} = \frac{\Delta}{\pi} \frac{|\delta D|}{\epsilon_d - D} \frac{V_{kd}}{\epsilon_q - \epsilon_k} \quad (2.464)$$

Close to the band edge, we get

$$\delta V = \frac{\Delta}{\pi} \frac{|\delta D|}{\epsilon_d - D} \frac{V}{\epsilon_q - D} \approx \frac{\Delta}{\pi} \frac{|\delta D|}{D^2} V \quad (2.465)$$

Therefore,

$$\delta \Delta \sim V \delta V = \frac{\Delta V^2}{\pi D^2} |\delta D| \implies \frac{d\Delta}{dD} \sim \left(\frac{\Delta}{D} \right)^2 \quad (2.466)$$

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. 2.459 gives

$$\epsilon_d = -\frac{\Delta}{\pi} \ln D + \text{constant} \quad (2.467)$$

Defining the constant as

$$\text{constant} = \epsilon_d^* + \frac{\Delta}{\pi} \ln \Delta \quad (2.468)$$

we get

$$\epsilon_d = -\frac{\Delta}{\pi} \ln D + \epsilon_d^* + \frac{\Delta}{\pi} \ln \Delta \quad (2.469)$$

$$\implies \epsilon_d = \epsilon_d^* - \frac{\Delta}{\pi} \ln \frac{D}{\Delta} \quad (2.470)$$

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. 2.470). 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 $D = -a\bar{\epsilon}_d$, $a > 1$. We can then express the SWT coupling constant \tilde{J} by replacing ϵ_d with $\bar{\epsilon}_d$ in eq. 2.108. For simplicity set $U = \infty$. Then,

$$\tilde{J} = -\frac{|V|^2}{\bar{\epsilon}_d} = \frac{a|V|^2}{D} \quad (2.471)$$

We can then do the poor man's scaling with this coupling. From eq. 2.252,

$$\begin{aligned} T_K &\sim D \sqrt{\tilde{J}N(0)^2} \exp\left(-\frac{1}{2\tilde{J}N(0)^2}\right) = \sqrt{\Delta D} \exp\left(-\frac{D}{2\Delta}\right) \\ &\sim D \sqrt{\frac{\Delta}{D}} \exp\left(\frac{\epsilon_d}{2\Delta}\right) \end{aligned} \quad (2.472)$$

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. 1a. Assuming $U \rightarrow \infty$ and ϵ_d outside the conduction band, we can do a SWT and the T_K obtained is q. 2.252,

$$J = -\frac{V^2}{\epsilon_d} \quad (2.473)$$

$$g = J\rho = -\frac{\Delta}{\epsilon_d} \quad (2.474)$$

$$\Rightarrow T_K = D \sqrt{\frac{\Delta}{\epsilon_d}} \exp\left(\frac{\epsilon_d}{2\Delta}\right) \quad (2.475)$$

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 $\bar{D} = a\epsilon_d(\bar{D}) \equiv \bar{\epsilon}_d$ where a is a constant of order unity. It satisfies the equation

$$\bar{\epsilon}_d = \epsilon_d^* - \frac{\Delta}{\pi} \ln \frac{a\bar{\epsilon}_d}{\Delta} \quad (2.476)$$

which is just eq. 2.470 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

$$\chi_d = \frac{\Delta}{2\pi} \left(\frac{g\mu_B}{\epsilon_d}\right)^2 \left[1 + \frac{2\Delta}{\pi\epsilon_d} \ln \frac{\epsilon_d}{D} + \dots\right] \quad (2.477)$$

Figure 1: Renormalization in the energy levels when $\epsilon_d^* \gg \Delta$

From the scaling, we know that D can be decreased to \bar{D} . We can hence substitute $D = a\bar{\epsilon}_d$, $\epsilon_d = \bar{\epsilon}_d$. With this in mind, the susceptibility becomes

$$\begin{aligned}\chi_d &= \frac{\Delta}{2\pi} \left(\frac{g\mu_B}{\bar{\epsilon}_d} \right)^2 \left[1 + \frac{2\Delta}{\pi\bar{\epsilon}_d} \ln a + \dots \right] \\ &= \frac{\Delta}{2\pi} \left(\frac{g\mu_B}{\bar{\epsilon}_d} \right)^2 \left[1 + \mathcal{O}\left(\frac{2\Delta}{\pi\bar{\epsilon}_d}\right) \right]\end{aligned}\quad (2.478)$$

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)

$$\chi_d(T) = \frac{\Delta}{2\pi} \left(\frac{g\mu_B}{\bar{\epsilon}_d} \right)^2 + \frac{1}{4T} \left[1 + \frac{1}{2} \exp\left(\frac{T^*}{T}\right) \right]^{-1} \quad (2.479)$$

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:

$$T \gg T_{FL} \implies e^{\frac{T^*}{T}} \gg 1 \implies \left[1 + \frac{1}{2} \exp\left(\frac{T^*}{T}\right) \right]^{-1} \approx 0 \quad (2.480)$$

The susceptibility in this low temperature range can thus be written as

$$\chi_d = \frac{\Delta}{2\pi} \left(\frac{g\mu_B}{\bar{\epsilon}_d} \right)^2 \quad (2.481)$$

This is analogous to the result obtained in eq. 2.366, 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. 2.366 then becomes

$$\chi_d = \frac{g^2 \mu_B^2}{2} \rho_d(0) = \frac{g^2 \mu_B^2}{2} \frac{\Delta}{\pi} \frac{1}{\bar{\epsilon}_d^2 + \Delta^2} \quad (2.482)$$

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. 2.476, we can drop the π and a because they are of order 1.

$$\bar{\epsilon}_d = \epsilon_d^* - \Delta \ln \frac{\bar{\epsilon}_d}{\Delta} \quad (2.483)$$

Dividing through by Δ and defining $x_1 = \frac{\bar{\epsilon}_d}{\Delta}$, $x_2 = \frac{\epsilon_d^*}{\Delta}$, we get

$$x_1 + \ln x_1 = x_2 \quad (2.484)$$

Since $O(\ln x_1) \leq O(x_1)$, we can write

$$O(x_1) = O(x_2) \quad (2.485)$$

$$\implies O\left(\frac{\bar{\epsilon}_d}{\Delta}\right) = O\left(\frac{\epsilon_d^*}{\Delta}\right) \quad (2.486)$$

$$\implies O(\bar{\epsilon}_d) = O(\epsilon_d^*) \quad (2.487)$$

$$(2.488)$$

Since $\bar{\epsilon}_d$ and ϵ_d^* are of the same order, we can say:

$$\epsilon_d^* \gg \Delta \implies \bar{\epsilon}_d \gg \Delta \quad (2.489)$$

Applying this to eq. 2.482 means

$$\chi_d \approx \frac{g^2 \mu_B^2}{2} \frac{\Delta}{\pi} \frac{1}{\bar{\epsilon}_d^2} \quad (2.490)$$

which is the same as eq. 2.481. 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,

$$m = \frac{1}{\beta} \frac{\partial \ln Z}{\partial B} \implies \chi = \lim_{B \rightarrow 0} \frac{\partial m}{\partial B} = \lim_{B \rightarrow 0} \frac{1}{Z^2 \beta} \left[Z \frac{\partial^2 Z}{\partial B^2} - \left(\frac{\partial Z}{\partial B} \right)^2 \right] \quad (2.491)$$

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

$$Z = 1 + \exp(\beta h) + \exp(-\beta h) + 1 = 2(1 + \cosh \beta h) \quad (2.492)$$

$$\implies \frac{\partial Z}{\partial B} = g\mu_B \beta \sinh \beta h \quad (2.493)$$

$$\implies \frac{\partial^2 Z}{\partial B^2} = \frac{1}{2} (g\mu_B)^2 \beta^2 \cosh \beta h \quad (2.494)$$

Since $\lim_{h \rightarrow 0} \sinh \beta h = 0$ and $\lim_{h \rightarrow 0} \cosh \beta h = 1$, we get

$$\chi = \frac{\beta g^2 \mu_B^2}{2Z(h=0)} \quad (2.495)$$

Setting $g\mu_B = k_B = 1$, we get

$$\chi T = \frac{1}{2\mathcal{D}} \quad (2.496)$$

where $Z(h=0) = 2 + 2 = 4 = \mathcal{D}$ 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 $Z(h=0) = 1 + 2 = 3 = \mathcal{D}$.

For $\epsilon_d = k_B T^* > k_B T$ such that $k_B T^* \gg \Delta$, we can find the magnetic moment in a perturbative fashion. At the zeroth order, we can neglect the hybridisation Δ . Then,

$$m^{(0)} = \frac{1}{\beta} \frac{\partial \ln Z(h)}{\partial B} \quad (2.497)$$

where

$$Z(h) = 1 + e^{-\beta(k_B T^* - h)} + e^{-\beta(k_B T^* + h)} = 1 + e^{-\frac{\beta}{\beta^*}} 2 \cosh \beta h \quad (2.498)$$

Therefore,

$$\chi^{(0)} = \lim_{h \rightarrow 0} \frac{1}{\beta Z} \frac{\partial^2 Z}{\partial B^2} = \lim_{h \rightarrow 0} \frac{g^2 \mu_B^2}{4\beta Z} \frac{\partial^2 Z}{\partial h^2} = \frac{g^2 \mu_B^2}{4} \beta \frac{2e^{-\frac{\beta}{\beta^*}}}{1 + 2e^{-\frac{\beta}{\beta^*}}} \quad (2.499)$$

Again setting $g\mu_B = k_B = 1$, we get,

$$\chi^{(0)} = \frac{1}{4T} \frac{2e^{-\frac{\beta}{\beta^*}}}{1 + 2e^{-\frac{\beta}{\beta^*}}} = \frac{1}{4T} \frac{2}{e^{\frac{\beta}{\beta^*}} + 2} \quad (2.500)$$

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. 2.53

$$m^{(1)} = \frac{g\mu_B}{2} (n_{\uparrow} - n_{\downarrow}) = \frac{g\mu_B}{2\pi} \left[\tan^{-1} \frac{\Delta}{k_B T^* - h} - \tan^{-1} \frac{\Delta}{k_B T^* + h} \right] \quad (2.501)$$

Since $\Delta \ll T^*$, we can expand the arctan in a Taylor series. Up to first order, we get

$$m^{(1)} = \frac{g\mu_B}{2\pi} \left[\frac{\Delta}{k_B T^* - h} - \frac{\Delta}{k_B T^* + h} \right] = \frac{g\mu_B \Delta}{\pi} \frac{h}{k_B (T^*)^2 - h^2} \quad (2.502)$$

Differentiating with B gives

$$\chi^{(1)} = \lim_{h \rightarrow 0} \frac{\partial m^{(1)}}{\partial B} = \frac{g^2 \mu_B^2}{2} \frac{\Delta}{\pi} \frac{1}{k_B^2 T^{*2}} = \frac{\Delta}{2\pi T^{*2}} \quad (2.503)$$

Combining the zeroth and first order terms, the susceptibility in the regime $T \lesssim T^*$ is

$$\chi = \frac{1}{4T} \frac{2}{e^{\frac{\beta}{\beta^*}} + 2} + \frac{\Delta}{2\pi T^{*2}} \quad (2.504)$$

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

$$\chi \approx \frac{1}{4T} \frac{2}{e^{\frac{\beta}{\beta^*}}} + \frac{\Delta}{2\pi T^{*2}} \approx \frac{\Delta}{2\pi T^{*2}} \quad (2.505)$$

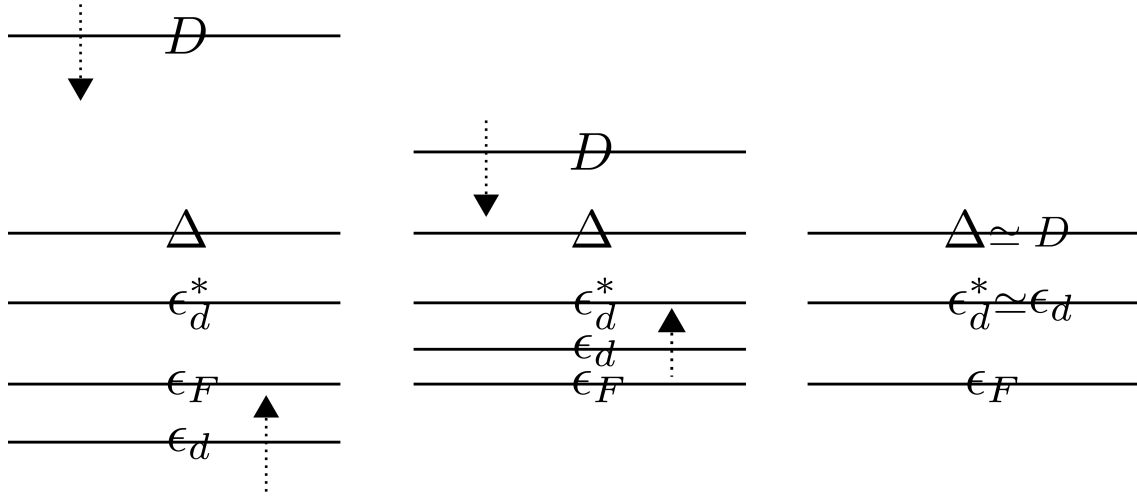
$$\implies \chi T \propto T \quad (2.506)$$

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 .

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

Next we consider the mixed valence regime, described by $|\epsilon_d^*| < \Delta$. It is clear that since the impurity level is within an interval of the hybridisation from the Fermi surface, the charge fluctuations can cause transitions between the various states of the impurity. This means that the occupation number of the impurity site is not a good quantum number in this regime, and the average number of impurity electrons will be fractional. This definition is a bit arbitrary because any observed sample will display an eigenstate in which the impurity states have contributions from both $\langle n_d \rangle = 0$ and $\langle n_d \rangle = 1$, so any sample will be mixed in that sense. However, if we are not in the mixed valence regime ($|\epsilon_d| \gg \Delta$), then the contribution from any one state will far outweigh the other. If $\epsilon_d > 0$, then the impurity level is far above the Fermi level and it will most probably not be occupied and the majority of the contribution will come from $\langle n_d \rangle = 0$. Similarly, if $\epsilon_d < 0$, then the impurity level is far below the Fermi level and the average occupation will be close to 1. The regime of mixed valence is one in which these two contributions are comparable.

Since we have $|\epsilon_d^*| \lesssim \Delta$, as we renormalize, the decreasing cutoff will first match Δ or $k_B T$, whichever is greater. From eq. 2.466, 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

Figure 2: Renormalization in energy levels when $|\epsilon_d^*| \lesssim \Delta$

at $D = \max\{\Delta, k_B T\}$. For the simpler situation in which $T = 0$, the renormalization will stop at $D = \Delta$. From eq. 2.470, putting $D = \Delta$, we get

$$(\epsilon_d)_{MV} = \epsilon_d^* \quad (2.507)$$

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

$$\sim \frac{k_B T}{\epsilon_d} \quad (2.508)$$

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.

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

For $\epsilon_d^* \ll -\Delta$, the scaling will stop when the impurity level again goes out of the Fermi surface. But this time, it goes out from below. This again decouples the singly-occupied state from the conduction band and the scaling stops. This happens at say $\tilde{D} = -\tilde{\epsilon}_d = \tilde{T}$. Since the singly-occupied impurity level is now well below $-D$, we have $\langle n_d \rangle = 1$ and we


 Figure 3: Renormalization in energy levels when $\epsilon_d^* \ll -\Delta$

are comfortably in the Kondo limit and the SWT and a consequent poor man's scaling can be performed, which will give eqs. 2.471 through 2.475. 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. 2.496, but with a degeneracy of 2. To go to lower temperatures, we can do a Poor Man's scaling which suggests that the Hamiltonian at $T \ll T_K$ is one with a large coupling between the impurity and the conduction electrons.

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

Jefferson's calculation

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

$$H = \sum_{k\sigma} \epsilon_{k\sigma} n_{k\sigma} + \epsilon_d n_d + \sum_{k\sigma} \left(V_{kd}^- c_{k\sigma}^\dagger c_{d\sigma} + V_{kd}^+ c_{d\sigma}^\dagger c_{k\sigma} \right) = H_0 + V \quad (2.509)$$

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

$$H\psi = E\psi \quad (2.510)$$

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

$$P = \sum |\phi\rangle \langle\phi| = \sum_{|k| < D - \delta D, \sigma = \pm 1, n_{d\sigma} = 0, 1} |n_{k\sigma}, n_{d\sigma'}\rangle \quad (2.511)$$

Its orthogonal subspace has a projection operator

$$Q = 1 - P = \sum_{D-\delta D < |k| < D, \sigma=\pm 1, n_{d\sigma}=0,1} |n_{k\sigma}, n_{d\sigma'}\rangle \quad (2.512)$$

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

$$P\{\psi\}_d = \{\phi\} \quad (2.513)$$

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

$$P\psi_0 \Big|_{|k| < D-\delta D} = \psi_0 \Big|_{|k| < D-\delta D} \quad (2.514)$$

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:

$$\Omega\{\phi\} = \{\psi\} \quad (2.515)$$

Since Ω can only act on states in the model subspace, we define

$$\Omega\{\phi\}^\perp = 0 \quad (2.516)$$

This allows us to write

$$\Omega P\phi = \Omega\phi \quad (2.517)$$

$$\Omega P\phi^\perp = \Omega \times 0 = 0 = \Omega\phi^\perp \quad (2.518)$$

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

$$\Omega P = \Omega \quad (2.519)$$

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

$$H\Omega\phi = E\Omega\phi \quad (2.520)$$

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

$$PH\Omega\phi = EP\Omega\phi = E\phi \quad (2.521)$$

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

$$H_{\text{eff}} = PH\Omega = PH_0P + PV\Omega = PH_0P + PV\Omega \quad (2.522)$$

To solve for the Ω , apply eq. 2.519 on the Schrödinger equation $(E - H_0)\psi = V\psi$:

$$\Omega V\psi = (E\Omega P - \Omega P H_0)\psi \quad (2.523)$$

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

$$\Omega V\psi = (E - \Omega H_0 P)\psi \quad (2.524)$$

Subtracting the Schrödinger equation from the last equation gives

$$\begin{aligned} (\Omega - 1) V\psi &= (H_0 - \Omega H_0 P) \psi \\ \implies (\Omega - 1) V\Omega\phi &= (H_0 - \Omega H_0 P) \Omega\phi \\ \implies (\Omega - 1) V\Omega\phi &= (H_0\Omega - \Omega H_0) \phi \\ \implies (\Omega - 1) V\Omega &= [H_0, \Omega] \end{aligned} \quad (2.525)$$

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

$$\Omega = \sum_n c_n V^n = \sum_n \Lambda_n \quad (2.526)$$

The zeroth term in the main equation becomes

$$[H_0, \Lambda_0] = 0 \implies \Lambda_0 = P \quad (2.527)$$

The first order equation is

$$[H_0, \Lambda_1] = (\Lambda_0 - 1) V \Lambda_0 = (P - 1) V P = -QVP \quad (2.528)$$

The second order equation is

$$[H_0, \Lambda_2] = -V\Lambda_1 + \Lambda_0 V\Lambda_1 + \Lambda_1 V\Lambda_0 = -QV\Lambda_1 + \Lambda_1 VP \quad (2.529)$$

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.

$$A_1 = -QVP \quad (2.530)$$

$$A_2 = -QV\Lambda_1 + \Lambda_1 VP \quad (2.531)$$

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

$$\langle h| A_n |l\rangle = (E_h - E_l) \langle h| \Lambda_n |l\rangle \implies \langle h| \Lambda_n |l\rangle = \frac{\langle h| A_n |l\rangle}{E_h - E_l} \quad (2.532)$$

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

$$\langle h| SA |l\rangle = \frac{\langle h| A |l\rangle}{E_l - E_h} \quad (2.533)$$

we can write the solution

$$\Lambda_n = -S(A_n) \quad (2.534)$$

The expression of SA can be written as

$$\begin{aligned}
 SA &= \sum_{h,l} |h\rangle \langle l| \frac{\langle h| A |l\rangle}{E_l - E_H} \\
 &= \sum_{h,l} \frac{1}{E_l - E_h} |h\rangle \langle h| A |l\rangle \langle l| \\
 &= \sum_l \frac{1}{E_l - H_0} \left(\sum_h |h\rangle \langle h| \right) A |l\rangle \langle l| \\
 &= \sum_l G_l A P_l
 \end{aligned} \tag{2.535}$$

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

S has the property

$$\begin{aligned}
 \langle h| SQA |l\rangle &= \frac{\langle h| QA |l\rangle}{E_l - E_h} = \frac{\langle h| A |l\rangle}{E_l - E_h} = \langle h| SA |l\rangle \\
 \implies S(QA) &= S(A)
 \end{aligned} \tag{2.536}$$

The lowest order solutions are thus

$$\Lambda_1 = S(QVP) = S(VP) \tag{2.537}$$

$$\Lambda_2 = S(QV\Lambda_1) - S(\Lambda_1VP) = S(VS(VP)) - S(S(VP)VP) \tag{2.538}$$

We can now expand the effective Hamiltonian in powers of V . From eq. 2.522, the interacting part of the effective Hamiltonian becomes

$$\begin{aligned}
 H_{\text{eff}} - PH_0P &= PV\Omega \\
 &\approx PV(\Lambda_0 + \Lambda_1 + \Lambda_2) \\
 &= PV[P + S(VP) + S(VS(VP)) - S(S(VP)VP)] \\
 &= PVP + PVS(VP) + PVS(VS(VP)) - PVS(S(VP)VP)
 \end{aligned} \tag{2.539}$$

Therefore,

$$H_{\text{eff}} = PHP + PVS(VP) + PVS(VS(VP)) - PVS(S(VP)VP) \tag{2.540}$$

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

$$PVSVP = PV \sum_l G_l V P P_l = PV \sum_l G_l V P_l \tag{2.541}$$

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

$$\begin{aligned}
 PVS V SVP &= PVS V \sum_l G_l V P_l = PV \sum_l S V G_l V P_l \\
 &= PV \sum_{l,l'} G_{l'} V G_l V P_l P_{l'} = PV \sum_l G_l V G_l V P_l
 \end{aligned} \tag{2.542}$$

The fourth term is

$$\begin{aligned}
 PVS(S(VP)VP) &= PVS\left(\sum_l G_l V P P_l V P\right) = PV \sum_{l,l'} G_{l'} G_l V P_l V P P_{l'} \\
 &= PV \sum_{l'} G_{l'} \left(\sum_l G_l V P_l \right) V P_{l'}
 \end{aligned} \tag{2.543}$$

The effective Hamiltonian up to third order in V is

$$\begin{aligned}
 H_{\text{eff}} &= PH_0P + PV \sum_l G_l V P_l + PV \sum_l G_l V G_l V P_l \\
 &\quad - PV \sum_{l,l'} G_{l'} G_l V P_l V P_{l'}
 \end{aligned} \tag{2.544}$$

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:

$$|k_1\rangle \langle k_2| = c_{k_1}^\dagger c_{k_2} \tag{2.545}$$

$$P_k = |k, n_{d\sigma}\rangle \langle k, n_{d\sigma}| = c_k^\dagger c_k c_{d\sigma}^\dagger c_{d\sigma} = n_{k\sigma} n_{d\sigma} \tag{2.546}$$

The first term becomes

$$PH_0P = \sum_{k\sigma} \epsilon_{k\sigma} n_{k\sigma} + \epsilon_d n_d + \sum_{k\sigma} \left(V_{kd} c_{k\sigma}^\dagger c_{d\sigma} + \text{h.c.} \right) \tag{2.547}$$

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

$$\begin{aligned}
 PV \sum_l G_l V P_l &= V \sum_{q\sigma} \left(\frac{V_q}{\epsilon_d - \epsilon_q} c_{q\sigma}^\dagger c_{d\sigma} + \frac{V_q^*}{\epsilon_q - \epsilon_d} c_{d\sigma}^\dagger c_{q\sigma} \right) \\
 &= \sum_{q\sigma}^+ \frac{|V_q|^2 c_{d\sigma}^\dagger c_{q\sigma} c_{q\sigma}^\dagger c_{d\sigma}}{\epsilon_d - \epsilon_q} + \sum_{q\sigma}^- \frac{|V_q|^2 c_{q\sigma}^\dagger c_{d\sigma} c_{d\sigma}^\dagger c_{q\sigma}}{\epsilon_q - \epsilon_d} \\
 &= \sum_{q\sigma}^+ \frac{|V_q|^2 n_{d\sigma} (1 - n_{q\sigma})}{\epsilon_d - \epsilon_q} + \sum_{q\sigma}^- \frac{|V_q|^2 n_{q\sigma} (1 - n_{d\sigma})}{\epsilon_q - \epsilon_d}
 \end{aligned} \tag{2.548}$$

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

$$\begin{aligned}
 PV \sum_l G_l V P_l &= \sum_q^+ \frac{|V_q|^2 n_{d\sigma}}{\epsilon_d - \epsilon_q} + \sum_q^- \frac{|V_q|^2 (1 - n_{d\sigma})}{\epsilon_q - \epsilon_d} \\
 &= n_d \left(\sum_q^+ \frac{|V_q|^2}{\epsilon_d - \epsilon_q} + 2 \sum_q^- \frac{|V_q|^2}{\epsilon_d - \epsilon_q} \right) \\
 &= n_d \delta \epsilon_d
 \end{aligned} \tag{2.549}$$

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

$$|k, n_{d\sigma}\rangle \rightarrow \begin{cases} |q_e, n_d = 0\rangle \rightarrow \begin{cases} |q_e, n_d = 1\rangle \\ |q_e, q'_h, n_d = 1\rangle \end{cases} \\ |q_h, n_d = 1\rangle \rightarrow \begin{cases} |q_h, q'_e, n_d = 0\rangle \\ |q_h, n_d = 0\rangle \end{cases} \end{cases} \quad (2.550)$$

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

$$|k, n_d = 0\rangle \xrightarrow{\Delta E = \epsilon_k - \epsilon_q} |n_d = 1\rangle \rightarrow |q_e, n_d = 0\rangle \xrightarrow{\Delta E = \epsilon_q - \epsilon_d} |k', n_d = 1\rangle \quad (2.551)$$

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

$$|n_{d\sigma} = 1\rangle \xrightarrow{\Delta E = \epsilon_k - \epsilon_q} |k\sigma, n_d = 0\rangle \rightarrow \begin{cases} |q_h \uparrow, n_{d\uparrow} = 1\rangle \\ |q_h \downarrow, n_{d\downarrow} = 1\rangle \end{cases} \xrightarrow{\Delta E = \epsilon_q - \epsilon_d} |n_d = 0\rangle \quad (2.552)$$

Combining the two processes gives

$$\begin{aligned} \sum_q^+ \sum_{k\sigma} \frac{|V_q|^2 c_{d\sigma}^\dagger c_{q\sigma} c_{q\sigma}^\dagger c_{d\sigma} c_{d\sigma}^\dagger c_{k\sigma}}{(\epsilon_q - \epsilon_d)(\epsilon_k - \epsilon_q)} + \sum_{q\sigma'}^- \sum_{k\sigma} \frac{|V_q|^2 c_{q\sigma'}^\dagger c_{d\sigma'} c_{d\sigma'}^\dagger c_{q\sigma'} c_{q\sigma'}^\dagger c_{k\sigma} c_{d\sigma}}{(\epsilon_q - \epsilon_d)(\epsilon_k - \epsilon_q)} \\ = \sum_{k\sigma} \left(c_{k\sigma}^\dagger c_{d\sigma} \delta V_k^- + c_{d\sigma}^\dagger c_{k\sigma} \delta V_k^- \right) \end{aligned} \quad (2.553)$$

where

$$\begin{aligned} \delta V^+ &= \sum_q^+ \frac{|V_q|^2}{(\epsilon_q - \epsilon_d)(\epsilon_k - \epsilon_q)} \\ \delta V^- &= \sum_q^- 2 \frac{|V_q|^2}{(\epsilon_q - \epsilon_d)(\epsilon_k - \epsilon_q)} \end{aligned} \quad (2.554)$$

The total Hamiltonian can be written in the form

$$\begin{aligned} H_{\text{eff}} &= \sum_{k\sigma} \epsilon_{k\sigma} n_{k\sigma} + (\epsilon_d + \delta\epsilon_d) n_d \\ &+ \sum_{k\sigma} \left\{ (V_k^- + \delta V_k^-) c_{k\sigma}^\dagger c_{d\sigma} + (V_k^+ + \delta V_k^+) c_{d\sigma}^\dagger c_{k\sigma} \right\} \end{aligned} \quad (2.555)$$

We now evaluate the changes:

$$\begin{aligned} \delta\epsilon_d &= \left(\sum_q^+ \frac{|V_q|^2}{\epsilon_d - \epsilon_q} + 2 \sum_q^- \frac{|V_q|^2}{\epsilon_d - \epsilon_q} \right) \\ &\approx |V|^2 \rho |\delta D| \left(\frac{1}{\epsilon_d - D} + \frac{2}{\epsilon_d + D} \right) \\ &= |V|^2 \rho |\delta D| \frac{D - 3\epsilon_d}{D^2 - \epsilon_d^2} \end{aligned} \quad (2.556)$$

I used the approximation

$$\sum_{q=D-\delta D}^D f(q) = \int_{D-\delta D}^D dE \rho(E) f(E) \approx \rho f(D) \delta D \quad (2.557)$$

Also,

$$\begin{aligned} \delta V_k^+ &= \sum_q^+ \frac{|V_q|^2}{(\epsilon_q - \epsilon_d)(\epsilon_k - \epsilon_q)} \\ &\approx |V|^2 \rho |\delta D| \frac{1}{(D - \epsilon_d)(\epsilon_k - D)} \\ \delta V_k^- &= 2 \sum_q^- \frac{|V_q|^2}{(\epsilon_q - \epsilon_d)(\epsilon_k - \epsilon_q)} \\ &\approx -|V|^2 \rho |\delta D| \frac{2}{(D + \epsilon_d)(\epsilon_k + D)} \end{aligned} \quad (2.558)$$

We now make the following assumptions:

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

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

3 Unitary Renormalization Group Method

This section is adapted from ref.[19].

3.1 Description of the problem

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

We take a general Hamiltonian,

$$\mathcal{H} = H_e \hat{n}_{q\beta} + H_h (1 - \hat{n}_{q\beta}) + c_{q\beta}^\dagger T + T^\dagger c_{q\beta} \quad (3.1)$$

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

$$\mathcal{H} = \begin{pmatrix} |1\rangle & |0\rangle \\ H_1 & T \\ T^\dagger & H_0 \end{pmatrix} \quad (3.2)$$

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.

$$\tilde{\mathcal{H}} \equiv U\mathcal{H}U^\dagger = \begin{pmatrix} |1\rangle & |0\rangle \\ \tilde{H}_1 & 0 \\ 0 & \tilde{H}_0 \end{pmatrix} \quad (3.3)$$

U_q is defined by

$$\tilde{\mathcal{H}} = U_q\mathcal{H}U_q^\dagger \text{ such that } [\tilde{\mathcal{H}}, n_q] = 0 \quad (3.4)$$

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

$$\mathcal{H}|\psi_i\rangle = \tilde{H}_i|\psi_i\rangle, i \in \{0, 1\} \quad (3.5)$$

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 $q\beta$:

$$|\psi_i\rangle = \sum_{j=0,1} |j\rangle \langle j|\psi_i\rangle \equiv |1\rangle |\phi_1^i\rangle + |0\rangle |\phi_0^i\rangle \quad (3.6)$$

where $|\phi_j^i\rangle = \langle j|\psi_i\rangle$. If we substitute the expansion 3.2 into the eigenvalue equation 3.5, we get

$$\left[H_e \hat{n}_{q\beta} + H_h (1 - \hat{n}_{q\beta}) + c_{q\beta}^\dagger T + T^\dagger c_{q\beta} \right] |\psi_i\rangle = \tilde{H}_i |\psi_i\rangle \quad (3.7)$$

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

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

This gives

$$\left[c_{q\beta}^\dagger T + T^\dagger c_{q\beta} \right] |\psi_i\rangle = \left(\tilde{H}_i - \mathcal{H}^i - \mathcal{H}^d \right) |\psi_i\rangle \quad (3.8)$$

3.2 Obtaining the decoupling transformation

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

$$\left[c_{q\beta}^\dagger T + T^\dagger c_{q\beta} \right] |\psi_i\rangle = (\hat{\omega}_i - \mathcal{H}^d) |\psi_i\rangle \quad (3.9)$$

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 3.6, we can write

$$\hat{\omega}_i |\psi_i\rangle = \hat{\omega}_i^1 |1\rangle |\phi_1^i\rangle + \hat{\omega}_i^0 |0\rangle |\phi_0^i\rangle \quad (3.10)$$

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

$$\left[\mathcal{H}^d + c_{q\beta}^\dagger T + T^\dagger c_{q\beta} \right] |\psi_i(\omega_i)\rangle = (\omega_i^1 - \mathcal{H}^d) |1\rangle |\phi_1^i\rangle + (\omega_i^0 - \mathcal{H}^d) |0\rangle |\phi_0^i\rangle \quad (3.11)$$

If we now substitute the expansion 3.6 and gather the terms that result in $\hat{n}_{q\beta} = 1$, we get

$$c_{q\beta}^\dagger T |0\rangle |\phi_0^i\rangle = (\omega_i^1 - \mathcal{H}^d) |1\rangle |\phi_1^i\rangle \quad (3.12)$$

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

$$T^\dagger c_{q\beta} |1\rangle |\phi_1^i\rangle = (\omega_i^0 - \mathcal{H}^d) |0\rangle |\phi_0^i\rangle \quad (3.13)$$

We now define two many-particle transition operators:

$$\begin{aligned} \eta^\dagger(\omega_i^1) &= \frac{1}{\omega_i^1 - \mathcal{H}^d} c_{q\beta}^\dagger T \equiv G_1 c_{q\beta}^\dagger T \\ \eta(\omega_i^0) &= \frac{1}{\omega_i^0 - \mathcal{H}^d} T^\dagger c_{q\beta} \equiv G_0 T^\dagger c_{q\beta} \end{aligned} \quad (3.14)$$

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

$$\eta(\hat{\omega}) = G T^\dagger c_{q\beta} = \frac{1}{\hat{\omega}_i - \mathcal{H}^d} T^\dagger c_{q\beta} \quad (3.15)$$

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:

$$\eta^\dagger(\omega_i^0) = \eta^\dagger(\omega_i^1) \implies \frac{1}{\omega_i^1 - \mathcal{H}^d} c_{q\beta}^\dagger T = c_{q\beta}^\dagger T \frac{1}{\omega_i^0 - \mathcal{H}^d} \quad (3.16)$$

Henceforth we will assume that this constraint has been imposed.

In terms of these operators, eq. 3.13 becomes

$$\begin{aligned} |1\rangle |\phi_1^i\rangle &= \eta^\dagger |0\rangle |\phi_0^i\rangle \\ |0\rangle |\phi_0^i\rangle &= \eta |1\rangle |\phi_1^i\rangle \end{aligned} \quad (3.17)$$

These allow us to write

$$\begin{aligned} |\psi_1\rangle &= |1\rangle |\phi_1^i\rangle + |0\rangle |\phi_0^i\rangle = (1 + \eta) |1\rangle |\phi_1^i\rangle \\ |\psi_0\rangle &= (1 + \eta^\dagger) |0\rangle |\phi_0^i\rangle \end{aligned} \quad (3.18)$$

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

$$U_1 = 1 + \eta \quad (3.19)$$

3.3 Properties of the many-body transition operators

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

$$\eta^2 = \eta^{\dagger 2} = 0 \quad [c^{\dagger 2} = c^2 = 0] \quad (3.20)$$

Second is:

$$\begin{aligned} |1\rangle |\phi_1^i\rangle &= \eta^\dagger |0\rangle |\phi_0^i\rangle = \eta^\dagger \eta |1\rangle |\phi_1^i\rangle \implies \eta^\dagger \eta = \hat{n}_{q\beta} \\ |0\rangle |\phi_0^i\rangle &= \eta |1\rangle |\phi_1^i\rangle = \eta \eta^\dagger |\phi_0^i\rangle \implies \eta \eta^\dagger = 1 - \hat{n}_{q\beta} \end{aligned} \quad (3.21)$$

and hence the anticommutator

$$\implies \{\eta, \eta^\dagger\} = 1 \quad (3.22)$$

Note that the three equations in 3.21 work only when applied on the eigenstate $|\psi_i\rangle$ and not any arbitrary state.

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

3.4 Form of the unitary operators

Although we have found the correct similarity transformations U_i (eqs. 3.19), 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

$$U_1 = 1 + \eta \quad (3.23)$$

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

$$U_1 = e^\eta \quad (3.24)$$

using the fact that $\eta^2 = 0$. It is shown in ref. [22] that corresponding to a similarity transformation e^ω , there exists a unitary transformation e^G where

$$G = \tanh^{-1} (\omega - \omega^\dagger) \quad (3.25)$$

Applying that to the problem at hand gives

$$U_1^\dagger = \exp (\tanh^{-1} (\eta - \eta^\dagger)) \quad (3.26)$$

Let $x = \tanh y$. Then,

$$x = \frac{e^{2y} + 1}{e^{2y} - 1} \implies y = \frac{1}{2} \log \frac{1+x}{1-x} \implies e^y = e^{\tanh^{-1} x} = \sqrt{\frac{1+x}{1-x}} \quad (3.27)$$

Therefore,

$$\begin{aligned} \exp (\tanh^{-1} (\eta - \eta^\dagger)) &= \frac{1 + \eta - \eta^\dagger}{\sqrt{(1 + \eta^\dagger - \eta)(1 - \eta^\dagger + \eta)}} \\ &= \frac{1 + \eta - \eta^\dagger}{\sqrt{1 + \{\eta, \eta^\dagger\}}} \\ &= \frac{1}{\sqrt{2}} (1 + \eta - \eta^\dagger) \end{aligned} \quad (3.28)$$

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

$$U_1 = \frac{1}{\sqrt{2}} (1 + \eta^\dagger - \eta) \quad (3.29)$$

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

$$\begin{aligned} \exp\left(\frac{\pi}{4}(\eta^\dagger - \eta)\right) &= 1 + (\eta^\dagger - \eta) \frac{\pi}{4} + \frac{1}{2!} (\eta^\dagger - \eta)^2 \left(\frac{\pi}{4}\right)^2 + \frac{1}{3!} (\eta^\dagger - \eta)^3 \left(\frac{\pi}{4}\right)^3 + \dots \\ &= 1 + (\eta^\dagger - \eta) \frac{\pi}{4} - \frac{1}{2!} \left(\frac{\pi}{4}\right)^2 - \frac{1}{3!} (\eta^\dagger - \eta) \left(\frac{\pi}{4}\right)^3 + \frac{1}{4!} \left(\frac{\pi}{4}\right)^4 + \dots \\ &= \cos \frac{\pi}{4} + (\eta^\dagger - \eta) \sin \frac{\pi}{4} \\ &= \frac{1}{\sqrt{2}} (1 + \eta^\dagger - \eta) \end{aligned} \quad (3.30)$$

There we used

$$(\eta^\dagger - \eta)^2 = \eta^{\dagger 2} + \eta^2 - \{\eta^\dagger, \eta\} = -1 \quad \left[\because \eta^2 = \eta^{\dagger 2} = 0 \right] \quad (3.31)$$

and hence

$$(\eta^\dagger - \eta)^3 = -1 (\eta^\dagger - \eta) \quad (3.32)$$

and so on.

3.5 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. 3.29,

$$\begin{aligned} U_1 \mathcal{H} U_1^\dagger &= \frac{1}{2} (1 + \eta^\dagger - \eta) \mathcal{H} (1 + \eta - \eta^\dagger) \\ &= \frac{1}{2} (1 + \eta^\dagger - \eta) (\mathcal{H} + \mathcal{H}\eta - \mathcal{H}\eta^\dagger) \\ &= \frac{1}{2} (\mathcal{H} + \mathcal{H}\eta - \mathcal{H}\eta^\dagger + \eta^\dagger \mathcal{H} + \eta^\dagger \mathcal{H}\eta - \eta^\dagger \mathcal{H}\eta^\dagger - \eta \mathcal{H} - \eta \mathcal{H}\eta + \eta \mathcal{H}\eta^\dagger) \\ &= \frac{1}{2} (\mathcal{H}^d + \mathcal{H}^i + \mathcal{H}^I + \mathcal{H}\eta - \mathcal{H}\eta^\dagger + \eta^\dagger \mathcal{H} + \eta^\dagger \mathcal{H}\eta - \eta^\dagger \mathcal{H}\eta^\dagger - \eta \mathcal{H} - \eta \mathcal{H}\eta + \eta \mathcal{H}\eta^\dagger) \\ &= \frac{1}{2} (\mathcal{H}^d + \mathcal{H}^i + \mathcal{H}^I + [\eta^\dagger - \eta, \mathcal{H}] + \eta^\dagger \mathcal{H}\eta - \eta^\dagger \mathcal{H}\eta^\dagger - \eta \mathcal{H}\eta + \eta \mathcal{H}\eta^\dagger) \end{aligned} \quad (3.33)$$

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:

$$\tilde{\mathcal{H}} = \frac{1}{2} \left(\underbrace{\mathcal{H}^d + \mathcal{H}^i + [\eta^\dagger - \eta, \mathcal{H}] + \eta^\dagger \mathcal{H}\eta + \eta \mathcal{H}\eta^\dagger}_{\text{group 1}} + \overbrace{\mathcal{H}^I - \eta^\dagger \mathcal{H}\eta^\dagger - \eta \mathcal{H}\eta}^{\text{group 2}} \right) \quad (3.34)$$

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.

$$\eta \mathcal{H} \eta = \eta c_q^\dagger T \eta \quad (3.35)$$

and

$$\eta^\dagger \mathcal{H} \eta^\dagger = \eta^\dagger T^\dagger c_q \eta^\dagger \quad (3.36)$$

Group 2 becomes

$$\text{group 2} = \mathcal{H}^I - \eta^\dagger T^\dagger c_q \eta^\dagger - \eta c_q^\dagger T \eta = c_q^\dagger T + T^\dagger c_q - \eta^\dagger T^\dagger c_q \eta^\dagger - \eta c_q^\dagger T \eta \quad (3.37)$$

To simplify this, we use the relation

$$\begin{aligned} \eta c_q^\dagger T \eta &= \frac{1}{\omega_i^0 - \mathcal{H}^d} T^\dagger c_q c_q^\dagger T \eta \\ &= T^\dagger c_q \frac{1}{\omega_i^1 - \mathcal{H}^d} c_q^\dagger T \eta \quad [\text{eq. 3.16}] \\ &= T^\dagger c_q \eta^\dagger \eta \quad [\text{eq. 3.15}] \\ &= T^\dagger c_q \hat{n}_q \quad [\text{eq. 3.21}] \end{aligned} \quad (3.38)$$

which gives

$$\eta c_q^\dagger T \eta = T^\dagger c_q \quad (3.39)$$

Taking the Hermitian conjugate of eq. 3.39 gives

$$\eta^\dagger T^\dagger c_q \eta^\dagger = c_q^\dagger T \quad (3.40)$$

Substituting the expressions 3.39 and 3.40 into the expression for group 2, 3.37, shows that it vanishes. This leaves us only with group 1:

$$\tilde{\mathcal{H}} = \frac{1}{2} \left(\mathcal{H}^d + \mathcal{H}^i + \overbrace{\eta^\dagger \mathcal{H} \eta + \eta \mathcal{H} \eta^\dagger}^{\text{group A}} + \underbrace{[\eta^\dagger - \eta, \mathcal{H}]}_{\text{group B}} \right) \quad (3.41)$$

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

$$\eta^\dagger [H_e \hat{n}_{q\beta} + H_h (1 - \hat{n}_{q\beta})] \eta + \eta [H_e \hat{n}_{q\beta} + H_h (1 - \hat{n}_{q\beta})] \eta^\dagger = \eta^\dagger H_h \eta + \eta H_e \eta^\dagger \quad (3.42)$$

This can be shown (**clear with AM**) to be equal to the diagonal part:

$$\text{group A} = \eta^\dagger H_h \eta + \eta H_e \eta^\dagger = H_e \hat{n}_{q\beta} + H_h (1 - \hat{n}_{q\beta}) = \mathcal{H}^d + \mathcal{H}^i \quad (3.43)$$

It can also be shown (**clear with AM**) that

$$\text{group B} = [\eta^\dagger - \eta, \mathcal{H}] = 2 [c_{q\beta}^\dagger T, \eta] \quad (3.44)$$

Putting it all together,

$$\tilde{\mathcal{H}} = \mathcal{H}^d + \mathcal{H}^i + [c_{q\beta}^\dagger T, \eta] \quad (3.45)$$

The renormalizing in the Hamiltonian is

$$\Delta\mathcal{H} = \tilde{\mathcal{H}} - \mathcal{H}^d - \mathcal{H}^i = [c_{q\beta}^\dagger T, \eta] \quad (3.46)$$

Because of eq. 3.44, (**clear with AM**) it can also be written as

$$\Delta\mathcal{H} = \frac{1}{2} [\eta^\dagger - \eta, \mathcal{H}_X] = \frac{1}{2} [\eta^\dagger - \eta, \mathcal{H}] \quad (3.47)$$

This form will be useful later when we make the connection with one-shot Schrieffer-Wolff transformation and CUT RG. To check that this indeed commutes with $\hat{n}_{q\beta}$,

$$\begin{aligned} [\tilde{\mathcal{H}}, \hat{n}_{q\beta}] &= [[c_{q\beta}^\dagger T, \eta], \hat{n}_{q\beta}] \\ &= [c_{q\beta}^\dagger T \eta, \hat{n}_{q\beta}] - [\eta c_{q\beta}^\dagger T, \hat{n}_{q\beta}] \\ &= c_{q\beta}^\dagger T \eta \hat{n}_{q\beta} - \hat{n}_{q\beta} c_{q\beta}^\dagger T \eta \quad \left[2^{\text{nd}} [\cdot] \text{ is 0, } \because c_{q\beta}^\dagger \hat{n}_{q\beta} = \hat{n}_{q\beta} \eta = 0 \right] \\ &= c_{q\beta}^\dagger T \eta - c_{q\beta}^\dagger T \eta \\ &= 0 \end{aligned} \quad (3.48)$$

3.6 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. 3.12 and 3.13 gives

$$c_{q\beta}^\dagger T |0\rangle |\phi_0^i\rangle = (\omega_i^1 - \mathcal{H}_1^d) |1\rangle |\phi_1^i\rangle = 0 \implies c_{q\beta}^\dagger T = 0 \quad (3.49)$$

3.7 Multiple off-diagonal terms

There is a subtle assumption in the definitions eq. 3.14. 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: $T = T_1 + T_2$.

$$\begin{aligned} \eta &= \frac{1}{\omega_0 - \mathcal{H}_d} (T_1^\dagger + T_2^\dagger) c = \left[\frac{1}{\omega^0 - E_1^0} T_1^\dagger c + \frac{1}{\omega^0 - E_2^0} T_2^\dagger c \right] \\ \eta^\dagger &= \frac{1}{\omega^1 - \mathcal{H}_d} c^\dagger (T_1 + T_2) = \left[\frac{1}{\omega^1 - E_1^1} c^\dagger T_1 + \frac{1}{\omega^1 - E_2^1} c^\dagger T_2 \right] \end{aligned} \quad (3.50)$$

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:

$$\omega^0 - E_1^0 = \omega^1 - E_1^1, \quad \omega^0 - E_2^0 = \omega^1 - E_2^1 \quad (3.51)$$

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 .

$$\begin{aligned}\eta &= \sum_i \frac{1}{\omega_i^0 - E_i^0} T_i^\dagger c \\ \eta^\dagger &= \sum_i \frac{1}{\omega_i^1 - E_1^1} c^\dagger T_i\end{aligned}\tag{3.52}$$

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

$$\begin{aligned}\eta^\dagger - \eta &= \sum_i \frac{1}{\omega_i^0 - E_i^0} (c^\dagger T_i - T_i^\dagger c) \\ \Delta\mathcal{H} &= \frac{1}{2} [\eta^\dagger - \eta, c^\dagger T + T^\dagger c] \\ &= \frac{1}{2} \sum_{ij} \frac{1}{\omega_i^0 - E_i^0} [c^\dagger T_i - T_i^\dagger c, c^\dagger T_j + T_j^\dagger c] \\ &= \frac{1}{2} \sum_{ij} \frac{1}{\omega_i^0 - E_i^0} [\hat{n} (T_i T_j^\dagger + T_j T_i^\dagger) - (1 - \hat{n}) (T_i^\dagger T_j + T_j^\dagger T_i)] \\ &= \frac{1}{2} \sum_{ij} \left(\frac{1}{\omega_i^0 - E_i^0} + \frac{1}{\omega_j^0 - E_j^0} \right) [\hat{n} T_i T_j^\dagger - (1 - \hat{n}) T_i^\dagger T_j]\end{aligned}\tag{3.53}$$

3.8 Equivalence of the two unitaries and preservation of partial trace

In the subsection 3.4, we determined the form of the operator U_1 that unitarily decouples the node $q\beta$ from the other degrees of freedom. Eq. 3.29 was derived by reading off the transformation of $|1\rangle$ to $|\psi_1\rangle$, the first equation in 3.18. We could easily have chosen the other equation in the same equation set,

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

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

$$U_0 = \frac{1}{\sqrt{2}} (1 + \eta - \eta^\dagger)\tag{3.54}$$

This η will however be different from the η in eq. 3.29. 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 :

$$\begin{aligned}\text{Starting from } |\psi_1\rangle: \eta_1 &= \frac{1}{\omega_1^0 - \mathcal{H}^d} T^\dagger c_{q\beta} \quad \text{and} \quad \eta_1^\dagger = \frac{1}{\omega_1^1 - \mathcal{H}^d} T^\dagger c_{q\beta} \\ \text{Starting from } |\psi_0\rangle: \eta_0 &= \frac{1}{\omega_0^0 - \mathcal{H}^d} T^\dagger c_{q\beta} \quad \text{and} \quad \eta_0^\dagger = \frac{1}{\omega_0^1 - \mathcal{H}^d} T^\dagger c_{q\beta}\end{aligned}\tag{3.55}$$

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

$$\begin{aligned} U_1 &= \frac{1}{\sqrt{2}} \left(1 + \eta_1^\dagger - \eta_1 \right) \\ U_0 &= \frac{1}{\sqrt{2}} \left(1 + \eta_0 - \eta_0^\dagger \right) \end{aligned} \quad (3.56)$$

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

$$\omega_1^0 - \mathcal{H}_0^d = -(\omega_0^0 - \mathcal{H}_0^d) \quad (3.57)$$

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.

$$\begin{aligned} \eta_1 &= \frac{1}{\tilde{H}_1 - \mathcal{H}^i - \mathcal{H}^d} T^\dagger c_{q\beta} \\ \eta_0 &= \frac{1}{\tilde{H}_0 - \mathcal{H}^i - \mathcal{H}^d} T^\dagger c_{q\beta} \\ \implies \eta_1 + \eta_0 &= \left[\frac{1}{\tilde{H}_1 - \mathcal{H}^i - \mathcal{H}^d} + \frac{1}{\tilde{H}_0 - \mathcal{H}^i - \mathcal{H}^d} \right] T^\dagger c_{q\beta} = 0 \\ \implies \tilde{H}_1 - \mathcal{H}^i - \mathcal{H}^d &= -[\tilde{H}_0 - \mathcal{H}^i - \mathcal{H}^d] \\ \implies \tilde{H}_1 + \tilde{H}_0 &= 2\mathcal{H}_0 \end{aligned} \quad (3.58)$$

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

$$\tilde{H} = \begin{pmatrix} E_1 & 0 \\ 0 & E_0 \end{pmatrix} \quad (3.59)$$

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 3.58 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 3.58 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 $t_{\text{new}} = t_{\text{old}}$.

3.9 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. 3.16), 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.

$$\begin{aligned}\omega_1^0 - \omega_1^1 &= \mathcal{H}_d^0 - \mathcal{H}_d^1 \\ \omega_0^0 - \omega_0^1 &= \mathcal{H}_d^0 - \mathcal{H}_d^1 \\ \omega_1^0 + \omega_0^0 &= 2\mathcal{H}_d^0\end{aligned}\tag{3.60}$$

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.

3.10 Prescription

Given a Hamiltonian

$$\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_0 + c^\dagger T + T^\dagger c\tag{3.61}$$

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. 3.45, 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

$$\Delta\mathcal{H} = \left[c_{q\beta}^\dagger \text{Tr}(\mathcal{H}c_{q\beta}), \eta \right] = c_{q\beta}^\dagger \text{Tr}(\mathcal{H}c_{q\beta}) \eta - \eta c_{q\beta}^\dagger \text{Tr}(\mathcal{H}c_{q\beta})\tag{3.62}$$

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

$$\Delta\mathcal{H} = c_{q\beta}^\dagger \text{Tr}(\mathcal{H}c_{q\beta}) \eta_1 - \eta_1 c_{q\beta}^\dagger \text{Tr}(\mathcal{H}c_{q\beta})\tag{3.63}$$

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*.

$$\Delta_1\mathcal{H} = c_{q\beta}^\dagger \text{Tr}(\mathcal{H}c_{q\beta}) \eta_1\tag{3.64}$$

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

$$\Delta_0\mathcal{H} = -\eta_1 c_{q\beta}^\dagger \text{Tr}(\mathcal{H}c_{q\beta})\tag{3.65}$$

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:

$$\Delta\mathcal{H} = c_{q\beta}^\dagger \text{Tr}(\mathcal{H}c_{q\beta}) \eta_1 + \eta_0 c_{q\beta}^\dagger \text{Tr}(\mathcal{H}c_{q\beta}) \quad (3.66)$$

We can make one more manipulation: using eq. 3.16, we get

$$\Delta\mathcal{H} = c_{q\beta}^\dagger \text{Tr}(\mathcal{H}c_{q\beta}) \eta_1 + \text{Tr}(c_{q\beta}^\dagger \mathcal{H}) c_{q\beta} \eta_0^\dagger \quad (3.67)$$

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

$$\Delta\mathcal{H} = c_{q\beta}^\dagger \text{Tr}(\mathcal{H}c_{q\beta}) \frac{1}{\omega_1^0 - \mathcal{H}_0^d} \text{Tr}(c_{q\beta}^\dagger \mathcal{H}) c_{q\beta} + \text{Tr}(c_{q\beta}^\dagger \mathcal{H}) c_{q\beta} \frac{1}{\omega_0^1 - \mathcal{H}_1^d} c_{q\beta}^\dagger \text{Tr}(\mathcal{H}c_{q\beta}) \quad (3.68)$$

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

$$\Delta\mathcal{H} = \sum_{q\beta} \left[c_{q\beta}^\dagger \text{Tr}(\mathcal{H}c_{q\beta}) \frac{1}{\omega_1^0 - \mathcal{H}_0^d} \text{Tr}(c_{q\beta}^\dagger \mathcal{H}) c_{q\beta} + \text{Tr}(c_{q\beta}^\dagger \mathcal{H}) c_{q\beta} \frac{1}{\omega_0^1 - \mathcal{H}_1^d} c_{q\beta}^\dagger \text{Tr}(\mathcal{H}c_{q\beta}) \right] \quad (3.69)$$

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.

4 Star Graph URG

The star graph problem consists of N spin-like degrees of freedom (labelled 1 through N) individually talking to a spin at the center (labelled 0). Each spin i ($i \in [0, N]$) has an on-site energy ϵ_i . The coupling strength between 0 and i ($i \in [1, N]$) 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.

$$\mathcal{H} = \epsilon_0 S_0^z + \sum_{i=1}^N \left[\epsilon_i S_i^z + J_i \vec{S}_0 \cdot \vec{S}_i \right] \quad (4.1)$$

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

$$\mathcal{H} = \epsilon_0 S_0^z + \sum_{i=1}^N \left[\epsilon_i S_i^z + J_i \left(S_0^z S_i^z + \frac{1}{2} (S_0^+ S_i^- + S_0^- S_i^+) \right) \right] \quad (4.2)$$

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

$$\mathcal{H}^d = \sum_{i=0}^N \epsilon_i S_i^z + \sum_{i=1}^N J_i S_0^z S_i^z \quad (4.3)$$

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

$$\mathcal{H}^D = \epsilon_0 S_0^z + \epsilon_N S_N^z + J_N S_0^z S_N^z \quad (4.4)$$

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

$$\mathcal{H}_X = \frac{1}{2} J_N (S_N^+ S_0^- + S_N^- S_0^+) \quad (4.5)$$

4.1 Calculation of Renormalization

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

$$\Delta \mathcal{H} = [c_{q\beta}^\dagger T, \eta] \quad (4.6)$$

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

$$\Delta \mathcal{H} = [S_N^+ T, \eta] \quad (4.7)$$

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

$$\eta = \frac{1}{\omega - \mathcal{H}^d} T^\dagger c_{q\beta} \rightarrow \frac{1}{\omega - \mathcal{H}^d} \frac{1}{2} J_N S_0^+ S_N^- \quad (4.8)$$

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

$$\eta = \frac{1}{\omega - \epsilon_0 S_0^z - \epsilon_N S_N^z - J_N S_0^z S_N^z} \frac{1}{2} J_N S_0^+ S_N^- = \frac{1}{\omega - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \frac{1}{2} J_N S_0^+ S_N^- \quad (4.9)$$

In the final step, I substituted $S_N^z = -\frac{1}{2}$ and $S_0^z = \frac{1}{2}$ in the denominator, because there is $S_0^+ S_N^-$ in front of the Greens function. The renormalization thus becomes

$$\Delta \mathcal{H} = \frac{1}{4} J_N^2 S_N^+ S_0^- \frac{1}{\omega - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} S_0^+ S_N^- - \frac{1}{4} J_N^2 \frac{1}{\omega - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} S_0^+ S_N^- S_N^+ S_0^- \quad (4.10)$$

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

$$\begin{aligned}\Delta\mathcal{H} &= \frac{1}{4}J_N^2 \frac{1}{\omega - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \left[\left(\frac{1}{2} + S_N^z \right) \left(\frac{1}{2} - S_0^z \right) - \left(\frac{1}{2} - S_N^z \right) \left(\frac{1}{2} + S_0^z \right) \right] \\ &= \frac{1}{4}J_N^2 \frac{1}{\omega - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} [S_N^z - S_0^z]\end{aligned}\quad (4.11)$$

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

$$\begin{aligned}\Delta\epsilon_N &= \frac{1}{4}J_N^2 \frac{1}{\omega - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \\ \Delta\epsilon_0 &= -\frac{1}{4}J_N^2 \frac{1}{\omega - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N}\end{aligned}\quad (4.12)$$

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

$$\Delta\epsilon_0 = -\frac{1}{4}J^2 \frac{1}{\omega - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon + \frac{1}{4}J}\quad (4.13)$$

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

$$\Delta\epsilon_0 = -\frac{1}{4}J^2 \frac{1}{\tilde{\omega} - \frac{1}{2}\epsilon_0}\quad (4.14)$$

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 4.2

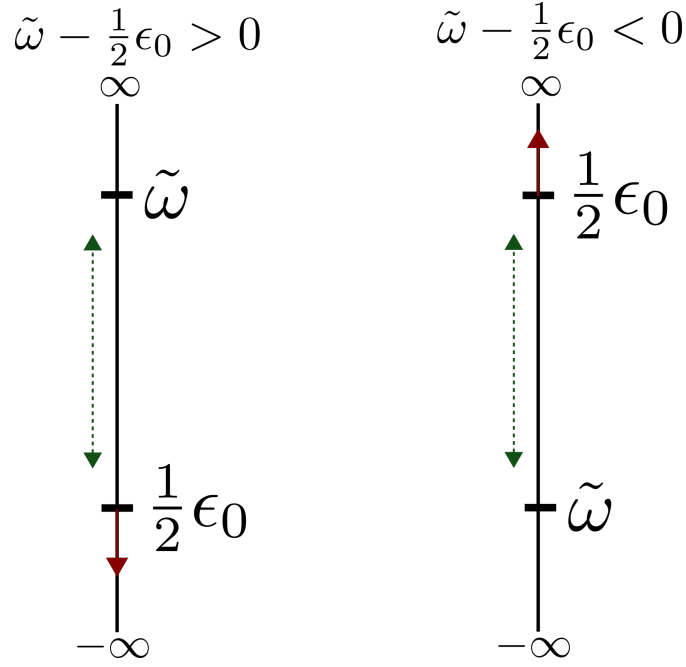


Figure 4: RG flow for the two cases. The green line is the distance between the bare values of the two couplings, and hence also the magnitude of the denominator. The red arrow denotes the direction in which ϵ_0 will flow. Upward flow is increase. In both cases, the flow is such that the distance between 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.

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. 3.14.

$$\eta^\dagger = \frac{1}{\omega' - \mathcal{H}_d} S_N^+ S_0^- = \frac{1}{\omega' - \frac{1}{2}\epsilon + \frac{1}{2}\epsilon_0 + \frac{1}{4}J} S_N^+ S_0^- \quad (4.15)$$

Comparing with eq. 4.9, and requiring $(\eta)^\dagger = \eta^\dagger$, we get the following equation relating ω and ω' :

$$\omega' - \frac{1}{2}\epsilon + \frac{1}{2}\epsilon_0 + \frac{1}{4}J = \omega + \frac{1}{2}\epsilon - \frac{1}{2}\epsilon_0 + \frac{1}{4}J \implies \omega = \omega' - \epsilon + \epsilon_0 \quad (4.16)$$

Substituting this in eq. 4.13 gives

$$\Delta\epsilon_0 = -\frac{1}{4}J^2 \frac{1}{\omega' - \frac{1}{2}\epsilon + \frac{1}{2}\epsilon_0 + \frac{1}{4}J} \quad (4.17)$$

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

$$\Delta\epsilon_0 = \frac{1}{4}J^2 \frac{1}{\tilde{\omega} - \frac{1}{2}\epsilon_0} \quad (4.18)$$

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 4.2.

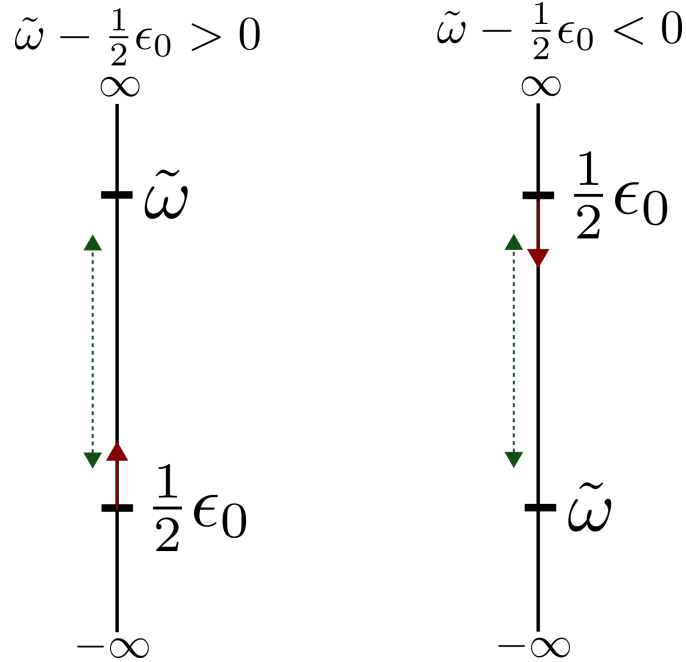


Figure 5: RG flow for the two cases with the new $-\tilde{\omega} = \omega' - \frac{1}{2}\epsilon + \frac{1}{4}J$. Now we can see that in both cases, the flow is such that the distance (green dotted line) between the couplings decreases. A fixed point is reached when this distance vanishes.

4.3 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

$$\mathcal{H}^* = 2\tilde{\omega}S_0^z + \epsilon \sum_i S_i^z + J \sum_i \vec{S}_i \cdot \vec{S}_0, \quad \text{if } \tilde{\omega}\epsilon_0 > 0 \quad (4.19)$$

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.

$$\mathcal{H}^* = \epsilon \sum_i S_i^z + J \sum_i \vec{S}_i \cdot \vec{S}_0, \quad \text{if } \tilde{\omega}\epsilon_0 < 0 \quad (4.20)$$

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

$$\begin{aligned} \mathcal{H}^* &= 2\tilde{\omega}S_0^z + J \sum_i \vec{S}_i \cdot \vec{S}_0, & \text{if } \tilde{\omega}\epsilon_0 > 0 \\ \mathcal{H}^* &= J \sum_i \vec{S}_i \cdot \vec{S}_0, & \text{if } \tilde{\omega}\epsilon_0 < 0 \end{aligned} \quad (4.21)$$

4.4 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. 6. The second kind are those where the two couplings have different signs, and so ϵ_0 flows to 0. These are shown in fig. 7.

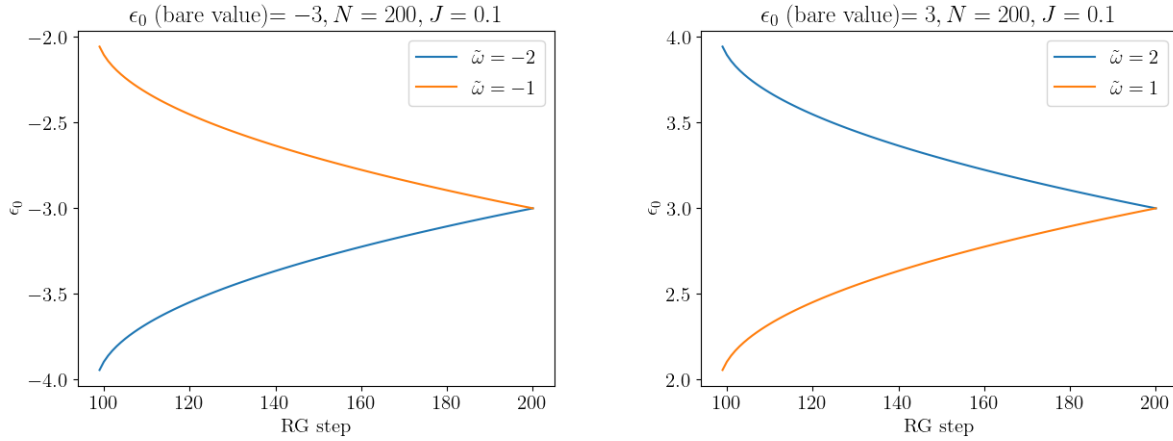


Figure 6: Flows where ϵ_0 and $\tilde{\omega}$ have same sign. The left and right panels show flows starting from negative and positive values respectively. The two plots in each panel correspond to different values of $\tilde{\omega}$, one greater than the bare ϵ_0 , the other less than that. The fixed point value is $2\tilde{\omega}$.

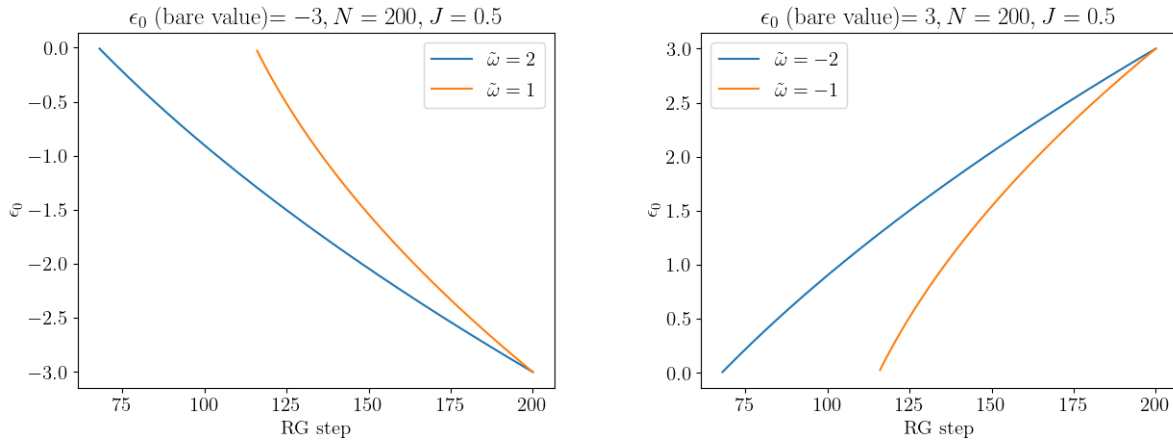


Figure 7: Flows where ϵ_0 and $\tilde{\omega}$ have opposite sign. The left and right panels show flows starting from negative and positive values respectively. The two plots in each panel correspond to different values of $\tilde{\omega}$, one greater than the bare ϵ_0 , the other less than that. The fixed point value is 0.

5 Kondo Model URG

$$\mathcal{H} = \sum_{k\alpha} \epsilon_k \hat{n}_{k\alpha} + J_z \sum_{k,k'} S_d^z \left(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow} \right) + J_t \sum_{k,k'} \left(S_d^+ c_{k\downarrow}^\dagger c_{k'\uparrow} + S_d^- c_{k\uparrow}^\dagger c_{k'\downarrow} \right) \quad (5.1)$$

The goal is to disentangle an electron $q\beta$ from the Hamiltonian, q being the momentum and β the spin. We take a pair of electrons $q\beta, q\bar{\beta}$ on the shell to preserve SU(2) symmetry of the Hamiltonian. The diagonal part of the Hamiltonian is

$$\mathcal{H}_d = \epsilon_q \hat{n}_{q\beta} + J_z S_d^z \beta \left(\hat{n}_{q\beta} - \hat{n}_{q\bar{\beta}} \right) \quad (5.2)$$

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

$$\mathcal{H}_d = \epsilon_q \tau_{q\beta} + 2J_z S_d^z s_q^z \quad (5.3)$$

where $s_q^z = \frac{1}{2}(\tau_{q\uparrow} - \tau_{q\downarrow})$. A constant $\frac{1}{2}\epsilon_q$ has been dropped while transforming the first term. The second term transforms exactly because we can just write the bare Hamiltonian term $S_d^z (\hat{n}_{q\uparrow} - \hat{n}_{q\downarrow})$ as $S_d^z (\tau_{q\uparrow} - \tau_{q\downarrow})$.

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

$$\mathcal{H}^I = J_z \sum_k S_d^z \beta \left(c_{k\beta}^\dagger c_{q\beta} + c_{q\beta}^\dagger c_{k\beta} \right) + J_t \sum_k \left(c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} + c_{q\beta}^\dagger c_{d\beta} c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} \right) \quad (5.4)$$

These are the terms that come in the numerator.

5.1 Particle sector

The particle sector involves integrating out those states which are occupied.

$$c_{q\beta}^\dagger T \eta \quad (5.5)$$

where

$$\begin{aligned} \eta &= \frac{1}{\omega - \mathcal{H}_d} \left[J_z \sum_k \beta S_d^z c_{k\beta}^\dagger c_{q\beta} + J_t \sum_k c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \right] \\ &= \sum_k \left[\frac{1}{\omega + \frac{1}{2}\epsilon_q + \frac{1}{2}J_z (\hat{n}_{d\beta} - \hat{n}_{d\bar{\beta}}) \hat{n}_{q\bar{\beta}}} J_z S_d^z \beta c_{k\beta}^\dagger c_{q\beta} + \frac{1}{\omega + \frac{1}{2}\epsilon_q + \frac{1}{2}J_z \hat{n}_{q\bar{\beta}}} J_t c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \right] \end{aligned} \quad (5.6)$$

The renormalization is therefore

$$\begin{aligned} &\sum_{kk'} J_z \beta S_d^z c_{q\beta}^\dagger c_{k'\beta} \frac{J_z \beta S_d^z c_{k\beta}^\dagger c_{q\beta}}{\omega + \frac{1}{2}\epsilon_q + \frac{1}{2}J_z (\hat{n}_{d\beta} - \hat{n}_{d\bar{\beta}}) \hat{n}_{q\bar{\beta}}} + \sum_{kk'} J_t c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\bar{\beta}} \frac{J_t c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta}}{\omega + \frac{1}{2}\epsilon_q + \frac{1}{2}J_z \hat{n}_{q\bar{\beta}}} \\ &+ \sum_{kk'} J_t c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\bar{\beta}} \frac{J_z \beta S_d^z c_{k\beta}^\dagger c_{q\beta}}{\omega + \frac{1}{2}\epsilon_q + \frac{1}{2}J_z (\hat{n}_{d\beta} - \hat{n}_{d\bar{\beta}}) \hat{n}_{q\bar{\beta}}} + \sum_{kk'} J_z \beta S_d^z c_{q\beta}^\dagger c_{k'\beta} \frac{J_t c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta}}{\omega + \frac{1}{2}\epsilon_q + \frac{1}{2}J_z \hat{n}_{q\bar{\beta}}} \end{aligned} \quad (5.7)$$

The total renormalization will have three types of terms: J_z^2, J_t^2 and $J_z J_t$. The first type (J_z^2) is just a number, so we ignore it. The remaining terms are

$$\sum_{kk'} \left[\frac{\frac{1}{2} J_z J_t \hat{n}_{q\beta} \left(c_{d\bar{\beta}}^\dagger c_{d\beta} c_{k'\bar{\beta}}^\dagger c_{k\beta} + \text{h.c.} \right)}{\omega + \frac{1}{2} \epsilon_q + \frac{1}{2} J_z \hat{n}_{q\bar{\beta}}} + \frac{J_t^2 \hat{n}_{q\beta} \hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta}) c_{k'\bar{\beta}} c_{k\bar{\beta}}^\dagger}{\omega + \frac{1}{2} \epsilon_q + \frac{1}{2} J_z \hat{n}_{q\bar{\beta}}} \right] \quad (5.8)$$

We choose the configuration $\hat{n}_{q\beta} = \hat{n}_{q\bar{\beta}} = 1$. This means we must be below the Fermi energy, so we choose $-\epsilon_q$.

$$\sum_{kk'} \left[\frac{\frac{1}{2} J_z J_t \left(c_{d\bar{\beta}}^\dagger c_{d\beta} c_{k'\bar{\beta}}^\dagger c_{k\beta} + \text{h.c.} \right)}{\omega - \frac{1}{2} \epsilon_q + \frac{1}{2} J_z} + \frac{J_t^2 \hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta}) c_{k'\bar{\beta}} c_{k\bar{\beta}}^\dagger}{\omega - \frac{1}{2} \epsilon_q + \frac{1}{2} J_z} \right] \quad (5.9)$$

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

$$\hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta}) = \left(\frac{1}{2} + \bar{\beta} S_d^z \right) \quad (5.10)$$

and

$$\sum_{kk'} \left(c_{d\bar{\beta}}^\dagger c_{d\beta} c_{k'\bar{\beta}}^\dagger c_{k\beta} + \text{h.c.} \right) = - \sum_{kk'} \left(c_{d\bar{\beta}}^\dagger c_{d\beta} c_{k\beta}^\dagger c_{k'\bar{\beta}} + \text{h.c.} \right) = - (S_d^+ s^- + S_d^- s^+) \quad (5.11)$$

5.2 Hole sector

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

$$T^\dagger c_{q\beta} \eta_0^\dagger = T^\dagger c_{q\beta} \frac{1}{\omega' - \mathcal{H}_d} c_{q\beta}^\dagger T \quad (5.12)$$

where η_0 is defined in eq. 3.55.

$$\eta_0^\dagger = \frac{1}{\omega' - \frac{1}{2} \epsilon_q - \frac{1}{2} J_z \beta S_d^z} \frac{1}{2} J_z \beta S_d^z c_{q\beta}^\dagger c_{k'\beta} + \frac{1}{\omega' - \frac{1}{2} \epsilon_q + \frac{1}{2} J_z} J_t c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\bar{\beta}} \quad (5.13)$$

Evaluating the terms similarly gives

$$\sum_{kk'} \left[\frac{-\frac{1}{2} J_z J_t \left(c_{d\bar{\beta}}^\dagger c_{d\beta} c_{k\beta}^\dagger c_{k'\bar{\beta}} + \text{h.c.} \right)}{\omega' - \frac{1}{2} \epsilon_q + \frac{1}{2} J_z} + \frac{J_t^2 \hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}}) c_{k\bar{\beta}}^\dagger c_{k'\bar{\beta}}}{\omega' - \frac{1}{2} \epsilon_q + \frac{1}{2} J_z} \right] \quad (5.14)$$

5.3 Scaling equations

Adding the two sectors, we get

$$\begin{aligned} \Delta \mathcal{H} = & -\frac{1}{2} J_z J_t (S_d^+ s^- + S_d^- s^+) \left(\frac{1}{\omega - \frac{1}{2} \epsilon_q + \frac{1}{2} J_z} + \frac{1}{\omega' - \frac{1}{2} \epsilon_q + \frac{1}{2} J_z} \right) \\ & - J_t^2 S_d^z \sum_{kk'} \left(\frac{\bar{\beta} c_{k\bar{\beta}}^\dagger c_{k'\bar{\beta}}}{\omega - \frac{1}{2} \epsilon_q + \frac{1}{2} J_z} + \frac{\bar{\beta} c_{k\bar{\beta}}^\dagger c_{k'\bar{\beta}}}{\omega' - \frac{1}{2} \epsilon_q + \frac{1}{2} J_z} \right) \end{aligned} \quad (5.15)$$

There we changed cc^\dagger into $c^\dagger c$ and dropped the constant piece generated in the process. We also dropped the impurity-free $\frac{1}{2}$ in $\frac{1}{2} + S_d^z$. At this point, we choose $\omega' = \omega$.

$$\Delta\mathcal{H} = -J_z J_t (S_d^+ s^- + S_d^- s^+) \frac{1}{\omega - \frac{1}{2}\epsilon_q + \frac{1}{2}J_z} - 2J_t^2 S_d^z \sum_{kk'} \bar{\beta} c_{k\bar{\beta}}^\dagger c_{k'\bar{\beta}} \frac{1}{\omega - \frac{1}{2}\epsilon_q + \frac{1}{2}J_z} \quad (5.16)$$

Summing over β gives

$$\sum_{\beta} \Delta\mathcal{H} = -2J_z J_t (S_d^+ s^- + S_d^- s^+) \frac{1}{\omega - \frac{1}{2}\epsilon_q + \frac{1}{2}J_z} - 2J_t^2 S_d^z s^z \frac{1}{\omega - \frac{1}{2}\epsilon_q + \frac{1}{2}J_z} \quad (5.17)$$

There we used $\sum_{\beta} \bar{\beta} \sum_{kk'} c_{k\bar{\beta}}^\dagger c_{k'\bar{\beta}} = \sum_{kk'} (c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow}) = s^z$. We can now write down the flow equations for J_z and J_t :

$$\begin{aligned} \Delta J_z &= -2J_t^2 \frac{1}{\omega - \frac{1}{2}\epsilon_q + \frac{1}{2}J_z} \\ \Delta J_t &= -2J_z J_t \frac{1}{\omega - \frac{1}{2}\epsilon_q + \frac{1}{2}J_z} \end{aligned} \quad (5.18)$$

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

$$\Delta J = -2J^2 \frac{1}{\omega - \frac{1}{2}\epsilon_q + \frac{1}{2}J} \quad (5.19)$$

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).

$$\Delta J \approx 2J^2 \frac{1}{\epsilon_q} \quad (5.20)$$

Note that these scaling equations are for decoupling a pair of electrons $q, \uparrow\downarrow$. To decouple a shell of electrons, we need to sum over q .

5.4 Numerical Solutions

The symmetric scaling equation 5.19 was solved numerically with the choice $\omega = -\frac{\epsilon_q}{2}$, for both positive and negative bare values of J .

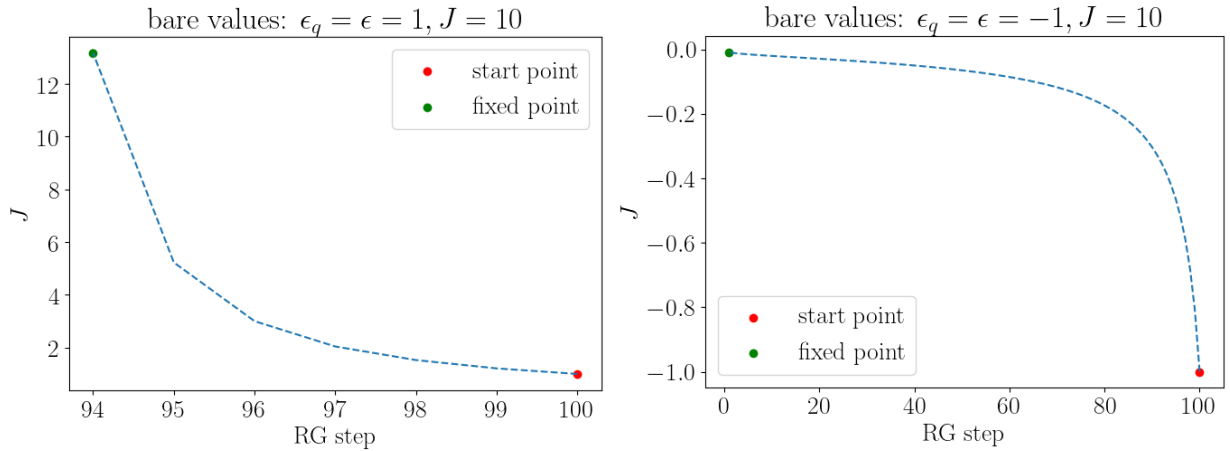


Figure 8: Flow of the Kondo coupling J towards the strong-coupling fixed point (right panel) and the weak coupling saddle-point (left panel). Both plots are for the choice $\omega = -\frac{1}{2}\epsilon_q$.

6 Anderson Model URG

6.1 Setting up the various terms in the URG

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

$$\mathcal{H} = \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{k\sigma} \left(V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right) + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \quad (6.1)$$

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.

$$\mathcal{H} = \sum_{k\sigma} \epsilon_k \tau_{k\sigma} + \sum_{k\sigma} \left(V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right) + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \quad (6.2)$$

The renormalization is

$$\left[c_{q\beta}^\dagger T, \eta \right] \quad (6.3)$$

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

$$\mathcal{H}_d = \epsilon_q \tau_{q\beta} + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \quad (6.4)$$

Since this is the first step of the RG, the shell being decoupled is the highest one, which we call Λ_N .

6.2 Calculation of renormalization

The η is

$$\begin{aligned} \eta &= \frac{1}{\omega - \mathcal{H}_d} T^\dagger c_{q\beta} = \frac{1}{\omega - \epsilon_q \tau_{q\beta} - \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} - U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow}} V_q^* c_{d\beta}^\dagger c_{q\beta} \\ &= \frac{1}{\omega + \frac{1}{2}\epsilon_q - \epsilon_d - (\epsilon_d + U) \hat{n}_{d\bar{\beta}}} V_q^* c_{d\beta}^\dagger c_{q\beta} \end{aligned} \quad (6.5)$$

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 is

$$\Delta\mathcal{H} = c_{q\beta}^\dagger T \eta - \eta c_{q\beta}^\dagger T = \frac{|V_q|^2}{\omega + \frac{1}{2}\epsilon_q - \epsilon_d - (\epsilon_d + U) \hat{n}_{d\bar{\beta}}} [(1 - \hat{n}_{d\beta}) \hat{n}_{q\beta} - (1 - \hat{n}_{q\beta}) \hat{n}_{d\beta}] \quad (6.6)$$

Similarly, the renormalization at an energy $-\epsilon_q$ is obtained simply by replacing $\epsilon_q \rightarrow -\epsilon_q$:

$$\Delta\mathcal{H} = \frac{|V_q|^2}{\omega' - \frac{1}{2}\epsilon_q - \epsilon_d - (\epsilon_d + U) \hat{n}_{d\bar{\beta}}} [(1 - \hat{n}_{d\beta}) \hat{n}_{q\beta} - (1 - \hat{n}_{q\beta}) \hat{n}_{d\beta}] \quad (6.7)$$

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

$$\Delta\mathcal{H} = -\frac{|V_q|^2 \hat{n}_{d\beta}}{\omega + \frac{1}{2}\epsilon_q - \epsilon_d - (\epsilon_d + U) \hat{n}_{d\bar{\beta}}} - \frac{|V_q|^2 (1 - \hat{n}_{d\beta})}{-\omega' + \frac{1}{2}\epsilon_q + \epsilon_d + (\epsilon_d + U) \hat{n}_{d\bar{\beta}}} \quad (6.8)$$

As an ansatz, we assume $\omega = -\omega'$.

$$\Delta\mathcal{H} = -\frac{|V_q|^2 \hat{n}_{d\beta}}{\omega + \frac{1}{2}\epsilon_q - \epsilon_d - (\epsilon_d + U) \hat{n}_{d\bar{\beta}}} - \frac{|V_q|^2 (1 - \hat{n}_{d\beta})}{\omega + \frac{1}{2}\epsilon_q + \epsilon_d + (\epsilon_d + U) \hat{n}_{d\bar{\beta}}} \quad (6.9)$$

6.3 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. 6.9, we can see that there are renormalizations to all three configuration energies of the impurity: the doublon energy E_2 corresponding to the state $\hat{n}_{d\beta}\hat{n}_{d\bar{\beta}}$, the single energy E_1 corresponding to $(\hat{n}_{d\beta}(1-\hat{n}_{d\bar{\beta}}) + \hat{n}_{d\bar{\beta}}(1-\hat{n}_{d\beta}))$, and the holon energy E_0 corresponding to $(1-\hat{n}_{d\beta})(1-\hat{n}_{d\bar{\beta}}) + \hat{n}_{d\bar{\beta}}(1-\hat{n}_{d\beta})$.

$$\begin{aligned}\Delta E_2 &= -2 \sum_q \frac{|V_q|^2}{\omega + \frac{1}{2}\epsilon_q - 2\epsilon_d - U} \\ \Delta E_1 &= - \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d} - \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d} \\ \Delta E_0 &= -2 \sum_q \frac{|V_q|^2}{\omega + \frac{1}{2}\epsilon_q}\end{aligned}\tag{6.10}$$

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

$$\begin{aligned}\Delta\epsilon_d &= - \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d} - \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d} + 2 \sum_q \frac{|V_q|^2}{\omega + \frac{1}{2}\epsilon_q} \\ \Delta U &= -2 \sum_q \frac{|V_q|^2}{\omega + \frac{1}{2}\epsilon_q - 2\epsilon_d - U} - 2 \sum_q \frac{|V_q|^2}{\omega + \frac{1}{2}\epsilon_q} + 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d} + 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d}\end{aligned}\tag{6.11}$$

6.4 Connection to Poor Man's scaling

To obtain the results of Poor Man's scaling [23][24], we can look at various regimes. First we look at the case when both ϵ_d and U are small such that both the singly-occupied and doubly-occupied subspaces of the impurity are comfortably inside the bandwidth, $U, \epsilon_d \ll \epsilon_q$. We can then ignore the ϵ_d and U in the denominator compared to the ϵ_q .

$$\begin{aligned}\Delta\epsilon_d &= \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} + \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} - 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} \\ \Delta U &= 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} + 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} - 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} - 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q}\end{aligned}\tag{6.12}$$

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

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

$$\begin{aligned}\Delta\epsilon_d &= \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} - 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} \\ \Delta U &= 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q} - 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q}\end{aligned}\tag{6.13}$$

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

$$\begin{aligned}\Delta U &= 0 \\ \delta\epsilon_d &= -\frac{\Delta}{\pi} \frac{1}{\omega - \frac{1}{2}D}\end{aligned}\tag{6.14}$$

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

$$\delta\epsilon_d = \frac{\Delta}{\pi} \frac{\delta D}{D}\tag{6.15}$$

This is the one-loop scaling equation.

6.5 Particle-Hole symmetry

The Anderson model Hamiltonian, eq. 7.7, has an impurity particle-hole symmetry for a certain condition of the couplings. To see this, we apply the particle-hole transformation $c_k \rightarrow c_k^\dagger, c_d \rightarrow -c_d^\dagger$ to the Hamiltonian. Since we are looking at the impurity symmetry, we will only look at the terms involving the impurity. The particle-hole symmetry of the conduction bath is a separate thing and that requires a specific lattice. Hence we will not consider kinetic energy term in this discussion. The rest of the terms transform as

$$\epsilon_d \sum_\sigma \hat{n}_{d\sigma} \rightarrow 2\epsilon_d - \epsilon_d \sum_\sigma \hat{n}_{d\sigma}\tag{6.16}$$

$$U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \rightarrow U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} - U \sum_\sigma \hat{n}_{d\sigma} + U\tag{6.17}$$

$$\sum_{k\sigma} V(k) c_{k\sigma}^\dagger c_{d\sigma} + hc \rightarrow \sum_{k\sigma} -V(k) c_{k\sigma} c_{d\sigma}^\dagger + hc = \sum_{k\sigma} V^*(k) c_{k\sigma}^\dagger c_{d\sigma} + hc\tag{6.18}$$

$$S^z \sum_{kq} s_{kq}^z \rightarrow (-S^z) \sum_{kq} (-s_{kq}^z) = S^z \sum_{kq} s_{kq}^z\tag{6.19}$$

$$S^\pm \sum_{kq} s_{kq}^\mp \rightarrow (-S^\pm) \sum_{kq} (-s_{kq}^\mp) = S^\pm \sum_{kq} s_{kq}^\mp\tag{6.20}$$

The transformation of the spin terms, eqs. 6.19 and 6.20, can be understood from the fact that since a spin degree of freedom can be written in terms of the number operator as $\hat{S} = \hat{n} - \frac{1}{2}$, it must transform by flipping its sign: $\hat{S} = \hat{n} - \frac{1}{2} \rightarrow \frac{1}{2} - \hat{n} = -\hat{S}$. The spin terms are thus invariant under the particle-hole transformation. The impurity-bath hopping term can be made symmetric by making $V(k)$ real; then we would have, from eq. 6.18,

$$V(k) \left(c_{k\sigma}^\dagger c_{d\sigma} + c_{d\sigma}^\dagger c_{k\sigma} \right) \rightarrow V(k) \left(c_{d\sigma}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger c_{d\sigma} \right)\tag{6.21}$$

The impurity diagonal terms, ϵ_d and U , require a specific condition. Combining eqs. 6.16 and 6.17,

$$\epsilon_d \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \rightarrow (-\epsilon_d - U) \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow}\tag{6.22}$$

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

$$\epsilon_d = -\epsilon_d - U \implies \epsilon_d + \frac{1}{2}U = 0 \quad (6.23)$$

This same condition can be obtained in a more physical way. If we consider the singly-occupied state of the impurity as the reference state, the doubly-occupied state is the particle-excitation and the vacant state is the hole excitation. The energy of this particle state is $E_2 = 2\epsilon_d + U$ and that of the hole state is $E_0 = 0$. Particle-hole symmetry then requires the particle and hole levels to be degenerate, which means $E_2 = E_0$, and we recover the condition eq. 6.23.

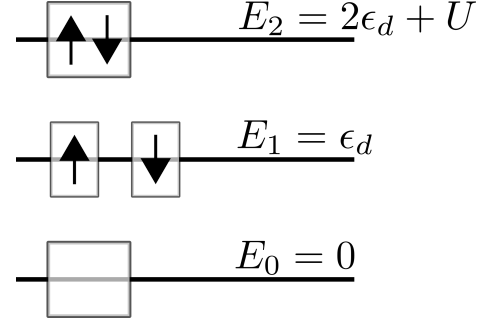


Figure 9: Particle and hole excitations of the impurity

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

$$\Delta \left(\epsilon_d + \frac{1}{2}U \right) = 0 \quad (6.24)$$

The quantity $\gamma = \epsilon_d + \frac{1}{2}U$ is thus an RG-invariant for the particle-hole symmetric model; it does not change under the RG flow. It is often referred to as the asymmetry parameter; it quantifies the asymmetry in the model. We need to check if our equations satisfy this. Looking at the RG equations for ϵ_d and U , we can find the RG equation for the asymmetry parameter. The slightly easier way is to just note that the renormalization in E_2 should be equal to the renormalization in E_0 , in order for p-h symmetry to hold.

$$\begin{aligned} \Delta E_2 &= 2 \frac{\Delta}{\pi} \frac{1}{\omega - D + \epsilon_d + U} \\ \Delta E_0 &= 2 \frac{\Delta}{\pi} \frac{1}{\omega - D - \epsilon_d} \end{aligned} \quad (6.25)$$

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

7 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.

7.1 Spin-spin interaction

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

$$\mathcal{H}_I = \sum_{k,k',\sigma_i} u c_{d\sigma_2}^\dagger c_{d\sigma_4} c_{k'\sigma_3} c_{k\sigma_1}^\dagger \delta_{(\sigma_1+\sigma_2=\sigma_3+\sigma_4)} \quad (7.1)$$

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

$$\mathcal{H}_I = \underbrace{\sum_{k,k',\sigma,\sigma'} u_1 \hat{n}_{d\sigma'} c_{k\sigma}^\dagger c_{k'\sigma}}_{\text{spin-preserving scattering}} + \overbrace{\sum_{k,k',\sigma} u_2 c_{d\bar{\sigma}}^\dagger c_{d\sigma} c_{k\sigma}^\dagger c_{k'\bar{\sigma}}}^{\text{spin-flip scattering}} \quad (7.2)$$

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

$$\mathcal{H}_{I,N} = \sum_{k,k',\sigma,\sigma'} u_P \hat{n}_{d\sigma'} c_{k\sigma}^\dagger c_{k'\sigma} + \sum_{k,k',\sigma} u_A c_{d\bar{\sigma}}^\dagger c_{d\sigma} c_{k\sigma}^\dagger c_{k'\bar{\sigma}} \quad (7.3)$$

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

$$u_{\uparrow\uparrow} \hat{n}_{d\uparrow} c_{k\uparrow}^\dagger c_{k'\uparrow} + u_{\downarrow\downarrow} \hat{n}_{d\downarrow} c_{k\downarrow}^\dagger c_{k'\downarrow} + u_{\uparrow\downarrow} \hat{n}_{d\uparrow} c_{k\downarrow}^\dagger c_{k'\downarrow} + u_{\downarrow\uparrow} \hat{n}_{d\downarrow} c_{k\uparrow}^\dagger c_{k'\uparrow} \quad (7.4)$$

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

$$\begin{aligned} \mathcal{H}_I &= J_z \frac{\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow}}{2} \sum_{kk'} \left(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow} \right) + J_t \sum_{kk'} \left[c_{d\uparrow}^\dagger c_{d\downarrow} c_{k\downarrow}^\dagger c_{k'\uparrow} + c_{d\downarrow}^\dagger c_{d\uparrow} c_{k\uparrow}^\dagger c_{k'\downarrow} \right] \\ &= 2J_z S_d^z s^z + J_t (S_d^+ s^- + S_d^- s^+) \end{aligned} \quad (7.5)$$

The spin-like operators are defined as

$$\begin{aligned} S_d^z &\equiv \frac{1}{2} (\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow}) & S_d^+ &\equiv c_{d\uparrow}^\dagger c_{d\downarrow} & S_d^- &\equiv c_{d\downarrow}^\dagger c_{d\uparrow} \\ s_{kk'}^z &\equiv \frac{1}{2} (c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow}) & s_{kk'}^+ &\equiv c_{k\uparrow}^\dagger c_{k'\downarrow} & s_{kk'}^- &\equiv c_{k\downarrow}^\dagger c_{k'\uparrow} \\ s^a &\equiv \sum_{kk'} s_{kk'}^a \end{aligned} \quad (7.6)$$

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

$$\mathcal{H} = \sum_{k\sigma} \left(\epsilon_k \hat{n}_{k\sigma} + V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right) + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + 2J_z S_d^z s^z + J_t (S_d^+ s^- + S_d^- s^+) \quad (7.7)$$

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

$$\mathcal{H}_I = J \left[S_d^z s^z + \frac{1}{2} (S_d^+ s^- + S_d^- s^+) \right] = J \mathbf{S}_d \cdot \mathbf{s} \quad (7.8)$$

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

$$\begin{aligned} \mathcal{H}_N = & H_{N-1} + H_{\text{imp}} + \epsilon_q \hat{n}_{q\beta} + 2J_z S_d^z s_q^z + V_q c_{q\beta}^\dagger c_{d\beta} + \text{h.c.} + \\ & \sum_{k < \Lambda_N} \left[J_z S_d^z \beta \left(c_{k\beta}^\dagger c_{q\beta} + c_{q\beta}^\dagger c_{k\beta} \right) + J_t \left(c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} + c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\bar{\beta}} \right) \right] \\ & + J_t \left(c_{d\beta}^\dagger c_{d\bar{\beta}} c_{q\bar{\beta}}^\dagger c_{q\beta} + c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{q\bar{\beta}} \right) \end{aligned} \quad (7.9)$$

where $s_q^z = \frac{1}{2} (\hat{n}_{q\uparrow} - \hat{n}_{q\downarrow})$ 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

$$H_{N-1} = \sum_{k < \Lambda_N, \sigma} \left[(\epsilon_k + \sigma J_z S_d^z) \hat{n}_{k\sigma} + V_k c_{k\sigma}^\dagger c_{d\sigma} + \text{h.c.} \right] + H_{I, N-1} \quad (7.10)$$

The diagonal (number-preserving) part is

$$\mathcal{H}_D = H_{N-1}^D + \epsilon_q (\hat{n}_{q\beta} + \hat{n}_{q\bar{\beta}}) + 2J_z S_d^z s_q^z + H_{\text{imp}} \quad (7.11)$$

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

$$\mathcal{H}_D = \epsilon_q \hat{n}_{q\beta} + 2J_z S_d^z s_q^z + H_{\text{imp}} \quad (7.12)$$

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

$$\sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} = \sum_{k\sigma} \epsilon_k \hat{\tau}_{k\sigma} + \mathcal{C} \quad (7.13)$$

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^D . Eq. 7.12 becomes

$$\mathcal{H}_D = \epsilon_q \tau_{q\beta} + 2J_z S_d^z s_q^z + H_{\text{imp}} \quad (7.14)$$

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

$$\begin{aligned} \mathcal{H}_X = & \underbrace{V_1^* c_{d\beta}^\dagger c_{q\beta} \hat{n}_{d\bar{\beta}}}_{T_1^\dagger} + \underbrace{V_0^* c_{d\beta}^\dagger c_{q\beta} (1 - \hat{n}_{d\bar{\beta}})}_{T_2^\dagger} + \underbrace{\sum_{k < \Lambda_N} J_0^z \hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}}) c_{k\beta}^\dagger c_{q\beta}}_{T_3^\dagger} \\ & + \underbrace{\sum_{k < \Lambda_N} J_1^z \hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta}) c_{k\beta}^\dagger c_{q\beta}}_{T_4^\dagger} + \underbrace{\sum_{k < \Lambda_N} J^t c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta}}_{T_5^\dagger} + \underbrace{J^t c_{d\beta}^\dagger c_{d\bar{\beta}} c_{q\bar{\beta}}^\dagger c_{q\beta}}_{T_6^\dagger} + \text{h.c.} \end{aligned} \quad (7.15)$$

7.2 Calculation of renormalization

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 generator will have five parts:

$$\eta = \sum_{i=1}^5 \frac{1}{\omega_i^0 - E_i^0} T_i^\dagger c_{q\beta} \quad (7.16)$$

where

$$\begin{aligned} T_1 &= V_1 c_{d\beta} \hat{n}_{d\bar{\beta}} \\ T_2 &= V_0 c_{d\beta} (1 - \hat{n}_{d\bar{\beta}}) \\ T_3 &= \sum_{k < \Lambda_N} J_0^z \hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}}) c_{k\beta} \\ T_4 &= \sum_{k < \Lambda_N} J_1^z \hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta}) c_{k\beta} \\ T_5 &= \sum_{k < \Lambda_N} J^t c_{d\bar{\beta}}^\dagger c_{d\beta} c_{k\bar{\beta}} \end{aligned} \quad (7.17)$$

Therefore,

$$\sum_{ij} \left(\frac{1}{\omega - E_i^0} + \frac{1}{\omega - E_j^0} \right) T_i T_j^\dagger \quad (7.18)$$

$$= \left(\frac{1}{\omega - E_1^0} + \frac{1}{\omega - E_1^0} \right) T_1 T_1^\dagger + \left(\frac{1}{\omega - E_1^0} + \frac{1}{\omega - E_4^0} \right) T_1 T_4^\dagger + \left(\frac{1}{\omega - E_1^0} + \frac{1}{\omega - E_5^0} \right) T_1 T_5^\dagger \quad (7.19)$$

$$+ \left(\frac{1}{\omega - E_2^0} + \frac{1}{\omega - E_2^0} \right) T_2 T_2^\dagger \quad (7.20)$$

$$+ \left(\frac{1}{\omega - E_3^0} + \frac{1}{\omega - E_3^0} \right) T_3 T_3^\dagger \quad (7.21)$$

$$+ \left(\frac{1}{\omega - E_4^0} + \frac{1}{\omega - E_1^0} \right) T_4 T_1^\dagger + \left(\frac{1}{\omega - E_4^0} + \frac{1}{\omega - E_4^0} \right) T_4 T_4^\dagger + \left(\frac{1}{\omega - E_4^0} + \frac{1}{\omega - E_5^0} \right) T_4 T_5^\dagger \quad (7.22)$$

$$+ \left(\frac{1}{\omega - E_5^0} + \frac{1}{\omega - E_1^0} \right) T_5 T_1^\dagger + \left(\frac{1}{\omega - E_5^0} + \frac{1}{\omega - E_4^0} \right) T_5 T_4^\dagger + \left(\frac{1}{\omega - E_5^0} + \frac{1}{\omega - E_5^0} \right) T_5 T_5^\dagger \quad (7.23)$$

$$= \frac{2}{\xi_1} |V_1|^2 \hat{n}_{d\beta} \hat{n}_{d\bar{\beta}} + \left(\frac{1}{\xi_1} + \frac{1}{\xi_4} \right) \sum_k V_1^* J_1^z c_{d\beta}^\dagger c_{k\beta} \hat{n}_{d\bar{\beta}} \quad (7.24)$$

$$+ \left(\frac{1}{\xi_1} + \frac{1}{\xi_5} \right) \sum_k V_1^* J^t \hat{n}_{d\beta} c_{k\bar{\beta}} c_{d\bar{\beta}}^\dagger \quad (7.25)$$

$$+ \left(\frac{1}{\omega - E_2^0} + \frac{1}{\omega - E_2^0} \right) T_2 T_2^\dagger \quad (7.26)$$

$$+ \left(\frac{1}{\omega - E_3^0} + \frac{1}{\omega - E_3^0} \right) T_3 T_3^\dagger \quad (7.27)$$

$$+ \left(\frac{1}{\omega - E_4^0} + \frac{1}{\omega - E_1^0} \right) T_4 T_1^\dagger + \left(\frac{1}{\omega - E_4^0} + \frac{1}{\omega - E_4^0} \right) T_4 T_4^\dagger + \left(\frac{1}{\omega - E_4^0} + \frac{1}{\omega - E_5^0} \right) T_4 T_5^\dagger \quad (7.28)$$

$$+ \left(\frac{1}{\omega - E_5^0} + \frac{1}{\omega - E_1^0} \right) T_5 T_1^\dagger + \left(\frac{1}{\omega - E_5^0} + \frac{1}{\omega - E_4^0} \right) T_5 T_4^\dagger + \left(\frac{1}{\omega - E_5^0} + \frac{1}{\omega - E_5^0} \right) T_5 T_5^\dagger \quad (7.29)$$

$$(7.30)$$

7.3 Particle sector

The renormalization in the Hamiltonian in the particle sector is

$$\begin{aligned} \Delta^+ \mathcal{H}_N = \sum_{q\beta} \left[V_q^* c_{d\beta}^\dagger c_{q\beta} + J_z \beta S_d^z \sum_k c_{k\beta}^\dagger c_{q\beta} + J_t \sum_k c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \right] \times \frac{1}{\hat{\omega}^+ - \mathcal{H}_D} \\ \times \left[V_q c_{q\beta}^\dagger c_{d\beta} + J_z \beta S_d^z \sum_k c_{q\beta}^\dagger c_{k\beta} + J_t \sum_k c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\bar{\beta}} \right] \end{aligned} \quad (7.31)$$

The entire renormalization expression has nine terms- one of order $|V_q|^2$, four of order $V_q J$ and four of order J^2 . The particle sector intermediate state has a particle excitation, so the state will be occupied. Hence $\tau_{q\beta} = \frac{1}{2}$ in the intermediate state. We make this substitution in eq. 7.12:

$$\mathcal{H}_D^+ = \frac{1}{2} \epsilon_q + 2J_z S_d^z s_q^z + H_{imp} \quad (7.32)$$

1.

$$\Delta_1^+ \mathcal{H}_N = \sum_{q\beta} |V_q|^2 c_{d\beta}^\dagger c_{q\beta} \frac{1}{\hat{\omega}^+ - \mathcal{H}_D^+} c_{q\beta}^\dagger c_{d\beta} \quad (7.33)$$

The intermediate state is characterized by $\hat{n}_{d\beta} = 0, \hat{n}_{q\beta} = 1 - \hat{n}_{q\bar{\beta}} = 1$. Therefore, at the propagator, we have

$$\begin{aligned} H_1 = \mathcal{H}_D^+ &= \epsilon_q \frac{1}{2} + \beta J_z S_d^z (\hat{n}_{q\beta} - \hat{n}_{q\bar{\beta}}) + H_{imp} \\ &= \epsilon_q \frac{1}{2} - \frac{1}{2} J_z \hat{n}_{d\bar{\beta}} + \epsilon_d \hat{n}_{d\bar{\beta}} \end{aligned} \quad (7.34)$$

H_1 is the intermediate state Hamiltonian. As a simplification, we replace $\hat{\omega}^+$ with its eigenvalue ω^+ .

$$\begin{aligned} \Delta_1^+ \mathcal{H}_N &= \sum_{q\beta} |V_q|^2 c_{d\beta}^\dagger c_{q\beta} \frac{1}{\hat{\omega}^+ - H_1} c_{q\beta}^\dagger c_{d\beta} \\ &= \sum_{q\beta} |V_q|^2 c_{d\beta}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{d\beta} \frac{1}{\omega^+ - \frac{1}{2} \epsilon_q - \epsilon_d \hat{n}_{d\bar{\beta}} + \frac{1}{2} J_z \hat{n}_{d\bar{\beta}}} \end{aligned} \quad (7.35)$$

Since $q\beta$ is on the upper band edge, we can assume it is unoccupied in the initial state, and set $c_{q\beta}c_{q\beta}^\dagger = 1$. Then,

$$\begin{aligned}\Delta_1^+ \mathcal{H}_N &= \sum_{q\beta} |V_q|^2 \hat{n}_{d\beta} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q + \left(\frac{J_z}{2} - \epsilon_d\right) \hat{n}_{d\bar{\beta}}} \\ &= \sum_{q\beta} |V(q)|^2 \hat{n}_{d\beta} \left[\frac{\hat{n}_{d\bar{\beta}}}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} + \frac{(1 - \hat{n}_{d\bar{\beta}})}{\omega^+ - \frac{1}{2}\epsilon_q} \right] \\ &= \sum_{q\beta} |V(q)|^2 \hat{n}_{d\beta} \left[\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q} + \hat{n}_{d\bar{\beta}} \left(\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} - \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q} \right) \right]\end{aligned}\quad (7.36)$$

2.

$$\Delta_2^+ \mathcal{H}_N = \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_z \beta S_d^z c_{q\beta}^\dagger c_{k\beta} \quad (7.37)$$

This can be simplified by noting that since the propagator is diagonal, the only operator that changes \hat{n}_d and S_d^z is the $c_{d\beta}^\dagger$, and therefore

$$c_{d\beta}^\dagger J_z \beta S_d^z = c_{d\beta}^\dagger \frac{1}{2} (-J_z) \hat{n}_{d\bar{\beta}} \quad (7.38)$$

The expression simplifies to

$$\Delta_2^+ \mathcal{H}_N = \frac{1}{2} (-J_z) \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{q\beta} \hat{n}_{d\bar{\beta}} \frac{1}{\omega^+ - \mathcal{H}_D^+} c_{q\beta}^\dagger c_{k\beta} \quad (7.39)$$

Intermediate ($\hat{n}_{q\beta} = 1 - \hat{n}_{q\bar{\beta}} = 1, \hat{n}_{d\bar{\beta}} = 1, \hat{n}_{d\beta} = 0$) energy is

$$H_1 = \mathcal{H}_D^+ = \frac{1}{2}\epsilon_q + J_z \beta S_d^z + \epsilon_d = \frac{1}{2}\epsilon_q - \frac{1}{2}J_z + \epsilon_d \quad (7.40)$$

The first term $\frac{1}{2}\epsilon_q + J_z \beta S_d^z$ is the total dispersion of the electron $q\beta$. The ϵ_d is the impurity energy and the third term is the total background energy.

$$\begin{aligned}\Delta_2^+ \mathcal{H}_N &= -\frac{1}{2}J_z \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{q\beta} \hat{n}_{d\bar{\beta}} c_{q\beta}^\dagger c_{k\beta} \frac{1}{\omega^+ - H_1} \\ &= -\frac{1}{2}J_z \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{k\beta} \frac{\hat{n}_{d\bar{\beta}}}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z}\end{aligned}\quad (7.41)$$

3.

$$\Delta_3^+ \mathcal{H}_N = \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_t c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\bar{\beta}} \quad (7.42)$$

Intermediate ($\hat{n}_{d\beta} = 0, \hat{n}_{q\beta} = 1 - \hat{n}_{q\bar{\beta}} = \hat{n}_{d\bar{\beta}} = 1$) energy is

$$H_1 = \frac{1}{2}\epsilon_q - \frac{1}{2}J_z + \epsilon_d \quad (7.43)$$

$$\begin{aligned}
\Delta_3^+ \mathcal{H}_N &= \sum_{q\beta k} J_t V_q^* c_{d\beta}^\dagger c_{q\beta} c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\bar{\beta}} \frac{1}{\omega^+ - H_1} \\
&= -J_t \sum_{q\beta k} V_q^* \hat{n}_{d\beta} (1 - \hat{n}_{q\beta}) c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}} \frac{1}{\omega^+ - H_1} \\
&= -J_t \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{k\beta} \frac{\hat{n}_{d\bar{\beta}}}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z}
\end{aligned} \tag{7.44}$$

4.

$$\Delta_4^+ \mathcal{H}_N = \sum_{q\beta k\sigma} J_z \beta S_d^z c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} V_q c_{q\beta}^\dagger c_{d\beta} \tag{7.45}$$

The first step is a simplification:

$$J_z \beta S_d^z c_{d\beta} = \frac{1}{2} (-J_z) \hat{n}_{d\bar{\beta}} c_{d\beta} \tag{7.46}$$

Intermediate ($\hat{n}_{d\beta} = 0, \hat{n}_{q\beta} = 1 - \hat{n}_{q\bar{\beta}} = \hat{n}_{d\bar{\beta}} = 1$) energy is

$$H_1 = \frac{1}{2}\epsilon_q - \frac{1}{2}J_z + \epsilon_d \tag{7.47}$$

$$\begin{aligned}
\Delta_4^+ \mathcal{H}_N &= -\frac{1}{2}J_z \sum_{q\beta k} V_q \hat{n}_{d\bar{\beta}} c_{k\beta}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{d\beta} \frac{1}{\omega^+ - H_1} \\
&= \sum_{q\beta k} -\frac{1}{2}J_z V_q \hat{n}_{d\bar{\beta}} (1 - \hat{n}_{q\beta}) c_{k\beta}^\dagger c_{d\beta} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} \\
&= -\frac{1}{2}J_z \sum_{q\beta k} V_q c_{k\beta}^\dagger c_{d\beta} \frac{\hat{n}_{d\bar{\beta}}}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z}
\end{aligned} \tag{7.48}$$

5.

$$\Delta_5^+ \mathcal{H}_N = \sum_{q\beta k\sigma} J_t c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} V_q c_{q\beta}^\dagger c_{d\beta} \tag{7.49}$$

Intermediate ($\hat{n}_{d\beta} = 0, \hat{n}_{q\beta} = 1 - \hat{n}_{q\bar{\beta}} = \hat{n}_{d\bar{\beta}} = 1$) energy is

$$H_1 = \frac{1}{2}\epsilon_q - \frac{1}{2}J_z + \epsilon_d \tag{7.50}$$

$$\begin{aligned}
\Delta_5^+ \mathcal{H}_N &= \sum_{q\beta k} J_t V_q c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{d\beta} \frac{1}{\omega^+ - H_1} \\
&= -\sum_{q\beta k} J_t V_q (1 - \hat{n}_{q\beta}) \hat{n}_{d\beta} c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} \\
&= -J_t \sum_{q\beta k} V_q c_{k\beta}^\dagger c_{d\beta} \frac{\hat{n}_{d\bar{\beta}}}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z}
\end{aligned} \tag{7.51}$$

6.

$$\Delta_6^+ \mathcal{H}_N = \sum_{k'q\beta k} J_z S_d^z \beta c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_z S_d^z \beta c_{q\beta}^\dagger c_{k'\beta} \quad (7.52)$$

The first step is a simplification:

$$(\beta S_d^z)^2 = \frac{1}{4} (\hat{n}_{d\beta} - \hat{n}_{d\bar{\beta}})^2 = \frac{1}{4} (\hat{n}_{d\beta} + \hat{n}_{d\bar{\beta}} - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}) = \frac{1}{4} (\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}) \quad (7.53)$$

Note that this term projects onto the singly-occupied subspace; both the doubly- and zero-occupied states will give zero for this term. Intermediate ($\hat{n}_{q\beta} = 1 - \hat{n}_{q\bar{\beta}} = 1$) energy is

$$H_1 = \frac{1}{2}\epsilon_q + \beta J_z S_d^z + H_{imp} \quad (7.54)$$

Since the $(S^z)^2$ term filters out only the single-occupied subspace, we can write $H_{imp} = \epsilon_d$.

$$\begin{aligned} \Delta_6^+ \mathcal{H}_N &= \frac{1}{4} J_z^2 \sum_{k'q\beta k} (\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}) c_{k\beta}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{k'\beta} \frac{1}{\omega^+ - H_1} \\ &= \frac{1}{4} J_z^2 \sum_{k'q\beta k} (\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}) (1 - \hat{n}_{q\beta}) c_{k\beta}^\dagger c_{k'\beta} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - H_{imp} - \beta J_z S_d^z} \\ &= \frac{1}{4} J_z^2 \sum_{k'q\beta k} c_{k\beta}^\dagger c_{k'\beta} \frac{(\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow})}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d - \beta J_z S_d^z} \\ &= \frac{1}{4} J_z^2 \sum_{k'q\beta k} c_{k\beta}^\dagger c_{k'\beta} \left[\frac{\hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}})}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d - \frac{1}{2}J_z} + \frac{\hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta})}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} \right] \end{aligned} \quad (7.55)$$

In the last step, we used the fact that $\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}$ is not zero only in the singly occupied subspace, hence we can expand it into $\hat{n}_\uparrow (1 - \hat{n}_\downarrow) + \hat{n}_\downarrow (1 - \hat{n}_\uparrow)$.

7.

$$\Delta_7^+ \mathcal{H}_N = \sum_{q\beta k k'} \beta J_z S_d^z c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_t c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\bar{\beta}} \quad (7.56)$$

The first step is a simplification:

$$\beta S_d^z c_{d\bar{\beta}}^\dagger c_{d\beta} = \beta S_d^z S_{d\bar{\beta}}^+ = \beta \frac{1}{2} \bar{\beta} S_{d\bar{\beta}}^+ = -\frac{1}{2} c_{d\bar{\beta}}^\dagger c_{d\beta} \quad (7.57)$$

Intermediate ($\hat{n}_{d\beta} = 0, \hat{n}_{q\beta} = 1 - \hat{n}_{q\bar{\beta}} = \hat{n}_{d\bar{\beta}} = 1$) energy is

$$H_1 = \frac{1}{2}\epsilon_q + \beta J_z S_d^z + \epsilon_d = \frac{1}{2}\epsilon_q - \frac{1}{2}J_z + \epsilon_d \quad (7.58)$$

$$\begin{aligned} \Delta_7^+ \mathcal{H}_N &= \sum_{q\beta k k'} \frac{1}{2} J_z J_t c_{k\beta}^\dagger c_{q\beta} c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\bar{\beta}} \frac{-1}{\omega^+ - H_1} \\ &= -\frac{1}{2} J_z J_t \sum_{q\beta k k'} (1 - \hat{n}_{q\beta}) c_{d\bar{\beta}}^\dagger c_{d\beta} c_{k\beta}^\dagger c_{k'\bar{\beta}} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} \\ &= -\frac{1}{2} J_z J_t \sum_{q\beta k k'} c_{d\bar{\beta}}^\dagger c_{d\beta} c_{k\beta}^\dagger c_{k'\bar{\beta}} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} \end{aligned} \quad (7.59)$$

8.

$$\Delta_8^+ \mathcal{H}_N = \sum_{q\beta k k'} J_t c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_z \beta S_d^z c_{q\beta}^\dagger c_{k'\beta} \quad (7.60)$$

The first step is a simplification:

$$c_{d\beta}^\dagger c_{d\bar{\beta}} \beta S_d^z = S_{d\beta}^+ \beta S_d^z = \beta \frac{1}{2} \bar{\beta} S_{d\bar{\beta}}^+ = -\frac{1}{2} c_{d\beta}^\dagger c_{d\bar{\beta}} \quad (7.61)$$

Intermediate ($\hat{n}_{d\beta} = 0, \hat{n}_{q\beta} = 1 - \hat{n}_{q\bar{\beta}} = \hat{n}_{d\bar{\beta}} = 1$) energy is

$$H_1 = \frac{1}{2} \epsilon_q + \beta J_z S_d^z + \epsilon_d = \frac{1}{2} \epsilon_q - \frac{1}{2} J_z + \epsilon_d \quad (7.62)$$

$$\begin{aligned} \Delta_8^+ \mathcal{H}_N &= - \sum_{q\beta k k'} \frac{1}{2} J_z J_t c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{k'\beta} \frac{1}{\omega^+ - H_1} \\ &= -\frac{1}{2} J_z J_t \sum_{q\beta k k'} (1 - \hat{n}_{q\beta}) c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{k'\beta} \frac{1}{\omega^+ - \frac{1}{2} \epsilon_q - \epsilon_d + \frac{1}{2} J_z} \\ &= -\frac{1}{2} J_z J_t \sum_{q\beta k k'} c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{k'\beta} \frac{1}{\omega^+ - \frac{1}{2} \epsilon_q - \epsilon_d + \frac{1}{2} J_z} \end{aligned} \quad (7.63)$$

9.

$$\Delta_9^+ \mathcal{H}_N = \sum_{q\beta k k'} J_t c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_t c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\bar{\beta}} \quad (7.64)$$

Intermediate ($\hat{n}_{d\beta} = 0, \hat{n}_{q\beta} = 1 - \hat{n}_{q\bar{\beta}} = \hat{n}_{d\bar{\beta}} = 1$) energy is

$$H_1 = \frac{1}{2} \epsilon_q - \frac{1}{2} J_z + \epsilon_d \quad (7.65)$$

$$\begin{aligned} \Delta_9^+ \mathcal{H}_N &= \sum_{q\beta k k'} J_t^2 c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\bar{\beta}} \frac{1}{\omega^+ - H_1} \\ &= J_t^2 \sum_{q\beta k k'} (1 - \hat{n}_{q\beta}) \hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}}) c_{k\bar{\beta}}^\dagger c_{k'\bar{\beta}} \frac{1}{\omega^+ - \frac{1}{2} \epsilon_q - \epsilon_d + \frac{1}{2} J_z} \\ &= J_t^2 \sum_{q\beta k k'} c_{k\bar{\beta}}^\dagger c_{k'\bar{\beta}} \frac{\hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta})}{\omega^+ - \frac{1}{2} \epsilon_q - \epsilon_d + \frac{1}{2} J_z} \end{aligned} \quad (7.66)$$

7.4 Scaling equations for particle sector

The scaling equations are obtained as follows. The first term gives the renormalization in ϵ_d and U . The renormalization in U will come with a factor of 2 because $\sum_\beta \hat{n}_{d\beta} \hat{n}_{d\bar{\beta}} = 2\hat{n}_{d\uparrow} \hat{n}_{d\downarrow}$. Terms 2 and 3 renormalize V^* . Terms 4 and 5 renormalize V . Since these renormalizations are same, we write just one them. Also, in the terms 2 through 5, the renormalization is actually that of $V \hat{n}_{d\bar{\beta}}$, not strictly of V . In other words, if we split V as $V = V [\hat{n}_{d\bar{\beta}} + (1 - \hat{n}_{d\bar{\beta}})] = V^1 \hat{n}_{d\bar{\beta}} + V^0 (1 - \hat{n}_{d\bar{\beta}})$, then these terms will renormalize V^1 . However, we do not make this distinction here because in the particle sector, we will get a renormalization in V^0 , and that will turn out to be the same, so we can just talk about

the renormalization in V instead of splitting it. Terms 7 and 8 renormalize J_t and term 9 renormalizes the anti-parallel part of J_z , that is, the part in which the conduction electron has spin $\bar{\beta}$. The other term, with spin β will renormalize in the hole sector. Term 6 can be ignored for now because it will get canceled by an opposite term in the hole sector, see 7.7. Otherwise it will renormalize J_z .

$$\Delta^+ \epsilon_d = \sum_q |V(q)|^2 \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q} \quad (7.67)$$

$$\Delta^+ U = \sum_q 2|V(q)|^2 \left(\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} - \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q} \right) \quad (7.68)$$

$$\Delta^+ V = - \left(\frac{1}{2}J_z + J_t \right) \sum_q V_q \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} \quad (7.69)$$

$$\Delta^+ J_t = -J_z J_t \sum_q \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} \quad (7.70)$$

$$\Delta^+ J_z = -J_t^2 \sum_q \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} \quad (7.71)$$

7.5 Hole sector

The renormalization in the Hamiltonian in the hole sector is

$$\begin{aligned} \Delta^- \mathcal{H}_N = \sum_{q\beta} \left[V_q c_{q\beta}^\dagger c_{d\beta} + J_z \beta S_d^z \sum_{k\sigma} \hat{n}_{d\sigma} c_{k\beta} c_{q\beta}^\dagger + J_t \sum_{k\sigma} c_{d\bar{\beta}}^\dagger c_{q\beta}^\dagger c_{d\beta} c_{k\bar{\beta}} \right] \times \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} \\ \times \left[V_q^* c_{d\beta}^\dagger c_{q\beta} + J_z \beta S_d^z \sum_{k\sigma} \hat{n}_{d\sigma} c_{q\beta} c_{k\beta}^\dagger + J_t \sum_{k\sigma} c_{d\beta}^\dagger c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} c_{q\beta} \right] \end{aligned} \quad (7.72)$$

\mathcal{H}_D^- is the energy of the hole state. Since the hole state consists of a missing electron, the diagonal part can be evaluated by substituting $\tau_{q\beta} = -\frac{1}{2}$ and $\epsilon_q = -\epsilon_q$ in eq. 7.12.

$$\mathcal{H}_D^- = \frac{1}{2}\epsilon_q + J_z S_d^z s_q^z + H_{\text{imp}} \quad (7.73)$$

1.

$$\Delta_1^- \mathcal{H}_N = \sum_{q\beta} |V_q|^2 c_{q\beta}^\dagger c_{d\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} c_{d\beta}^\dagger c_{q\beta} \quad (7.74)$$

The intermediate ($\hat{n}_{q\beta} = 0, \hat{n}_{d\beta} = 1$) energy is

$$H_1 = \epsilon_d + (\epsilon_d + U) \hat{n}_{d\bar{\beta}} + \frac{1}{2}\epsilon_q - \beta J_z S_d^z = \frac{1}{2}\epsilon_q - \frac{1}{2}J_z (1 - \hat{n}_{d\bar{\beta}}) + \epsilon_d + (\epsilon_d + U) \hat{n}_{d\bar{\beta}} \quad (7.75)$$

$$\Delta_1^- \mathcal{H}_N = \sum_{q\beta} |V_q|^2 \hat{n}_{q\beta} (1 - \hat{n}_{d\beta}) \frac{1}{\omega^- - H_1} \quad (7.76)$$

For hole excitations, the initial state must be filled, so we can set $\hat{n}_{q\beta} = 1$.

$$\begin{aligned}
\Delta_1^- \mathcal{H}_N &= \sum_{q\beta} |V_q|^2 \hat{n}_{q\beta} (1 - \hat{n}_{d\beta}) \frac{1}{\omega^- - \frac{1}{2}\epsilon_q + \frac{1}{2}J_z (1 - \hat{n}_{d\bar{\beta}}) - \epsilon_d - (\epsilon_d + U) \hat{n}_{d\bar{\beta}}} \\
&= \sum_{q\beta} |V_q|^2 (1 - \hat{n}_{d\beta}) \left[\frac{\hat{n}_{d\bar{\beta}}}{\omega^- - \frac{1}{2}\epsilon_q - 2\epsilon_d - U} + \frac{1 - \hat{n}_{d\bar{\beta}}}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} \right] \\
&= \sum_{q\beta} |V(q)|^2 \left[\hat{n}_{d\bar{\beta}} \left(\frac{1}{\omega^- - \frac{1}{2}\epsilon_q - 2\epsilon_d - U} - \frac{2}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} \right) \right. \\
&\quad \left. + \hat{n}_{d\uparrow}\hat{n}_{d\downarrow} \left(\frac{1}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} - \frac{1}{\omega^- - \frac{1}{2}\epsilon_q - 2\epsilon_d - U} \right) \right]
\end{aligned} \tag{7.77}$$

2.

$$\Delta_2^- \mathcal{H}_N = \sum_{q\beta k} V_q c_{q\beta}^\dagger c_{d\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_z \beta S_d^z c_{k\beta}^\dagger c_{q\beta} \tag{7.78}$$

The first step is a simplification:

$$c_{d\beta} J_z \beta S_d^z = c_{d\beta} \frac{1}{2} J_z (1 - \hat{n}_{d\bar{\beta}}) \tag{7.79}$$

The intermediate ($\hat{n}_{q\beta} = 0, \hat{n}_{d\beta} = 1$) energy is

$$H_1 = -\frac{1}{2}\epsilon_q + \epsilon_d + (\epsilon_d + U) \hat{n}_{d\bar{\beta}} - \frac{1}{2}J_z (1 - \hat{n}_{d\bar{\beta}}) \tag{7.80}$$

$$\begin{aligned}
\Delta_2^- \mathcal{H}_N &= \sum_{q\beta k} \frac{1}{2} J_z (1 - \hat{n}_{d\bar{\beta}}) V_q c_{q\beta}^\dagger c_{d\beta} (1 - \hat{n}_{d\bar{\beta}}) c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega^- - H_1} \\
&= - \sum_{q\beta k} \hat{n}_{q\beta} c_{k\beta}^\dagger c_{d\beta} \frac{V_q \frac{1}{2} J_z (1 - \hat{n}_{d\bar{\beta}})}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d - (\epsilon_d + U) \hat{n}_{d\bar{\beta}} + \frac{1}{2}J_z (1 - \hat{n}_{d\bar{\beta}})} \\
&= -\frac{1}{2} J_z \sum_{q\beta k} V_q \hat{n}_{q\beta} c_{k\beta}^\dagger c_{d\beta} \frac{(1 - \hat{n}_{d\bar{\beta}})}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z}
\end{aligned} \tag{7.81}$$

3.

$$\Delta_3^- \mathcal{H}_N = \sum_{q\beta k} V_q c_{q\beta}^\dagger c_{d\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_t c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \tag{7.82}$$

The intermediate ($\hat{n}_{q\beta} = \hat{n}_{d\bar{\beta}} = 0, \hat{n}_{d\beta} = 1$) energy is

$$H_1 = \epsilon_d - \frac{1}{2}\epsilon_q - \frac{1}{2}J_z \beta S_d^z = \epsilon_d - \frac{1}{2}\epsilon_q - \frac{1}{2}J_z \tag{7.83}$$

$$\begin{aligned}
\Delta_3^- \mathcal{H}_N &= \sum_{q\beta k} J_t V_q c_{q\beta}^\dagger c_{d\beta} c_{d\bar{\beta}}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \frac{1}{\omega^- - H_1} \\
&= \sum_{q\beta k} J_t V_q \hat{n}_{q\beta} (1 - \hat{n}_{d\beta}) c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} \frac{-1}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} \\
&= -J_t \sum_{q\beta k} V_q c_{k\bar{\beta}}^\dagger c_{d\beta} \frac{1 - \hat{n}_{d\bar{\beta}}}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z}
\end{aligned} \tag{7.84}$$

4.

$$\Delta_4^- \mathcal{H}_N = \sum_{q\beta k} \frac{1}{2} J_z \beta S_d^z c_{q\beta}^\dagger c_{k\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} V_q^* c_{d\beta}^\dagger c_{q\beta} \quad (7.85)$$

There is a simplification:

$$\frac{1}{2} J_z \beta S_d^z c_{d\beta}^\dagger = \frac{1}{2} J_z (1 - \hat{n}_{d\bar{\beta}}) c_{d\beta}^\dagger \quad (7.86)$$

The intermediate ($\hat{n}_{q\beta} = 0, \hat{n}_{d\beta} = 1$) energy is

$$H_1 = -\frac{1}{2} \epsilon_q + \epsilon_d + (\epsilon_d + U) \hat{n}_{d\bar{\beta}} - \frac{1}{2} J_z (1 - \hat{n}_{d\bar{\beta}}) \quad (7.87)$$

$$\begin{aligned} \Delta_4^- \mathcal{H}_N &= \sum_{q\beta k} V_q^* c_{q\beta}^\dagger c_{k\beta} c_{d\beta}^\dagger c_{q\beta} \frac{\frac{1}{2} J_z (1 - \hat{n}_{d\bar{\beta}})}{\omega^- - H_1} \\ &= \sum_{q\beta k} \hat{n}_{q\beta} V_q^* c_{k\beta} c_{d\beta}^\dagger \frac{\frac{1}{2} J_z (1 - \hat{n}_{d\bar{\beta}})}{\omega^- + \frac{1}{2} \epsilon_q - \epsilon_d - (\epsilon_d + U) \hat{n}_{d\bar{\beta}} + \frac{1}{2} J_z (1 - \hat{n}_{d\bar{\beta}})} \\ &= -\frac{1}{2} J_z \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{k\beta} \frac{1 - \hat{n}_{d\bar{\beta}}}{\omega^- + \frac{1}{2} \epsilon_q - \epsilon_d + \frac{1}{2} J_z} \end{aligned} \quad (7.88)$$

5.

$$\Delta_5^- \mathcal{H}_N = \sum_{q\beta k} J_t c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\bar{\beta}} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} V_q^* c_{d\beta}^\dagger c_{q\beta} \quad (7.89)$$

The intermediate ($\hat{n}_{q\beta} = \hat{n}_{d\bar{\beta}} = 0, \hat{n}_{d\beta} = 1$) energy is

$$H_1 = -\frac{1}{2} \epsilon_q + \epsilon_d - \frac{1}{2} J_z \quad (7.90)$$

$$\begin{aligned} \Delta_5^- \mathcal{H}_N &= \sum_{q\beta k} J_t V_q^* c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\bar{\beta}} c_{d\beta}^\dagger c_{q\beta} \frac{1}{\hat{\omega}^- - H_1} \\ &= -J_t \sum_{q\beta k} V_q^* \hat{n}_{q\beta} (1 - \hat{n}_{d\beta}) c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}} \frac{1}{\omega^- - \frac{1}{2} \epsilon_q - \epsilon_d + \frac{1}{2} J_z} \\ &= -J_t \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{k\beta} \frac{1 - \hat{n}_{d\bar{\beta}}}{\omega^- - \frac{1}{2} \epsilon_q - \epsilon_d + \frac{1}{2} J_z} \end{aligned} \quad (7.91)$$

6.

$$\Delta_6^- \mathcal{H}_N = \sum_{q\beta k k'} J_z \beta S_d^z c_{q\beta}^\dagger c_{k'\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_z \beta S_d^z c_{k\beta}^\dagger c_{q\beta} \quad (7.92)$$

From eq. 7.53,

$$(\beta S_d^z)^2 = \frac{1}{4} (\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}) \quad (7.93)$$

The intermediate ($\hat{n}_{q\beta} = 0$) energy is

$$H_1 = H_{\text{imp}} - \frac{1}{2} \epsilon_q - \beta J_z S_d^z \quad (7.94)$$

$$\begin{aligned}
 \Delta_6^- \mathcal{H}_N &= \sum_{q\beta k k'} \frac{J_z^2}{4} (\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}) c_{q\beta}^\dagger c_{k'\beta} c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega^- - H_1} \\
 &= \frac{J_z^2}{4} \sum_{q\beta k k'} \hat{n}_{q\beta} (\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}) c_{k'\beta} c_{k\beta}^\dagger \frac{1}{\omega^- - \frac{1}{2}\epsilon_q - H_{\text{imp}} + \beta J_z S_d^z} \\
 &= -\frac{J_z^2}{4} \sum_{q\beta k k'} c_{k\beta}^\dagger c_{k'\beta} \left[\frac{\hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}})}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} + \frac{\hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta})}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d - \frac{1}{2}J_z} \right] \\
 &\quad + \frac{J_z^2}{4} \sum_{q\beta k} \left[\frac{\hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}})}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} + \frac{\hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta})}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d - \frac{1}{2}J_z} \right]
 \end{aligned} \tag{7.95}$$

7.

$$\Delta_7^- \mathcal{H}_N = \sum_{q\beta k k'} J_z \beta S_d^z c_{q\beta}^\dagger c_{k'\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D} J_t c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \tag{7.96}$$

Simplification:

$$\beta S_d^z c_{d\beta}^\dagger c_{d\bar{\beta}} = \beta S_d^z S_{d\beta}^+ = \beta \frac{1}{2} \beta S_{d\beta}^+ = \frac{1}{2} c_{d\beta}^\dagger c_{d\bar{\beta}} \tag{7.97}$$

 The intermediate ($\hat{n}_{q\beta} = \hat{n}_{d\bar{\beta}} = 0, \hat{n}_{d\beta} = 1$) energy is

$$H_1 = \epsilon_d - \frac{1}{2}\epsilon_q - \frac{1}{2}J_z \tag{7.98}$$

$$\begin{aligned}
 \Delta_7^- \mathcal{H}_N &= \sum_{q\beta k k'} \frac{1}{2} J_z J_t c_{q\beta}^\dagger c_{k'\beta} c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \frac{1}{\omega^- - H_1} \\
 &= \sum_{q\beta k k'} \frac{1}{2} J_z J_t \hat{n}_{q\beta} c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{k'\beta} \frac{-1}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} \\
 &= -\frac{1}{2} J_z J_t \sum_{q\beta k k'} c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{k'\beta} \frac{1}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} \\
 &= -\frac{1}{2} J_z J_t \sum_{q\beta k k'} c_{d\bar{\beta}}^\dagger c_{d\beta} c_{k\beta}^\dagger c_{k'\bar{\beta}} \frac{1}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z}
 \end{aligned} \tag{7.99}$$

8.

$$\Delta_8^- \mathcal{H}_N = \sum_{q\beta k k'} J_t c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\bar{\beta}} \frac{1}{\hat{\omega}^- - \mathcal{H}_D} J_z \beta S_d^z c_{k\beta}^\dagger c_{q\beta} \tag{7.100}$$

Simplification:

$$c_{d\bar{\beta}}^\dagger c_{d\beta} \beta S_d^z = S_{d\bar{\beta}}^+ S_{d\beta}^z \beta = \beta \frac{1}{2} S_{d\bar{\beta}}^+ \beta = \frac{1}{2} c_{d\bar{\beta}}^\dagger c_{d\beta} \tag{7.101}$$

 The intermediate ($\hat{n}_{q\beta} = \hat{n}_{d\bar{\beta}} = 0, \hat{n}_{d\beta} = 1$) energy is

$$H_1 = -\frac{1}{2}\epsilon_q - \frac{1}{2}J_z + \epsilon_d \tag{7.102}$$

$$\begin{aligned}
 \Delta_8^- \mathcal{H}_N &= \sum_{q\beta k k'} \frac{1}{2} J_z J_t c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\bar{\beta}} c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega^- - H_1} \\
 &= \sum_{q\beta k k'} \frac{1}{2} J_z J_t \hat{n}_{q\beta} c_{d\bar{\beta}}^\dagger c_{d\beta} c_{k'\bar{\beta}}^\dagger c_{k\beta} \frac{-1}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d - \frac{1}{2}J_z} \\
 &= -\frac{1}{2} J_z J_t \sum_{q\beta k k'} c_{d\bar{\beta}}^\dagger c_{d\beta} c_{k'\bar{\beta}}^\dagger c_{k\beta} \frac{1}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z}
 \end{aligned} \tag{7.103}$$

9.

$$\Delta_9^- \mathcal{H}_N = \sum_{q\beta k k'} J_t c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\bar{\beta}} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_t c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\beta}^\dagger c_{q\beta} \tag{7.104}$$

The intermediate ($\hat{n}_{q\beta} = \hat{n}_{d\bar{\beta}} = 0, \hat{n}_{d\beta} = 1$) energy is

$$H_1 = -\frac{1}{2}\epsilon_q - \frac{1}{2}J_z + \epsilon_d \tag{7.105}$$

$$\begin{aligned}
 \Delta_9^- \mathcal{H}_N &= \sum_{q\beta k k'} J_t^2 c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\bar{\beta}} c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega^- - H_1} \\
 &= \sum_{q\beta k k'} J_t^2 \hat{n}_{q\beta} c_{d\bar{\beta}}^\dagger c_{d\beta} c_{k'\bar{\beta}}^\dagger c_{k\beta} \frac{1}{\omega^- - H_1} \\
 &= -\sum_{q\beta k k'} J_t^2 \hat{n}_{q\beta} \hat{n}_{d\bar{\beta}} c_{d\beta} c_{k'\bar{\beta}}^\dagger c_{d\beta}^\dagger c_{k\beta} \frac{1}{\omega^- - H_1} \\
 &= \sum_{q\beta k k'} J_t^2 \hat{n}_{q\beta} \hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta}) c_{k'\bar{\beta}}^\dagger c_{k\beta} \frac{1}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} \\
 &= -J_t^2 \sum_{q\beta k k'} c_{k\beta}^\dagger c_{k'\bar{\beta}} \frac{\hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}})}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} + J_t^2 \sum_{qk\beta} \frac{\hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta})}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z}
 \end{aligned} \tag{7.106}$$

7.6 Scaling equations for hole sector

The scaling equations are obtained similarly as in the particle sector. The important things to note are the following. The first two terms in term 6 here cancel the term 6 of the particle sector. The last two terms in term 6 and the last term in term 9 renormalize U and ϵ_d .

$$\begin{aligned}
 \Delta^- \epsilon_d &= \sum_q |V(q)|^2 \left(\frac{1}{\omega^- - \frac{1}{2}\epsilon_q - 2\epsilon_d - U} - \frac{2}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} \right) + \\
 &\quad \sum_{qk} \left[\frac{\frac{1}{4}J_z^2 + J_t^2}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} + \frac{\frac{1}{4}J_z^2}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d - \frac{1}{2}J_z} \right] \\
 \Delta^- U &= 2 \sum_q |V(q)|^2 \left(\frac{1}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} - \frac{1}{\omega^- - \frac{1}{2}\epsilon_q - 2\epsilon_d - U} \right) - \\
 &\quad 2 \sum_{qk} \left[\frac{\frac{1}{4}J_z^2 + J_t^2}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} + \frac{\frac{1}{4}J_z^2}{\omega^- - \frac{1}{2}\epsilon_q - \epsilon_d - \frac{1}{2}J_z} \right]
 \end{aligned}$$

$$\begin{aligned}\Delta^- V &= - \left(\frac{1}{2} J_z + J_t \right) \sum_q V_q \frac{1}{\omega^- - \frac{1}{2} \epsilon_q - \epsilon_d + \frac{1}{2} J_z} \\ \Delta^- J_t &= - J_z J_t \sum_q \frac{1}{\omega^- - \frac{1}{2} \epsilon_q - \epsilon_d + \frac{1}{2} J_z} \\ \Delta^- J_z &= - J_t^2 \sum_q \frac{1}{\omega^- - \frac{1}{2} \epsilon_q - \epsilon_d + \frac{1}{2} J_z}\end{aligned}$$

7.7 Vanishing of $\Delta^6 \mathcal{H}$

If take the scattering term $J_z \beta S_d^z c_{q\beta}^\dagger c_{k'\beta}$ and construct the η and η^\dagger operators from them,

$$\begin{aligned}\eta &= \frac{1}{\omega^- - \frac{1}{2} \epsilon_q - \epsilon_d + \beta J_z S_d^z} J_z \beta S_d^z c_{k'\beta}^\dagger c_{q\beta} \\ \eta^\dagger &= \frac{1}{\omega^+ - \frac{1}{2} \epsilon_q - H_{\text{imp}} - \beta J_z S_d^z} J_z \beta S_d^z c_{q\beta}^\dagger c_{k'\beta}\end{aligned}\tag{7.107}$$

From the expression of η , we can take its Hermitian conjugate to get another expression for η^\dagger :

$$\eta^\dagger = J_z \beta S_d^z c_{q\beta}^\dagger c_{k'\beta} \frac{1}{\omega^- - \frac{1}{2} \epsilon_q - \epsilon_d + \beta J_z S_d^z}\tag{7.108}$$

Comparing the two expressions gives

$$\frac{1}{\omega^- - \frac{1}{2} \epsilon_q - \epsilon_d + \beta J_z S_d^z} = \frac{1}{\omega^+ - \frac{1}{2} \epsilon_q - H_{\text{imp}} - \beta J_z S_d^z}\tag{7.109}$$

Substituting this equation into either Δ_6^+ or Δ_6^- gives $\Delta_6^+ \mathcal{H} = -\Delta_6^- \mathcal{H}$, so $\Delta_6 \mathcal{H} = 0$.

7.8 Total RG Equations

Just as in the previous section, we replace ω_j^\pm with $\omega + E_j$ in the first term in each sector. For the rest of the equations, we set $\omega^+ = \omega^- = \omega$. We can ignore the sixth term in each sector since they add up to zero as shown in the previous section. We then get, after adding

contributions from both sectors,

$$\begin{aligned}
\Delta\epsilon_d &= \sum_{\epsilon_q=D} |V(q)|^2 \frac{1}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d} + \sum_{\epsilon_q=-D} |V(q)|^2 \left(\frac{1}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d - U} - \frac{2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} \right) \\
&\quad + \sum_{\substack{\epsilon_q=-D \\ k < q}} \left[\frac{\frac{1}{4}J_z^2 + J_t^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} + \frac{\frac{1}{4}J_z^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d - \frac{1}{2}J_z} \right] \\
\Delta U &= \sum_{\epsilon_q=D} 2|V(q)|^2 \frac{1}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d + U + \frac{1}{2}J_z} - \sum_{\epsilon_q=D} 2|V(q)|^2 \frac{1}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d} \\
&\quad + \sum_{\epsilon_q=-D} 2|V(q)|^2 \frac{1}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} - \sum_{\epsilon_q=-D} 2|V(q)|^2 \frac{1}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d - U} \\
&\quad - \sum_{\substack{\epsilon_q=-D, \\ k < q}} 2 \left[\frac{\frac{1}{4}J_z^2 + J_t^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} + \frac{\frac{1}{4}J_z^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d - \frac{1}{2}J_z} \right] \\
\Delta V &= - \left(\frac{1}{2}J_z + J_t \right) \left(\sum_{\epsilon_q=D} + \sum_{\epsilon_q=-D} \right) V_q \frac{1}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} \\
\Delta J_t &= -J_z J_t \left(\sum_{\epsilon_q=D} + \sum_{\epsilon_q=-D} \right) \frac{1}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} \\
\Delta J_z &= -J_t^2 \left(\sum_{\epsilon_q=D} + \sum_{\epsilon_q=-D} \right) \frac{1}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z}
\end{aligned} \tag{7.110}$$

7.9 Particle-Hole symmetry

As discussed in the previous section, the particle-hole symmetry condition is $\epsilon_d + U = -\epsilon_d$. We henceforth also assume that $\sum_D = \sum_{-D}$ and drop the indices on the summations. The RG equations for ϵ_d and U then look like,

$$\begin{aligned}
\Delta\epsilon_d &= 2 \sum_q |V(q)|^2 \frac{1}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d} - 2 \sum_q |V(q)|^2 \frac{1}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} \\
&\quad + \sum_{q,k} \left[\frac{\frac{1}{4}J_z^2 + J_t^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} + \frac{\frac{1}{4}J_z^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d - \frac{1}{2}J_z} \right] \\
\frac{1}{2}\Delta U &= 2 \sum_q |V(q)|^2 \frac{1}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} - 2 \sum_q |V(q)|^2 \frac{1}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d} \\
&\quad - \sum_{q,k} \left[\frac{\frac{1}{4}J_z^2 + J_t^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{2}J_z} + \frac{\frac{1}{4}J_z^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d - \frac{1}{2}J_z} \right]
\end{aligned} \tag{7.111}$$

The asymmetry parameter $\gamma = \epsilon_d + \frac{1}{2}U$ is thus invariant under the flow.

$$\implies \Delta \left(\epsilon_d + \frac{1}{2}U \right) = 0 \tag{7.112}$$

Starting from a particle-hole symmetric model keeps you on a symmetric flow.

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

In the limit of $\epsilon_d, J \ll D \ll U$, the equation for ϵ_d becomes, up to lowest order in J ,

$$\delta\epsilon_d = - \sum_q \frac{|V_q|^2}{\omega^+ - \frac{1}{2}\epsilon_q} \quad (7.113)$$

This is the same form that we had in the pure SIAM, and we can again repeat what we did in 6.4.

7.11 $SU(2)$ 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:

$$2\Delta J_z = 2\Delta J_t = \Delta J = -J^2 \sum_{|\epsilon_q|=D} \frac{1}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J} \quad (7.114)$$

In order to reach the Kondo RG equations, we need to make the appropriate physical change; the difference between the Anderson model and the Kondo model is that the impurity charge fluctuations are frozen at single occupation in the latter. This means that the ground state of the impurity is now at ϵ_d . We can take account of this change by now measuring ω from the single occupation energy itself, ϵ_d . Hence we should redefine $\omega - \epsilon_d \rightarrow \tilde{\omega}$.

$$2\Delta J_z = 2\Delta J_t = \Delta J = -J^2 \sum_{|\epsilon_q|=D} \frac{1}{\tilde{\omega} - \frac{1}{2}\epsilon_q + \frac{1}{4}J} \quad (7.115)$$

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

$$\Delta J = -J^2 \sum_{|\epsilon_q|=D} \frac{1}{-\epsilon_q + \frac{1}{4}J} \quad (7.116)$$

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

$$\Delta J = -J^2 \sum_{|\epsilon_q|=D} \frac{1}{-\epsilon_q} \quad (7.117)$$

For an isotropic dispersion, we can use $\epsilon_q = D$. The sum can then be evaluated as

$$\sum_{|\epsilon_q|=D} = \sum_{\epsilon_q=D} + \sum_{\epsilon_q=-D} = 2\rho(D)|\Delta D| \quad (7.118)$$

The flow equation of J becomes

$$\Delta J = 2J^2\rho(D)\frac{|\Delta D|}{D} \quad (7.119)$$

This is the familiar one-loop Kondo flow equation obtained from Poor man's scaling. To get the continuum version, we must note that since we are decreasing the bandwidth, we have to set $\Delta D = -|\Delta D|$. Therefore,

$$\frac{dJ}{d \ln D} = -2J^2 \rho(D) \quad (7.120)$$

8 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 [25],[26]

$$\psi^k = \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow}^\dagger \end{pmatrix} \quad (8.1)$$

and the charge isospin [27] for the mobile conduction electrons

$$\vec{C} = \frac{1}{2} \sum_{kk'\alpha\beta} \psi_\alpha^{k\dagger} \vec{\sigma}_{\alpha\beta} \psi_\beta^{k'} \quad (8.2)$$

The various components of the isospin are

$$C_{kk'}^z = \frac{1}{2} \sum_\alpha \psi_\alpha^{k\dagger} \sigma_{\alpha\alpha}^z \psi_\alpha^{k'} = \frac{1}{2} \left(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow} \right) = \frac{1}{2} \left(c_{k\uparrow}^\dagger c_{k'\uparrow} + c_{k\downarrow}^\dagger c_{k'\downarrow} - \delta_{kk'} \right) \quad (8.3)$$

$$= \frac{1}{2} \sum_\sigma \left(c_{k\sigma}^\dagger c_{k'\sigma} - \frac{1}{2} \delta_{kk'} \right) \quad (8.4)$$

$$C_{kk'}^x = \frac{1}{2} \sum_\alpha \psi_\alpha^{k\dagger} \sigma_{\alpha\bar{\alpha}}^x \psi_{\bar{\alpha}}^{k'} = \frac{1}{2} \left(c_{k\uparrow}^\dagger c_{k'\downarrow}^\dagger + c_{k\downarrow}^\dagger c_{k'\uparrow}^\dagger \right) \quad (8.5)$$

$$C_{kk'}^y = \frac{1}{2} \sum_\alpha \psi_\alpha^{k\dagger} \sigma_{\alpha\bar{\alpha}}^y \psi_{\bar{\alpha}}^{k'} = -i \frac{1}{2} \left(c_{k\uparrow}^\dagger c_{k'\downarrow}^\dagger - c_{k\downarrow}^\dagger c_{k'\uparrow}^\dagger \right) \quad (8.6)$$

$$(8.7)$$

There are similar operators for the impurity electron:

$$\begin{aligned} \psi_d &= \begin{pmatrix} c_{d\uparrow} \\ c_{d\downarrow}^\dagger \end{pmatrix} \\ C_d^z &= \frac{1}{2} \left(c_{d\uparrow}^\dagger c_{d\uparrow} + c_{d\downarrow}^\dagger c_{d\downarrow} - 1 \right) = \frac{1}{2} (\hat{n}_d - 1) \\ C_d^x &= \frac{1}{2} \left(c_{d\uparrow}^\dagger c_{d\downarrow}^\dagger + c_{d\downarrow}^\dagger c_{d\uparrow}^\dagger \right) \\ C_d^y &= -i \frac{1}{2} \left(c_{d\uparrow}^\dagger c_{d\downarrow}^\dagger - c_{d\downarrow}^\dagger c_{d\uparrow}^\dagger \right) \end{aligned} \quad (8.8)$$

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

$$4K_z \sum_{kk'} C_d^z C_{kk'}^z + K_t \sum_{kk'} (C_d^+ C_{kk'}^- + C_d^- C_{kk'}^+) \quad (8.9)$$

where $C^\pm \equiv C^x \pm iC^y$. For $4K_z = 2K_t = K$, we get an $SU(2)$ -charge symmetric model:

$$K \sum_{kk'} C_d^z C_{kk'}^z + \frac{1}{2} K \sum_{kk'} (C_d^+ C_{kk'}^- + C_d^- C_{kk'}^+) = K \vec{C}_d \cdot \vec{C} \quad (8.10)$$

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

$$\begin{aligned} \mathcal{H}_d &= \epsilon_q \tau_{q\beta} + H_{imp} + K_z (\hat{n}_d - 1) \tau_{q\beta} \\ \mathcal{H}_X &= V_q c_{q\beta}^\dagger c_{d\beta} + \text{h.c.} + K_z (\hat{n}_d - 1) \sum_k \left(c_{q\beta}^\dagger c_{k\beta} + \text{h.c.} \right) + K_t \sum_k \left(c_{d\beta}^\dagger c_{d\bar{\beta}}^\dagger c_{q\beta} c_{k\bar{\beta}} + \text{h.c.} \right) \end{aligned} \quad (8.11)$$

As usual, we have considered only one mobile electron on the shell we are decoupling, and we only keep 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. 8.4, 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 that

$$\begin{aligned} C_{q\neq k}^z &= \frac{1}{2} \left(c_{q\uparrow}^\dagger c_{k\uparrow} + c_{k\uparrow}^\dagger c_{q\uparrow} - c_{k\downarrow}^\dagger c_{q\downarrow} - c_{q\downarrow}^\dagger c_{k\downarrow} \right) \\ &= \frac{1}{2} \left(c_{q\uparrow}^\dagger c_{k\uparrow} + c_{k\uparrow}^\dagger c_{q\uparrow} + c_{q\downarrow}^\dagger c_{k\downarrow} + c_{k\downarrow}^\dagger c_{q\downarrow} \right) \\ &= \frac{1}{2} \sum_\sigma (c_{q\sigma}^\dagger c_{k\sigma} + \text{h.c.}) \end{aligned} \quad (8.12)$$

8.1 Hole sector

This will involve terms which start from an empty state (hole). This renormalization is given by

$$T^\dagger c_{q\beta} G c_{q\beta}^\dagger T \quad (8.13)$$

where

$$\begin{aligned} G c_{q\beta}^\dagger T &= \frac{1}{\omega_0 - \mathcal{H}_d} \sum_{q\beta} \left[V_q c_{q\beta}^\dagger c_{d\beta} + K_z (\hat{n}_d - 1) \sum_k c_{q\beta}^\dagger c_{k\beta} + K_t \sum_k c_{q\beta}^\dagger c_{k\bar{\beta}}^\dagger c_{d\beta} c_{d\bar{\beta}} \right] \\ &= \sum_{q\beta} \left[\frac{V_q}{\omega_0 - \frac{1}{2}\epsilon_q - \epsilon_d \hat{n}_{d\bar{\beta}} - \frac{1}{2}K_z (\hat{n}_{d\bar{\beta}} - 1)} c_{q\beta}^\dagger c_{d\beta} + \frac{K_z (\hat{n}_d - 1)}{\omega_0 - \frac{1}{2}\epsilon_q - H_{imp} - \frac{1}{2}K_z (\hat{n}_d - 1)} \sum_k c_{q\beta}^\dagger c_{k\beta} \right. \\ &\quad \left. + \frac{K_t}{\omega_0 - \frac{1}{2}\epsilon_q + \frac{1}{2}K_z} \sum_k c_{q\beta}^\dagger c_{k\bar{\beta}}^\dagger c_{d\beta} c_{d\bar{\beta}} \right] \end{aligned}$$

The renormalization is, therefore,

$$\begin{aligned}
& \sum_{q\beta} \left[V_1^* c_{d\beta}^\dagger \hat{n}_{d\bar{\beta}} c_{q\beta} + V_0^* c_{d\beta}^\dagger (1 - \hat{n}_{d\bar{\beta}}) c_{q\beta} + K_z^+ \hat{n}_{d\beta} \hat{n}_{d\bar{\beta}} \sum_k c_{k\beta}^\dagger c_{q\beta} - K_z^- (1 - \hat{n}_{d\beta}) (1 - \hat{n}_{d\bar{\beta}}) \sum_k c_{k\beta}^\dagger c_{q\beta} + K_t \sum_k c_{k\beta}^\dagger c_{q\beta} \right. \\
&= \sum_{q\beta} \left[\frac{|V_q|^2 \hat{n}_{d\beta} (1 - \hat{n}_{q\beta})}{\omega_0 - \frac{1}{2}\epsilon_q - \epsilon_d \hat{n}_{d\bar{\beta}} - \frac{1}{2}K_z (\hat{n}_{d\bar{\beta}} - 1)} - \sum_k \frac{V_q^* K_z c_{d\beta}^\dagger c_{k\beta} (1 - \hat{n}_{d\bar{\beta}}) (1 - \hat{n}_{q\beta})}{\omega_0 - \frac{1}{2}\epsilon_q + \frac{1}{2}K_z} \right. \\
&- \sum_k \frac{V_q^* K_t \hat{n}_{d\beta} (1 - \hat{n}_{q\beta}) c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}}}{\omega_0 - \frac{1}{2}\epsilon_q + K_z} - \sum_k \frac{K_z V_q (1 - \hat{n}_{d\bar{\beta}}) (1 - \hat{n}_{q\beta}) c_{k\beta}^\dagger c_{d\beta}}{\omega_0 - \frac{1}{2}\epsilon_q + \frac{1}{2}K_z} \\
&+ \sum_{kk'} \frac{K_z^2 (1 - \hat{n}_d)^2 (1 - \hat{n}_{q\beta}) c_{k\beta}^\dagger c_{k'\beta}}{\omega_0 - \frac{1}{2}\epsilon_q - H_{imp} - \frac{1}{2}K_z (\hat{n}_d - 1)} - \sum_{kk'} \frac{K_z K_t (1 - \hat{n}_{q\beta}) c_{k\beta}^\dagger c_{k'\bar{\beta}} c_{d\beta} c_{d\bar{\beta}}}{\omega_0 - \frac{1}{2}\epsilon_q + \frac{1}{2}K_z} \\
&- \sum_k \frac{K_t V_q (1 - \hat{n}_{q\beta}) \hat{n}_{d\beta} c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}}}{\omega_0 - \frac{1}{2}\epsilon_q + \frac{1}{2}K_z} - \sum_{kk'} \frac{K_z K_t (1 - \hat{n}_{q\beta}) c_{d\beta}^\dagger c_{d\bar{\beta}}^\dagger c_{k\beta} c_{k'\bar{\beta}}}{\omega_0 - \frac{1}{2}\epsilon_q + \frac{1}{2}K_z} \\
&\left. + \sum_{kk'} \frac{K_t^2 \hat{n}_{d\beta} \hat{n}_{d\bar{\beta}} (1 - \hat{n}_{q\beta}) c_{k'\bar{\beta}} c_{k\bar{\beta}}^\dagger}{\omega_0 - \frac{1}{2}\epsilon_q + \frac{1}{2}K_z} \right]
\end{aligned}$$

8.2 Particle sector

This will involve terms which start from an occupied state (particle). This renormalization is given by

$$c_{q\beta}^\dagger T G T^\dagger c_{q\beta} \quad (8.14)$$

where

$$\begin{aligned}
GT^\dagger c_{q\beta} &= \sum_{q\beta} \frac{1}{\omega - \mathcal{H}_d} \left[V_q^* c_{d\beta}^\dagger c_{q\beta} + K_z (\hat{n}_d - 1) \sum_k c_{k\beta}^\dagger c_{q\beta} + K_t \sum_k c_{d\beta}^\dagger c_{d\bar{\beta}}^\dagger c_{q\beta} c_{k\bar{\beta}} \right] \\
&= \sum_{q\beta} \left[\frac{V_q^* c_{d\beta}^\dagger c_{q\beta}}{\omega_1 - \frac{1}{2}\epsilon_q - \epsilon_d - (\epsilon_d + U) \hat{n}_{d\bar{\beta}} + \frac{1}{2}K_z \hat{n}_{d\bar{\beta}}} + \frac{K_z (\hat{n}_d - 1) \sum_k c_{k\beta}^\dagger c_{q\beta}}{\omega_1 - \frac{1}{2}\epsilon_q - H_{imp} + \frac{1}{2}K_z (\hat{n}_d - 1)} \right. \\
&\quad \left. + \frac{K_t \sum_k c_{d\beta}^\dagger c_{d\bar{\beta}}^\dagger c_{q\beta} c_{k\bar{\beta}}}{\omega_1 - \frac{1}{2}\epsilon_q - 2\epsilon_d - U + \frac{1}{2}K_z} \right] \quad (8.15)
\end{aligned}$$

The renormalization is, therefore,

$$\begin{aligned}
& \sum_{q\beta} \left[V_q c_{q\beta}^\dagger c_{d\beta} + K_z (\hat{n}_d - 1) \sum_k c_{q\beta}^\dagger c_{k\beta} + K_t \sum_k c_{q\beta}^\dagger c_{k\bar{\beta}}^\dagger c_{d\beta} c_{d\bar{\beta}} \right] GT^\dagger c_{q\beta} \\
&= \sum_{q\beta} \left[\frac{|V_q|^2 \hat{n}_{q\beta} (1 - \hat{n}_{d\beta})}{\omega_1 - \frac{1}{2}\epsilon_q - \epsilon_d - (\epsilon_d + U - \frac{1}{2}K_z) \hat{n}_{d\bar{\beta}}} - \sum_k \frac{V_q K_z c_{k\beta}^\dagger c_{d\beta} \hat{n}_{d\bar{\beta}} \hat{n}_{q\beta}}{\omega_1 - \frac{1}{2}\epsilon_q - 2\epsilon_d - U + \frac{1}{2}K_z} \right. \\
&- \sum_k \frac{V_q K_t \hat{n}_{q\beta} (1 - \hat{n}_{d\beta}) c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}}}{\omega_1 - \frac{1}{2}\epsilon_q - 2\epsilon_d - U + \frac{1}{2}K_z} - \sum_k \frac{K_z V_q^* \hat{n}_{d\bar{\beta}} \hat{n}_{q\beta} c_{d\beta}^\dagger c_{k\beta}}{\omega_1 - \frac{1}{2}\epsilon_q - 2\epsilon_d - U + \frac{1}{2}K_z}
\end{aligned}$$

$$\begin{aligned}
& + \sum_{kk'} \frac{K_z^2 (\hat{n}_d - 1)^2 \hat{n}_{q\beta} c_{k\beta} c_{k'\beta}^\dagger}{\omega_1 - \frac{1}{2}\epsilon_q - H_{imp} + \frac{1}{2}K_z (\hat{n}_d - 1)} - \sum_{kk'} \frac{K_z K_t \hat{n}_{q\beta} c_{d\beta}^\dagger c_{d\beta}^\dagger c_{k\beta} c_{k'\beta}}{\omega_1 - \frac{1}{2}\epsilon_q - 2\epsilon_d - U + \frac{1}{2}K_z} \\
& - \sum_k \frac{K_t V_q^* \hat{n}_{q\beta} (1 - \hat{n}_{d\beta}) c_{k\beta}^\dagger c_{d\beta}}{\omega_1 - \frac{1}{2}\epsilon_q - 2\epsilon_d - U + \frac{1}{2}K_z} - \sum_{kk'} \frac{K_z K_t \hat{n}_{q\beta} c_{k\beta}^\dagger c_{k'\beta}^\dagger c_{d\beta} c_{d\beta}}{\omega_1 - \frac{1}{2}\epsilon_q - 2\epsilon_q - U + \frac{1}{2}K_z} \\
& + \sum_{kk'} \frac{K_t^2 (1 - \hat{n}_{d\beta}) (1 - \hat{n}_{d\beta}) \hat{n}_{q\beta} c_{k\beta}^\dagger c_{k'\beta}}{\omega_1 - \frac{1}{2}\epsilon_q - 2\epsilon_d - U + \frac{1}{2}K_z} \Big]
\end{aligned}$$

8.3 Scaling Equations

To get the scaling equations, we perform similar steps as in the spin-Kondo URG. First of all, we substitute $\hat{n}_{q\beta}$ with 1 and 0 in the particle and hole sectors respectively. Secondly, in the RG equations that involve $\hat{n}_{d\beta}$ in the denominator, we replace the quantum fluctuations with $E_j + \omega$, where E_j is the impurity part of the energy of the initial state and ω is a redefined quantum fluctuation scale. Thirdly, by using the constraint $\eta = (\eta^\dagger)^\dagger$, we can relate the denominators of the RG equations of the V s and K s. The term with K_z^2 in either sector mostly cancel each other, leaving a renormalization of ϵ_d and U at K^2 order.

$$\sum_{kk'q\beta} \frac{K_z^2 (1 - \hat{n}_d)^2 [c_{k\beta}^\dagger c_{k'\beta} + c_{k'\beta} c_{k\beta}^\dagger]}{\omega_0 - \frac{1}{2}\epsilon_q - H_{imp} - \frac{1}{2}K_z (\hat{n}_d - 1)} = \sum_{kk'q\beta} \frac{K_z^2 (1 - \hat{n}_d)^2 \delta_{kk'}}{\omega_0 - \frac{1}{2}\epsilon_q - H_{imp} - \frac{1}{2}K_z (\hat{n}_d - 1)} \quad (8.16)$$

Since $(1 - \hat{n}_d)^2 = (1 - \hat{n}_{d\uparrow})(1 - \hat{n}_{d\downarrow}) + \hat{n}_{d\uparrow}\hat{n}_{d\downarrow}$, we can write down the renormalization in ΔE_0 and ΔE_2 and hence in ϵ_d and U .

$$\begin{aligned}
\Delta E_0 &= \sum_{kq\beta} \frac{K_z^2}{\omega_0 - \frac{1}{2}\epsilon_q + \frac{1}{2}K_z} \\
\Delta E_2 &= \sum_{kk'q\beta} \frac{K_z^2}{\omega_0 - \frac{1}{2}\epsilon_q - 2\epsilon_d - U - \frac{1}{2}K_z}
\end{aligned} \quad (8.17)$$

Making the substitution $\omega_0 = \omega$ The penultimate term in the hole sector, gets canceled by a piece from the final term in particle sector, and the remaining piece gives the renormalization in K_z .

$$\Delta \epsilon_d = \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d + \frac{1}{2}K_z} + \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d - U + \frac{1}{2}K_z} - \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d - \frac{1}{2}K_z} \quad (8.18)$$

$$+ \frac{8K_z^2}{\omega - \frac{1}{2}\epsilon_q} \quad (8.19)$$

$$\Delta U = \frac{|V|^2}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d + U - \frac{1}{2}K_z} + \frac{|V|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d - \frac{1}{2}K_z} - \frac{|V|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d - U + \frac{1}{2}K_z} \quad (8.20)$$

$$- \frac{|V|^2}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d + \frac{1}{2}K_z} - \frac{16K_z^2}{\omega - \frac{1}{2}\epsilon_q} \quad (8.21)$$

$$\Delta V = \frac{-V_q^* K_t + V_q K_z}{\omega - \frac{1}{2}\epsilon_q + \frac{1}{2}K_z} \quad (8.22)$$

$$\Delta K_z = \frac{-K_t^2}{\omega - \frac{1}{2}\epsilon_q + \frac{1}{2}K_z} \quad (8.23)$$

$$\Delta K_t = \frac{-2K_z K_t}{\omega - \frac{1}{2}\epsilon_q + \frac{1}{2}K_z} \quad (8.24)$$

$$(8.25)$$

9 Connection between URG and Other Canonical Transformations

9.1 Poor Man's Scaling

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

$$\mathcal{H}|\Psi\rangle = E|\Psi\rangle \quad (9.1)$$

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

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

$$|\Psi\rangle = \sum_i |\phi_0^i\rangle + \sum_i |\phi_1^i\rangle \quad (9.2)$$

The Hamiltonian can also be split as

$$\mathcal{H} = H_0 + V_+ + V_- \quad (9.3)$$

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:

$$\begin{aligned} V_+ \{|0\rangle\} &\mapsto \{|1\rangle\}, & V_+ |1\rangle &\rightarrow 0 \\ V_- \{|1\rangle\} &\mapsto \{|0\rangle\}, & V_- |0\rangle &\rightarrow 0 \end{aligned} \quad (9.4)$$

The Schrodinger equation can thus be split into

$$\begin{aligned} H_0 \sum_i |\phi_0^i\rangle + V_- \sum_i |\phi_1^i\rangle &= E \sum_i |\phi_0^i\rangle \\ H_0 \sum_i |\phi_1^i\rangle + V_+ \sum_i |\phi_0^i\rangle &= E \sum_i |\phi_1^i\rangle \end{aligned} \quad (9.5)$$

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

$$H_0 \sum_i |\phi_0^i\rangle + V_- \frac{1}{E_1 - H_0} V_+ \sum_i |\phi_0^i\rangle = E \sum_i |\phi_0^i\rangle \quad (9.6)$$

The effective Hamiltonian in this subspace is therefore

$$\tilde{\mathcal{H}}_0 = H_0 + V_- \frac{1}{E - H_0} V_+ \quad (9.7)$$

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

$$\tilde{\mathcal{H}}_1 = H_0 + V_+ \frac{1}{E - H_0} V_- \quad (9.8)$$

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

$$\tilde{\mathcal{H}}(E) = H_0 + \underbrace{V_- \frac{1}{E - H_0} V_+ + V_+ \frac{1}{E - H_0} V_-}_{\text{renormalization}} \quad (9.9)$$

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 $V_- = V_+^\dagger \equiv V$.

$$\Delta\mathcal{H}(E) = V \frac{1}{E - H_0} V^\dagger + V^\dagger \frac{1}{E - H_0} V \quad (9.10)$$

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

$$\begin{aligned} V \frac{1}{E - H_0} V^\dagger &= \sum_{ijk} |\phi_0^i\rangle \langle \phi_0^i| V |\phi_1^j\rangle \langle \phi_1^j| \frac{1}{E - H_0} |\phi_1^j\rangle \langle \phi_1^j| V^\dagger |\phi_0^k\rangle \langle \phi_0^k| \\ &= \sum_{ijk} |\phi_0^i\rangle V_{ij} \langle \phi_1^j| \frac{1}{E - H_0} |\phi_1^j\rangle V_{kj}^\dagger \langle \phi_0^k| \end{aligned} \quad (9.11)$$

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

$$V \frac{1}{E - H_0} V^\dagger = \sum_{ijk} |\phi_0^i\rangle \langle \phi_0^k| \frac{V_{ij} V_{kj}^\dagger}{\omega_1 - E_1^j} \quad (9.12)$$

The second term similarly gives

$$V^\dagger \frac{1}{E - H_0} V = \sum_{ijk} |\phi_1^i\rangle \langle \phi_1^k| \frac{V_{ji}^\dagger V_{jk}}{\omega_0 - E_0^j} \quad (9.13)$$

The total renormalization becomes

$$\Delta\mathcal{H}(E) = \sum_{ijk} \left(\frac{1}{\omega_1 - E_1^j} |\phi_0^i\rangle \langle \phi_0^k| V_{ij} V_{kj}^\dagger + \frac{1}{\omega_0 - E_0^j} |\phi_1^i\rangle \langle \phi_1^k| V_{ji}^\dagger V_{jk} \right) \quad (9.14)$$

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.

$$\Delta\mathcal{H}(E) = \sum_{ijk} \left(\frac{1}{E_0^k - E_1^j} |\phi_0^i\rangle \langle \phi_0^k| V_{ij} V_{kj}^\dagger + \frac{1}{E_1^k - E_0^j} |\phi_1^i\rangle \langle \phi_1^k| V_{ji}^\dagger V_{jk} \right) \quad (9.15)$$

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

$$\begin{aligned} \Delta\mathcal{H} &= \frac{1}{2} \sum_{ijk} \frac{1}{\omega_1 - E_1^j} \left(|\phi_0^i\rangle \langle \phi_0^k| V_{ij} V_{kj}^\dagger + |\phi_0^k\rangle \langle \phi_0^i| V_{kj} V_{ij}^\dagger \right) \\ &+ \frac{1}{2} \sum_{ijk} \frac{1}{\omega_0 - E_0^j} \left(|\phi_1^i\rangle \langle \phi_1^k| V_{ji}^\dagger V_{jk} + |\phi_1^k\rangle \langle \phi_1^i| V_{jk} V_{ji}^\dagger \right) \\ &= \frac{1}{2} \sum_{ijk} \left(\frac{1}{E_0^k - E_1^j} |\phi_0^i\rangle \langle \phi_0^k| V_{ij} V_{kj}^\dagger + \frac{1}{E_0^k - E_1^j} |\phi_0^k\rangle \langle \phi_0^i| V_{kj} V_{ij}^\dagger \right) \\ &+ \frac{1}{2} \sum_{ijk} \left(\frac{1}{E_1^k - E_0^j} |\phi_1^i\rangle \langle \phi_1^k| V_{ji}^\dagger V_{jk} + \frac{1}{E_1^k - E_0^j} |\phi_1^k\rangle \langle \phi_1^i| V_{jk} V_{ji}^\dagger \right) \end{aligned} \quad (9.16)$$

Therefore,

$$\begin{aligned} \Delta\mathcal{H} &= \frac{1}{2} \sum_{ijk} \left(\frac{1}{E_0^k - E_1^j} + \frac{1}{E_0^i - E_1^j} \right) |\phi_0^i\rangle \langle \phi_0^k| V_{ij} V_{kj}^\dagger \\ &+ \frac{1}{2} \sum_{ijk} \left(\frac{1}{E_1^k - E_0^j} + \frac{1}{E_1^i - E_0^j} \right) |\phi_1^i\rangle \langle \phi_1^k| V_{ji}^\dagger V_{jk} \end{aligned} \quad (9.17)$$

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

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

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

$$|\Psi\rangle = |\Psi_0\rangle + |\Psi_1\rangle \quad (9.18)$$

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

$$\mathcal{H} = \mathcal{H}^d + V_0 + V_+ + V_- \quad (9.19)$$

\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. 9.19 and 9.18 in eq. 9.1 gives

$$(\mathcal{H}^d + V_0 + V_+ + V_-) (|\Psi_0\rangle + |\Psi_1\rangle) = E (|\Psi_0\rangle + |\Psi_1\rangle) \quad (9.20)$$

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

$$\begin{aligned} (\mathcal{H}_0^d + V_0) |\Psi_0\rangle + V_- |\Psi_1\rangle &= E |\Psi_0\rangle \\ (\mathcal{H}_1^d + V_0) |\Psi_1\rangle + V_+ |\Psi_0\rangle &= E |\Psi_1\rangle \end{aligned} \quad (9.21)$$

The second equation can be written as

$$|\Psi_1\rangle = \eta^\dagger |\Psi_0\rangle \quad (9.22)$$

where

$$(\eta^\dagger)_{\text{PMS}} = \frac{1}{E - \mathcal{H}_1^d - V_0} V_+ \quad (9.23)$$

Substituting this in the first equation gives

$$(\mathcal{H}_0^d + V_0 + V_- \eta^\dagger) |\Psi_0\rangle = E |\Psi_0\rangle \quad (9.24)$$

This new Hamiltonian,

$$\tilde{\mathcal{H}}_0 = \mathcal{H}_0^d + V_0 + V_- \eta^\dagger \quad (9.25)$$

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

$$\Delta V_0 = V_- \eta^\dagger \quad (9.26)$$

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

$$|\Psi_0\rangle = \eta |\Psi_1\rangle \quad (9.27)$$

where

$$(\eta)_{\text{PMS}} = \frac{1}{E - \mathcal{H}_0^d - V_0} V_- \quad (9.28)$$

,so

$$(\mathcal{H}_1^d + V_0 + V_+ \eta) |\Psi_1\rangle = E |\Psi_1\rangle \quad (9.29)$$

The renormalized Hamiltonian in the high energy subspace is thus

$$\tilde{\mathcal{H}}_1 = \mathcal{H}_1^d + V_0 + V_+ \eta \quad (9.30)$$

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

$$\begin{aligned} \tilde{\mathcal{H}} &= \tilde{\mathcal{H}}_1 \hat{n} + \tilde{\mathcal{H}}_0 (1 - \hat{n}) \\ &= \mathcal{H}_0^d + \mathcal{H}_1^d + V_0 + V_+ \eta + V_- \eta^\dagger \end{aligned} \quad (9.31)$$

The total renormalization is

$$(\Delta\mathcal{H})_{\text{PMS}} = V_+ (\eta)_{\text{PMS}} + V_- (\eta^\dagger)_{\text{PMS}} \quad (9.32)$$

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. 9.31. This, along with the properties of η , have been shown in section 3. The important feature of eq. 9.31 is that there is no term in the transformed Hamiltonian which scatters between $|\Psi_0\rangle$ and $|\Psi_0\rangle$ - the two subspaces have been truly decoupled.

$$[U\mathcal{H}U^\dagger, n_q] = 0 \quad (9.33)$$

We can write down the renormalized Schrodinger equation in the low energy subspace, from eq. 9.24,

$$\tilde{\mathcal{H}}_0 |\Psi_0\rangle = E |\Psi_0\rangle \quad (9.34)$$

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. 9.1.

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

$$\mathcal{H} |\Phi\rangle = \mathcal{H}' |\Phi\rangle \quad (9.35)$$

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

The operators η and its conjugate change accordingly:

$$\begin{aligned} (\eta)_{\text{URG}} &= \frac{1}{\tilde{\mathcal{H}} - \mathcal{H}_0^d - V_0} V_- \\ &= \frac{1}{\hat{\omega} - \mathcal{H}_0^d} V_- \end{aligned} \quad (9.36)$$

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

$$(\eta^\dagger)_{\text{URG}} = \frac{1}{\hat{\omega} - \mathcal{H}_1^d} V_+ \quad (9.37)$$

The renormalization is again

$$(\Delta\mathcal{H})_{\text{URG}} = V_+ (\eta)_{\text{URG}} + V_- (\eta^\dagger)_{\text{URG}} \quad (9.38)$$

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

$$U = 1 - \eta + \eta^\dagger, [\hat{n}_q, U\mathcal{H}U^\dagger] = 0 \quad (9.39)$$

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

$$(\hat{\omega} - \mathcal{H}_1^d) V_+ |\Psi_0\rangle \text{ or } (\hat{\omega} - \mathcal{H}_1^d) V_- |\Psi_1\rangle \quad (9.40)$$

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,

$$\mathcal{H} = \sum_{k\sigma} \left(\epsilon_k \tau_{k\sigma} + V c_{k\sigma}^\dagger c_{d\sigma} + \text{h.c.} \right) \quad (9.41)$$

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

$$\Delta V_0 = c_{d\beta}^\dagger c_{q\beta} \frac{1}{(E - V_0) - \hat{\mathcal{H}}_0^d} c_{q\beta}^\dagger c_{d\beta} \quad (9.42)$$

The intermediate energy (at the propagator) is

$$\hat{\mathcal{H}}_0^d = \sum_{k, \sigma} \epsilon_k \tau_{k\sigma} + \epsilon_d \hat{n}_{d\bar{\beta}} \quad (9.43)$$

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.

$$\Delta V_0 = c_{d\beta}^\dagger c_{q\beta} \frac{1}{(E - V_0) - \sum_{k, \sigma} \epsilon_k \tau_{k\sigma} - \epsilon_d \hat{n}_{d\bar{\beta}}} c_{q\beta}^\dagger c_{d\beta} \quad (9.44)$$

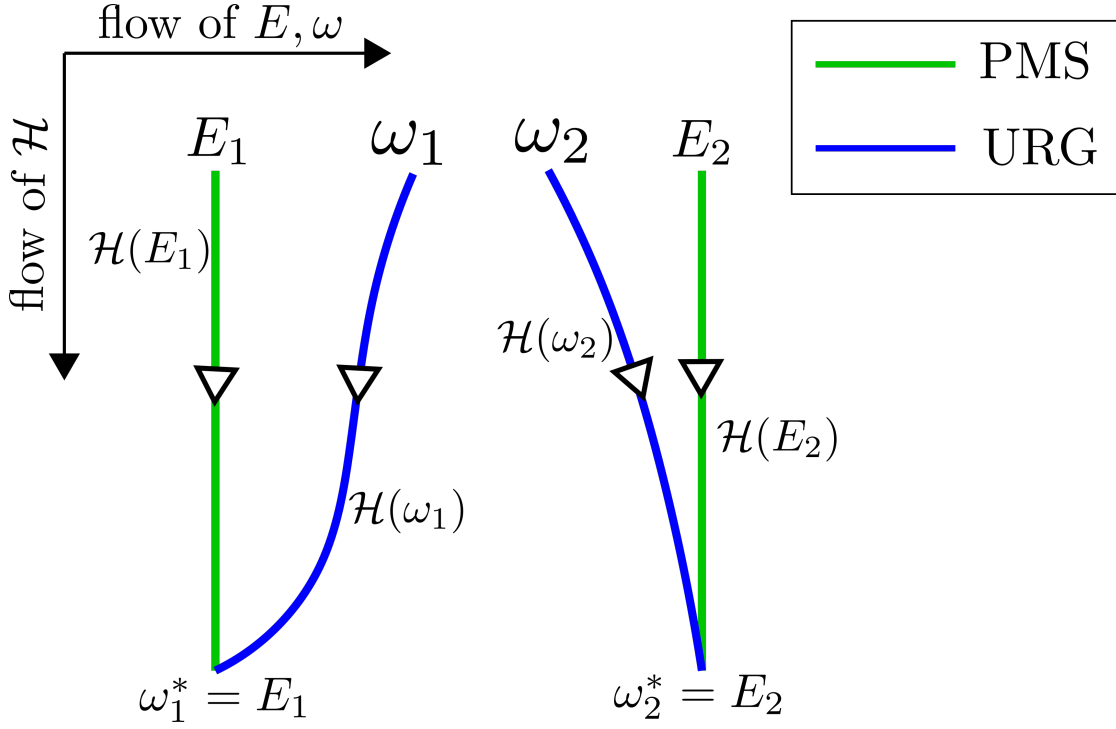


Figure 10: Flows of PMS(green) and URG(blue)

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

$$E - V_0 = \sum_{k < q, \sigma} \epsilon_k \tau_{k\sigma} - \frac{1}{2} \epsilon_q + \epsilon_d + (\epsilon_d + U) \hat{n}_{d\bar{\beta}} \quad (9.45)$$

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

$$\begin{aligned} \Delta V_0 &= c_{d\beta}^\dagger c_{q\beta} \frac{1}{-\frac{1}{2}\epsilon_q - \epsilon_q \tau_{q\beta} + \epsilon_d + U \hat{n}_{d\bar{\beta}}} c_{q\beta}^\dagger c_{d\beta} \\ &= c_{d\beta}^\dagger c_{q\beta} \frac{1}{-\epsilon_q + \epsilon_d + U \hat{n}_{d\bar{\beta}}} c_{q\beta}^\dagger c_{d\beta} \\ &= c_{d\beta}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{d\beta} \frac{1}{-\epsilon_q + \epsilon_d + U \hat{n}_{d\bar{\beta}}} \\ &= -c_{d\beta}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{d\beta} \frac{1}{\epsilon_q - \epsilon_d - U \hat{n}_{d\bar{\beta}}} \\ &= (1 - \hat{n}_{q\beta}) \left(\frac{-\hat{n}_{d\beta} \hat{n}_{d\bar{\beta}}}{\epsilon_q - \epsilon_d - U} + \frac{-\hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}})}{\epsilon_q - \epsilon_d} \right) \end{aligned} \quad (9.46)$$

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

and the second term renormalizes that of the singly-occupied state:

$$\begin{aligned}\Delta E_2 &= \frac{-1}{\epsilon_q - \epsilon_d - U} \\ \Delta E_1 &= \frac{-1}{\epsilon_q - \epsilon_d}\end{aligned}\tag{9.47}$$

The renormalization in the hole sector is

$$\begin{aligned}\Delta V_0 &= c_{q\beta}^\dagger c_{d\beta} \frac{1}{(E - V_0) - \hat{\mathcal{H}}_0^d} c_{d\beta}^\dagger c_{q\beta} \\ &= c_{q\beta}^\dagger c_{d\beta} \frac{1}{(E - V_0) - \sum_{k,\sigma} \epsilon_k \tau_{k\sigma} - \epsilon_d - (\epsilon_d + U) \hat{n}_{d\bar{\beta}}} c_{d\beta}^\dagger c_{q\beta}\end{aligned}\tag{9.48}$$

This time we substitute

$$\begin{aligned}E - V_0 &= \sum_{k < q, \sigma} \epsilon_k \tau_{k\sigma} + \tau_{q\beta} \epsilon_q^- + \epsilon_d \hat{n}_{d\bar{\beta}} \\ &= \sum_{k < q, \sigma} \epsilon_k \tau_{k\sigma} + \frac{1}{2} \epsilon_q^- + \epsilon_d \hat{n}_{d\bar{\beta}}\end{aligned}\tag{9.49}$$

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

$$\begin{aligned}\Delta V_0 &= c_{q\beta}^\dagger c_{d\beta} \frac{1}{-\frac{1}{2}\epsilon_q - \epsilon_q^- \tau_{q\beta} - \epsilon_d - U \hat{n}_{d\bar{\beta}}} c_{d\beta}^\dagger c_{q\beta} \\ &= c_{q\beta}^\dagger c_{d\beta} c_{d\beta}^\dagger c_{q\beta} \frac{1}{-\epsilon_q - \epsilon_d - U \hat{n}_{d\bar{\beta}}} \\ &= \hat{n}_{q\beta} \left(\frac{-(1 - \hat{n}_{d\beta}) \hat{n}_{d\bar{\beta}}}{\epsilon_q + \epsilon_d + U} + \frac{-(1 - \hat{n}_{d\beta}) (1 - \hat{n}_{d\bar{\beta}})}{\epsilon_q + \epsilon_d} \right)\end{aligned}\tag{9.50}$$

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

$$\begin{aligned}\Delta E_0 &= -\frac{1}{\epsilon_q + \epsilon_d} \\ \Delta E_1 &= -\frac{1}{\epsilon_q + \epsilon_d + U} - \frac{1}{\epsilon_q - \epsilon_d} \\ \Delta E_2 &= -\frac{1}{\epsilon_q - \epsilon_d - U}\end{aligned}\tag{9.51}$$

These results are also obtained in ref. [11]. The complete process is depicted in fig. 11.

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

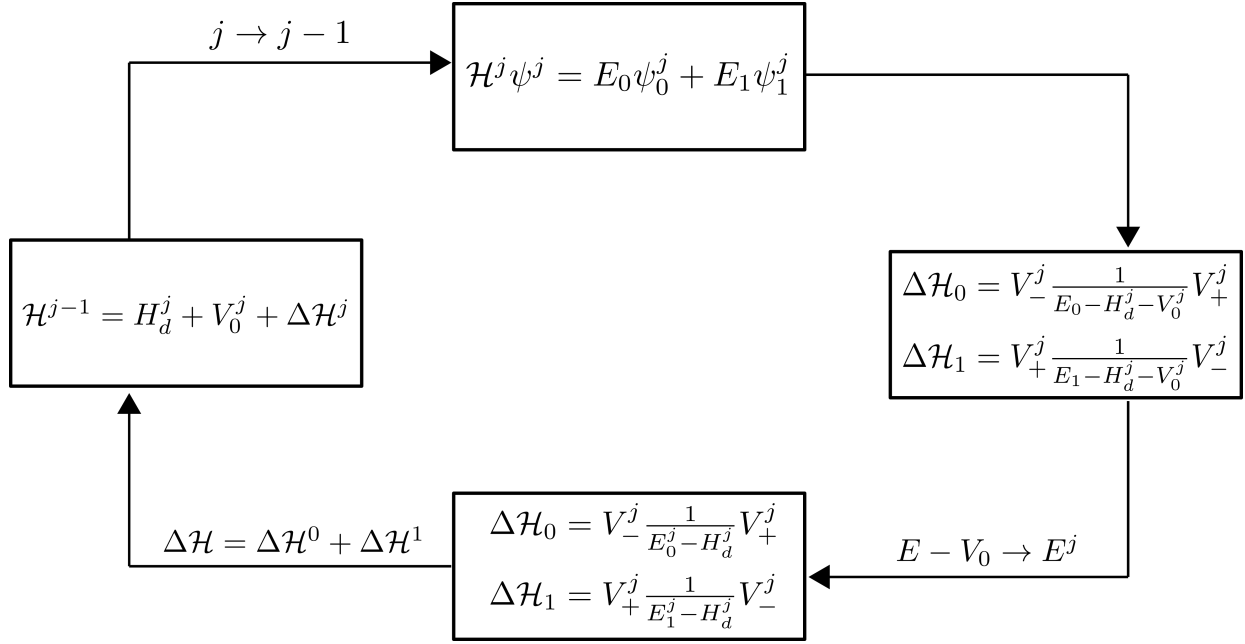


Figure 11: Flow chart of "Poor Man's" scaling algorithm

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. 9.1, 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.

9.2 Schrieffer-Wolff transformation

9.2.1 Formal Differences

We have a general Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_X \quad (9.52)$$

\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.

$$\begin{aligned} U\mathcal{H}U^\dagger &= e^S (\mathcal{H}_0 + \mathcal{H}_X) e^{-S} \\ &= (\cosh(S) + \sinh(S)) (\mathcal{H}_0 + \mathcal{H}_X) (\cosh(S) - \sinh(S)) \\ &= H_1 + H_2 \end{aligned} \quad (9.53)$$

where H_1 is diagonal and H_2 is off-diagonal.

$$\begin{aligned} H_1 &= \cosh(S) \mathcal{H}_0 \cosh(S) - \sinh(S) \mathcal{H}_0 \sinh(S) - \cosh(S) \mathcal{H}_X \sinh(S) \\ &\quad + \sinh(S) \mathcal{H}_X \cosh(S) \\ H_2 &= -\cosh(S) \mathcal{H}_0 \sinh(S) + \sinh(S) \mathcal{H}_0 \cosh(S) + \cosh(S) \mathcal{H}_X \cosh(S) \\ &\quad - \sinh(S) \mathcal{H}_X \sinh(S) \end{aligned} \quad (9.54)$$

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

$$H_2 = -\mathcal{H}_0 S + S\mathcal{H}_0 + \mathcal{H}_X + O(S^3) = [S, \mathcal{H}_0] + \mathcal{H}_X \quad (9.55)$$

The second order decoupling condition is thus

$$[S, \mathcal{H}_0] = -\mathcal{H}_X \quad (9.56)$$

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

$$\begin{aligned} H_1 &= \left(1 + \frac{1}{2}S^2\right) \mathcal{H}_0 \left(1 + \frac{1}{2}S^2\right) - S\mathcal{H}_0 S - \left(1 + \frac{1}{2}S^2\right) \mathcal{H}_X S + S\mathcal{H}_X \left(1 + \frac{1}{2}S^2\right) \\ &= \mathcal{H}_0 + \frac{1}{2} \{S^2, \mathcal{H}_0\} - S\mathcal{H}_0 S - \mathcal{H}_X S + S\mathcal{H}_X + O(S^3) \\ &= \mathcal{H}_0 + \frac{1}{2} S [S, \mathcal{H}_0] - \frac{1}{2} [S, \mathcal{H}_0] S + [S, \mathcal{H}_X] + O(S^3) \\ &= \mathcal{H}_0 + \frac{1}{2} [S, [S, \mathcal{H}_0]] + [S, \mathcal{H}_X] + O(S^3) \\ &= \mathcal{H}_0 + \frac{1}{2} [S, -\mathcal{H}_X] + [S, \mathcal{H}_X] + O(S^3) \\ &= \mathcal{H}_0 + \frac{1}{2} [S, \mathcal{H}_X] + O(S^3) \end{aligned} \quad (9.57)$$

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

$$\begin{aligned}
 e^S &= \exp\left(\frac{\pi}{4}(\eta^\dagger - \eta)\right) \\
 &= 1 + (\eta^\dagger - \eta) \frac{\pi}{4} + \frac{1}{2!} (\eta^\dagger - \eta)^2 \left(\frac{\pi}{4}\right)^2 + \frac{1}{3!} (\eta^\dagger - \eta)^3 \left(\frac{\pi}{4}\right)^3 + \dots \\
 &= 1 + (\eta^\dagger - \eta) \frac{\pi}{4} - \frac{1}{2!} \left(\frac{\pi}{4}\right)^2 - \frac{1}{3!} (\eta^\dagger - \eta) \left(\frac{\pi}{4}\right)^3 + \frac{1}{4!} \left(\frac{\pi}{4}\right)^4 + \dots \\
 &= \cos \frac{\pi}{4} + (\eta^\dagger - \eta) \sin \frac{\pi}{4} \\
 &= \frac{1}{\sqrt{2}} (1 + \eta^\dagger - \eta)
 \end{aligned} \tag{9.58}$$

There we used

$$(\eta^\dagger - \eta)^2 = \eta^{\dagger 2} + \eta^2 - \{\eta^\dagger, \eta\} = -1 \quad \left[\because \eta^2 = \eta^{\dagger 2} = 0 \right] \tag{9.59}$$

and hence

$$(\eta^\dagger - \eta)^3 = -1 (\eta^\dagger - \eta) \tag{9.60}$$

and so on. This simplification allows us to write

$$\cosh S = \frac{1}{2} [e^S + e^{-S}] = \frac{1}{2\sqrt{2}} (1 + \eta^\dagger - \eta + 1 - \eta^\dagger + \eta) = \frac{1}{\sqrt{2}} \tag{9.61}$$

and

$$\sinh S = \frac{1}{2} [e^S - e^{-S}] = \frac{1}{2\sqrt{2}} (1 + \eta^\dagger - \eta - 1 + \eta^\dagger - \eta) = \frac{1}{\sqrt{2}} (\eta^\dagger - \eta) \tag{9.62}$$

The off-diagonal part now becomes

$$H_2 = \frac{1}{2} (\mathcal{H}_X - \eta^\dagger \mathcal{H}_X \eta^\dagger - \eta \mathcal{H}_X \eta + [\eta^\dagger - \eta, \mathcal{H}_0]) \tag{9.63}$$

The vanishing of this quantity is now the decoupling condition, and is also given in eq 16 of ref. [19].

To look for a decoupling condition similar to eq. 9.56, we can re-express the cosh and sinh in eq. 9.61 in terms of S , by substituting $\eta^\dagger - \eta = \frac{4}{\pi} S$:

$$\cosh S = \frac{1}{\sqrt{2}}, \text{ and } \sinh S = \frac{4}{\sqrt{2}\pi} S \tag{9.64}$$

That gives

$$H_2 = \frac{1}{2} \left(\frac{4}{\pi} [S, \mathcal{H}_0] + \mathcal{H}_X - \frac{16}{\pi^2} S \mathcal{H}_X S \right) \tag{9.65}$$

The decoupling condition becomes

$$[S, \mathcal{H}_0] = -\frac{\pi}{4} \mathcal{H}_X + \frac{4}{\pi} S \mathcal{H}_X S \tag{9.66}$$

	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 1: Comparison of perturbative and non-perturbative canonical transformations

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.

$$U \mathcal{H} U^\dagger = H_1 = \frac{1}{2} \mathcal{H}_0 - \frac{4}{\pi^2} S \mathcal{H}_0 S + \frac{2}{\pi} [S, \mathcal{H}_X] \quad (9.67)$$

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

9.2.2 Renormalization due to SWT and Comparison with PMS and URG

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

$$S = \sum_{ij} [s |\phi_1^i\rangle \langle \phi_0^j| - s^\dagger |\phi_0^j\rangle \langle \phi_1^i|] \quad (9.68)$$

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

$$-\mathcal{H}_X = [S, H_0] = S H_0 - H_0 S \quad (9.69)$$

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

$$-\langle \phi_0^a| V + V^\dagger |\phi_1^b\rangle = \langle \phi_0^a| S H_0 - H_0 S |\phi_1^b\rangle \quad (9.70)$$

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

$$\begin{aligned}
 -V_{ab} &= \langle \phi_0^a | \sum_i [S | \phi_1^i \rangle \langle \phi_1^i | H_0 - H_0 | \phi_0^i \rangle \langle \phi_0^i | S] | \phi_1^b \rangle \\
 &= \sum_i [S_{ai} E_1^i \delta_{bi} - E_0^i \delta_{ai} S_{ib}] \\
 &= S_{ab} E_1^b - E_0^a S_{ab} \\
 \implies S_{ab} &= \frac{V_{ab}}{E_0^a - E_1^b}
 \end{aligned} \tag{9.71}$$

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

$$\begin{aligned}
 S &= \sum_{ij} [S_{ij} | \phi_0^i \rangle \langle \phi_1^j | - S_{ij}^\dagger | \phi_1^j \rangle \langle \phi_0^i |] \\
 &= \sum_{ij} \frac{1}{E_0^i - E_1^j} [V_{ij} | \phi_0^i \rangle \langle \phi_1^j | - V_{ij}^\dagger | \phi_1^j \rangle \langle \phi_0^i |]
 \end{aligned} \tag{9.72}$$

The renormalization is thus

$$\begin{aligned}
 \Delta \mathcal{H} &= \frac{1}{2} [S, \mathcal{H}_X] \\
 &= \frac{1}{2} \sum_{ij,kl} \left[\frac{1}{E_0^i - E_1^j} (V_{ij} | \phi_0^i \rangle \langle \phi_1^j | - V_{ij}^\dagger | \phi_1^j \rangle \langle \phi_0^i |), V_{kl} | \phi_0^k \rangle \langle \phi_1^l | + V_{kl}^\dagger | \phi_1^l \rangle \langle \phi_0^k | \right] \\
 &= \frac{1}{2} \sum_{ij,kl} \left[\frac{1}{E_0^i - E_1^j} (V_{ij} V_{kl}^\dagger | \phi_0^i \rangle \langle \phi_0^k | \delta_{jl} - V_{ij}^\dagger V_{kl} | \phi_1^j \rangle \langle \phi_1^l | \delta_{ik} \right. \\
 &\quad \left. - V_{kl}^\dagger V_{ij} | \phi_1^l \rangle \langle \phi_1^j | \delta_{ki} + V_{kl} V_{ij}^\dagger | \phi_0^k \rangle \langle \phi_0^i | \delta_{lj}) \right] \\
 &= \frac{1}{2} \sum_{ijk} \left[\frac{1}{E_0^i - E_1^j} (V_{ij} V_{kj}^\dagger | \phi_0^i \rangle \langle \phi_0^k | - V_{ij}^\dagger V_{ik} | \phi_1^j \rangle \langle \phi_1^k | - V_{ik}^\dagger V_{ij} | \phi_1^k \rangle \langle \phi_1^j | + V_{kj} V_{ij}^\dagger | \phi_0^k \rangle \langle \phi_0^i |) \right] \\
 &= \frac{1}{2} \sum_{ijk} \left[\left(\frac{1}{E_0^i - E_1^j} + \frac{1}{E_0^k - E_1^j} \right) V_{ij} V_{kj}^\dagger | \phi_0^i \rangle \langle \phi_0^k | - \left(\frac{1}{E_0^i - E_1^j} + \frac{1}{E_0^i - E_1^k} \right) V_{ij}^\dagger V_{ik} | \phi_1^j \rangle \langle \phi_1^k | \right]
 \end{aligned} \tag{9.73}$$

This is the same as the PMS result eq. 9.17. It is easy to see that since this transformation is unitary, it has zero trace so as to preserve the trace of the Hamiltonian:

$$\begin{aligned}
 \text{Tr} [\mathcal{H}] &= \sum_l (\langle \phi_0^l | + \langle \phi_1^l |) \Delta \mathcal{H} (| \phi_0^l \rangle + | \phi_1^l \rangle) \\
 &= \frac{1}{2} \sum_{jl} \frac{2}{E_0^l - E_1^j} V_{lj} V_{lj}^\dagger - \frac{1}{2} \sum_{ji} \frac{2}{E_0^i - E_1^l} V_{il}^\dagger V_{il} \\
 &= 0
 \end{aligned} \tag{9.74}$$

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

$$\Delta \mathcal{H} = \frac{1}{2} [\eta^\dagger - \eta, \mathcal{H}] \tag{9.75}$$

where

$$\begin{aligned}
 \eta &= \frac{1}{\omega - \mathcal{H}^d} \sum_{ij} V_{ij} |\phi_0^i\rangle \langle \phi_1^j| = \sum_{ij} \frac{1}{\omega_1^j - E_0^i} V_{ij} |\phi_0^i\rangle \langle \phi_1^j| \\
 \Rightarrow \eta^\dagger &= \sum_{ij} \frac{1}{\omega_1^j - E_0^i} V_{ij}^\dagger |\phi_1^j\rangle \langle \phi_0^i| \\
 \Rightarrow \eta^\dagger - \eta &= \sum_{ij} \frac{1}{\omega_1^j - E_0^i} \left(V_{ij}^\dagger |\phi_1^j\rangle \langle \phi_0^i| - V_{ij} |\phi_0^i\rangle \langle \phi_1^j| \right)
 \end{aligned} \tag{9.76}$$

This can be thought of as the generator for the unitary transformations of URG. Comparing with the generator S of eq. 9.72, the prescription to go from URG to SWT is to replace $\omega_1^j \rightarrow E_1^j$. Doing a similar calculation gives

$$\begin{aligned}
 \Delta \mathcal{H}_{URG} &= \frac{1}{2} \sum_{ijk} \left[\left(\frac{1}{E_0^i - \omega_1^j} + \frac{1}{E_0^k - \omega_1^j} \right) V_{ij} V_{kj}^\dagger |\phi_0^i\rangle \langle \phi_0^k| \right. \\
 &\quad \left. - \left(\frac{1}{E_0^i - \omega_1^j} + \frac{1}{E_0^i - \omega_1^k} \right) V_{ij}^\dagger V_{ik} |\phi_1^j\rangle \langle \phi_1^k| \right]
 \end{aligned} \tag{9.77}$$

9.2.3 SIAM URG vs SIAM SWT

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

$$-\epsilon_q (A + B\hat{n}_{d\bar{\beta}}) + \epsilon_d (A + B\hat{n}_{d\bar{\beta}}) + U (A + B) \hat{n}_{d\bar{\beta}} = -V \tag{9.78}$$

which gives

$$S = V \left[\frac{1 - \hat{n}_{d\bar{\beta}}}{\epsilon_q - \epsilon_d} + \frac{\hat{n}_{d\bar{\beta}}}{\epsilon_q - \epsilon_d - U} \right] (c_{q\beta}^\dagger c_{d\beta} - \text{h.c.}) \tag{9.79}$$

The remaining diagonal part constitutes the effective Hamiltonian.

$$\begin{aligned}
 U\mathcal{H}U^\dagger &= H_1 = \mathcal{H}_0 + \frac{1}{2} \{ \mathcal{H}_0, S^2 \} - S\mathcal{H}_0S + [S, \mathcal{H}_X] \\
 &= \mathcal{H}_0 + \frac{1}{2} [[\mathcal{H}_0, S], S] + [S, \mathcal{H}_X] \\
 &= \mathcal{H}_0 + \frac{1}{2} [\mathcal{H}_X, S] + [S, \mathcal{H}_X] \\
 &= \mathcal{H}_0 + \frac{1}{2} [S, \mathcal{H}_X]
 \end{aligned} \tag{9.80}$$

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

$$\begin{aligned}
 \mathcal{H}_0 &= \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \epsilon_d \hat{n}_d + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \sum_{k\sigma \neq q\beta} \left(c_{k\sigma}^\dagger c_{d\sigma} + \text{h.c.} \right) \\
 \mathcal{H}_X &= c_{q\beta}^\dagger c_{d\beta} + \text{h.c.}
 \end{aligned} \tag{9.81}$$

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

$$\begin{aligned} \frac{1}{2} [S, \mathcal{H}_X] \Big|_{\hat{n}_{q\beta}=0} &= |V|^2 \left[\frac{1 - \hat{n}_{d\bar{\beta}}}{\epsilon_q - \epsilon_d} + \frac{\hat{n}_{d\bar{\beta}}}{\epsilon_q - \epsilon_d - U} \right] [\hat{n}_{q\beta} (1 - \hat{n}_{d\beta}) - \hat{n}_{d\beta} (1 - \hat{n}_{q\beta})] \Big|_{\hat{n}_{q\beta}=0} \\ &= -\hat{n}_{d\beta} |V|^2 \left[\frac{1 - \hat{n}_{d\bar{\beta}}}{\epsilon_q - \epsilon_d} + \frac{\hat{n}_{d\bar{\beta}}}{\epsilon_q - \epsilon_d - U} \right] \end{aligned} \quad (9.82)$$

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 $\epsilon_q \rightarrow -\epsilon_q$.

$$\frac{1}{2} [S, \mathcal{H}_X] \Big|_{\hat{n}_{q\beta}=1} = -(1 - \hat{n}_{d\beta}) |V|^2 \left[\frac{1 - \hat{n}_{d\bar{\beta}}}{\epsilon_q + \epsilon_d} + \frac{\hat{n}_{d\bar{\beta}}}{\epsilon_q + \epsilon_d + U} \right] \quad (9.83)$$

These two results - the renormalization in the particle and hole sectors - is identical to the result (see [11]) 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.

$$\begin{aligned} \Delta E_2 &= -2 \sum_q \frac{|V_q|^2}{\epsilon_q - \epsilon_d - U} \\ \Delta E_1 &= - \sum_q \frac{|V_q|^2}{\epsilon_q - \epsilon_d} - \sum_q \frac{|V_q|^2}{\epsilon_q + \epsilon_d + U} \\ \Delta E_0 &= -2 \sum_q \frac{|V_q|^2}{\epsilon_q + \epsilon_d} \end{aligned} \quad (9.84)$$

This can be compared with the URG result, eq. 6.10,

$$\begin{aligned} \Delta E_2 &= 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d + U} \\ \Delta E_1 &= \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d - U} + \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q + \epsilon_d} \\ \Delta E_0 &= 2 \sum_q \frac{|V_q|^2}{\omega - \frac{1}{2}\epsilon_q - \epsilon_d} \end{aligned} \quad (9.85)$$

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 3.6). 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.

9.3 Kondo model from a one-shot URG

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

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

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

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

$$\mathcal{H}^I = \sum_{k\sigma} \left[V_k c_{k\sigma}^\dagger c_{d\sigma} + \text{h.c.} \right] \quad (9.86)$$

The diagonal part is the rest of the Hamiltonian.

$$\begin{aligned} \mathcal{H}^d &= \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \epsilon_d \hat{n}_d + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \\ &= \sum_{k\sigma} \epsilon_k \tau_{k\sigma} + \epsilon_d \hat{n}_d + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \end{aligned} \quad (9.87)$$

Following eq. 3.47, the renormalization is

$$\Delta\mathcal{H} = \frac{1}{2} [\eta^\dagger - \eta, \mathcal{H}_X] \quad (9.88)$$

The transition operator η is

$$\begin{aligned} \eta &= \frac{1}{\omega - \mathcal{H}^d} \sum_{k\sigma} V_k^* c_{d\sigma}^\dagger c_{k\sigma} \\ &= \sum_{k\sigma} \frac{1}{\omega + \frac{1}{2}\epsilon_k - \epsilon_d - (\epsilon_d + U) \hat{n}_{d\bar{\sigma}}} V_k^* c_{d\sigma}^\dagger c_{k\sigma} \\ &= \sum_{k\sigma} \left[\frac{\hat{n}_{d\bar{\sigma}}}{\omega_1 + \frac{1}{2}\epsilon_k - 2\epsilon_d - U} + \frac{1 - \hat{n}_{d\bar{\sigma}}}{\omega_0 + \frac{1}{2}\epsilon_k - \epsilon_d} \right] V_k^* c_{d\sigma}^\dagger c_{k\sigma} \\ &= \sum_{k\sigma} \left[\frac{\hat{n}_{d\bar{\sigma}}}{E_k^1} + \frac{1 - \hat{n}_{d\bar{\sigma}}}{E_k^0} \right] V_k^* c_{d\sigma}^\dagger c_{k\sigma} \end{aligned} \quad (9.89)$$

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

$$\eta^\dagger - \eta = \sum_{k\sigma} \left[\frac{\hat{n}_{d\bar{\sigma}}}{E_k^1} + \frac{1 - \hat{n}_{d\bar{\sigma}}}{E_k^0} \right] \left(V_k c_{k\sigma}^\dagger c_{d\sigma} - V_k^* c_{d\sigma}^\dagger c_{k\sigma} \right) \quad (9.90)$$

The renormalization is

$$\Delta\mathcal{H}(\omega_1, \omega_0) = \frac{1}{2} \sum_{kq\sigma\alpha} \left[\left(\frac{\hat{n}_{d\bar{\sigma}}}{E_k^1} + \frac{1 - \hat{n}_{d\bar{\sigma}}}{E_k^0} \right) \left(V_k c_{k\sigma}^\dagger c_{d\sigma} - V_k^* c_{d\sigma}^\dagger c_{k\sigma} \right), V_q c_{q\alpha}^\dagger c_{d\alpha} + V_q^* c_{d\alpha}^\dagger c_{q\alpha} \right] \quad (9.91)$$

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

$$\begin{aligned} \Delta_1 &= \frac{1}{2} \sum_{kq\sigma=\alpha} \left[\left(\frac{\hat{n}_{d\bar{\sigma}}}{E_k^1} + \frac{1 - \hat{n}_{d\bar{\sigma}}}{E_k^0} \right) \left(V_k c_{k\sigma}^\dagger c_{d\sigma} - V_k^* c_{d\sigma}^\dagger c_{k\sigma} \right), V_q c_{q\sigma}^\dagger c_{d\sigma} + V_q^* c_{d\sigma}^\dagger c_{q\sigma} \right] \\ &= \frac{1}{2} \sum_{kq\sigma} \left(\frac{\hat{n}_{d\bar{\sigma}}}{E_k^1} + \frac{1 - \hat{n}_{d\bar{\sigma}}}{E_k^0} \right) \left[V_k c_{k\sigma}^\dagger c_{d\sigma} - V_k^* c_{d\sigma}^\dagger c_{k\sigma}, V_q c_{q\sigma}^\dagger c_{d\sigma} + V_q^* c_{d\sigma}^\dagger c_{q\sigma} \right] \\ &= \frac{1}{2} \sum_{kq\sigma} \left(\frac{\hat{n}_{d\bar{\sigma}}}{E_k^1} + \frac{1 - \hat{n}_{d\bar{\sigma}}}{E_k^0} \right) \left\{ V_k V_q^* \left[c_{k\sigma}^\dagger c_{d\sigma}, V_q^* c_{d\sigma}^\dagger c_{q\sigma} \right] - V_k^* V_q \left[c_{d\sigma}^\dagger c_{k\sigma}, c_{q\sigma}^\dagger c_{d\sigma} \right] \right\} \\ &= \frac{1}{2} \sum_{kq\sigma} \left(\frac{\hat{n}_{d\bar{\sigma}}}{E_k^1} + \frac{1 - \hat{n}_{d\bar{\sigma}}}{E_k^0} \right) \left\{ V_k V_q^* \left[c_{k\sigma}^\dagger c_{d\sigma}, V_q^* c_{d\sigma}^\dagger c_{q\sigma} \right] + V_k^* V_q \left[c_{q\sigma}^\dagger c_{d\sigma}, c_{d\sigma}^\dagger c_{k\sigma} \right] \right\} \\ &= \frac{1}{2} \sum_{kq\sigma} \left[\hat{n}_{d\bar{\sigma}} \left(\frac{1}{E_k^1} + \frac{1}{E_q^1} \right) + (1 - \hat{n}_{d\bar{\sigma}}) \left(\frac{1}{E_k^0} + \frac{1}{E_q^0} \right) \right] V_k V_q^* \left[c_{k\sigma}^\dagger c_{d\sigma}, c_{d\sigma}^\dagger c_{q\sigma} \right] \\ &= \sum_{kq\sigma} \left[\frac{1}{2} V_k V_q^* \left(\frac{1}{E_k^0} + \frac{1}{E_q^0} \right) + \hat{n}_{d\bar{\sigma}} \frac{1}{2} V_k V_q^* \left(\frac{1}{E_k^1} + \frac{1}{E_q^1} - \frac{1}{E_k^0} - \frac{1}{E_q^0} \right) \right] \left(c_{k\sigma}^\dagger c_{q\sigma} - c_{d\sigma}^\dagger c_{d\sigma} \delta_{kq} \right) \end{aligned} \quad (9.92)$$

We can now define two new energy scales:

$$W_{kq} = \frac{1}{2} V_k V_q^* \left(\frac{1}{E_k^0} + \frac{1}{E_q^0} \right), \quad J_{kq} = \frac{1}{2} V_k V_q^* \left(\frac{1}{E_k^1} + \frac{1}{E_q^1} - \frac{1}{E_k^0} - \frac{1}{E_q^0} \right) \quad (9.93)$$

The renormalization Δ_1 becomes

$$\begin{aligned} \Delta_1 &= \sum_{kq\sigma} [W_{kq} + \hat{n}_{d\bar{\sigma}} J_{kq}] \left(c_{k\sigma}^\dagger c_{q\sigma} - c_{d\sigma}^\dagger c_{d\sigma} \delta_{kq} \right) \\ &= \sum_{kq\sigma} [W_{kq} + \hat{n}_{d\bar{\sigma}} J_{kq}] c_{k\sigma}^\dagger c_{q\sigma} - \sum_{k\sigma} [W_{kk} + \hat{n}_{d\bar{\sigma}} J_{kk}] \hat{n}_{d\sigma} \\ &= \sum_{kq\sigma} \left[W_{kq} + \frac{1}{2} \hat{n}_d J_{kq} \right] c_{k\sigma}^\dagger c_{q\sigma} - \sum_{kq\sigma} \sigma J_{kq} S_d^z c_{k\sigma}^\dagger c_{q\sigma} - \sum_{k\sigma} [W_{kk} + \hat{n}_{d\bar{\sigma}} J_{kk}] \hat{n}_{d\sigma} \end{aligned} \quad (9.94)$$

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

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

$$\begin{aligned}
 \Delta_2 &= \frac{1}{2} \sum_{kq\bar{\sigma}=\alpha} \left[\left(\frac{\hat{n}_{d\bar{\sigma}}}{E_k^1} + \frac{1 - \hat{n}_{d\bar{\sigma}}}{E_k^0} \right) \left(V_k c_{k\sigma}^\dagger c_{d\sigma} - V_k^* c_{d\sigma}^\dagger c_{k\sigma} \right), V_q c_{q\bar{\sigma}}^\dagger c_{d\bar{\sigma}} + V_q^* c_{d\bar{\sigma}}^\dagger c_{q\bar{\sigma}} \right] \\
 &= \frac{1}{2} \sum_{kq\sigma} \left(V_k c_{k\sigma}^\dagger c_{d\sigma} - V_k^* c_{d\sigma}^\dagger c_{k\sigma} \right) \left[\frac{\hat{n}_{d\bar{\sigma}}}{E_k^1} + \frac{1 - \hat{n}_{d\bar{\sigma}}}{E_k^0}, V_q c_{q\bar{\sigma}}^\dagger c_{d\bar{\sigma}} + V_q^* c_{d\bar{\sigma}}^\dagger c_{q\bar{\sigma}} \right] \\
 &= \frac{1}{2} \sum_{kq\sigma} \left(V_k c_{k\sigma}^\dagger c_{d\sigma} - V_k^* c_{d\sigma}^\dagger c_{k\sigma} \right) \left(V_q^* c_{d\bar{\sigma}}^\dagger c_{q\bar{\sigma}} - V_q c_{q\bar{\sigma}}^\dagger c_{d\bar{\sigma}} \right) \left(\frac{1}{E_k^1} - \frac{1}{E_k^0} \right) \\
 &= \frac{1}{2} \sum_{kq\sigma} \left(V_k V_q^* c_{k\sigma}^\dagger c_{d\sigma} c_{d\bar{\sigma}}^\dagger c_{q\bar{\sigma}} - V_k V_q c_{k\sigma}^\dagger c_{d\sigma} c_{q\bar{\sigma}}^\dagger c_{d\bar{\sigma}} - V_k^* V_q^* c_{d\sigma}^\dagger c_{k\sigma} c_{d\bar{\sigma}}^\dagger c_{q\bar{\sigma}} + V_k^* V_q c_{d\sigma}^\dagger c_{k\sigma} c_{q\bar{\sigma}}^\dagger c_{d\bar{\sigma}} \right) \\
 &\quad \times \left(\frac{1}{E_k^1} - \frac{1}{E_k^0} \right)
 \end{aligned} \tag{9.95}$$

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

$$\begin{aligned}
 &\frac{1}{2} \sum_{kq\sigma} \left(V_k V_q^* c_{k\sigma}^\dagger c_{d\sigma} c_{d\bar{\sigma}}^\dagger c_{q\bar{\sigma}} + V_k^* V_q c_{k\sigma}^\dagger c_{d\sigma} c_{q\bar{\sigma}}^\dagger c_{d\bar{\sigma}} \right) \times \left(\frac{1}{E_k^1} - \frac{1}{E_k^0} \right) \\
 &= \frac{1}{2} \sum_{kq\sigma} V_k V_q^* c_{k\sigma}^\dagger c_{d\sigma} c_{d\bar{\sigma}}^\dagger c_{q\bar{\sigma}} \left(\frac{1}{E_k^1} - \frac{1}{E_k^0} \right) + \frac{1}{2} \sum_{kq\sigma} V_k^* V_q c_{k\sigma}^\dagger c_{d\sigma} c_{q\bar{\sigma}}^\dagger c_{d\bar{\sigma}} \left(\frac{1}{E_k^1} - \frac{1}{E_k^0} \right) \\
 &= \frac{1}{2} \sum_{kq\sigma} V_k V_q^* c_{k\sigma}^\dagger c_{d\sigma} c_{d\bar{\sigma}}^\dagger c_{q\bar{\sigma}} \left(\frac{1}{E_k^1} - \frac{1}{E_k^0} \right) + \frac{1}{2} \sum_{qk\sigma} V_q^* V_k c_{q\bar{\sigma}}^\dagger c_{d\bar{\sigma}} c_{k\sigma}^\dagger c_{d\sigma} \left(\frac{1}{E_q^1} - \frac{1}{E_q^0} \right) \\
 &= - \sum_{kq\sigma} J_{kq} c_{k\sigma}^\dagger c_{q\bar{\sigma}} c_{d\bar{\sigma}}^\dagger c_{d\sigma}
 \end{aligned} \tag{9.96}$$

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

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

where K_{kq} is yet another energy scale.

$$K_{kq} = \frac{1}{4} \left(\frac{1}{E_k^1} - \frac{1}{E_k^0} + \frac{1}{E_q^1} - \frac{1}{E_q^0} \right) \quad (9.97)$$

The third term gives

$$\frac{1}{2} \sum_{kq\sigma} V_k^* V_q^* c_{d\sigma}^\dagger c_{k\sigma} c_{d\bar{\sigma}}^\dagger c_{q\bar{\sigma}} \left(\frac{1}{E_k^1} - \frac{1}{E_k^0} \right) = \sum_{kq\sigma} K_{kq} c_{d\sigma}^\dagger c_{k\sigma} c_{d\bar{\sigma}}^\dagger c_{q\bar{\sigma}} \quad (9.98)$$

The total renormalization can thus be written as

$$\begin{aligned} \Delta\mathcal{H}(\omega_1, \omega_0) = & - \sum_{k\sigma} [W_{kk} + \hat{n}_{d\bar{\sigma}} J_{kk}] \hat{n}_{d\sigma} && [\text{renormalization in } \epsilon_d, U] \\ & + \sum_{kq\sigma} \left[W_{kq} + \frac{1}{2} \hat{n}_d J_{kq} \right] c_{k\sigma}^\dagger c_{q\sigma} && [\text{potential scattering}] \\ & - \sum_{kq\sigma} J_{kq} \left[S_d^z \sigma c_{k\sigma}^\dagger c_{q\sigma} + \sum_{kq\sigma} J_{kq} c_{k\sigma}^\dagger c_{q\bar{\sigma}} c_{d\bar{\sigma}}^\dagger c_{d\sigma} \right] && [\text{spin Kondo}] \\ & + \sum_{kq\sigma} K_{kq} c_{k\sigma}^\dagger c_{d\sigma} c_{q\bar{\sigma}}^\dagger c_{d\bar{\sigma}} + \text{h.c.} && [\text{charge Kondo}] \end{aligned} \quad (9.99)$$

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.

$$\begin{aligned} W_{kq}^{SWT} &= \frac{1}{2} V_k V_q^* \left(\frac{1}{\epsilon_k - \epsilon_d} + \frac{1}{\epsilon_q - \epsilon_d} \right) \\ J_{kq}^{SWT} &= \frac{1}{2} V_k V_q^* \left(\frac{1}{\epsilon_k - \epsilon_d - U} + \frac{1}{\epsilon_q - \epsilon_d - U} - \frac{1}{\epsilon_k - \epsilon_d} - \frac{1}{\epsilon_q - \epsilon_d} \right) \\ W_{kq}^{URG}(\omega) &= \frac{1}{2} V_k V_q^* \left(\frac{1}{\omega_0 + \frac{1}{2}\epsilon_k - \epsilon_d} + \frac{1}{\omega_0 + \frac{1}{2}\epsilon_q - \epsilon_d} \right) \\ J_{kq}^{URG}(\omega) &= \frac{1}{2} V_k V_q^* \left(\frac{1}{\omega_1 + \epsilon_k - \epsilon_d - U} + \frac{1}{\omega_1 + \epsilon_q - \epsilon_d - U} - \frac{1}{\omega_0 + \epsilon_k - \epsilon_d} - \frac{1}{\omega_0 + \epsilon_q - \epsilon_d} \right) \end{aligned} \quad (9.100)$$

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. 9.89, 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.

9.4 CUT RG

9.4.1 FOrmalism

The following equation generates a family of unitary Hamiltonians.

$$\frac{d\mathcal{H}(l)}{dl} = [\mathcal{H}, \eta(l)] \quad (9.101)$$

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

$$\eta(l) = \frac{dU}{dl}U^\dagger = -U\frac{dU^\dagger}{dl} \left[UU^\dagger = 1 \implies \frac{d(UU^\dagger)}{dl} = 0 \right] \quad (9.102)$$

This will give

$$\begin{aligned} \frac{d\mathcal{H}(l)}{dl} &= \frac{dU}{dl}\mathcal{H}(0)U^\dagger(l) + U\mathcal{H}(0)\frac{dU^\dagger}{dl} \\ &= \frac{dU}{dl}U^\dagger\mathcal{H}(l) + \mathcal{H}(l)U\frac{dU^\dagger}{dl} \\ &= \eta(l)\mathcal{H}(l) - \mathcal{H}(l)\eta(l) \\ &= [\eta(l), \mathcal{H}(l)] \end{aligned} \quad (9.103)$$

This proves that the family of Hamiltonians $\mathcal{H}(l)$ satisfy the flow equation eq. 9.101. $\eta(l)$ 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,

$$\frac{d\mathcal{H}}{dl} = [[\mathcal{H}_d(l), \mathcal{H}_X(l)], \mathcal{H}(l)] \quad (9.104)$$

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

$$\mathcal{H} = \mathcal{H}_d + \mathcal{H}_X \quad (9.105)$$

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

$$\sum_{kq} g_q b_{-q}^\dagger c_{k+q,\sigma}^\dagger c_{k\sigma} + \text{h.c.} \quad (9.106)$$

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

$$\eta(l) = [\mathcal{H}_d, \mathcal{H}] = [\mathcal{H}_d, \mathcal{H}_X] \quad (9.107)$$

It is easy to compute the commutators.

$$\begin{aligned} \left[\sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma}, \sum_{kq\sigma} b_{-q}^\dagger c_{k+q,\sigma}^\dagger c_{k\sigma} \right] &= \sum_{kq\sigma} g_q (\epsilon_{k+q} - \epsilon_k) g_q b_{-q}^\dagger c_{k+q,\sigma}^\dagger c_{k\sigma} \\ \left[\sum_q \hbar\omega_q b_q^\dagger b_q, \sum_{kq} g_q b_{-q}^\dagger c_{k+q,\sigma}^\dagger c_{k\sigma} \right] &= \sum_{kq} g_q \hbar\omega_q b_{-q}^\dagger c_{k+q,\sigma}^\dagger c_{k\sigma} \end{aligned} \quad (9.108)$$

Therefore,

$$\eta = \sum_{kq\sigma} g_q (\epsilon_{k+q} - \epsilon_k + \hbar\omega_q) b_{-q}^\dagger c_{k+q,\sigma}^\dagger c_{k\sigma} - \text{h.c.} \quad (9.109)$$

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

$$\frac{d\mathcal{H}}{dl} = [\eta, \mathcal{H}] \quad (9.110)$$

The flow equation for the electron-phonon coupling is

$$\frac{dg_q}{dl} = -\xi^2 g_q \implies g_q(l) = g_q(0) \exp(-\xi^2 l) \quad (9.111)$$

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

$$V_{k,-k,q}(\infty) = V_{k,-k,-q}(0) - \frac{g_q^2 \omega_q}{\omega_q^2 + (\epsilon_{k+q} - \epsilon_k)^2} \quad (9.112)$$

9.4.2 Comparison with URG

From the structure of the flow equations, it is clear that the off-diagonal terms connected by the largest energy difference decay the fastest. 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. This separation of scales does exist in URG and PMS in a different fashion. There, the separation of scale 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 at most block diagonal at this stage. On the other hand, URG progressively decouples single electrons, meaning all scattering terms corresponding to that electron vanish at each step.

One last thing to note is that URG, being unitarily implemented with a well-defined generator, does not accommodate for spontaneous symmetry breaking (SSB). In order to see SSB, the symmetry-breaking term has to be added to the bare model explicitly; if this term grows under the RG, then the ground state will be symmetry-broken. CUT RG, however, does allow for SSB through the idea that the generator is not uniquely defined. If the generator commutes with a particular symmetry, then the family of Hamiltonians will also have the symmetry [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].

9.4.3 CUT RG from URG

We will now see that the renormalization in URG can also be put into a similar form. From eq. 3.47, we can write the URG renormalization as

$$\Delta\mathcal{H} = \frac{1}{2} [\eta^\dagger - \eta, \mathcal{H}] \quad (9.113)$$

The URG generator can be recast (starting from the definitions of η , eqs. 3.14) as

$$\begin{aligned} \eta^\dagger - \eta &= G_1 c^\dagger T - G_0 T^\dagger c \\ &= \frac{1}{\omega_1 - \omega_0} [G_1 (\omega_1 - \omega_0) c^\dagger T - G_0 (\omega_1 - \omega_0) T^\dagger c] \\ &= \frac{1}{\omega_1 - \omega_0} [G_1 \omega_1 c^\dagger T - c^\dagger T \omega_0 G_0 - T^\dagger c \omega_1 G_1 + G_0 \omega_0 T^\dagger c] \end{aligned} \quad (9.114)$$

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. 3.16. 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.

$$\begin{aligned} \eta^\dagger - \eta &= \frac{1}{\omega_1 - \omega_0} [G_1 (\omega_1 - G_1^{-1}) c^\dagger T + c^\dagger T - c^\dagger T (\omega_0 - G_0^{-1}) G_0 - c^\dagger T \\ &\quad - T^\dagger c (\omega_1 - G_1^{-1}) G_1 - T^\dagger c + G_0 (\omega_0 - G_0^{-1}) T^\dagger c + T^\dagger c] \\ &= \frac{1}{\omega_1 - \omega_0} [G_1 (\omega_1 - G_1^{-1}) c^\dagger T - c^\dagger T (\omega_0 - G_0^{-1}) G_0 \\ &\quad - T^\dagger c (\omega_1 - G_1^{-1}) G_1 + G_0 (\omega_0 - G_0^{-1}) T^\dagger c] \end{aligned} \quad (9.115)$$

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 $(\omega_j - G_j^{-1}) G_j = G_j (\omega_j - G_j^{-1})$:

$$\begin{aligned}\eta^\dagger - \eta &= \frac{1}{\omega_1 - \omega_0} [G_1 (\omega_1 - G_1^{-1}) c^\dagger T - c^\dagger T G_0 (\omega_0 - G_0^{-1}) \\ &\quad - T^\dagger c G_1 (\omega_1 - G_1^{-1}) + G_0 (\omega_0 - G_0^{-1}) T^\dagger c] \\ &= \frac{1}{\omega_1 - \omega_0} [G_1 (\omega_1 - G_1^{-1}) c^\dagger T - G_1 c^\dagger T (\omega_0 - G_0^{-1}) \\ &\quad - G_0 T^\dagger c (\omega_1 - G_1^{-1}) + G_0 (\omega_0 - G_0^{-1}) T^\dagger c]\end{aligned}\quad (9.116)$$

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,

$$\begin{aligned}\eta^\dagger - \eta &= \frac{1}{\omega_1 - \omega_0} [G_1 \mathcal{H}_1^d c^\dagger T - G_1 c^\dagger T \mathcal{H}_0^d - G_0 T^\dagger c \mathcal{H}_1^d + G_0 \mathcal{H}_0^d T^\dagger c] \\ &= \frac{1}{\omega_1 - \omega_0} [G \mathcal{H}^d c^\dagger T - G c^\dagger T \mathcal{H}^d - G T^\dagger c \mathcal{H}^d + G \mathcal{H}^d T^\dagger c] \\ &= \frac{1}{\omega_1 - \omega_0} G [\mathcal{H}^d, c^\dagger T + T^\dagger c]\end{aligned}\quad (9.117)$$

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,

$$\eta^\dagger - \eta = \frac{1}{\omega_1 - \omega_0} G [\mathcal{H}^d, \mathcal{H}^I] \quad (9.118)$$

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

$$\Delta \mathcal{H}(\omega, D) = \frac{1}{\omega_1 - \omega_0} [G [\mathcal{H}^d, \mathcal{H}^I], \mathcal{H}] \quad (9.119)$$

This can be compared to the analogous equation for CUT (eq. 9.104),

$$\Delta \mathcal{H}(\lambda) = \Delta \lambda [[\mathcal{H}_d, \mathcal{H}_X], \mathcal{H}] \quad (9.120)$$

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.

$$G c^\dagger T = G_1 c^\dagger T = \frac{1}{\omega_1 - \mathcal{H}_1^d} c^\dagger T \approx -\frac{1}{\mathcal{H}_1^d} c^\dagger T \quad (9.121)$$

where we dropped ω_1 for small quantum fluctuations. Similarly,

$$G T^\dagger c = G_0 T^\dagger c = T^\dagger c \frac{1}{\omega_1 - \mathcal{H}_1^d} \approx -\frac{1}{\mathcal{H}_1^d} T^\dagger c \quad (9.122)$$

This gives

$$\Delta\mathcal{H}(\omega, D) = \frac{1}{\mathcal{H}_1^d} \frac{1}{\omega_0 - \omega_1} [[\mathcal{H}^d, \mathcal{H}^I], \mathcal{H}] \quad (9.123)$$

We can thus make the connection,

$$\Delta\lambda \sim \frac{1}{\mathcal{H}_1^d} \frac{1}{\omega_0 - \omega_1} \quad (9.124)$$

Note that in going from eq. 9.119 to the simplified form eq. 9.123, 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.

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