Unitary Renormalization Group Approach to Single-Impurity Anderson Model

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Contents

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. 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 the 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 ieratively 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 Weigman [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.

- *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 $T >> T_K$. 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 requite 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 the in the process. This allows us to calculate exact quantities for simple systems like the Kondo model.

- *Tractable low-energy effective Hamiltonians* The final Hamiltonians obtained at the fixed point are usually tractable and allow us to extract information.

The work is organized as follows. Section 1 goes over the available work on the Anderson and Kondo model. Section 2 lays out the URG formalism and prescription. Section 4 solves the Kondo model using the URG method. Section 5 contains the URG analysis of the SIAM.

1 Preliminaries

1.1 $T-$matrix and $S-$matrix

$T-$matrix is defined as[7]

$$V\psi = T\phi \tag{1.1}$$

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

$$H_0\phi = E\phi \tag{1.2}$$
$$(H_0 + V)\psi = E\psi \tag{1.3}$$

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

$$\psi = \phi + G_0 V\psi \tag{1.4}$$

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

$$\psi = \phi + G_0 T\phi$$
$$\implies \psi = (1 + G_0 T)\phi \tag{1.5}$$

Eq. 1.4 can also be written as

$$\psi = (1 - G_0 V)^{-1}\phi \tag{1.6}$$

Comparing the last two equations gives

$$1 = (1 - G_0 V)(1 + G_0 T)$$
$$\implies T = V + V G_0 T \tag{1.7}$$

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

$$T = V + V G_0 V + V G_0 V G_0 V + \dots \tag{1.8}$$

From scattering theory, we can write

$$\psi = (2\pi)^{-\frac{3}{2}} \left[e^{ikx} + f\frac{e^{ikr}}{r} \right] \tag{1.9}$$

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

$$f(k',k) \sim \langle k'| T |k\rangle \tag{1.10}$$

By definition, the $S-$matrix is

$$S(\omega) = e^{2i\pi\delta(\omega)} \tag{1.11}$$

Also,

$$S = 1 - 2i\pi\rho T \tag{1.12}$$

Therefore,

$$T = \frac{1}{2i\pi\rho}\left(1 - e^{2i\pi\delta(\omega)}\right) = -\frac{e^{i\delta}\sin\delta}{\pi\rho} \tag{1.13}$$

1.2 An identity

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

$$HA = A(\lambda + H) \tag{1.14}$$

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

$$(E - H)A = AE - A(\lambda + H) = A(E - \lambda - H) \tag{1.15}$$
$$\implies A(E - \lambda - H)^{-1} = (E - H)^{-1}A \tag{1.16}$$

1.3 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 $\{n_{k_1\uparrow}, n_{k_1\downarrow}, n_{k_2\uparrow}, n_{k_2\downarrow}, n_{k_3\uparrow}, n_{k_3\downarrow}, ..., \}$, where $n_{k\sigma} \in \{0, 1\}$ is the number of particles with momentum k and spin σ. In the ground state,

$$n_{k\sigma} = \begin{cases} 1 & k \leq k_F \\ 0 & k > k_F \end{cases} \tag{1.17}$$

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.

$$\Psi^* \xrightarrow{\text{turn interactions off}} \Phi \tag{1.18}$$

$$\Phi^* \xrightarrow{\text{turn interactions off}} \Psi \tag{1.19}$$

If some state Γ^*, instead of flowing into an ideal excited state, gets lost while the interactions are being turned off, then we arent 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,

$$|IGS\rangle \otimes |k_+\rangle \xrightarrow{\text{turn interactions on}} |RGS\rangle \otimes |k_+\rangle^* \tag{1.20}$$

$$|IGS\rangle \otimes |k_-\rangle \xrightarrow{\text{turn interactions on}} |RGS\rangle \otimes |k_-\rangle^* \tag{1.21}$$

$$\tag{1.22}$$

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

$$c_{k_+}^\dagger |IGS\rangle \xrightarrow{\text{turn interactions on}} \eta_{k_+}^\dagger |RGS\rangle \tag{1.23}$$

$$c_{k_-} |IGS\rangle \xrightarrow{\text{turn interactions on}} \eta_{k_-} |RGS\rangle \tag{1.24}$$

$\eta^\dagger$ 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

$$\delta n_k = n_k - n_k^0 \tag{1.25}$$

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.

$$\mathcal{E}^0[n_k] = \sum_k n_k \epsilon_k \tag{1.26}$$

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

$$\mathcal{E}[n_k] = \mathcal{E}[n_k^0] + \sum_k \frac{\partial \mathcal{E}}{\partial n_k} \delta n_k \tag{1.27}$$

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

$$\delta \mathcal{E} \equiv \mathcal{E}[n_k] - \mathcal{E}[n_k^0] = \sum_k \xi_k \delta n_k \tag{1.28}$$

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

$$n_k^2 - n_k^1 = \begin{cases} 0 & k \neq q \\ 1 & k = q \end{cases} \tag{1.29}$$

Then, up to first order,

$$\mathcal{E}[n_k^2] - \mathcal{E}[n_k^1] = \sum_k \xi_k \left(n_k^2 - n_k^1 \right) = \xi_q \tag{1.30}$$

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 xi_k itself is, in general, a functional of n_k. Consequently, we expand it upto first order.

$$\xi_k = \xi_k^0 + \sum_q \frac{\partial \xi_k}{\partial n_q} \delta n_q \tag{1.31}$$

Eq. 1.28 then becomes

$$\delta \mathcal{E} = \sum_k \xi_k^0 \delta n_k + \sum_{k,q} f(k,q) \delta n_k \delta n_q \tag{1.32}$$

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,

$$f(\xi) = \left[e^{(\xi-\mu)\beta} + 1\right]^{-1} \tag{1.33}$$

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

$$F[\delta n_k] = \delta\mathcal{E}[\delta n_k] - TS[\delta n_k] \tag{1.34}$$

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

$$\xi_k(T) = \xi_k^0 + \sum_q f(k,q)\langle \delta n_q \rangle \tag{1.35}$$

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

$$\frac{\mathrm{d}F}{\mathrm{d}\delta n_q}\bigg|_{\delta n_q = \langle \delta n_q \rangle} = 0 \tag{1.36}$$

1.4   The model

$$H = \epsilon_d \hat{n}_d + \sum_k \epsilon_k \hat{n}_k + \sum_{k\sigma} t\left(c_{k\sigma}^\dagger c_{d\sigma} + c_{d\sigma}^\dagger c_{k\sigma}\right) + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} \tag{1.37}$$

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 allows 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.

1.5 Atomic limit ($t = 0$)

$$H_{\text{atomic}} = E_d + E_{CB} + U n_{d\uparrow} n_{d\downarrow} \tag{1.38}$$

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

$$H_{\text{atomic}} = \epsilon_d n_d + U n_{d\uparrow} n_{d\downarrow} \tag{1.39}$$

For a magnetic solution, we need

$$(\epsilon_\uparrow = \epsilon_\downarrow =)\epsilon_d < (\epsilon_0, \epsilon_{\uparrow\downarrow})0, 2\epsilon_d + U \tag{1.40}$$

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

$$\epsilon_d > -U \tag{1.41}$$

1.6 Non-interacting limit ($U = 0$):

$$H_{\text{non-int}} = \epsilon_d n_d + \sum_k \epsilon_k n_k + \sum_{k\sigma} t \left(c_{k\sigma}^\dagger c_{d\sigma} + c_{d\sigma}^\dagger c_{k\sigma} \right) \tag{1.42}$$

1.6.1 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

$$G_d^0(E) = \frac{1}{E - \epsilon_d} \tag{1.43}$$

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

$$G_d^0 \Sigma_c G_d^0, \text{ where } \Sigma_c = t \left(\sum_k G_k^0 \right) t = \sum_k \frac{t^2}{E - \epsilon_k} \tag{1.44}$$

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

$$\begin{aligned}
G_d(E) &= G_d^0 + G_d^0 \Sigma_c G_d^0 + G_d^0 \Sigma_c G_d^0 \Sigma_c G_d^0 + G_d^0 \Sigma_c G_d^0 \Sigma_c G_d^0 \Sigma_c G_d^0 + \dots \\
&= G_d^0 \left[1 + \left(\Sigma_c G_d^0 \right)^2 + \dots \right] = G_d^0 \frac{1}{1 - \Sigma_c G_d^0} = \frac{1}{E - \epsilon_d - \Sigma_c(E)}
\end{aligned} \tag{1.45}$$

Now,

$$\frac{1}{t^2} \Sigma_c(E) = \sum_k \frac{1}{E - \epsilon_k} = \lim_{\eta \to 0} \int_{-W}^{W} d\epsilon \rho(\epsilon) \frac{1}{E - \epsilon + i\eta} \tag{1.46}$$

$$\implies \frac{1}{t^2} \text{Re} \left[\Sigma_c(E) \right] = \int_{-W}^{W} d\epsilon \rho(\epsilon) \frac{1}{E - \epsilon}, \text{ and} \tag{1.47}$$

$$\frac{1}{t^2} \text{Im} \left[\Sigma_c(E) \right] = \int_{-W}^{W} d\epsilon \rho(\epsilon) (-i\pi) \delta(E - \epsilon) \tag{1.48}$$

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

$$\Sigma_c(E) = \text{Im}\left[\Sigma_c(E)\right] = -i\pi t^2 \rho(E) = -i\Delta \tag{1.49}$$

Therefore,

$$G_d(E) = \frac{1}{E - \epsilon_d + i\Delta} \tag{1.50}$$

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

$$\rho_d^0(E) = -\frac{1}{\pi}\text{Im}\left[G_d^0\right] = -\frac{1}{\pi}\lim_{\eta \to 0}\frac{1}{E - \epsilon_d + i\eta} = \delta(E - \epsilon_d) \tag{1.51}$$

$$\rho_d(E) = -\frac{1}{\pi}\text{Im}\left[G_d\right] = -\frac{1}{\pi}\lim_{\eta \to 0}\frac{1}{E - \epsilon_d + i(\eta + \Delta)} = \frac{1}{\pi}\frac{\Delta}{(E - \epsilon_d)^2 + \Delta^2} \tag{1.52}$$

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:

$$\langle n_d \rangle = 2\int d\epsilon \rho_d(\epsilon) = \frac{2\Delta}{\pi}\int \frac{d\epsilon}{(\epsilon - \epsilon_d)^2 + \Delta^2} = \frac{2}{\pi}\cot^{-1}\left(\frac{\epsilon_d}{\Delta}\right) \tag{1.53}$$

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

$T-$matrix is defined by

$$T = V + VGT \tag{1.54}$$

We also have

$$\begin{aligned}
G = G_0 + G_0VG &= G_0 + G_0T\frac{1}{1 + GT}G \\
&= G_0 + G_0T(1 - GT + ...)(G_0 + G_0VG_0 + ...) \\
&= G_0 + G_0TG_0
\end{aligned} \tag{1.55}$$

The conduction electron Green's function can be calculated as

$$\begin{aligned}
G_c(k, k', E) = \delta_{k,k'}G_c^0(k, E) &+ G_c^0(k)tG_d^0tG_c^0(k') + \\
&G_c^0(k)tG_d^0t\sum_q G_c^0(q)tG_d^0tG_c^0(k') + ...
\end{aligned} \tag{1.56}$$

Noting that

$$t\sum_q G_c^0(q)t = \Sigma_c, \tag{1.57}$$

we have

$$G_c(k, k', E) = \delta_{k,k'}G_c^0(k, E) + G_c^0(k)t^2G_d(E)G_c^0(k') \tag{1.58}$$

Comparing with the final form of G in eq. 1.55, we can write

$$T(k, k', E) = t^2G_d(E) = \frac{t^2}{E - \epsilon_d + i\Delta} = -\frac{t^2}{\Delta}\frac{1}{\frac{\epsilon_d - E}{\Delta} - i} \tag{1.59}$$

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

$$\text{Im}[T] = -\frac{t^2\Delta}{(E - \epsilon_d)^2 + \Delta^2} = -\pi t^2 \rho_d \tag{1.60}$$

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

$$\rho_d = -\frac{1}{\pi}\text{Im}\,[G_d] = -\frac{1}{\pi t^2}\text{Im}\,[t^2 G_d] = -\frac{1}{\pi t^2}\text{Im}\,[T] \tag{1.61}$$

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

$$T = e^{2i\delta} - 1 = e^{i\delta}\left(e^{i\delta} - e^{-i\delta}\right) \sim \frac{1}{\cot\delta - i} \tag{1.62}$$

Comparing with eq. 1.59, we can write

$$\delta(E) = \cot^{-1}\left(\frac{\epsilon_d - E}{\Delta}\right) \tag{1.63}$$

When $E = \epsilon_d$, the phase shift is π, and the scattering is head on (the conduction electron is reflected back). Comparing with eq. 1.53,

$$\frac{2}{\pi}\delta(0) = \langle n_d \rangle \tag{1.64}$$

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

1.6.3 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.

$$H_{\text{dot}} = \sum_{m\sigma} \epsilon_m n_{m\sigma} + U\frac{N(N+1)}{2} \tag{1.65}$$

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.

$$H_{\text{dot}} = \sum_{m\sigma} \left(\epsilon_m - eV\right) n_{m\sigma} + U\frac{N(N+1)}{2} \tag{1.66}$$

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

$$\Delta E = UN + \epsilon_N - eV \tag{1.67}$$

Tuning the voltage can make these two levels degenerate.

$$eV^* = UN + \epsilon_N \tag{1.68}$$

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,

$$G(V) = G_0 \rho(0) = \frac{2e^2}{h}\frac{\Delta^2}{\left(\epsilon_m - eV\right)^2 + \Delta^2} \tag{1.69}$$

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

1.7   Total Hamiltonian: Mean field treatment

$$n_{d\uparrow} n_{d\downarrow} \approx n_{d\uparrow} \langle n_{d\downarrow} \rangle + n_{d\downarrow} \langle n_{d\uparrow} \rangle + \text{constant} \tag{1.70}$$

$$H \approx \sum_k \epsilon_k n_k + \sum_\sigma \left[\epsilon_d + U \langle n_{d\bar\sigma} \rangle \right] n_{d\sigma} + t \sum_{k\sigma} \left(c_{k\sigma}^\dagger c_{d\sigma} + c_{d\sigma}^\dagger c_{k\sigma} \right) \tag{1.71}$$

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

$$\rho_{d\sigma} = \frac{1}{\pi} \frac{\Delta}{(E - \epsilon_{d\sigma})^2 + \Delta^2} \implies \langle n_{d\sigma} \rangle = \int \rho_{d\sigma} = \frac{1}{\pi} \cot^{-1} \left(\frac{\epsilon_{d\sigma}}{\Delta} \right) \tag{1.72}$$

An alternative way of writing that is

$$\frac{\epsilon_{d\sigma}}{\Delta} = \frac{\epsilon_d + U \langle n_{d\sigma} \rangle}{\Delta} = \cot \left(\pi \langle n_{d\sigma} \rangle \right) \implies \langle n_{d\sigma} \rangle = \frac{\Delta}{U} \left[\cot \left(\pi \langle n_{d\bar\sigma} \rangle \right) - \frac{\epsilon_d}{\Delta} \right] \tag{1.73}$$

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

$$\begin{aligned}
\langle n_{d\uparrow} - n_{d\downarrow} \rangle \equiv m &= \frac{\Delta}{U} \left[\cot \left(\pi \langle n_{d\downarrow} \rangle \right) - \cot \left(\pi \langle n_{d\uparrow} \rangle \right) \right] \\
&= \frac{\Delta}{U} \left[\cot \frac{\pi}{2} (n_d - m) - \cot \frac{\pi}{2} (n_d + m) \right]
\end{aligned} \tag{1.74}$$

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

$$\cot(a + x) \approx \cot a - x \left(\sin a \right)^{-2} \implies \cot(a - x) - \cot(a + x) \approx 2x \left(\sin a \right)^{-2} \tag{1.75}$$

we get

$$m = \frac{\Delta}{U} \left[-\pi \frac{m}{\sin^2 \frac{\pi}{2} n_d} \right] \implies 1 = \lim_{m \to 0} \frac{U}{\pi \Delta} \frac{1}{1 + \cot^2 \frac{\pi n_d}{2}} \tag{1.76}$$

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. 1.76,

$$1 = \frac{U_c}{\pi} \frac{\Delta}{\Delta^2 + \left(\frac{U_c n_d}{2} + \epsilon_d \right)^2} \tag{1.77}$$

Magnetism will prevail for $U \geq U_c$. Comparing with eq. 1.73,

$$1 = U_c \rho_d(E = 0) \tag{1.78}$$

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

$$U_c = \pi \Delta \tag{1.79}$$

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

$$\langle n_{d\uparrow} \rangle = \frac{1 + m}{2} \tag{1.80}$$

$$\langle n_{d\downarrow} \rangle = \frac{1 - m}{2} \tag{1.81}$$

$$\epsilon_{d\sigma} = \epsilon_d + U \langle n_{d\bar\sigma} \rangle = \epsilon_d + \frac{U}{2} \pm \frac{U}{2} m = \pm \frac{U}{2} m \tag{1.82}$$

$$\rho_d = \rho_{d\uparrow} + \rho_{d\downarrow} = \frac{\Delta}{\pi} \left[\frac{1}{\Delta^2 + \left(E - \frac{Um}{2} \right)^2} + \frac{1}{\Delta^2 + \left(E + \frac{Um}{2} \right)^2} \right] \tag{1.83}$$

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

1.8   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 $T \to 0$. Thus, the singlet phase shift at ϵ_F approaches $\frac{\pi}{2}$ as $T \to 0$.

1.9 Derivation of the Kondo Hamiltonian

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

$$\begin{aligned}
\text{low energy (L)} &\rightarrow \begin{cases} |\uparrow\rangle \\ |\downarrow\rangle \end{cases} \\
\text{high energy (H)} &\rightarrow \begin{cases} |\rangle \\ |\uparrow\downarrow\rangle \end{cases}
\end{aligned} \tag{1.84}$$

$$H = H_0 + V = \begin{array}{c} \\ \text{low} \\ \text{high} \end{array} \overset{\begin{array}{cc} \text{low} & \text{high} \end{array}}{\begin{pmatrix} H^L & v^\dagger \\ v & H^H \end{pmatrix}} \tag{1.85}$$

$$H_0 = \sum_k \epsilon_k n_k + \epsilon_d n_d + U n_{d\uparrow} n_{d\downarrow}, V = \sum_{k\sigma} \left(V_k c_{k\sigma}^\dagger c_{d\sigma} + V_k^* c_{d\sigma}^\dagger c_{k\sigma} \right) \tag{1.86}$$

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

$$\overline{H} = e^{-S} H e^S = H_0 + (V + [H_0, S]) + \frac{1}{2} \left([V, S] + [[H_0, S], S] \right) \tag{1.87}$$

Defining S such that the first order term vanishes,

$$V = [S, H_0] \tag{1.88}$$

$$\overline{H} = H_0 + \frac{1}{2}[V, S] \tag{1.89}$$

Take $S = \begin{pmatrix} 0 & -s^\dagger \\ s & 0 \end{pmatrix}$. From eq. 1.88,

$$\begin{aligned}
V &= \begin{pmatrix} 0 & -s^\dagger \\ s & 0 \end{pmatrix} \begin{pmatrix} H^L & 0 \\ 0 & H^H \end{pmatrix} - \begin{pmatrix} H^L & 0 \\ 0 & H^H \end{pmatrix} \begin{pmatrix} 0 & -s^\dagger \\ s & 0 \end{pmatrix} \\
&= \begin{pmatrix} 0 & -s^\dagger H^H + H^L s^\dagger \\ s H^L - H^H s & 0 \end{pmatrix}
\end{aligned} \tag{1.90}$$

Comparing with the definition of V, we can write

$$v_{ij}^\dagger = s_{ij}^\dagger \left(E_i^L - E_j^H \right), v_{ij} = s_{ij} \left(E_j^L - E_i^H \right) \tag{1.91}$$

$$\implies s_{ij}^\dagger = \frac{v_{ij}^\dagger}{E_i^L - E_j^H}, s_{ij} = \frac{v_{ij}}{E_j^L - E_i^H} \tag{1.92}$$

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

$$[V, S] = \begin{pmatrix} 0 & v^\dagger \\ v & 0 \end{pmatrix} \begin{pmatrix} 0 & -s^\dagger \\ s & 0 \end{pmatrix} - \begin{pmatrix} 0 & -s^\dagger \\ s & 0 \end{pmatrix} \begin{pmatrix} 0 & v^\dagger \\ v & 0 \end{pmatrix} = \begin{pmatrix} v^\dagger s + s^\dagger v & 0 \\ 0 & -vs^\dagger - sv^\dagger \end{pmatrix} \tag{1.93}$$

Hence,

$$\overline{H} = H_0 + \frac{[V, S]}{2} = \begin{pmatrix} H^L + \frac{1}{2}\left(v^\dagger s + s^\dagger v \right) & 0 \\ 0 & H^H - vs^\dagger - sv^\dagger \end{pmatrix} \tag{1.94}$$

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

$$\mathcal{H} = \langle L| \overline{H} |L\rangle = H^L + \frac{1}{2} \left(v^\dagger s + s^\dagger v \right) \tag{1.95}$$

16

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

$$\Delta H = \frac{1}{2}\left(v^\dagger s + s^\dagger v\right) = \frac{1}{2}\left(v^\dagger \sum_{HL} s_{HL} |H\rangle \langle L| + \text{h.c.}\right)$$

$$= \frac{1}{2}\sum_{HL}\left[v^\dagger |H\rangle \langle L| \frac{v_{HL}}{E_L - E_H} + |L\rangle \langle H| \frac{v_{LH}^\dagger}{E_L - E_H} v\right] \tag{1.96}$$

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

$$\Delta H_{ll'} = \langle l | \Delta H | l'\rangle = \frac{1}{2}\sum_H v_{lH}^\dagger v_{Hl'}\left(\frac{1}{E_{l'} - E_H} + \frac{1}{E_l - E_H}\right) \tag{1.97}$$

This can also be written as

$$\Delta H_{ll'} = \frac{1}{2}\left[T_{ll'}(E_l) + T_{ll'}(E_{l'})\right] \tag{1.98}$$

where

$$T_{ll'}(E) = \sum_H \frac{v_{lH}^\dagger v_{Hl'}}{E - E_H} = \sum_H \frac{V_{lH}^\dagger V_{Hl'}}{E - E_H} \tag{1.99}$$

$T(E)$, 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

$$\Delta H_{ll'} = \sum_H v_{lH}^\dagger v_{Hl'} \frac{1}{E_L - E_H}$$

$$\implies \Delta H = V\left(\sum_H \frac{1}{\Delta_{LH}} |H\rangle \langle H|\right) V \tag{1.100}$$

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,

$$\Delta_{LH_1} = \epsilon_d - 0 = \epsilon_d, \Delta_{LH_2} = \epsilon_d - (2\epsilon_d + U) = -\epsilon_d - U \tag{1.101}$$

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,

$$\Delta H = V\frac{|0\rangle \langle 0|}{\epsilon_d}V - V\frac{|\uparrow\downarrow\rangle \langle \uparrow\downarrow|}{\epsilon_d + U}V$$

$$= \sum_{k_1,k_2,\sigma_1,\sigma_2} V(k_1)V^*(k_2)\left[\frac{c_{d\sigma_2}^\dagger c_{k_2\sigma_2}|0\rangle \langle 0| c_{k_1\sigma_1}^\dagger c_{d\sigma_1}}{\epsilon_d} - \frac{c_{k_1\sigma_1}^\dagger c_{d\sigma_1}|\uparrow\downarrow\rangle \langle \uparrow\downarrow| c_{d\sigma_2}^\dagger c_{k_2\sigma_2}}{\epsilon_d + U}\right]$$

$$= \sum_{k_1,k_2,\sigma_1,\sigma_2} V(k_1)V^*(k_2)\frac{c_{d\sigma_2}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_1}|d\sigma_1, h_{k_1\sigma_1}\rangle \langle d\sigma_1, h_{k_1\sigma_1}|}{\epsilon_d}$$

$$- \sum_{k_1,k_2,\sigma_1,\sigma_2} V(k_1)V^*(k_2)\frac{c_{k_1\sigma_1}^\dagger c_{d\sigma_1} c_{d\sigma_2}^\dagger c_{k_2\sigma_2}|d\overline{\sigma_2}, e_{k_2\sigma_2}\rangle \langle d\overline{\sigma_2}, e_{k_2\sigma_2}|}{\epsilon_d + U}$$

$$= \sum_{k_1,k_2,\sigma_1,\sigma_2} V(k_1)V^*(k_2)\left[\frac{c_{d\sigma_2}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_1}}{\epsilon_d} - \frac{c_{k_1\sigma_1}^\dagger c_{d\sigma_1} c_{d\sigma_2}^\dagger c_{k_2\sigma_2}}{\epsilon_d + U}\right] P_{n_d=1} \tag{1.102}$$

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

$$
\begin{aligned}
c_{d\sigma_2}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_1} &= \sum_{\sigma_3,\sigma_4} c_{d\sigma_3}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_4} \delta_{\sigma_1\sigma_3}\delta_{\sigma_4\sigma_2} \\
&= \frac{1}{2}\sum_{\sigma_3,\sigma_4} c_{d\sigma_3}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_4} \left(\delta_{\sigma_1\sigma_2}\delta_{\sigma_3\sigma_4} + \vec{\sigma}_{\sigma_1\sigma_2}\cdot\vec{\sigma}_{\sigma_3\sigma_4}\right) \\
&= \frac{1}{2}c_{k_2\sigma_1} c_{k_1\sigma_1}^\dagger n_d + c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2}\cdot \sum_{\sigma_3,\sigma_4} c_{d\sigma_3}^\dagger \frac{\vec{\sigma}_{\sigma_3\sigma_4}}{2} c_{d\sigma_4}
\end{aligned}
\tag{1.103}
$$

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 $n_d = 1$.

$$
c_{d\sigma_2}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_1} = -\frac{1}{2}c_{k_1\sigma_1}^\dagger c_{k_2\sigma_1} - c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2}\cdot \sum_{\sigma_3,\sigma_4} c_{d\sigma_3}^\dagger \frac{\vec{\sigma}_{\sigma_3\sigma_4}}{2} c_{d\sigma_4}
\tag{1.104}
$$

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

$$
c_{d\sigma_2}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_1} = -\frac{1}{2}c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2}\cdot \vec{\sigma}_d
\tag{1.105}
$$

Similarly,

$$
c_{k_1\sigma_1}^\dagger c_{d\sigma_1} c_{d\sigma_2}^\dagger c_{k_2\sigma_2} = -\frac{1}{2}c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2}\cdot \vec{\sigma}_d
\tag{1.106}
$$

Finally, putting all this together,

$$
\begin{aligned}
\Delta H &= \frac{1}{2}\sum_{k_1,k_2,\sigma_1,\sigma_2} V(k_1)V^*(k_2)\left[\frac{1}{\epsilon_d + U} - \frac{1}{\epsilon_d}\right] c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2}\cdot \vec{\sigma}_d \\
&= \frac{1}{2}\sum_{k_1,k_2,\sigma_1,\sigma_2} J(k_1,k_2) c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2}\cdot \vec{\sigma}_d
\end{aligned}
\tag{1.107}
$$

where

$$
J(k_1,k_2) = V(k_1)V^*(k_2)\left[\frac{1}{\epsilon_d + U} - \frac{1}{\epsilon_d}\right]
\tag{1.108}
$$

Assuming $V(k) \equiv t$,

$$
H_K = \sum_k \epsilon_k n_k + \frac{J}{2}\vec{\sigma}_e\cdot\vec{\sigma}_d
\tag{1.109}
$$

where

$$
\vec{\sigma}_e = \sum_{k_1,k_2,\sigma_1,\sigma_2} c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2} = \sum_{\sigma_1,\sigma_2} c_{\sigma_1}^\dagger(\vec{r}=0)\vec{\sigma}_{\sigma_1\sigma_2} c_{\sigma_2}(\vec{r}=0)
\tag{1.110}
$$

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

1.10   Obtaining the resistivity minimum and log-dependence

The next few sections follow the approach in [10]. The model we are working with is

$$
H_K = H_0 + V = \sum_k \epsilon_k n_k + \frac{J}{2}\sum_{k_1,k_2,\sigma_1,\sigma_2} c_{k_1\sigma_1}^\dagger \vec{\sigma}_d\cdot\vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2}
\tag{1.111}
$$

18

$$\sum_{\sigma_1,\sigma_2} c_{k_1\sigma_1}^\dagger \vec{\sigma}_d \cdot \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2} = \sigma_d^z \left(c_{k_1\uparrow}^\dagger c_{k_2\uparrow} - c_{k_1\downarrow}^\dagger c_{k_2\downarrow} \right) + \sigma_d^x \left(c_{k_1\downarrow}^\dagger c_{k_2\uparrow} + c_{k_1\uparrow}^\dagger c_{k_2\downarrow} \right)$$
$$-i\sigma_d^y \left(c_{k_1\uparrow}^\dagger c_{k_2\downarrow} - c_{k_1\downarrow}^\dagger c_{k_2\uparrow} \right) \tag{1.112}$$

$$= \sigma_d^z \left(c_{k_1\uparrow}^\dagger c_{k_2\uparrow} - c_{k_1\downarrow}^\dagger c_{k_2\downarrow} \right) + c_{k_1\downarrow}^\dagger c_{k_2\uparrow} \sigma_d^+ + c_{k_1\uparrow}^\dagger c_{k_2\downarrow} \sigma_d^- \tag{1.113}$$

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

$$H_K = \sum_k \epsilon_k n_k + \frac{J}{2} \sum_{k_1,k_2} \left[\sigma_d^z \left(c_{k_1\uparrow}^\dagger c_{k_2\uparrow} - c_{k_1\downarrow}^\dagger c_{k_2\downarrow} \right) + \sigma_d^+ c_{k_1\downarrow}^\dagger c_{k_2\uparrow} + \sigma_d^- c_{k_1\uparrow}^\dagger c_{k_2\downarrow} \right]$$
$$= \sum_k \epsilon_k n_k + J \sum_{k_1,k_2} \left[S_d^z \left(c_{k_1\uparrow}^\dagger c_{k_2\uparrow} - c_{k_1\downarrow}^\dagger c_{k_2\downarrow} \right) + S_d^+ c_{k_1\downarrow}^\dagger c_{k_2\uparrow} + S_d^- c_{k_1\uparrow}^\dagger c_{k_2\downarrow} \right] \tag{1.114}$$

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

$$T = V + VG_0V \tag{1.115}$$

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

1.10.1 First order scattering

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

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

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

$$T_{\text{nonflip}}^{(1)} = T_{k_\uparrow,d_\sigma\to q_\uparrow,d_\sigma} = \langle q_\uparrow, d_\sigma| V |k_\uparrow, d_\sigma\rangle = m_d J \tag{1.116}$$

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

$$\mathcal{P}_{k_\sigma,d_{\sigma'}\to q_\sigma,d_{\sigma'}} = 2\pi \sum_\epsilon \rho(\epsilon) T_{k_\uparrow,d_\sigma\to q_\uparrow,d_\sigma}^2 = 2\pi\rho(0)J^2 m_d^2 \tag{1.117}$$

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

$$\mathcal{P}_1 = 2\pi\rho(0)J^2 m_d^2 \tag{1.118}$$

For spin-flip, the matrix element is

$$T_{\text{flip}}^{(1)} = T_{k_\uparrow,d_\downarrow\to q_\downarrow,d_\uparrow} = \langle q_\downarrow, d_\uparrow| V |k_\uparrow, d_\downarrow\rangle = \lambda_+ J \tag{1.119}$$

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

$$\mathcal{P}_2 = \mathcal{P}_{k_\uparrow,d_\downarrow\to q_\downarrow,d_\uparrow} = 2\pi\rho(0)J \left[s_d(s_d+1) - m_d(m_d+1) \right] \tag{1.120}$$

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

$$\mathcal{P}^{(1)} = \frac{1}{2s_d+1} \sum_{m_d=-s_d}^{s_d} (\mathcal{P}_1 + \mathcal{P}_2) = \frac{2\pi\rho(0)J^2}{(2s_d+1)} \sum_{m_d=-s_d}^{s_d} (s_d(s_d+1) - m_d)$$
$$= 2\pi\rho(0)J^2 s_d(s_d+1) \tag{1.121}$$

1.10.2 Second order scattering

$$
\text{no-impurity-flip}\begin{cases} |k\uparrow,d_\sigma\rangle \to |q\uparrow,d_\sigma\rangle \to |k'\uparrow,d_\sigma\rangle \\ |k\uparrow,q\uparrow,d_\sigma\rangle \to |k\uparrow,k'\uparrow,d_\sigma\rangle \to |k'\uparrow,q\uparrow,d_\sigma\rangle \end{cases}
$$

$$
\text{pro-impurity-flip}\begin{cases} |k\uparrow,d_\downarrow\rangle \to |q\downarrow,d_\uparrow\rangle \to |k'\uparrow,d_\downarrow\rangle \\ |k\uparrow,q\downarrow,d_\uparrow\rangle \to |k\uparrow,k'\uparrow,d_\downarrow\rangle \to |k'\uparrow,q\downarrow,d_\uparrow\rangle \end{cases}
$$

$$
\left.\phantom{\begin{cases}a\\b\\c\\d\end{cases}}\right\}\text{no-cond-flip}
$$

$$
\text{flip-first}\begin{cases} |k\uparrow,d_\downarrow\rangle \to |q\downarrow,d_\uparrow\rangle \to |k'\downarrow,d_\uparrow\rangle \\ |k\uparrow,q\uparrow,d_\downarrow\rangle \to |k\uparrow,k'\downarrow,d_\uparrow\rangle \to |k'\downarrow,q\uparrow,d_\uparrow\rangle \end{cases}
$$

$$
\text{flip-later}\begin{cases} |k\uparrow,d_\downarrow\rangle \to |q\uparrow,d_\downarrow\rangle \to |k'\downarrow,d_\uparrow\rangle \\ |k\uparrow,q\downarrow,d_\downarrow\rangle \to |k\uparrow,k'\downarrow,d_\downarrow\rangle \to |k'\downarrow,q\downarrow,d_\uparrow\rangle \end{cases}
$$

$$
\left.\phantom{\begin{cases}a\\b\\c\\d\end{cases}}\right\}\text{pro-cond-flip}
$$

The second order transition matrix contribution is of the form

$$
T^{(2)}_{i\to j} = \langle j|\,V G_0 V\,|i\rangle = \sum_l \frac{\langle j|\,V\,|l\rangle\,\langle l|\,V\,|i\rangle}{E_i - E_l} \tag{1.122}
$$

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:

$$
\begin{aligned}
T^{(2)}_{11} &= \sum_q \frac{\langle k'_\uparrow d_\sigma|\,V\,|q_\uparrow d_\sigma\rangle\,\langle q_\uparrow d_\sigma|\,V\,|k_\uparrow d_\sigma\rangle}{\epsilon_k - \epsilon_q} \\
&= (Jm_d)^2 \sum_q \frac{1-P(q)}{\epsilon_k - \epsilon_q} = J^2 m_d^2 \sum_q \frac{1-P(q)}{\epsilon_k - \epsilon_q}
\end{aligned} \tag{1.123}
$$

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,

$$
T^{(2)}_{12} = \sum_q \frac{\langle q_\uparrow k'_\uparrow d_\sigma|\,V\,|k'_\uparrow k_\uparrow d_\sigma\rangle\,\langle k'_\uparrow k_\uparrow d_\sigma|\,V\,|q_\uparrow k_\uparrow d_\sigma\rangle}{\epsilon_q - \epsilon_{k'}}P(q) \tag{1.124}
$$

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

$$
T^{(2)}_{12} = -J^2 m_d^2 \sum_q \frac{P(q)}{\epsilon_q - \epsilon_k} = J^2 m_d^2 \sum_q \frac{P(q)}{\epsilon_k - \epsilon_q} \tag{1.125}
$$

For the third process,

$$
T^{(2)}_{13} = \sum_q \frac{\langle k'_\uparrow d_\downarrow|\,V\,|q_\downarrow d_\uparrow\rangle\,\langle q_\downarrow d_\uparrow|\,V\,|k_\uparrow d_\downarrow\rangle}{\epsilon_k - \epsilon_q} \tag{1.126}
$$

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

$$
T^{(2)}_{13} = \lambda_+^2 J^2 \sum_q \frac{1-P(q)}{\epsilon_k - \epsilon_q} \tag{1.127}
$$

20

For the fourth process,

$$T_{14}^{(2)} = \sum_q \frac{\langle q_\downarrow k'_\uparrow d_\uparrow | V | k'_\uparrow k_\uparrow d_\downarrow \rangle \langle k'_\uparrow k_\uparrow d_\downarrow | V | q_\downarrow k_\uparrow d_\uparrow \rangle}{\epsilon_q - \epsilon'_k}$$

$$= -\lambda_-^2 J^2 \sum_q \frac{P(q)}{\epsilon_q - \epsilon_k} \tag{1.128}$$

$$= \lambda_-^2 J^2 \sum_q \frac{P(q)}{\epsilon_k - \epsilon_q}$$

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

$$T_{\text{nonflip}}^{(2)} = \sum_{i=1}^{4} T_{1i}^{(2)} = J^2 \sum_q \frac{m_d^2 + \lambda_+^2 - P(q)\left(\lambda_+^2 - \lambda_-^2\right)}{\epsilon_k - \epsilon_q}$$

$$= J^2 \sum_q \frac{s(s+1) - m_d + 2m_d P(q)}{\epsilon_k - \epsilon_q} \tag{1.129}$$

$$= J^2 \left[s(s+1) - m_d\right](\alpha + \gamma) + 2J^2 m_d \gamma$$

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.

$$T_{\text{nonflip}}^{(2)} = 2J^2 m_d \gamma$$

$$= 2J^2 m_d \int d\epsilon N(\epsilon) \frac{P(\epsilon)}{\epsilon_k - \epsilon} = \frac{\sqrt{2} J^2 m_d m^{\frac{3}{2}}}{\pi^2 \hbar^3} \int d\epsilon \frac{\sqrt{\epsilon} P(\epsilon)}{\epsilon_k - \epsilon} \tag{1.130}$$

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

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

$$= \frac{\sqrt{2} J^2 m_d m^{\frac{3}{2}}}{\pi^2 \hbar^3} \sqrt{\epsilon_k} \ln \left| \frac{\epsilon_k + \epsilon_F + 2\sqrt{\epsilon_k \epsilon_F}}{\epsilon_k - \epsilon_F} \right| \tag{1.131}$$

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 $\epsilon_k = \epsilon_F$.

$$T_{\text{nonflip}}^{(2)} = \frac{\sqrt{2} J^2 m_d m^{\frac{3}{2}}}{\pi^2 \hbar^3} \sqrt{\epsilon_F} \ln \left| \frac{4T_F}{T} \right| \tag{1.132}$$

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

$$T_{\text{nonflip}}^{(2)} = 2J^2 m_d N(\epsilon_F) \ln \left| \frac{T_F}{T} \right| \tag{1.133}$$

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

$$T_{\text{nonflip}} = J m_d \left[1 + 2N(\epsilon_F) J \ln \frac{T_F}{T}\right] \tag{1.134}$$

21

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

$$T_{21}^{(2)} = -J^2(m_d+1)\lambda_+ \sum_q \frac{1-P_q}{\epsilon_k - \epsilon_q}$$

$$T_{23}^{(2)} = J^2 m_d \lambda_+ \sum_q \frac{1-P_q}{\epsilon_k - \epsilon_q}$$

$$T_{22}^{(2)} = J^2(m_d+1)\lambda_+ \sum_q \frac{P(q)}{\epsilon_k - \epsilon_q}$$

(1.135)

$$T_{24}^{(2)} = -\lambda_+ m_d J^2 \sum_q \frac{P(q)}{\epsilon_k - \epsilon_q}$$

$$T_{\text{flip}}^{(2)} = -J^2 \lambda_+ \left(\alpha - \gamma\right) \tag{1.136}$$

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

$$T_{\text{flip}}^{(2)} = 2J^2 \lambda_+ \sum_q \frac{P(q)}{\epsilon_k - \epsilon_q}$$

$$= 2J^2 \lambda_+ N(\epsilon_F) \ln\left|\frac{T_F}{T}\right| \tag{1.137}$$

Adding the first order contribution,

$$T_{\text{flip}} = \lambda_+ J \left[1 + 2N(\epsilon_F)J\ln\frac{T}{T_F}\right] \tag{1.138}$$

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

$$\mathcal{P} = \mathcal{P}^{(2)} \left[1 + 2JN(\epsilon_F)\ln\frac{T_F}{T}\right] \tag{1.139}$$

1.11   The Kondo resonance

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

$$T_{a\to b} = \sum_{s,m_s} |\langle s, m_s|a\rangle|^2 T_s \tag{1.140}$$

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

$$T_{|k\uparrow,d_\uparrow\rangle \to |k'\uparrow d_\uparrow\rangle} = T_1 \tag{1.141}$$

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

$$T_{|k\uparrow,d_\downarrow\rangle \to |k'\uparrow d_\downarrow\rangle} = \frac{T_1 + T_0}{2} \tag{1.142}$$

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

$$T_{|k\uparrow,d_\downarrow\rangle \to |k'\downarrow d_\uparrow\rangle} = \frac{T_1 - T_0}{2} \tag{1.143}$$

22

Therefore,

$$T_1 = T_{|k\uparrow,d_\downarrow\rangle \to |k'\uparrow d_\downarrow\rangle} + T_{|k\uparrow,d_\downarrow\rangle \to |k'\downarrow d_\uparrow\rangle} = T_{\text{nonflip}} + T_{\text{flip}}$$
$$T_0 = T_{|k\uparrow,d_\downarrow\rangle \to |k'\uparrow d_\downarrow\rangle} - T_{|k\uparrow,d_\downarrow\rangle \to |k'\downarrow d_\uparrow\rangle} = T_{\text{nonflip}} - T_{\text{flip}} \tag{1.144}$$

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

$$T_{\text{nonflip}} = J\left[m_d + \frac{J}{4}\left\{3(\alpha + \gamma) + 4m_d(\gamma - \alpha)\right\}\right] \tag{1.145}$$

$$T_{\text{flip}} = J\left[1 + J(\gamma - \alpha)\right] \tag{1.146}$$

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

$$T_1 = \frac{J}{2}\left[1 + \frac{J}{2}(\alpha + 5\gamma)\right]$$
$$T_0 = -\frac{3J}{2}\left[1 - \frac{3J}{2}\left(\alpha - \frac{\gamma}{3}\right)\right] \tag{1.147}$$

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

$$J\vec{S}_d \cdot \vec{\sigma}_e = 2J\vec{S}_d \cdot \vec{S}_e = J\left(S^2 - S_d^2 - S_e^2\right) = J\left(s(s+1) - \frac{3}{2}\right) = \begin{cases} -\frac{3J}{2} & \text{(singlet)} \\ \frac{J}{2} & \text{(triplet)} \end{cases} \tag{1.148}$$

Hence, the pre-factors are just the bare values of the interaction Hamiltonian, V. Hence, the equations 1.147 can be written as

$$T = V(1 + TG) \tag{1.149}$$

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

$$T_1 = \frac{J}{2}\left[1 + T_1(\alpha + 5\gamma)\right] \implies T_1 = \frac{J/2}{1 - \frac{J}{2}(\alpha + 5\gamma)}$$
$$T_0 = -\frac{3J}{2}\left[1 + T_0\left(\alpha - \frac{\gamma}{3}\right)\right] \implies T_0 = \frac{-3J/2}{1 + \frac{3J}{2}(\alpha - \gamma/3)} \tag{1.150}$$

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

$$T_1 = \frac{1}{2/J - 5\gamma - \alpha} \tag{1.151}$$

$$T_0 = \frac{1}{-2/3J + \gamma/2 - \alpha} \tag{1.152}$$

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

$$T_s = \frac{1}{\text{real part} + i\pi N(0)} \tag{1.153}$$

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

$$|T_s| \leq \frac{1}{\pi N_0} \tag{1.154}$$

From eq. 1.13, we can write

$$T_s = -\frac{e^{i\delta_s}\sin\delta_s}{\pi N(0)} \tag{1.155}$$

23

Eq. 1.60 allows us to write

$$\rho_{d\sigma}(0) = -\frac{\text{Im}[T]}{t^2\pi} = \frac{\sin^2\delta_s}{t^2\pi^2 N(0)} = \frac{\sin^2\delta_s}{\pi\Delta} = \frac{1}{\pi\Delta}\sin^2\left(\frac{\pi n_c}{2}\right) \tag{1.156}$$

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, 1.72,

$$\rho_{d\sigma}(0) = \frac{1}{\pi\Delta}\left[1 + \left(\frac{\epsilon_d + U n_c}{\Delta}\right)^2\right]^{-1} \tag{1.157}$$

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. 1.150 can be written as

$$T_1 = \frac{J/2}{1 - 2J\gamma - \frac{J}{2}(\alpha + \gamma)} \tag{1.158}$$

$$T_0 = \frac{-3J/2}{1 - 2J\gamma + \frac{3J}{2}(\alpha + \gamma)} \tag{1.159}$$

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

$$T_1 = \frac{1}{\frac{2}{J_{\text{eff}}} - (\alpha + \gamma)}$$
$$T_0 = \frac{-1}{\frac{2}{3J_{\text{eff}}} + \alpha + \gamma} \tag{1.160}$$

$\alpha + \gamma$ can be calculated as

$$\alpha + \gamma = \lim_{\eta \to 0} \int_0^\infty d\epsilon \frac{N(\epsilon)}{\epsilon_k - \epsilon + i\eta}$$
$$\sim \lim_{\epsilon_{\text{up}} \to \infty} \ln\left|\frac{\sqrt{\epsilon_k} - \sqrt{\epsilon_{\text{up}}}}{\sqrt{\epsilon_k} + \sqrt{\epsilon_{\text{up}}}}\right| - i\pi N(0) \tag{1.161}$$

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

$$\left|\frac{\sqrt{\epsilon_k} - \sqrt{\epsilon_{\text{up}}}}{\sqrt{\epsilon_k} + \sqrt{\epsilon_{\text{up}}}}\right| \approx \left|\frac{-\sqrt{\epsilon_{\text{up}}}}{\sqrt{\epsilon_{\text{up}}}}\right| = 1 \tag{1.162}$$

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

$$T_1 = \frac{1}{2J_{\text{eff}}^{-1} + i\pi N(0)} \sim \frac{1}{\frac{2}{\pi N(0) J_{\text{eff}}} + i} \tag{1.163}$$

Since

$$T_s \sim e^{i\delta_s}\sin\delta_s = \frac{1}{\cot\delta_s - i} \tag{1.164}$$

we can write

$$\cot\delta_1 = -\frac{2}{\pi N(0) J_{\text{eff}}} \implies \tan\delta_1 = -\frac{\pi}{2}N(0)J_{\text{eff}} \tag{1.165}$$

Similarly,

$$T_0 = \frac{-1}{\frac{2}{3J_{\text{eff}}} - i\pi N(0)} \sim \frac{-1}{\frac{2}{3J_{\text{eff}}\pi N(0)} - i} \tag{1.166}$$

giving

$$\cot \delta_0 = \frac{2}{3J_{\text{eff}}\pi N(0)} \implies \tan \delta_0 = \frac{3\pi}{2} J_{\text{eff}} N(0) \tag{1.167}$$

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

$$\psi \sim \psi_{\text{in}} - e^{2i\delta_d}\psi_{\text{out}} \tag{1.168}$$

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,

$$\psi = \frac{e^{i\delta}}{r} \left(e^{-i(k_F r + \delta_d)} - e^{i(k_F r + \delta_d)} \right) \sim \frac{e^{i\delta}}{r} \sin\left[k_F \left(r + \Delta r \right) \right] \tag{1.169}$$

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.

1.12   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 $E = 0$:

$$\Sigma(E) = \Sigma(0) + E\frac{\mathrm{d}\Sigma}{\mathrm{d}E}\bigg|_{E=0} + O(E^2) \tag{1.170}$$

Defining

$$Z^{-1} \equiv 1 - \frac{\mathrm{d}\Sigma}{\mathrm{d}E}\bigg|_{E=0} \tag{1.171}$$

we can write

$$\Sigma(E) = \Sigma(0) + \left(1 - Z^{-1}\right) E \tag{1.172}$$

The interacting Green's function for the impurity becomes

$$G_d(E) = \frac{1}{E - \epsilon_d - \Sigma - i\Delta} \tag{1.173}$$

where Δ is the result of the hybridisation. Substituting eq. 1.172 and gathering the terms gives

$$G_d(E) = \frac{Z}{E - Z(\epsilon_d + \Sigma(0)) - iZ\Delta} \tag{1.174}$$

Defining the renormalised parameters

$$\epsilon_d^* = Z(\epsilon_d + \Sigma(0)) \tag{1.175}$$
$$\Delta^* = Z\Delta \tag{1.176}$$

we have

$$G_d(E) = \frac{Z}{E - \epsilon_d^* - i\Delta^*} \tag{1.177}$$

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

$$Z = 1, \Sigma = 0 \implies \epsilon_d^* = \epsilon_d, \Delta^* = \Delta \tag{1.178}$$

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

$$\delta_d(0) = \cot^{-1} \frac{\epsilon_d^*}{\Delta^*} \tag{1.179}$$

Similarly, the renormalised version of eq. 1.52 is

$$\rho_d(0) = \frac{1}{\pi} \frac{\Delta^*}{\epsilon_d^{*2} + \Delta^{*2}} \tag{1.180}$$

Using eq. 1.179 gives

$$\rho_d(0) = \frac{1}{\pi} \frac{\Delta^*}{\Delta^{*2} \cot^2 \delta_d + \Delta^{*2}} = \frac{\sin^2 \delta_d}{\pi \Delta} \tag{1.181}$$

1.13   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,

$$H_K = \sum_{k>k_F} \epsilon_k n_k - \frac{3J}{2} \sum_{k,k'>k_F} c_{k'\sigma}^\dagger c_{k\sigma} \tag{1.182}$$

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

$$b_k^\dagger = \frac{1}{\sqrt{2}} \left(c_{k\uparrow}^\dagger c_{d\downarrow}^\dagger - c_{k\downarrow}^\dagger c_{d\uparrow}^\dagger \right) \tag{1.183}$$

Hence the total wavefunction of singlet+Fermi-sea is

$$|\Psi\rangle = \sum_{k>k_F} a_k b_k^\dagger |\Phi\rangle = |\Phi\rangle \otimes \sum_{k>k_F} a_k |S_k\rangle \tag{1.184}$$

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

$$a_q = \langle\Phi| \langle S_q| \sum_k a_k |S_k\rangle |\Phi\rangle = \langle\Phi| b_q |\Psi\rangle \tag{1.185}$$

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

$$E |\Psi\rangle = H_K |\Psi\rangle = |\Phi\rangle \otimes H_k \sum_{k>k_F} a_k |S_k\rangle$$

$$= |\Phi\rangle \otimes \sum_{k>k_F} a_k \left(\epsilon_k |S_k\rangle - \frac{3J}{2} \sum_{k'>k_F} |S_{k'}\rangle \right) \tag{1.186}$$

$$= \sum_{k>k_F} a_k \left(\epsilon_k b_k^\dagger - \frac{3J}{2} \sum_{k'>k_F} b_{k'}^\dagger \right) |\Phi\rangle$$

Multiplying b_q from left gives

$$Eb_q \left| \Psi \right> = \epsilon_q a_q \left| \Phi \right> - \frac{3J}{2} \sum_{k>k_F} a_k \left| \Phi \right> \tag{1.187}$$

Multiplying $\left< \Phi \right|$ from left and looking at eq. 1.185 gives

$$E \left< \Phi \right| b_q \left| \Psi \right> = Ea_q = a_q \epsilon_q - \frac{3J}{2} \sum_k a_k$$

$$\implies a_q = \frac{3J/2}{\epsilon_q - E} \sum_k a_k \tag{1.188}$$

$$\implies \sum_q a_q = \sum_q \frac{3J/2}{\epsilon_q - E} \sum_k a_k$$

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

$$1 = \frac{3J}{2} \sum_{q>k_F} \frac{1}{\epsilon_q - E} \tag{1.189}$$

Converting to integral,

$$1 = \frac{3J}{2} \int_{\epsilon_F}^{D} d\epsilon \frac{N(\epsilon)}{\epsilon - E} \tag{1.190}$$

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

$$\frac{2}{3JN(0)} = \ln \left| \frac{D-E}{\epsilon_F - E} \right| \approx \ln \left| \frac{D}{\epsilon_F - E} \right| \tag{1.191}$$

$$\implies E = \epsilon_F - De^{-\frac{2}{3N(0)J}}$$

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

$$E_b = De^{-\frac{2}{3N(0)J}} \tag{1.192}$$

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

$$k_B T_k \sim E_b \implies T_K = \frac{D}{k_B} e^{-\frac{2}{3N(0)J}} \tag{1.193}$$

1.14 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

$$T^{(2)} = VG_0V \tag{1.194}$$

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 $V \to V' = V + \Delta V$. The interaction part is

$$H' = J_z \sum_{k_1,k_2} S_d^z \left(c_{k_1\uparrow}^\dagger c_{k_2\uparrow} - c_{k_1\downarrow}^\dagger c_{k_2\downarrow} \right) + J_T \sum_{k_1,k_2} \left(S_d^+ c_{k_1\downarrow}^\dagger c_{k_2\uparrow} + S_d^- c_{k_1\uparrow}^\dagger c_{k_2\downarrow} \right) \tag{1.195}$$

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.

1.14.1   Renormalization of J_z

First consider the process

$$k \uparrow, d \downarrow \to q \downarrow d \uparrow \to k' \uparrow d \downarrow \tag{1.196}$$

The $T-$matrix term is

$$T_1 = J_T^2 \sum_q S_d^- c_{k'\uparrow}^\dagger c_{q\downarrow} \frac{1}{E - H_0} S_d^+ c_{q\downarrow}^\dagger c_{k\uparrow} \tag{1.197}$$

Using eq. 1.16, we can write

$$(E - H_0)^{-1} c_{q\downarrow}^\dagger c_{k\uparrow} = c_{q\downarrow}^\dagger c_{k\uparrow} (E - \lambda - H_0)^{-1} \tag{1.198}$$

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

$$T_1 = J_T^2 S_d^- S_d^+ \sum_q c_{k'\uparrow}^\dagger c_{q\downarrow} c_{q\downarrow}^\dagger c_{k\uparrow} (E - \epsilon_q + \epsilon_k - H_0)^{-1} \tag{1.199}$$

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

$$T_1 = J_T^2 S_d^- S_d^+ c_{k'\uparrow}^\dagger c_{k\uparrow} \sum_q (E - \epsilon_q + \epsilon_k - H_0)^{-1} \tag{1.200}$$

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

$$\sum_q (E - \epsilon_q + \epsilon_k - H_0)^{-1} = N|\delta D| \frac{1}{E - D + \epsilon_k} \tag{1.201}$$

N is the density of states. Also,

$$S^- S^+ = (S^x - iS^y)(S^x + iS^y) = \frac{1}{2} + i \left[S^x, S^y \right] = \frac{1}{2} - S^z \tag{1.202}$$

Putting it all together,

$$T_1 = J_T^2 \left(\frac{1}{2} - S_d^z \right) N|\delta D| c_{k'\uparrow}^\dagger c_{k\uparrow} \frac{1}{E - D + \epsilon_k} \tag{1.203}$$

For the second possible scattering,

$$q \downarrow k \uparrow d \uparrow \to k' \uparrow k \uparrow d \downarrow \to k' \uparrow q \downarrow d \uparrow \tag{1.204}$$

we get

$$T_2 = J_T^2 \sum_q S_d^+ S_d^- c_{q\downarrow}^\dagger c_{k\uparrow} \frac{1}{E - H_0} c_{k'\uparrow}^\dagger c_{q\downarrow} \tag{1.205}$$

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

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

$$= -J_T^2 \left(\frac{1}{2} + S_d^z\right) N|\delta D| c_{k'\uparrow}^\dagger c_{k\uparrow} \frac{1}{E - D - \epsilon_{k'}} \tag{1.206}$$

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 $\downarrow$:

$$k\downarrow, d\uparrow \rightarrow q\uparrow d\downarrow \rightarrow k'\downarrow d\uparrow \tag{1.207}$$

$$q\uparrow k\downarrow d\downarrow \rightarrow k'\downarrow k\downarrow d\uparrow \rightarrow k'\downarrow q\uparrow d\downarrow \tag{1.208}$$

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

$$T_3 = J_T^2 \left(\frac{1}{2} + S_d^z\right) N|\delta D| c_{k'\downarrow}^\dagger c_{k\downarrow} \frac{1}{E - D + \epsilon_k} \tag{1.209}$$

$$T_4 = -J_T^2 \left(\frac{1}{2} - S_d^z\right) N|\delta D| c_{k'\downarrow}^\dagger c_{k\downarrow} \frac{1}{E - D - \epsilon_{k'}} \tag{1.210}$$

The total second order contribution is

$$T^{(2)} = -J_T^2 S_d^z N|\delta D| \left(\frac{1}{E - D + \epsilon_k} + \frac{1}{E - D - \epsilon_{k'}}\right) \left(c_{k'\uparrow}^\dagger c_{k\uparrow} - c_{k'\downarrow}^\dagger c_{k\downarrow}\right) \tag{1.211}$$

Comparing this with the S_d^z term in the Hamiltonian

$$J_z S_d^z \left(c_{k'\uparrow}^\dagger c_{k\uparrow} - c_{k'\downarrow}^\dagger c_{k\downarrow}\right) \tag{1.212}$$

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

$$\delta J_d^z = -J_T^2 N|\delta D| \left(\frac{1}{E - D + \epsilon_k} + \frac{1}{E - D - \epsilon_{k'}}\right) \tag{1.213}$$

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

$$\frac{dJ_d^z}{dD} = -J_T^2 N \frac{2}{D} \tag{1.214}$$

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

1.14.2 Renormalization of J_T

Consider the scattering

$$k\uparrow d\downarrow \rightarrow q\downarrow d\uparrow \rightarrow k'\downarrow d\uparrow \tag{1.215}$$

$$T_1 = -J_T J_z S_d^z S_d^+ N|\delta D| c_{k'\downarrow}^\dagger c_{k\uparrow} \frac{1}{E - D + \epsilon_k} \tag{1.216}$$

The minus sign at the front comes from the term

$$-S_d^z c_{k'\downarrow}^\dagger c_{q\downarrow} \tag{1.217}$$

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

$$T_1 = -J_T J_z \frac{S_d^+}{2} N |\delta D| c_{k'\downarrow}^\dagger c_{k\uparrow} \frac{1}{E - D + \epsilon_k} \tag{1.218}$$

The second process is

$$q \uparrow k \uparrow d \downarrow \rightarrow k' \downarrow k \uparrow d \uparrow \rightarrow q \uparrow k' \downarrow d \uparrow \tag{1.219}$$

$$T_2 = -J_T J_z \frac{S_d^+}{2} N |\delta D| c_{k'\downarrow}^\dagger c_{k\uparrow} \frac{1}{E - D - \epsilon_{k'}} \tag{1.220}$$

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

$$+S_d^z c_{k'\uparrow}^\dagger c_{q\uparrow} \tag{1.221}$$

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

$$-S_d^z c_{k'\downarrow}^\dagger c_{q\downarrow} \tag{1.222}$$

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 proces.

$$T_3 = T_1 \tag{1.223}$$
$$T_4 = T_2 \tag{1.224}$$

The total contribution is

$$T^{(2)} = -J_T J_z S_d^+ N |\delta D| c_{k'\downarrow}^\dagger c_{k\uparrow} \left(\frac{1}{E - D - \epsilon_{k'}} + \frac{1}{E - D + \epsilon_k} \right) \tag{1.225}$$

Comparing with the S_d^+ term in the Hamiltonian

$$J_T S_d^+ c_{k'\downarrow}^\dagger c_{k\uparrow} \tag{1.226}$$

we can write

$$\delta J_T = -J_T J_z N |\delta D| \left(\frac{1}{E - D - \epsilon_{k'}} + \frac{1}{E - D + \epsilon_k} \right) \tag{1.227}$$

Again neglecting the terms in the denominator, we get

$$\frac{\mathrm{d}J_T}{\mathrm{d}D} = -J_T J_z N \frac{2}{D} \tag{1.228}$$

This is the scaling equation for J_T.

1.14.3 Flow of the couplings

Switching to the dimensionless couplings

$$g_1 = N J_z, g_2 = N J_T \tag{1.229}$$

the equations become

$$\frac{\mathrm{d}g_1}{\mathrm{d}D} = -\frac{2g_2^2}{D} \tag{1.230}$$

30

$$\frac{\mathrm{d}g_2}{\mathrm{d}D} = -\frac{2g_1 g_2}{D} \tag{1.231}$$

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

$$\frac{\mathrm{d}g_1}{\mathrm{d}g_2} = \frac{g_2}{g_1} \implies g_1^2 - g_2^2 = \text{constant} \tag{1.232}$$

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 $g_2 \to -g_2$, 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

$$g(D') = \frac{g_0}{1 - 2g_0 \ln \frac{D}{D'}}$$
$$\implies 2g(D') = \frac{1}{\ln \frac{D'}{T_K}} \tag{1.233}$$

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. 1.193, 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.

$$g(D') = \frac{g_0}{1 - 2g_0 \ln \frac{D}{D'}} = -\frac{|g_0|}{1 + 2|g_0| \ln \frac{D}{D'}} \tag{1.234}$$

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

1.14.4 Alternate way of obtaining the scaling equations

From eq. 1.98, the interaction part can be written as

$$\Delta H_{ll'} = \frac{1}{2} \left[T_{ll'}(E_l) + T_{ll'}(E_{l'}) \right] \tag{1.235}$$

where the transition matrix T is

$$T_{ll'}(E) = \sum_H \frac{V_{lH} V_{Hl'}}{E - E_H} \tag{1.236}$$

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

$$V = J\vec{S}_d \cdot \sum_{k,k',\alpha,\alpha'} c_{k\alpha}^\dagger \vec{\sigma}_{\alpha\alpha'} c_{k'\alpha'} \tag{1.237}$$

The first process is

$$ka \xrightarrow{\;\sigma^b\;} q\lambda \xrightarrow{\;\sigma^a\;} k'\beta \tag{1.238}$$

$$d\sigma \xrightarrow{\;S_d^b\;} d\sigma'' \xrightarrow{\;S_d^a\;} d\sigma' \tag{1.239}$$

The transition matrix element is

$$
\begin{aligned}
T_1 &= \sum_{q\in\{D-\delta D\},\lambda,\sigma''} \langle k'\beta,\sigma'|\,V\,|q\lambda,\sigma''\rangle \langle q\lambda,\sigma''|\,V\,|k\alpha,\sigma\rangle \frac{1}{E-E_q} \\
&= J^2 \sum_{\sigma''} (S_d^a)_{\sigma'\sigma''} (S_d^b)_{\sigma''\sigma} \sum_{\lambda} (\sigma^a)_{\beta\lambda}(\sigma^b)_{\lambda\alpha} \sum_{q\in\{D-\delta D\}} \frac{1}{E-E_q} \\
&\approx J^2 (S_d^a S_d^b)_{\sigma'\sigma} (\sigma^a\sigma^b)_{\beta\alpha} \frac{N|\delta D|}{E-D}
\end{aligned}
\tag{1.240}
$$

The second process is

$$ka \xrightarrow{\quad\quad} k\alpha \xrightarrow{\;\sigma^a\;} q\lambda \tag{1.241}$$

$$q\lambda \xrightarrow{\;\sigma^b\;} k'\beta \xrightarrow{\quad\quad} k'\beta \tag{1.242}$$

$$d\sigma \xrightarrow{\;S_d^b\;} d\sigma'' \xrightarrow{\;S_d^a\;} d\sigma' \tag{1.243}$$

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

$$
\begin{aligned}
T_2 &= \sum_{q\in\{D-|\delta D|\},\lambda,\sigma''} \langle q\lambda, k'\beta,\sigma'|\,V\,|k'\beta, k\alpha,\sigma''\rangle \langle k'\beta, k\alpha,\sigma''|\,V\,|q\lambda, k\alpha,\sigma\rangle \frac{1}{E-(E_k+E_{k'}-E_q)} \\
&\approx -J^2 (S_d^a S_d^b)_{\sigma'\sigma}(\sigma^b\sigma^a)_{\beta\alpha}\frac{N|\delta D|}{E-D}
\end{aligned}
\tag{1.244}
$$

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

$$
\begin{aligned}
T &= \frac{J^2 N|\delta D|}{D}(S_d^a S_d^b)_{\sigma'\sigma}[\sigma^b,\sigma^a]_{\beta\alpha} \\
&= \frac{J^2 N|\delta D|}{2D}[S_d^a,S_d^b]_{\sigma'\sigma}[\sigma^b,\sigma^a]_{\beta\alpha}
\end{aligned}
\tag{1.245}
$$

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

$$
\begin{aligned}
[S_d^a,S_d^b]_{\sigma'\sigma}[\sigma^b,\sigma^a]_{\beta\alpha} &= -[S_d^a,S_d^b]_{\sigma'\sigma}[\sigma^a,\sigma^b]_{\beta\alpha} \\
&= -i\epsilon_{abc}S_{\sigma\sigma'}^c 2i\epsilon_{abd}\sigma_{\beta\alpha}^d \\
&= 4\delta_{cd}S_{\sigma\sigma'}^c \sigma_{\beta\alpha}^d \\
&= 4\vec{S}_{\sigma\sigma'}\cdot\vec{\sigma}_{\beta\alpha}
\end{aligned}
\tag{1.246}
$$

Therefore,

$$T = \frac{2J^2 N|\delta D|}{D}\vec{S}_{\sigma\sigma'}\cdot\vec{\sigma}_{\beta\alpha} \tag{1.247}$$

The correction to the coupling J can be read off:

$$J(D-\delta D) = J(D) - \frac{2J^2 N\delta D}{D} \tag{1.248}$$

This gives the same scaling equations we found earlier.

1.15 Universality

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

$$\frac{\partial g}{\partial \ln D} = -2g^2 + 2g^3 \tag{1.249}$$

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

$$\ln \frac{D'}{D} = -\int_{g_0}^{g} \frac{dg}{2g^2 - 2g^3} = -\int_{g_0}^{g} \frac{dg}{2g^2}(1+g) \tag{1.250}$$

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

$$\ln \frac{k_B T_K}{D} = -\int_{g_0}^{1} \frac{dg}{2g^2}(1+g) = -\frac{1}{2g_0} + \frac{1}{2}\ln g_0 + O(1)$$
$$= -\frac{1}{2g_0} + \frac{1}{2}\ln 2g_0 + O(1) \tag{1.251}$$

This gives a better estimate of the Kondo temperature

$$T_K = \frac{D}{k_B}\sqrt{2g_0}\exp\left(-\frac{1}{2g_0}\right) \tag{1.252}$$

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

$$k_B T_K = D y(g) \tag{1.253}$$

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

$$\frac{\mathrm{d}T_K}{\mathrm{d}D} = 0 \tag{1.254}$$

Substituting the form of T_K, eq. 1.253, in this equation gives

$$y(g) + D\frac{\mathrm{d}y(g)}{\mathrm{d}D} = 0$$
$$\implies y + D\frac{\mathrm{d}y}{\mathrm{d}g}\frac{\mathrm{d}g}{\mathrm{d}D} = 0$$
$$\implies y - 2g^2\frac{\mathrm{d}y}{\mathrm{d}g} = 0 \tag{1.255}$$
$$\implies y = e^{-\frac{1}{2g}}$$

This gives almost the same solution as eq. 1.252:

$$T_K = \frac{D}{k_B}e^{-\frac{1}{2g}} \tag{1.256}$$

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. 1.233, up to second order, we can write

$$g(D') = g_0\left(1 + 2g_0^2\ln\frac{D}{D'}\right) \tag{1.257}$$

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

$$g_0 \to g = g_0 \left(1 + 2g_0 \ln \frac{T_F}{T} \right) \tag{1.258}$$

Since $g \equiv NJ$, we have recovered eq. 1.139. Since eq. 1.139 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.

1.16   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 [11]. For example,

$$S^z = \frac{\sigma^z}{2} = \sum_{ij} c_i^\dagger \frac{\sigma_{ij}^z}{2} c_j = \frac{1}{2} \left(c_\uparrow^\dagger c_\uparrow - c_\downarrow^\dagger c_\downarrow \right) \tag{1.259}$$

Similarly,

$$S^x = \frac{1}{2} \left(c_\uparrow^\dagger c_\downarrow + c_\downarrow^\dagger c_\uparrow \right)$$
$$S^y = \frac{-i}{2} \left(c_\uparrow^\dagger c_\downarrow - c_\downarrow^\dagger c_\uparrow \right) \tag{1.260}$$

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

$$|\uparrow\rangle = c_\uparrow^\dagger |0\rangle \tag{1.261}$$

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 [12]

$$\mu = -i\frac{\pi}{2}k_B T \tag{1.262}$$

The new Hamiltonian is

$$\widetilde{H} = H - \mu(n_d - 1) \tag{1.263}$$

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

$$Z = \text{Tr} \left[\exp\left(-\beta H \right) \right] = \sum_{\sigma_d = \uparrow, \downarrow} \sum_k \left[\exp\left(-\beta H \right) \right] \tag{1.264}$$

The modified partition function is

$$\begin{aligned}
\widetilde{Z} &= \text{Tr} \left[\exp\left(-\beta \left(H - \mu(n_d - 1) \right) \right) \right] \\
&= \text{Tr} \left[\exp\left(-\beta H - i\frac{\pi}{2}(n_d - 1) \right) \right] \\
&= \sum_{\sigma_d = \uparrow, \downarrow} \sum_k \left[\exp\left(-\beta H \right) \right] + \sum_k \exp\left(-\beta H + i\frac{\pi}{2} \right) + \sum_k \exp\left(-\beta H - i\frac{\pi}{2} \right) \\
&= Z \bigg|_{n_d=1} + iZ \bigg|_{n_d=0} - iZ \bigg|_{n_d=0}
\end{aligned} \tag{1.265}$$

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

$$Z \bigg|_{n_d=0} = Z \bigg|_{n_d=0} \tag{1.266}$$

34

Hence,
$$\widetilde{Z} = Z \tag{1.267}$$

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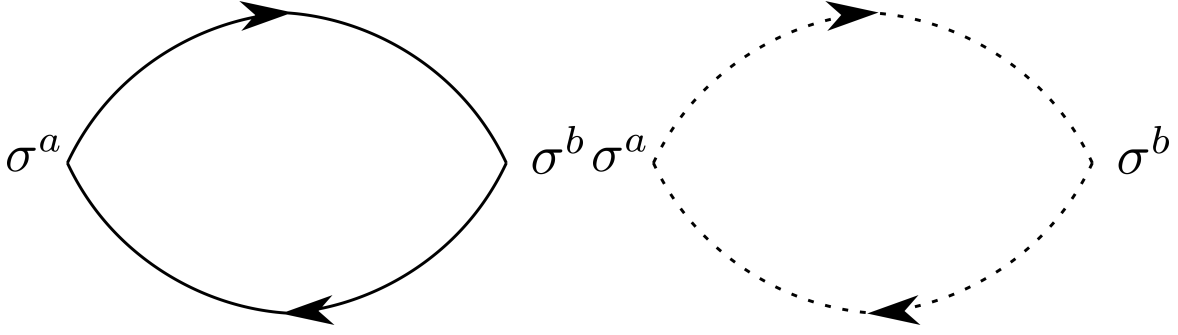
The dotted lines are the impurity Greens function, so that diagram gives the impurity contribution to the susceptibility. Similarly, the solid lines are the conduction electron Greens function. The first diagram gives

$$\chi_c = -k_B T \sum_{k,\omega_n,\phi_0} \langle \phi_0 | \, \sigma^a G(k, i\omega_n) \sigma^b G_k(i\omega_n) \, | \phi_0 \rangle \tag{1.268}$$

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

$$
\begin{aligned}
\chi_c &= -k_B T \sum_{k,\omega_n} \mathrm{Tr} \left[\sigma^a G(k, i\omega_n) \sigma^b G(k, i\omega_n) \right] \\
&= -2 k_B T \sum_{k,\omega_n} G^2(k, i\omega_n) \\
&= -2 k_B T \sum_{k,\omega_n} (i\omega_n - \epsilon_k)^{-2} \\
&= 2 \sum_k \frac{\mathrm{d}}{\mathrm{d}\epsilon_k} k_B T \sum_{\omega_n} (i\omega_n - \epsilon_k)^{-1}
\end{aligned}
\tag{1.269}
$$

Now, it can be shown that

$$k_B T \sum_{\omega_n} (i\omega_n - \epsilon_k)^{-1} = f(\epsilon_k) - \frac{1}{2} \tag{1.270}$$

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

$$\chi_c = 2 \sum_k \frac{\mathrm{d}f(\epsilon_k)}{\mathrm{d}\epsilon_k} = 2 \sum_k \rho(\epsilon_k) = 2N(0) \tag{1.271}$$

The second diagram gives

$$\chi_d^{(0)} = -k_B T \sum_{\omega_n} \mathrm{Tr} \left[\sigma^a G_d(i\omega_n) \sigma^b G_d(i\omega_n) \right] \tag{1.272}$$

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

$$G_d = \frac{1}{i\omega_n - \lambda_d} \tag{1.273}$$

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

$$\chi_d^{(0)} = 2\frac{\mathrm{d}f(\lambda_d)}{\mathrm{d}\lambda_d} = -2\beta\frac{e^{\beta\lambda_d}}{(1 + e^{\beta\lambda_d})^2} = \beta \tag{1.274}$$

The first order diagrams are The first diagram gives

$$\chi^{(1)} = \chi_c\left(-\frac{J}{2}\right)\chi_d = -\beta J N(0) \tag{1.275}$$

The second one gives

$$\chi_d^{(1)} = \chi_d\left(-\frac{J}{2}\right)\chi_c = -\beta J N(0) \tag{1.276}$$

The total susceptibility is

$$\chi_d = \chi_d^{(0)} + \chi_d^{(1)} = \beta\left(1 - 2JN(0)\right) \tag{1.277}$$

1.17   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

$$C_V = \gamma T \tag{1.278}$$

This suggests that the strong-coupling limit of the Kondo model is a Fermi liquid.
The singlet state $(s = 0)$ has an energy

$$E_g = J\left[2\vec{S}_e \cdot \vec{S}_d\right] = J\left[S^2 - S_d^2 - S_e^2\right] = J\left[s\left(s+1\right) - \frac{3}{2}\right] = -\frac{3J}{2} \tag{1.279}$$

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,

$$\frac{|0_\uparrow, d\downarrow\rangle - |0_\downarrow, d_\uparrow\rangle}{\sqrt{2}} \tag{1.280}$$

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

$$E_1 = -\frac{3}{2}J + \frac{3}{2}J = 0 \tag{1.281}$$

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 [13] 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

$$\psi \sim \frac{\sin\left[kr + \delta(E_k)\right]}{r} \tag{1.282}$$

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.

$$n = \sum_\sigma \frac{\delta}{\pi} \implies 1 = \frac{2\delta}{\pi} \implies \delta = \frac{\pi}{2} \tag{1.283}$$

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

$$k_F a = \delta(0) \implies \delta(0) = \frac{\pi}{2a}2 = \frac{\pi}{2} \tag{1.284}$$

where the formula for k_F was used.

In a Fermi gas, the energy levels are separated by

$$\Delta\epsilon = \frac{\partial\epsilon}{\partial k}\Delta k \tag{1.285}$$

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

$$\Delta\epsilon = \frac{\partial\epsilon}{\partial k}\frac{\pi}{L} \tag{1.286}$$

However, this changes in the presence of the impurity. Because of eq. 1.282, the boundary condition becomes

$$k_n L + \delta(\epsilon_k) = n\pi \implies k_n = \frac{n\pi}{L} - \frac{\delta}{L} = k_n^0 - \frac{\delta(\epsilon_k)}{L} \tag{1.287}$$

The energy becomes

$$\begin{aligned}\epsilon(k) &= \epsilon(k^0) + \frac{\partial\epsilon}{\partial k}(k - k_0) \\ &= \epsilon_k - \frac{\partial\epsilon}{\partial k}\frac{\delta(\epsilon_k)}{L}\end{aligned} \tag{1.288}$$

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

$$\widetilde{\epsilon}_\sigma(k) = \epsilon_k - \frac{\partial\epsilon}{\partial k}\frac{\delta_\sigma(\epsilon_k, \{n_{q,\sigma}\})}{L} \tag{1.289}$$

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,

$$\widetilde{\epsilon}_p = \underbrace{\epsilon_F}_{\text{Fermi gas}} + \overbrace{\frac{p_F^*}{m}(p - p_F)}^{\text{linear contribution for } p \text{ close to } p_F} + \underbrace{\sum_{q\sigma} f(p,q)\left(n_q - n_q^0\right)}_{\text{interacting between two quasiparticles at momenta } p \text{ and } q} \tag{1.290}$$

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

$$\delta_\sigma(\widetilde{\epsilon}, \{n_{q,\sigma}\}) = \delta_\sigma(\widetilde{\epsilon} = \epsilon_F, n_k = n_k^0) + \alpha\left(\widetilde{\epsilon} - \epsilon_F\right) + \Phi \sum_{q\sigma'}\left(n_{q\sigma'} - n_{q\sigma'}^0\right) \tag{1.291}$$

This is just a Taylor expansion of δ_σ around $\widetilde{\epsilon} = \epsilon_F$ and $n_q = n_q^0$. Φ and α play the same role as f and $\frac{p_F^*}{m}$ in eq. 1.290. Specifically, Φ represents the onsite interaction between quasiparticles of opposite spin and

$$\alpha = \frac{\mathrm{d}\delta_\sigma}{\mathrm{d}E} \tag{1.292}$$

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

$$\delta_\sigma(\widetilde{\epsilon}, \{n_{q,\sigma}\}) = \delta_\sigma(\widetilde{\epsilon} = \epsilon_F, n_k = n_k^0) + \alpha\left(\widetilde{\epsilon} - \epsilon_F\right) + \Phi \sum_{q} \delta n_{q,-\sigma} \tag{1.293}$$

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,

$$\delta_\uparrow^0 = \frac{\pi}{2} + \Phi \sum_{q} \delta n_{q\downarrow}^0 \tag{1.294}$$

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

$$\delta_\uparrow^0 = \frac{\pi}{2} \tag{1.295}$$

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

$$N(\mu = 0) = N^0 \tag{1.296}$$

$$N(E' = E + \mu) = N(E' = E) + \frac{\mathrm{d}N}{\mathrm{d}E'}(E' - E) = N^0 + \rho\Delta\mu \tag{1.297}$$

$$\implies \sum_{q} \delta n_q = N - N^0 = \rho\Delta\mu \tag{1.298}$$

Hence, from eq. 1.293,

$$\delta_\uparrow = \frac{\pi}{2} + \alpha\left(\epsilon_F' - \epsilon_F\right) + \Phi \sum_{q} \delta n_{q\downarrow} \tag{1.299}$$

$$= \delta_\uparrow^0 + \alpha\Delta\mu + \Phi\rho\Delta\mu$$

Hence the change in the phase is

$$0 = \Delta\delta_\uparrow = \Delta\mu\left(\alpha + \Phi\rho\right) \implies \alpha = -\Phi\rho \tag{1.300}$$

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

$$n_\sigma = \frac{kL}{\pi} + \frac{\delta_\sigma(E)}{\pi} = n^0 + \frac{\delta_\sigma(E)}{\pi} \tag{1.301}$$

Hence,

$$\rho = \frac{\mathrm{d}n_\sigma}{\mathrm{d}E} = \rho^0 + \frac{1}{\pi}\frac{\mathrm{d}\delta_\sigma}{\mathrm{d}E}$$
$$\implies \rho = \rho^0 + \frac{1}{\pi}\alpha \tag{1.302}$$

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

$$C_v^0 = \gamma T = \frac{\pi^2 k_B^2}{3}\mathcal{N}(0)T \tag{1.303}$$

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

$$C_v = \frac{\pi^2 k_B^2}{3}\left(\rho_\uparrow + \rho_\downarrow\right)T$$
$$= \frac{2\alpha}{\pi}\frac{\pi^2 k_B^2}{3}T \tag{1.304}$$

In presence of a magnetic field B, the magnetization is

$$m = \delta n \times \mu \tag{1.305}$$

where μ is the magnetic moment

$$\mu = -\frac{g}{2}\mu_B \tag{1.306}$$

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

$$\delta n = \langle n_\uparrow \rangle - \langle n_\downarrow \rangle = \frac{1}{\pi}\left(\delta_\uparrow - \delta_\downarrow\right) \tag{1.307}$$

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

$$E_\sigma^B = E - \sigma\frac{g\mu_B}{2}B \tag{1.308}$$

Hence,

$$\sum_k \delta n_{k\sigma} = N_\sigma(E_\sigma^B) - N(E) = \frac{\mathrm{d}N}{\mathrm{d}E^B}\left(E^B - E\right) = -\rho\frac{g\mu_B}{2}\sigma B \tag{1.309}$$

This modifies the phase shift at the Fermi surface,

$$\delta_\sigma(\epsilon_F) = \frac{\pi}{2} + \alpha\left(\epsilon_F - \frac{g\mu_B}{2}\sigma B - \epsilon_F\right) + \Phi\sum_q \delta n_{q,-\sigma}$$

$$= \frac{\pi}{2} - \sigma\frac{g\mu_B}{2}\alpha B + \Phi\rho\frac{g\mu_B}{2}\sigma B \tag{1.310}$$

$$= \frac{\pi}{2} - 2\alpha\frac{g\mu_B}{2}\sigma B$$

Hence,

$$\delta n = \frac{1}{\pi}(\delta_\uparrow - \delta_\downarrow) = -\frac{4\alpha B}{\pi}\frac{g\mu_B}{2} \tag{1.311}$$

The susceptibility is

$$\chi = \frac{\partial m}{\partial B} = \frac{\partial}{\partial B}\mu\delta n = \frac{4\alpha}{\pi}\left(\frac{g\mu_B}{2}\right)^2 \tag{1.312}$$

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

$$\mu = -\frac{g}{2}\mu_B \tag{1.313}$$

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

$$\delta n = n_\uparrow(0) - n_\downarrow(0) = n_\uparrow(\epsilon_F - \frac{g}{2}\mu_B B) - n_\downarrow(\epsilon_F + \frac{g}{2}\mu_B B) = -\frac{1}{2}\mathcal{N}(0)gB\mu_B \tag{1.314}$$

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

$$m = \delta n \times \mu = \mathcal{N}(0)\left(\frac{g}{2}\mu_B\right)^2 B \tag{1.315}$$

The magnetic susceptibility comes out to be

$$\chi^0 = \left.\frac{\partial m}{\partial B}\right|_{B\to 0} = \mathcal{N}(0)\left(\frac{g}{2}\mu_B\right)^2 \tag{1.316}$$

The Wilson ratio R can now be computed,

$$R = \frac{\chi/\chi_0}{C_v/C_v^0} = \frac{4\alpha/\pi\mathcal{N}(0)}{2\alpha/\pi\mathcal{N}(0)} = 2 \tag{1.317}$$

1.18 Numerical renormalization group calculation

Wilson's idea [14] 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

$$H = \sum_k \epsilon_k n_k + J\vec{S}_d \cdot \vec{\sigma}_e \tag{1.318}$$

where $\vec{\sigma}_e = \sum_{k_1,k_2,\alpha\beta} c^\dagger_{k_1\alpha}\vec{\sigma}_{\alpha\beta}c_{k_2,\beta}$ 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 $H_c|0\rangle$,

$$|1\rangle = (\lambda_1 H_c |0\rangle + \lambda_2 |0\rangle) \tag{1.319}$$

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:

$$|1\rangle = \frac{1}{\gamma_0} (H_c |0\rangle + \lambda |0\rangle) \tag{1.320}$$

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

$$\lambda = -\langle 0|H_c|0\rangle \tag{1.321}$$

Therefore,

$$|1\rangle = \frac{1}{\gamma_0} (H_c |0\rangle - \langle 0|H_c|0\rangle |0\rangle) \tag{1.322}$$

The general state can be shown to be

$$|n+1\rangle = \frac{1}{\gamma_n} (H_c |n\rangle - |n\rangle \langle n|H_c|n-1\rangle - |n-1\rangle \langle n-1|H_c|n\rangle) \tag{1.323}$$

From eq. 1.323, by multiplying $\langle n'|$ from left, we get

$$\delta_{n',n+1} = \frac{1}{\gamma_n} \left[(H_c)_{n',n} + (H_c)_{n,n-1} \delta_{n',n} + (H_c)_{n-1,n} \delta_{n',n-1} \right] \tag{1.324}$$

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

$$(H_c)_{n',n} = 0 \tag{1.325}$$

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

$$(H_c)_{n+1,n} = \gamma_n \tag{1.326}$$

Taking the complex conjugate of this gives

$$\gamma_n^* = \left(H_c^\dagger \right)_{n,n+1} = (H_c)_{n,n+1} \tag{1.327}$$

Defining

$$(H_c)_{n,n} = \epsilon_n \tag{1.328}$$

we can write

$$\begin{aligned}
H_c &= \sum_{n_1,n_2} |n_1\rangle \langle n_1| H_c |n_2\rangle \langle n_2| \\
&= \sum_n \epsilon_n |n\rangle \langle n| + \sum_n (\gamma_n |n\rangle \langle n+1| + \gamma_n^* |n+1\rangle \langle n|) \\
&= \sum_n \epsilon_n \hat{n}_n + \sum_n \left(\gamma_n c_n^\dagger c_{n+1} + \gamma_n^* c_{n+1}^\dagger c_n \right)
\end{aligned} \tag{1.329}$$

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.

1.18.1   Logarithmic discretization

First, note that up to first order

$$\epsilon_k = \epsilon_F + (k - k_F)\frac{\partial \epsilon_k}{\partial k} \tag{1.330}$$

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 $n = 1, 2, 3...$ The width of each interval is

$$d_n = \Lambda^{-n}\left(1 - \Lambda^{-1}\right) \tag{1.331}$$

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

$$\psi_{m,n}(k) = \frac{1}{\sqrt{d_n}}\exp\left(\frac{2\pi i m}{d_n}k\right) \tag{1.332}$$

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

$$a^\dagger_{m,n} = \sum_k \psi_m(k)c^\dagger_k \tag{1.333}$$

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

$$\phi_{m,n}(k) = \frac{1}{\sqrt{d_n}}\exp\left(-\frac{2\pi i m}{d_n}k\right) \tag{1.334}$$

$$b^\dagger_{m,n} = \sum_k \phi_m(k)c^\dagger_k \tag{1.335}$$

Then,

$$a^\dagger_{m,n} + b^\dagger_{m,n} = \frac{2}{\sqrt{d_n}}\sum_{\pm k\in[]}\cos\left(\frac{2\pi mk}{d_n}\right)c^\dagger_k \tag{1.336}$$

Summing over n involves summing over all momenta.

$$\sum_n \left(a^\dagger_{m,n} + b^\dagger_{m,n}\right) = \frac{2}{\sqrt{d_n}}\sum_k \cos\left(\frac{2\pi mk}{d_n}\right)c^\dagger_k$$

$$\implies \sum_n \left(a^\dagger_{0,n} + b^\dagger_{0,n}\right) = \frac{2}{\sqrt{d_n}}\sum_k c^\dagger_k \tag{1.337}$$

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

$$\sum_{k,q}c^\dagger_k c_q = \sum_k c^\dagger_k \sum_q c_q \tag{1.338}$$

Looking at eq. 1.337, 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

$$\epsilon_n = 0, \gamma = D'\Lambda^{\frac{-n}{2}} \tag{1.339}$$

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

$$H_N = D'\sum_{n=0}^{N-1}\Lambda^{-\frac{n}{2}}\left(c^\dagger_n c_{n+1} + c^\dagger_{n+1}c_n\right) + 2J\vec{S}_d \cdot \vec{S}_e \tag{1.340}$$

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

$$H_{N+1} = H_N + D'\Lambda^{-\frac{N}{2}} \left(c_N^\dagger c_{N+1} + c_{N+1}^\dagger c_N\right) \tag{1.341}$$

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

$$\overline{H}_N = \frac{H_N}{\Gamma_N} = \frac{\Lambda^{\frac{N-1}{2}}}{D'} H_N \tag{1.342}$$

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

$$\overline{H}_{N+1} = \frac{\Lambda^{\frac{N}{2}}}{D'} \left[H_N + \Lambda^{\frac{-N}{2}} D' \left(c_N^\dagger c_{N+1} + c_{N+1}^\dagger c_N\right)\right]$$
$$\implies \overline{H}_{N+1} = \Lambda^{\frac{1}{2}}\overline{H}_N + \left(c_N^\dagger c_{N+1} + c_{N+1}^\dagger c_N\right) \tag{1.343}$$

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

$$H = \lim_{N\to\infty} H_N = \lim_{N\to\infty} D'\Lambda^{\frac{1-N}{2}}\overline{H}_N \tag{1.344}$$

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

$$\overline{H}_N = \sum_m E_m |m\rangle \langle m| \tag{1.345}$$

The next Hamiltonian is then

$$\overline{H}_{N+1} = \Lambda^{\frac{1}{2}} \sum_m E_m |m\rangle \langle m| + \sum_{m.m'} \left(C(m,m')|m\rangle \langle m'| + \text{h.c.}\right) \tag{1.346}$$

This is the same equation as eq. 1.343, with $\overline{H}_N$ 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 $J = \infty$.

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

1.19.1 Local Fermi liquid

The fixed-point Hamiltonians [15] are found to represent interacting Fermi liquids. The effective Hamiltonian can be shown to resemble the Anderson model, but with modified parameters,

$$H_{\text{eff}} = \sum_k \epsilon_k n_k + \sum_k V_k c_d^\dagger c_k + \text{h.c.} + U n_{d\uparrow} n_{d\downarrow} \tag{1.347}$$

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 $T \to 0$, assuming only single excitations, the interacting term will not get invoked.

Under mean-field,

$$n_{d\uparrow} n_{d\downarrow} \approx n_{d\uparrow} \langle n_{d\downarrow} \rangle + \langle n_{d\uparrow} \rangle n_{d\downarrow} - \langle n_{d\uparrow} \rangle \langle n_{d\downarrow} \rangle$$
$$\implies \langle n_{d\uparrow} n_{d\downarrow} \rangle = \langle n_{d\uparrow} \rangle \langle n_{d\downarrow} \rangle$$
$$= \sum_{k,q} \langle n_{k\sigma} \rangle \langle n_{q,-\sigma} \rangle \tag{1.348}$$

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:

$$\langle n_q^> \rangle = \langle \psi^> | c_k^\dagger c_k | \psi^> \rangle = n_k^p \tag{1.349}$$

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

$$\langle n_q^< \rangle = \langle \psi^< | c_k^\dagger c_k | \psi^< \rangle = - \langle \psi^< | c_k c_k^\dagger | \psi^< \rangle = -n_k^h \tag{1.350}$$

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

$$\langle \delta n_{k,\sigma} \rangle = \begin{cases} n_k^p, & \epsilon_k > \epsilon_F \\ -n_k^h, & \epsilon_k < \epsilon_F \end{cases} \tag{1.351}$$

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

$$\epsilon_{k\sigma} = \epsilon_k + U \sum_q \langle \delta n_{q,-\sigma} \rangle \equiv \epsilon_k + U \langle \delta n_{-\sigma} \rangle \tag{1.352}$$

This is analogous to the Landau quasiparticle energy functional, eq. 1.35, 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

$$\rho_{d\sigma}(\omega) = \frac{\Delta}{\pi} \frac{1}{(\omega - \epsilon_d^*)^2 + \Delta^2} \tag{1.353}$$

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

1.19.2 Calculation of C_v

To calculate the specific heat, $C_v = \frac{\mathrm{d}\langle E\rangle}{\mathrm{d}T}$, 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:

$$\frac{\mathrm{d}\langle E\rangle}{\mathrm{d}T} = \sum_{k,\sigma} \epsilon_{k\sigma} \frac{\mathrm{d}\langle \delta n_{k\sigma}\rangle}{\mathrm{d}T} \tag{1.354}$$

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

$$\langle \delta n_{k\sigma}\rangle(T) = \frac{1}{e^{\beta \epsilon_{k\sigma}} + 1}$$

$$\implies \frac{\mathrm{d}\langle \delta n_{k\sigma}\rangle}{\mathrm{d}T} = \frac{e^{\beta \epsilon_{k\sigma}}}{\left(e^{\beta \epsilon_{k\sigma}} + 1\right)^2} \left[\frac{1}{k_B T^2}\epsilon_{k\sigma} - \frac{1}{k_B T}(2\epsilon_{k\sigma} - \epsilon_k)\frac{\mathrm{d}\langle \delta n_{k\sigma}\rangle}{\mathrm{d}T}\right] \tag{1.355}$$

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

$$\begin{aligned}
\frac{\mathrm{d}\langle E\rangle}{\mathrm{d}T} &= \sum_{k,\sigma} \epsilon_{k\sigma} \frac{e^{\beta \epsilon_{k\sigma}}}{\left(e^{\beta \epsilon_{k\sigma}} + 1\right)^2} \frac{1}{k_B T^2}\epsilon_{k\sigma} \\
&= \frac{1}{k_B T^2} \sum_{k,\sigma} \epsilon_{k\sigma}^2 \frac{e^{\beta \epsilon_{k\sigma}}}{\left(e^{\beta \epsilon_{k\sigma}} + 1\right)^2} \\
&= \frac{1}{k_B T^2} \sum_{\sigma} \int d\epsilon_\sigma \rho(\epsilon_\sigma) \epsilon_\sigma^2 \frac{e^{\beta \epsilon_{k\sigma}}}{\left(e^{\beta \epsilon_{k\sigma}} + 1\right)^2}
\end{aligned} \tag{1.356}$$

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

$$\begin{aligned}
\frac{\mathrm{d}\langle E\rangle}{\mathrm{d}T} &= \frac{1}{k_B T^2} \sum_{\sigma} \rho_\sigma(0) \int_{-\infty}^{\infty} d\epsilon_\sigma \epsilon_\sigma^2 \frac{e^{\beta \epsilon_{k\sigma}}}{\left(e^{\beta \epsilon_{k\sigma}} + 1\right)^2} \\
&= -\frac{1}{T} \sum_{\sigma} \rho_\sigma(0) \int_{-\infty}^{\infty} d\epsilon_\sigma \epsilon_\sigma^2 f'(\epsilon_\sigma) \\
&= -\frac{1}{T} \sum_{\sigma} \rho_\sigma(0) \int_{1}^{0} df \epsilon_\sigma^2
\end{aligned} \tag{1.357}$$

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

$$\epsilon = k_B T \ln\left(f^{-1} - 1\right) \implies \epsilon^2 = k_B^2 T^2 \left[\ln\left(f^{-1} - 1\right)\right]^2 \tag{1.358}$$

Therefore,

$$\frac{\mathrm{d}\langle E\rangle}{\mathrm{d}T} = -k_B^2 T \sum_{\sigma} \rho_\sigma(0) \int_{1}^{0} df \left[\ln\left(f^{-1} - 1\right)\right]^2 \tag{1.359}$$

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

$$\begin{aligned}
\frac{\mathrm{d}\langle E\rangle}{\mathrm{d}T} &= k_B^2 T \sum_{\sigma} \rho_d(0) \frac{\pi^2}{3} \\
&= 2k_B^2 T \rho_d(0) \frac{\pi^2}{3} \\
&= \gamma_{\mathrm{imp}} T
\end{aligned} \tag{1.360}$$

where

$$\gamma_{\text{imp}} \equiv \frac{C_v}{T} = \frac{2\pi^2}{3} k_B^2 \rho_d(0) \tag{1.361}$$

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

$$\frac{\gamma_{\text{imp}}}{\gamma^{(0)}} = \frac{\rho_d(0)}{\rho_d^{(0)}(0)} \tag{1.362}$$

1.19.3   Calculation of χ

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

$$\begin{aligned}
m &= \frac{g\mu_B}{2} \left(\delta n_\uparrow - \delta n_\downarrow \right) \\
&= \frac{g\mu_B}{2} \sum_\sigma \sigma \delta n_\sigma \\
&= \frac{g\mu_B}{2} \sum_{k\sigma} \sigma \frac{\partial n_\sigma}{\partial \epsilon_{k\sigma}} \delta \epsilon_{k\sigma} \\
&= \frac{g\mu_B}{2} \sum_{k\sigma} \sigma \rho_{k\sigma} \left(\sigma h + U \delta n_{-\sigma} \right) \\
&= \frac{g\mu_B}{2} \sum_\sigma \sigma \rho_\sigma \left(\sigma h + U \delta n_{-\sigma} \right)
\end{aligned} \tag{1.363}$$

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

$$\delta n_{-\sigma} = \sum_q \delta n_{q,-\sigma} = \sum_q \Delta \epsilon_F \rho_{q-\sigma} = \sigma h \rho_{-\sigma}(0) \tag{1.364}$$

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

$$\begin{aligned}
m &= \frac{g\mu_B}{2} h \sum_\sigma \sigma^2 \rho_\sigma(0) \left(1 + U \rho_{-\sigma}(0) \right) \\
&= \left(\frac{g\mu_B}{2} \right)^2 B \sum_\sigma \rho_\sigma(0) \left[1 + U \rho_{-\sigma}(0) \right]
\end{aligned} \tag{1.365}$$

The susceptibility is

$$\begin{aligned}
\chi_{\text{imp}} &= \lim_{h\to 0} \frac{\partial m}{\partial B} \\
&= \left(\frac{g\mu_B}{2} \right)^2 \rho_d(0) \left[1 + U \rho_d(0) \right] \sum_\sigma \\
&= \frac{(g\mu_B)^2}{2} \rho_d(0) \left[1 + U \rho_d(0) \right] \\
&= \chi^{(0)} \frac{\rho_d(0)}{\rho_d^{(0)}(0)} \left[1 + U \rho_d(0) \right]
\end{aligned} \tag{1.366}$$

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

The Wilson ratio is

$$R \equiv \frac{\chi_{\text{imp}}}{\chi^{(0)}} \frac{\gamma^{(0)}}{\gamma_{\text{imp}}} = 1 + U \rho_d(0) \tag{1.367}$$

1.19.4 Relation between the density of states and scattering phase shift

The Green's function is of the general form

$$G_d(\omega) = \frac{1}{\omega - \epsilon_d - i\Delta - \Sigma(\omega)} \tag{1.368}$$

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:

$$\Sigma(\omega) = \Sigma(0,0) + \omega\Sigma'(0) + O(i\omega^2)$$
$$\equiv \Sigma(0) + \left(1 - Z^{-1}\right)\omega \tag{1.369}$$

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

$$\begin{aligned}
G_d(\omega) &= \frac{1}{\omega - \epsilon_d - i\Delta - \Sigma(0) - \left(1 - Z^{-1}\right)\omega} \\
&= \frac{Z}{Z\omega - Z\epsilon_d - iZ\Delta - Z\Sigma(0) - Z\omega + \omega} \\
&= \frac{Z}{\omega - Z\left(\epsilon_d + \Sigma(0)\right) - iZ\Delta} \\
&\equiv \frac{Z}{\omega - \epsilon_d^* - i\Delta^*}
\end{aligned} \tag{1.370}$$

The density of states at the Fermi surface is given by

$$\begin{aligned}
\rho_d(0) &= \frac{1}{\pi}\text{Im } G_d(\omega)\Big|_{\omega=0} \\
&= \frac{1}{\pi}\frac{Z\Delta^*}{\left(\omega - \epsilon_d^*\right)^2 + \Delta^{*2}}\Big|_{\omega=0} \\
&= \frac{1}{\pi}\frac{Z\Delta^*}{\epsilon_d^{*2} + \Delta^{*2}}
\end{aligned} \tag{1.371}$$

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

$$\begin{aligned}
G &= G^{(0)} + G^{(0)}VG_d^{(0)}VG^{(0)} + G^{(0)}VG_d^{(0)}VG^{(0)}VG_d^{(0)}VG^{(0)} + \dots \\
&= G^{(0)} + G^{(0)}V\left[G_d^{(0)} + G_d^{(0)}VG^{(0)}VG_d^{(0)}\right]VG^{(0)} \\
&= G^{(0)} + G^{(0)}V^2G_dG^{(0)}
\end{aligned} \tag{1.372}$$

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

$$G = G_0 + G_0TG_0 \tag{1.373}$$

we can write

$$T = V^2G_d \tag{1.374}$$

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

$$e^{2i\delta(\omega)} = 1 - 2\pi i\rho T(\omega)$$
$$\implies T = V^2G_d = \frac{1}{2\pi i\rho}\left(1 - e^{2i\delta(\omega)}\right) = \frac{e^{i\delta(\omega)}}{2\pi i\rho}\left(-2i\sin\delta\right) \tag{1.375}$$
$$\implies G_d = -\frac{e^{i\delta(\omega)}}{V^2\pi\rho}\sin\delta$$

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

$$G_d = |G_d|e^{i\delta(\omega)} \tag{1.376}$$

From the expression for G_d in eq. 1.370, we can find the phase of G_d:

$$\delta(\omega) = \tan^{-1}\frac{\Delta^*}{\omega - \epsilon_d^*} \tag{1.377}$$
$$\implies \epsilon_d^* = -\Delta^*\cot\delta(0)$$

Substituting this in the density of states expression gives

$$\rho_d(0) = \frac{Z\sin^2\delta(0)}{\pi\Delta^*} \tag{1.378}$$

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

$$R = 1 + \frac{UZ\sin^2\delta(0)}{\pi\Delta^*} \tag{1.379}$$

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

$$R = 1 + \frac{U}{\pi\Delta}\sin^2\delta(0) \tag{1.380}$$

1.19.5   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

$$\begin{aligned}\Delta n_\uparrow &= \delta n_\uparrow(\epsilon_{k\uparrow} + \mu) - \delta n_\uparrow(\epsilon_{k\uparrow}) \\ &= \rho_d(0)\left(\Delta\mu + U\Delta n_\downarrow\right) \\ &= \rho_d(0)\left(\Delta\mu - U\rho_d(0)\Delta\mu\right) \\ &= \rho_d(0)\Delta\mu\left(1 - U\rho_d(0)\right)\end{aligned} \tag{1.381}$$

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 $\Delta n_\uparrow$. Hence,

$$1 - U\rho_d(0) = 0 \implies U\rho_d(0) = 1 \tag{1.382}$$

Substituting $\langle n_{d\sigma} \rangle = \frac{1}{2}$ and $\epsilon_d = -\frac{U}{2}$ in the density of states eq. 1.353 gives $\rho_d(0) = \frac{1}{\pi\Delta} = \frac{1}{U}$. This can be substituted in the Wilson ratio to give

$$R = 1 + \sin^2\delta(0) \tag{1.383}$$

1.19.6 Connection to the change in Luttinger's volume

From the Friedel sum rule[16], 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:

$$\widetilde{N} = \frac{1}{2\pi i} \operatorname{Tr}\, \ln S(0) = \int_\Gamma dz \partial_z \frac{1}{2\pi i} \operatorname{Tr}\, \ln S(0) \tag{1.384}$$

From the optical theorem, we can write

$$S = 1 + TG_0 = \frac{G}{G_0} \quad \text{[eq. 1.373]} \tag{1.385}$$

This allows us to write [17]

$$\widetilde{N} = \int_\Gamma dz \partial_z \frac{1}{2\pi i} \operatorname{Tr}\, \ln \frac{G}{G_0} \tag{1.386}$$

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

$$\begin{aligned}
\widetilde{N} &= \int_\Gamma dz \partial_z \frac{1}{2\pi i} \ln \operatorname{Det} \frac{G}{G_0} \\
&= -\int_\Gamma dz \partial_z \frac{1}{2\pi i} \ln \frac{\operatorname{Det} G_0}{\operatorname{Det} G} \\
&\equiv -\int_\Gamma dz \partial_z \frac{1}{2\pi i} \ln D \\
&= -\int_{\Gamma(D)} \frac{dD}{D}
\end{aligned} \tag{1.387}$$

From the work of Seki and Yunoki [18], 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 $T = 0$.

$$\widetilde{N} = -\int_{\Gamma(D)} \frac{dD}{D} = -\Delta V_L \tag{1.388}$$

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

$$\widetilde{N} = \frac{1}{\pi} \sum_\sigma \delta_\sigma(0) \tag{1.389}$$

$$\implies \delta(0) = \frac{\pi}{2} \widetilde{N} = -\frac{\pi}{2} \Delta V_L$$

$$\begin{aligned}
R &= 1 + \sin^2 \left(\frac{\pi}{2} \widetilde{N} \right) \\
&= 1 + \sin^2 \left(\frac{\pi}{2} \Delta V_L \right)
\end{aligned} \tag{1.390}$$

1.20 Microscopic approach

The average occupation for the non-interacting quasiparticles can be similarly written from eq. 1.401.

$$\langle \widetilde{n}_d \rangle = \frac{1}{2} - \frac{1}{\pi} \tan^{-1} \frac{\widetilde{\epsilon}_d}{\widetilde{\Delta}} = \frac{1}{2} - \frac{1}{\pi} \tan^{-1} \frac{\epsilon_d - \Sigma(0)}{\Delta} = \langle n_d \rangle \tag{1.391}$$

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

$$\gamma_{\text{imp}} = \frac{2\pi k_B^2}{3} \frac{\widetilde{\Delta}}{\widetilde{\epsilon}_d^2 + \widetilde{\Delta}^2} \tag{1.392}$$

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

$$\chi_{\text{m,imp}} = \frac{g^2 \mu_B^2}{2} \alpha' \rho_d(0) \tag{1.393}$$

$$\chi_{\text{c,imp}} = 2\alpha'' \rho_d(0) \tag{1.394}$$

where

$$\alpha' = \frac{1 - \partial_h \Sigma_\sigma(\epsilon_F, 0)}{1 - \partial_E \Sigma_\sigma(\epsilon_F, 0)} \tag{1.395}$$

$$\alpha'' = \frac{1 + \partial_\mu \Sigma_\sigma(\epsilon_F, 0)}{1 - \partial_E \Sigma_\sigma(\epsilon_F, 0)} \tag{1.396}$$

1.21 Renormalized perturbation theory

This is a perturbative expansion of the Hamiltonian in terms of the renormalized interaction $\widetilde{U}$, and the second order results obtained from this approach coincide with the phenomenological results at $T, h \to 0$.. 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

$$G_d^0 = \frac{1}{E - \epsilon_d + i\Delta} \tag{1.397}$$

Including the self energy gives

$$G_d = \frac{1}{E - \epsilon_d + i\Delta - \Sigma(E)} \tag{1.398}$$

As shown previously in section 1.12, the impurity Green's function can be shown to take the form

$$G_d = \frac{Z}{E - \widetilde{\epsilon}_d + i\widetilde{\Delta} - \widetilde{\Sigma}(E)} \tag{1.399}$$

where the ~ represents the renormalised quantities

$$\widetilde{\epsilon}_d = Z(\epsilon_d + \Sigma(0))$$
$$\widetilde{\Delta} = Z\Delta$$
$$\widetilde{\Sigma} = Z\Sigma^{\text{rem}}(E)$$
$$Z^{-1} = 1 - \Sigma(0)' \tag{1.400}$$
$$\widetilde{\Gamma}_{\sigma\sigma'}(E, E') = z^2 \Gamma_{\sigma\sigma'}(E, E')$$
$$\widetilde{U} = z^2 \Gamma_{\uparrow\downarrow}(0, 0)$$

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

$$\widetilde{G}_d = \frac{1}{E - \widetilde{\epsilon}_d + i\widetilde{\Delta}} \tag{1.401}$$

The Anderson hamiltonian

$$H = \epsilon_d n_d + U n_{d\uparrow} n_{d\downarrow} + \sum_k \epsilon_k n_k + \sum_k \left(V_k c_{d\sigma}^{\dagger} c_{k\sigma} + V_k^* c_{k\sigma}^{\dagger} c_{d\sigma} \right) \tag{1.402}$$

can be written in the form

$$H = \widetilde{H}_{qp} - \widetilde{H}_c \tag{1.403}$$

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

$$\widetilde{H}_{qp}^0 = \widetilde{\epsilon}_d \widetilde{n}_d + \sum_k \epsilon_k n_k + \sum_k \left(\widetilde{V}_k \widetilde{c}_{d\sigma}^{\dagger} c_{k\sigma} + \widetilde{V}_k^* c_{k\sigma}^{\dagger} \widetilde{c}_{d\sigma} \right) \tag{1.404}$$

$$\widetilde{H}_{qp}^I = \widetilde{U} \widetilde{n}_{d\uparrow} \widetilde{n}_{d\downarrow} \tag{1.405}$$

The renormalised parameters are defined in eq. 1.400. The renormalised operators are

$$\widetilde{c}_d^{\dagger} = \sqrt{z} c_d^{\dagger} \tag{1.406}$$
$$\widetilde{c}_d = \sqrt{z} c_d \tag{1.407}$$

The $\widetilde{H}_c$ that satisfies eq. 1.403 is

$$\widetilde{H}_c = \lambda_1 \widetilde{n}_d + \lambda_2 \widetilde{n}_{d\uparrow} \widetilde{n}_{d\downarrow} \tag{1.408}$$

where

$$\lambda_1 = z\Sigma(0, 0) \tag{1.409}$$
$$\lambda_2 = z^2 \left[\Gamma_{\uparrow\downarrow}(0, 0) - U \right] \tag{1.410}$$

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

$$\widetilde{\Sigma}(0) = 0$$
$$\widetilde{\Sigma}'(0) = 0 \tag{1.411}$$

Close to the Fermi surface, we also have

$$\widetilde{\Gamma}_{\uparrow\downarrow}(0) = \widetilde{U} \tag{1.412}$$

$$\widetilde{\Gamma}_{\sigma\sigma}(0) = 0 \tag{1.413}$$

$$\implies \Gamma_{\sigma\sigma'}(0) = \widetilde{U}(1 - \delta_{\sigma\sigma'}) \tag{1.414}$$

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

$$\lambda_i = \sum_n \lambda_i^{(n)} \widetilde{U}^n \tag{1.415}$$

$$z = \sum_n z^{(n)} \widetilde{U}^n \tag{1.416}$$

$$\tag{1.417}$$

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

$$G^0 = \frac{1}{E - \widetilde{\epsilon}_d + i\widetilde{\Delta}} \tag{1.418}$$

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

$$\langle n_{d\sigma} \rangle = \frac{1}{2} - \frac{1}{\pi} \tan^{-1} \frac{\epsilon_d + \Sigma(0, h)}{\Delta} \tag{1.419}$$

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

$$\langle n_{d\sigma} \rangle = \frac{1}{2} - \frac{1}{\pi} \tan^{-1} \frac{\widetilde{\epsilon}_d + \widetilde{\Sigma}(0, h)}{\widetilde{\Delta}} \tag{1.420}$$

For $T, h \to 0$, the counter-term cancels appropriate terms from the quasiparticle Hamiltonian leading to the vanishing of the effects of the self-energy, eq. 1.411. 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

$$\widetilde{\Sigma}(\omega, H, T) = \widetilde{U} \left(n_{d\sigma}^{(0)}(0, H, T) - n_{d\sigma}^{(0)}(0, 0, 0) \right) \tag{1.421}$$

This satisfies the constraint eq. 1.411. 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

$$m = \frac{g\mu_B}{2} \langle n_{d\uparrow} - n_{d\downarrow} \rangle \tag{1.422}$$

We can substitute the expression for the self-energy into eq. 1.420. That gives

$$\chi_d = \frac{1}{2} (g\mu_B)^2 \frac{\partial \langle n_{d\uparrow} - n_{d\downarrow} \rangle}{\partial h} = \frac{1}{2\pi} (g\mu_B)^2 \frac{\partial}{\partial h} \left(\tan^{-1} \frac{\widetilde{\epsilon}_{d\downarrow}}{\widetilde{\Delta}} - \tan^{-1} \frac{\widetilde{\epsilon}_{d\uparrow}}{\widetilde{\Delta}} \right) \tag{1.423}$$

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

$$\chi_d = \frac{1}{2\pi} (g\mu_B)^2 \frac{1}{1 + \left(\frac{\widetilde{\epsilon}_d}{\widetilde{\Delta}} \right)^2} \frac{1}{\widetilde{\Delta}} \frac{\partial}{\partial h} [\widetilde{\epsilon}_{d\downarrow} - \widetilde{\epsilon}_{d\uparrow}] \tag{1.424}$$

We can recognize that

$$\frac{1}{1 + \left(\frac{\widetilde{\epsilon}_d}{\widetilde{\Delta}}\right)^2} \frac{1}{\pi \widetilde{\Delta}} = \frac{1}{\pi} \frac{\widetilde{\Delta}}{\widetilde{\Delta}^2 + \widetilde{\epsilon}_d^2} = \rho_d(0) \tag{1.425}$$

Therefore,

$$\chi_d = \frac{1}{2} \left(g\mu_B\right)^2 \rho_d(0) \frac{\partial}{\partial h} \left[\widetilde{\epsilon}_{d\downarrow} - \widetilde{\epsilon}_{d\uparrow}\right] \tag{1.426}$$

Up to first order, we can write

$$\widetilde{\epsilon}_{d\downarrow} - \widetilde{\epsilon}_{d\uparrow} = \epsilon_{d\downarrow} - \epsilon_{d\uparrow} + \widetilde{U}\left(n_{d\downarrow}^{(0)} - n_{d\uparrow}^{(0)}\right) = 2\epsilon_d + h + \widetilde{U}\left(n_{d\downarrow}^{(0)} - n_{d\uparrow}^{(0)}\right) \tag{1.427}$$

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

$$\frac{\partial}{\partial h} \left[\widetilde{\epsilon}_{d\downarrow} - \widetilde{\epsilon}_{d\uparrow}\right] = 1 + \widetilde{U}\left(\frac{\partial n_{d\downarrow}^{(0)}}{\partial \epsilon_{d\downarrow}} \frac{\partial \epsilon_{d\downarrow}}{\partial h} - \frac{\partial n_{d\uparrow}^{(0)}}{\partial \epsilon_{d\uparrow}} \frac{\partial \epsilon_{d\uparrow}}{\partial h}\right) \tag{1.428}$$

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

$$\frac{\partial}{\partial h} \left[\widetilde{\epsilon}_{d\downarrow} - \widetilde{\epsilon}_{d\uparrow}\right] = 1 + \widetilde{U}\rho_d(0) \tag{1.429}$$

Substituting in to the parent equation, we get

$$\chi_d = \frac{1}{2} \left(g\mu_B\right)^2 \rho_d(0) \left(1 + \widetilde{U}\rho_d(0)\right) \tag{1.430}$$

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.

$$\left(\frac{\partial}{\partial E} + \frac{\partial}{\partial \mu}\right) \Sigma(E)\Big|_{E=0} = -\rho_{d\sigma}(0)\Gamma_{\uparrow\downarrow}(0,0) \tag{1.431}$$

$$\left(\frac{\partial}{\partial h} - \frac{\partial}{\partial E}\right) \Sigma(E)\Big|_{E=0} = -\rho_{d\sigma}(0)\Gamma_{\uparrow\downarrow}(0,0) \tag{1.432}$$

Multiplying both equations throughout by Z, we get

$$\left(\frac{\partial}{\partial E} + \frac{\partial}{\partial \mu}\right) \widetilde{\Sigma}(E)\Big|_{E=0} = -Z\rho_{d\sigma}(0)\Gamma_{\uparrow\downarrow}(0,0) = -\frac{1}{Z}\rho_{d\sigma}(0)\widetilde{U} \tag{1.433}$$

$$\left(\frac{\partial}{\partial h} - \frac{\partial}{\partial E}\right) \widetilde{\Sigma}(E)\Big|_{E=0} = -Z\rho_{d\sigma}(0)\Gamma_{\uparrow\downarrow}(0,0) = -\frac{1}{Z}\rho_{d\sigma}(0)\widetilde{U} \tag{1.434}$$

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

$$\widetilde{\rho}(0) \sim \frac{\widetilde{\Delta}}{\widetilde{\epsilon}_d^2 + \widetilde{\Delta}^2} = \frac{1}{Z} \frac{\Delta}{\epsilon_d^2 + \Delta^2} = \frac{1}{Z}\rho_d(0) \tag{1.435}$$

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

$$\frac{\partial \widetilde{\Sigma}(E)}{\partial \mu}\Big|_{E=0} = \frac{\partial \widetilde{\Sigma}(E)}{\partial h}\Big|_{E=0} = -\widetilde{\rho}_{d\sigma}(0)\widetilde{U} \tag{1.436}$$

53

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.

$$\widetilde{\gamma} \sim \widetilde{\rho}_d(0) \tag{1.437}$$

The susceptibilities are given by

$$\chi_m = -\left(\frac{g\mu_B}{2}\right)^2 \widetilde{\rho}_d \sum_\sigma \frac{\partial\left(\epsilon_k - h\sigma + \widetilde{\Sigma}\right)}{\partial h} = \frac{g^2\mu_B^2}{2}\widetilde{\rho}_d\left(1 - \frac{\partial\widetilde{\Sigma}}{\partial h}\right) \tag{1.438}$$

Substituting from eq. 1.436,

$$\chi_m = \frac{g^2\mu_B^2}{2}\widetilde{\rho}_d\left(1 + \widetilde{U}\widetilde{\rho}_d(0)\right) \tag{1.439}$$

Similarly,

$$\chi_c = \frac{dn}{d\mu} = \widetilde{\rho}_d(0)\sum_\sigma \frac{d\left(\epsilon_F + \widetilde{\Sigma}\right)}{d\mu} = 2\widetilde{\rho}_d(0)\left(1 + \frac{\partial\widetilde{\Sigma}}{\partial\mu}\right) = 2\widetilde{\rho}_d(0)\left(1 - \widetilde{U}\widetilde{\rho}_d(0)\right) \tag{1.440}$$

1.21.1 Friedel sum rule

Looking at eq. 1.398, we can write down the density of states and hence the average occupancy of the impurity site

$$\rho_{d\sigma} = \frac{-1}{\pi}\text{Im}\left[G_d\right] \tag{1.441}$$

$$\langle n_{d\sigma}\rangle = \int_{-\infty}^0 dE\ \rho_{d\sigma} = -\frac{1}{\pi}\text{Im}\int_{-\infty}^0 dE\ G_d(E) \tag{1.442}$$

Luttinger proved that

$$\int_{-\infty}^0 \Sigma' G dE = 0 \tag{1.443}$$

In order to use this, note that

$$\ln G_d^{-1} = \ln\left(E - \epsilon_d + i\Delta - \Sigma\right)$$
$$\implies \frac{d\ln G_d^{-1}}{dE} = \frac{1}{E - \epsilon_d + i\Delta - \Sigma}(1 - \Sigma') = G_d - \Sigma' G_d \tag{1.444}$$
$$\implies G_d = \Sigma' G_d - \frac{d\ln G_d}{dE}$$

Substituting this expression for G_d in eq. 1.442,

$$\langle n_{d\sigma}\rangle = -\frac{1}{\pi}\text{Im}\int_{-\infty}^0 \Sigma' G\ dE + \frac{1}{\pi}\text{Im}\int_{-\infty}^0 \frac{d\ln G_d}{dE}dE \tag{1.445}$$

The first integral is zero, courtesy Luttinger. We get

$$
\begin{aligned}
\langle n_{d\sigma} \rangle &= \frac{1}{\pi}\text{Im}\left[\ln\frac{1}{E - \epsilon_d + i\Delta - \Sigma}\right]_{-\infty}^{0} \\
&= -\frac{1}{\pi}\text{Im}\left[\ln\left(E - \epsilon_d + i\Delta - \Sigma\right)\right]_{-\infty}^{0} \\
&= -\frac{1}{\pi}\text{Im}\left[\ln e^{i\theta}\right]_{-\infty}^{0} \qquad\qquad \left[\tan\theta = \frac{\Delta}{E - \epsilon_d - \Sigma}\right] \\
&= -\frac{1}{\pi}\left[\theta(0) - \theta(-\infty)\right] \\
&= \frac{1}{\pi}\tan^{-1}\frac{\Delta}{\epsilon_d + \Sigma(0,h)} \\
&= \frac{1}{2} - \frac{1}{\pi}\tan^{-1}\frac{\epsilon_d + \Sigma(0,h)}{\Delta}
\end{aligned}
\tag{1.446}
$$

We can now relate the average occupancy with the density of states. From eq. 1.441,

$$
\begin{aligned}
\rho_{d\sigma} &= \frac{1}{\pi}\frac{\Delta}{\left(\epsilon_d + \Sigma(0)\right)^2 + \Delta^2} \\
&= \frac{1}{\pi\Delta}\left[1 + \left(\frac{\epsilon_d + \Sigma(0)}{\Delta}\right)^2\right]^{-1} \\
&= \frac{1}{\pi\Delta}\left[1 + \cot^2\pi\langle n_{d\sigma}\rangle\right]^{-1} \\
&= \frac{\sin^2\pi\langle n_{d\sigma}\rangle}{\pi\Delta}
\end{aligned}
\tag{1.447}
$$

1.22   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 fat 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 wont 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 $|1\sigma\rangle$ 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

$$
H = \sum_{k\sigma}\epsilon_{k\sigma}n_{k\sigma} + \epsilon_d\sum_{\sigma}n_{d\sigma} + Un_{d\uparrow}n_{d\downarrow} + \sum_{k\sigma}\left(V_{kd}c_{k\sigma}^{\dagger}c_{d\sigma} + V_{kd}^{*}c_{d\sigma}^{\dagger}c_{k\sigma}\right)
\tag{1.448}
$$

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

(a) Subcaption 1   (b) Subcaption 1
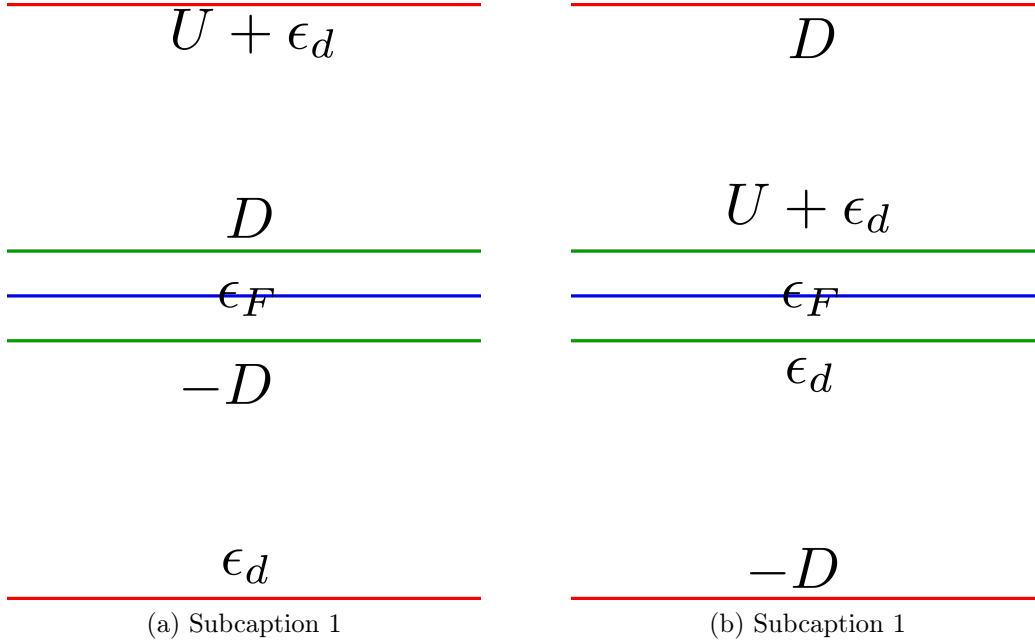
impossible.

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

$$H^{(0)} = \sum_{k<D-\delta D,\sigma} \epsilon_{k\sigma} n_{k\sigma} + \epsilon_d \sum_{\sigma} n_{d\sigma} + \sum_{k<D-\delta D,\sigma} \left(V_{kd} c_{k\sigma}^{\dagger} c_{d\sigma} + V_{kd}^{*} c_{d\sigma}^{\dagger} c_{k\sigma} \right) \tag{1.449}$$

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

$$H_{\sigma}^{(1,p)} = \sum_{k\in k^{+}} \alpha_{k\sigma} c_{d\sigma}^{\dagger} c_{k\sigma} c_{k\sigma}^{\dagger} c_{d\sigma} \tag{1.450}$$

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}.

$$\alpha_{k\sigma} = \frac{\langle 1_{d\sigma}| V_{kd}^{*} c_{d\sigma}^{\dagger} c_{k\sigma} |k\sigma\rangle \langle k\sigma| V_{kd} c_{k\sigma}^{\dagger} c_{d\sigma} |1_{d\sigma}\rangle}{E_{1_{d\sigma}} - E_{k\sigma}} = \frac{|V_{kd}|^{2}}{\epsilon_d - \epsilon_k} \tag{1.451}$$

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

$$H^{(1,h)} = \sum_{k\in k^{-},\sigma} \beta_{k\sigma} c_{k\sigma}^{\dagger} c_{d\sigma} c_{k\sigma} c_{d\sigma}^{\dagger} \tag{1.452}$$

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

$$\beta_{k\sigma} = \frac{\langle 0| V_{kd}^{*} c_{d\sigma} c_{k\sigma}^{\dagger} |k\sigma\rangle \langle k\sigma| V_{kd} c_{k\sigma} c_{d\sigma}^{\dagger} |0\rangle}{E_0 - E_{k\sigma}} = \frac{|V_{kd}|^{2}}{\epsilon_k - \epsilon_d} \tag{1.453}$$

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

$$H^{(1)} = \sum_{k^+,\sigma} \alpha_{k\sigma} T^+_{k\sigma} + \sum_{k^-,\sigma} \beta_{k\sigma} T^-_{k\sigma} \tag{1.454}$$

$T^{+,-}$ 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

$$\delta\epsilon_1 = \alpha_{k\sigma} = \sum_{k^+} \frac{|V_{kd}|^2}{\epsilon_d - \epsilon_k} \tag{1.455}$$

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

$$\delta\epsilon_1 = \sum_{k^+} \frac{|V_{kd}|^2}{\epsilon_d - \epsilon_k} = \int_{D-\delta D}^{D} dE N(E) \frac{|V(E)|^2}{\epsilon_d - E} \approx \frac{\Delta}{\pi} \frac{|\delta D|}{\epsilon_d - D} \tag{1.456}$$

The change in ϵ_0 is

$$\delta\epsilon_0 = \sum_\sigma \beta_{k\sigma} \approx -2\frac{\Delta}{\pi} \frac{|\delta D|}{\epsilon_d + D} \tag{1.457}$$

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

$$\delta\epsilon_d = \delta\epsilon_1 - \delta\epsilon_0 = \frac{\Delta|\delta D|}{\pi} \left[\frac{1}{\epsilon_d - D} + \frac{2}{\epsilon_d + D} \right] = \frac{\Delta}{\pi} \frac{|\delta D|}{D} = -\frac{\Delta}{\pi} \delta \ln D \tag{1.458}$$

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

$$\frac{d\epsilon_d}{d \ln D} = -\frac{\Delta}{\pi} \tag{1.459}$$

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:

$$\frac{|V_{kd}|^2}{\epsilon_k - U - \epsilon_d} \approx \frac{|V|^2}{-D - U - \epsilon_d} \tag{1.460}$$

$-(U + \epsilon_d)$ 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

$$\delta\epsilon_d = \frac{\Delta|\delta D|}{\pi} \left(\frac{1}{\epsilon_d - D} - \frac{1}{D + U + \epsilon_d} + \frac{2}{\epsilon_d + D} \right) \tag{1.461}$$

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.

$$H^{(2)} = \sum_{k^+,q,\sigma} \alpha_{k\sigma} T^+_{k\sigma} \gamma_{q,k,\sigma} c^\dagger_{d\sigma} c_{q\sigma} + \sum_{k^-,q,\sigma} \beta_{k\sigma} T^-_{k\sigma} \gamma_{q,k,\sigma} c_{d\sigma} c^\dagger_{q\sigma} \tag{1.462}$$

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

$$\alpha_{k\sigma}\gamma_{q,k,\sigma} = \frac{\langle 1_{d\sigma}| V_{kd}^* c_{d\sigma}^\dagger c_{k\sigma} |k\sigma\rangle \langle k\sigma| V_{kd} c_{k\sigma}^\dagger c_{d\sigma} |1_{d\sigma}\rangle \langle 1_{d\sigma}| V_{kd} c_{q\sigma} c_{d\sigma}^\dagger |q\sigma\rangle}{(E_{1_{d\sigma}} - E_{k\sigma})(E_q - E_k)}$$

$$= \alpha_{k\sigma}\frac{V_{kd}}{\epsilon_q - \epsilon_k} \tag{1.463}$$

The renormalization in V_{kd} is therefore

$$\delta V_{kd} = \frac{\Delta}{\pi}\frac{|\delta D|}{\epsilon_d - D}\frac{V_{kd}}{\epsilon_q - \epsilon_k} \tag{1.464}$$

Close to the band edge, we get

$$\delta V = \frac{\Delta}{\pi}\frac{|\delta D|}{\epsilon_d - D}\frac{V}{\epsilon_q - D} \approx \frac{\Delta}{\pi}\frac{|\delta D|}{D^2}V \tag{1.465}$$

Therefore,

$$\delta\Delta \sim V\delta V = \frac{\Delta V^2}{\pi D^2}|\delta D| \implies \frac{d\Delta}{dD} \sim \left(\frac{\Delta}{D}\right)^2 \tag{1.466}$$

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. 1.459 gives

$$\epsilon_d = -\frac{\Delta}{\pi}\ln D + \text{constant} \tag{1.467}$$

Defining the constant as

$$\text{constant} = \epsilon_d^* + \frac{\Delta}{\pi}\ln\Delta \tag{1.468}$$

we get

$$\epsilon_d = -\frac{\Delta}{\pi}\ln D + \epsilon_d^* + \frac{\Delta}{\pi}\ln\Delta \tag{1.469}$$

$$\implies \epsilon_d = \epsilon_d^* - \frac{\Delta}{\pi}\ln\frac{D}{\Delta} \tag{1.470}$$

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. 1.470). 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 $D = -a\widetilde{\epsilon}_d, a > 1$. We can then express the SWT coupling constant $\widetilde{J}$ by replacing ϵ_d with $\widetilde{\epsilon}_d$ in eq. 1.108. For simplicity set $U = \infty$. Then,

$$\widetilde{J} = -\frac{|V|^2}{\widetilde{\epsilon}_d} = \frac{a|V|^2}{D} \tag{1.471}$$

We can then do the poor man's scaling with this coupling. From eq. 1.252,

$$T_K \sim D\sqrt{\widetilde{J}N(0)^2}\exp\left(-\frac{1}{2\widetilde{J}N(0)^2}\right) = \sqrt{\Delta D}\exp\left(-\frac{D}{2\Delta}\right)$$

$$\sim D\sqrt{\frac{\Delta}{D}}\exp\left(\frac{\epsilon_d}{2\Delta}\right) \tag{1.472}$$
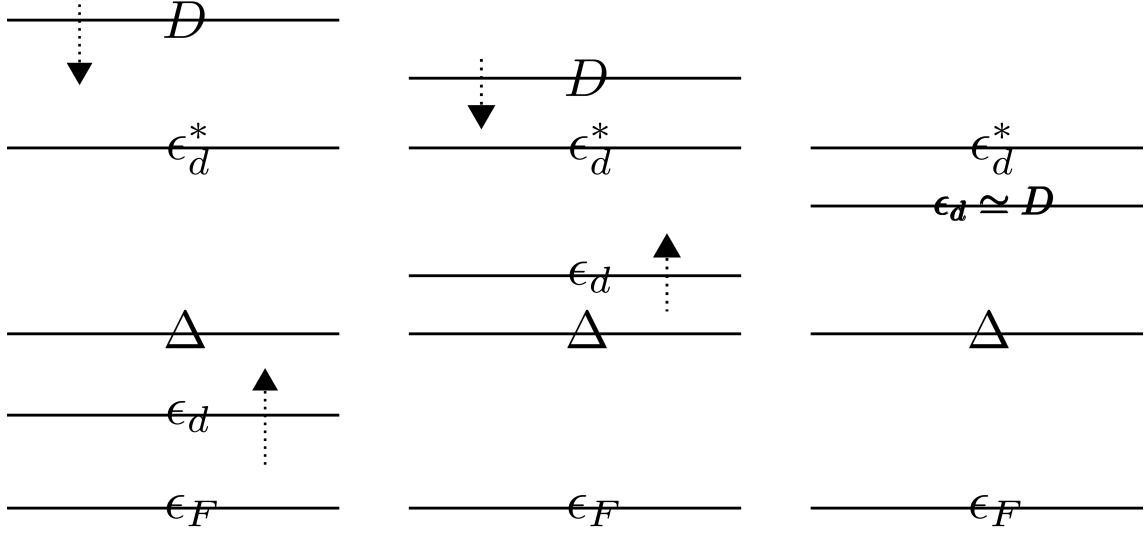
Figure 1: Renormalization in the energy levels when $\epsilon_d^* \gg \Delta$

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 $U \to \infty$ and ϵ_d outside the conduction band, we can do a SWT and the T_K obtained is q. 1.252,

$$J = -\frac{V^2}{\epsilon_d} \tag{1.473}$$

$$g = J\rho = -\frac{\Delta}{\epsilon_d} \tag{1.474}$$

$$\implies T_K = D\sqrt{\frac{\Delta}{\epsilon_d}}\exp\left(\frac{\epsilon_d}{2\Delta}\right) \tag{1.475}$$

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 ($U \to \infty$), all physical quantities will involve only one energy scale, T_K. This T_K itself might be different based on the starting Hamiltonian.

For $\epsilon_d^* \gg \Delta$, the renormalization will stop at $D \sim \epsilon_d$. Note that we had assumed $D \gg \epsilon_d$. That was the starting condition, that is, ϵ_d deep inside the Fermi surface. During the renormalization, D will keep on decreasing and ϵ_d will continuously increase. At some value of D, they will become equal and the impurity level will go outside the Fermi surface. At this point, none of the impurity levels can renormalize any more, because the relevant energy scales are greater than the cutoff. Hence the renormalization stops at this point. This point is given by $\overline{D} = a\epsilon_d(\overline{D}) \equiv \bar{\epsilon}_d$ where a is a constant of order unity. It satisfies the equation

$$\bar{\epsilon}_d = \epsilon_d^* - \frac{\Delta}{\pi}\ln\frac{a\bar{\epsilon}_d}{\Delta} \tag{1.476}$$

which is just eq. 1.470 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

$$\chi_d = \frac{\Delta}{2\pi}\left(\frac{g\mu_B}{\epsilon_d}\right)^2\left[1 + \frac{2\Delta}{\pi\epsilon_d}\ln\frac{\epsilon_d}{D} + ...\right] \tag{1.477}$$

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

$$
\begin{aligned}
\chi_d &= \frac{\Delta}{2\pi} \left(\frac{g\mu_B}{\bar{\epsilon}_d}\right)^2 \left[1 + \frac{2\Delta}{\pi\bar{\epsilon}_d} \ln a + ...\right] \\
&= \frac{\Delta}{2\pi} \left(\frac{g\mu_B}{\bar{\epsilon}_d}\right)^2 \left[1 + O\left(\frac{2\Delta}{\pi\bar{\epsilon}_d}\right)\right]
\end{aligned}
\tag{1.478}
$$

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 $\overline{D}$ can be associated with a temperature scale $k_b\overline{T} = \overline{D}$. At temperatures sufficiently below this temperature ($T \ll \overline{T}$), the susceptibility becomes (again from perturbation theory)

$$
\chi_d(T) = \frac{\Delta}{2\pi} \left(\frac{g\mu_B}{\bar{\epsilon}_d}\right)^2 + \frac{1}{4T} \left[1 + \frac{1}{2}\exp\left(\frac{T^*}{T}\right)\right]^{-1}
\tag{1.479}
$$

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:

$$
T \gg T_{FL} \implies e^{\frac{T^*}{T}} \gg 1 \implies \left[1 + \frac{1}{2}\exp\left(\frac{T^*}{T}\right)\right]^{-1} \approx 0
\tag{1.480}
$$

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

$$
\chi_d = \frac{\Delta}{2\pi} \left(\frac{g\mu_B}{\bar{\epsilon}_d}\right)^2
\tag{1.481}
$$

This is analogous to the result obtained in eq. 1.366, 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. 1.366 then becomes

$$
\chi_d = \frac{g^2\mu_B^2}{2}\rho_d(0) = \frac{g^2\mu_B^2}{2}\frac{\Delta}{\pi}\frac{1}{\bar{\epsilon}_d^2 + \Delta^2}
\tag{1.482}
$$

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

$$
\bar{\epsilon}_d = \epsilon_d^* - \Delta \ln \frac{\bar{\epsilon}_d}{\Delta}
\tag{1.483}
$$

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

$$
x_1 + \ln x_1 = x_2
\tag{1.484}
$$

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

$$
O(x_1) = O(x_2)
\tag{1.485}
$$

$$
\implies O\left(\frac{\bar{\epsilon}_d}{\Delta}\right) = O\left(\frac{\epsilon_d^*}{\Delta}\right)
\tag{1.486}
$$

$$
\implies O(\bar{\epsilon}_d) = O(\epsilon_d^*)
\tag{1.487}
$$

$$
\tag{1.488}
$$

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

$$\epsilon_d^* \gg \Delta \implies \bar{\epsilon}_d \gg \Delta \tag{1.489}$$

Applying this to eq. 1.482 means

$$\chi_d \approx \frac{g^2 \mu_B^2}{2} \frac{\Delta}{\pi} \frac{1}{\bar{\epsilon}_d^2} \tag{1.490}$$

which is the same as eq. 1.481. 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,

$$m = \frac{1}{\beta} \frac{\partial \ln Z}{\partial B} \implies \chi = \lim_{B \to 0} \frac{\partial m}{\partial B} = \lim_{B \to 0} \frac{1}{Z^2 \beta} \left[Z \frac{\partial^2 Z}{\partial B^2} - \left(\frac{\partial Z}{\partial B} \right)^2 \right] \tag{1.491}$$

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

$$Z = 1 + \exp(\beta h) + \exp(-\beta h) + 1 = 2(1 + \cosh \beta h) \tag{1.492}$$

$$\implies \frac{\partial Z}{\partial B} = g\mu_B \beta \sinh \beta h \tag{1.493}$$

$$\implies \frac{\partial^2 Z}{\partial B^2} = \frac{1}{2}(g\mu_B)^2 \beta^2 \cosh \beta h \tag{1.494}$$

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

$$\chi = \frac{\beta g^2 \mu_B^2}{2Z(h=0)} \tag{1.495}$$

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

$$\chi T = \frac{1}{2\mathcal{D}} \tag{1.496}$$

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,

$$m^{(0)} = \frac{1}{\beta} \frac{\partial \ln Z(h)}{\partial B} \tag{1.497}$$

61

where

$$Z(h) = 1 + e^{-\beta(k_B T^* - h)} + e^{-\beta(k_B T^* + h)} = 1 + e^{-\frac{\beta}{\beta^*}} 2\cosh\beta h \tag{1.498}$$

Therefore,

$$\chi^{(0)} = \lim_{h\to 0} \frac{1}{\beta Z} \frac{\partial^2 Z}{\partial B^2} = \lim_{h\to 0} \frac{g^2 \mu_B^2}{4\beta Z} \frac{\partial^2 Z}{\partial h^2} = \frac{g^2 \mu_B^2}{4} \beta \frac{2e^{-\frac{\beta}{\beta^*}}}{1 + 2e^{-\frac{\beta}{\beta^*}}} \tag{1.499}$$

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

$$\chi^{(0)} = \frac{1}{4T} \frac{2e^{-\frac{\beta}{\beta^*}}}{1 + 2e^{-\frac{\beta}{\beta^*}}} = \frac{1}{4T} \frac{2}{e^{\frac{\beta}{\beta^*}} + 2} \tag{1.500}$$

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. 1.53

$$m^{(1)} = \frac{g\mu_B}{2}(n_\uparrow - n_\downarrow) = \frac{g\mu_B}{2\pi}\left[\tan^{-1}\frac{\Delta}{k_B T^* - h} - \tan^{-1}\frac{\Delta}{k_B T^* + h}\right] \tag{1.501}$$

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

$$m^{(1)} = \frac{g\mu_B}{2\pi}\left[\frac{\Delta}{k_B T^* - h} - \frac{\Delta}{k_B T^* + h}\right] = \frac{g\mu_B \Delta}{\pi} \frac{h}{k_B (T^*)^2 - h^2} \tag{1.502}$$

Differentiating with B gives

$$\chi^{(1)} = \lim_{h\to 0} \frac{\partial m^{(1)}}{\partial B} = \frac{g^2 \mu_B^2}{2} \frac{\Delta}{\pi} \frac{1}{k_B^2 T^{*2}} = \frac{\Delta}{2\pi T^{*2}} \tag{1.503}$$

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

$$\chi = \frac{1}{4T} \frac{2}{e^{\frac{\beta}{\beta^*}} + 2} + \frac{\Delta}{2\pi T^{*2}} \tag{1.504}$$

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

$$\chi \approx \frac{1}{4T} \frac{2}{e^{\frac{\beta}{\beta^*}}} + \frac{\Delta}{2\pi T^{*2}} \approx \frac{\Delta}{2\pi T^{*2}} \tag{1.505}$$

$$\implies \chi T \propto T \tag{1.506}$$

We can now visualize the various phases as the temperature is changed. For $T \gg U, \epsilon_d$, all the four states 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 $\frac{1}{2\times3} = \frac{1}{6}$. At still lower temperatures $T^* \gg T$, the singly-occupied levels become disconnected and thee 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
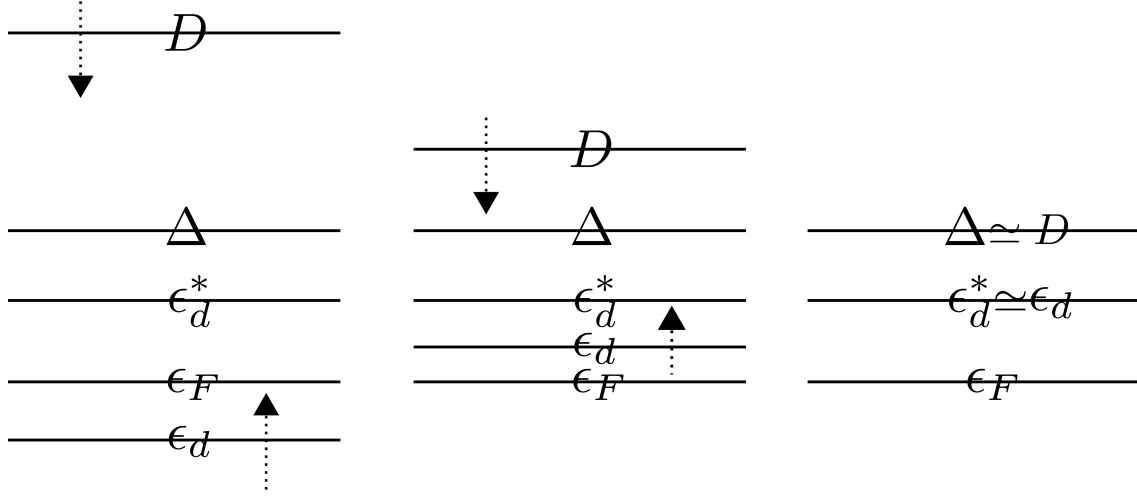
Figure 2: Renormalization in energy levels when $|\epsilon_d^*| \lesssim \Delta$

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. 1.466, 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 at $D = \max\{\Delta, k_B T\}$. For the simpler situation in which $T = 0$, the renormalization will stop at $D = \Delta$. From eq. 1.470, putting $D = \Delta$, we get

$$(\epsilon_d)_{\text{MV}} = \epsilon_d^* \tag{1.507}$$

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

$$\sim \frac{k_B T}{\epsilon_d} \tag{1.508}$$

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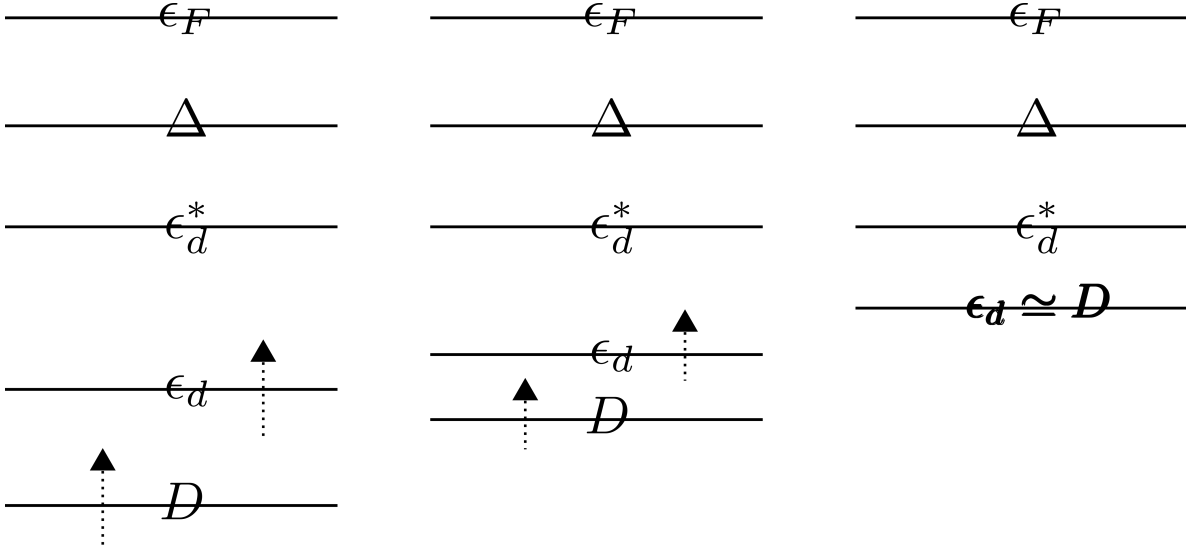
Figure 3: Renormalization in energy levels when $\epsilon_d^* \ll -\Delta$

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

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 $\widetilde{D} = -\widetilde{\epsilon}_d = \widetilde{T}$. Since the singly-occupied impurity level is now well below $-D$, we have $\langle n_d \rangle = 1$ and we are comfortably in the Kondo limit and the SWT and a consequent poor man's scaling can be performed, which will give eqs. 1.471 through 1.475. The result of the Schrieffer-Wolff transformation is a Hamiltonian that couples the impurity to the conduction electrons only through their spins; their 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. 1.496, 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.

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

Jefferson's calculation

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

$$
H = \sum_{k\sigma} \epsilon_{k\sigma} n_{k\sigma} + \epsilon_d n_d + \sum_{k\sigma} \left(V_{kd}^- c_{k\sigma}^\dagger c_{d\sigma} + V_{kd}^+ c_{d\sigma}^\dagger c_{k\sigma} \right) = H_0 + V \tag{1.509}
$$

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

$$
H\psi = E\psi \tag{1.510}
$$

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

$$
P = \sum |\phi\rangle \langle \phi| = \sum_{|k|<D-\delta D, \sigma=\pm 1, n_{d\sigma}=0,1} |n_{k\sigma}, n_{d\sigma'}\rangle \tag{1.511}
$$

Its orthogonal subspace has a projection operator

$$Q = 1 - P = \sum_{D-\delta D < |k| < D, \sigma = \pm 1, n_{d\sigma} = 0,1} |n_{k\sigma}, n_{d\sigma'}\rangle \tag{1.512}$$

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

$$P\{\psi\}_d = \{\phi\} \tag{1.513}$$

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

$$P\psi_0\Big|_{|k|<D-\delta D} = \psi_0\Big|_{|k|<D-\delta D} \tag{1.514}$$

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:

$$\Omega\{\phi\} = \{\psi\} \tag{1.515}$$

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

$$\Omega\{\phi\}^\perp = 0 \tag{1.516}$$

This allows us to write

$$\Omega P\phi = \Omega\phi \tag{1.517}$$
$$\Omega P\phi^\perp = \Omega \times 0 = 0 = \Omega\phi^\perp \tag{1.518}$$

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

$$\Omega P = \Omega \tag{1.519}$$

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

$$H\Omega\phi = E\Omega\Phi \tag{1.520}$$

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

$$PH\Omega\phi = EP\Omega\phi = E\phi \tag{1.521}$$

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

$$H_{\text{eff}} = PH\Omega = PH_0P + PV\Omega = PH_0P + PV\Omega \tag{1.522}$$

To solve for the Ω, apply eq. 1.519 on the Schrödinger equation $(E - H_0)\psi = V\psi$:

$$\Omega V\psi = (E\Omega P - \Omega PH_0)\psi \tag{1.523}$$

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

$$\Omega V\psi = (E - \Omega H_0 P)\psi \tag{1.524}$$

Subtracting the Schrödinger equation from the last equation gives

$$
\begin{aligned}
&(\Omega - 1)\, V\psi = (H_0 - \Omega H_0 P)\, \psi \\
\implies\ &(\Omega - 1)\, V\Omega\phi = (H_0 - \Omega H_0 P)\, \Omega\phi \\
\implies\ &(\Omega - 1)\, V\Omega\phi = (H_0\Omega - \Omega H_0)\, \phi \\
\implies\ &(\Omega - 1)\, V\Omega = [H_0, \Omega]
\end{aligned}
\tag{1.525}
$$

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

$$
\Omega = \sum_n c_n V^n = \sum_n \Lambda_n
\tag{1.526}
$$

The zeroth term in the main equation becomes

$$
[H_0, \Lambda_0] = 0 \implies \Lambda_0 = P
\tag{1.527}
$$

The first order equation is

$$
[H_0, \Lambda_1] = (\Lambda_0 - 1)\, V\Lambda_0 = (P - 1)\, VP = -QVP
\tag{1.528}
$$

The second order equation is

$$
[H_0, \Lambda_2] = -V\Lambda_1 + \Lambda_0 V\Lambda_1 + \Lambda_1 V\Lambda_0 = -QV\Lambda_1 + \Lambda_1 VP
\tag{1.529}
$$

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.

$$
A_1 = -QVP
\tag{1.530}
$$
$$
A_2 = -QV\Lambda_1 + \Lambda_1 VP
\tag{1.531}
$$

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

$$
\langle h|\, A_n\, |l\rangle = (E_h - E_l)\, \langle h|\, \Lambda_n\, |l\rangle \implies \langle h|\, \Lambda_n\, |l\rangle = \frac{\langle h|\, A_n\, |l\rangle}{E_h - E_l}
\tag{1.532}
$$

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

$$
\langle h|\, SA\, |l\rangle = \frac{\langle h|\, A\, |l\rangle}{E_l - E_h}
\tag{1.533}
$$

we can write the solution

$$
\Lambda_n = -S(A_n)
\tag{1.534}
$$

The expression of SA can be written as

$$
\begin{aligned}
SA &= \sum_{h,l} |h\rangle\, \langle l|\, \frac{\langle h|\, A\, |l\rangle}{E_l - E_H} \\
&= \sum_{h,l} \frac{1}{E_l - E_h}\, |h\rangle\, \langle h|\, A\, |l\rangle\, \langle l| \\
&= \sum_{l} \frac{1}{E_l - H_0} \left(\sum_h |h\rangle\, \langle h| \right) A\, |l\rangle\, \langle l| \\
&= \sum_l G_l A P_l
\end{aligned}
\tag{1.535}
$$

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

S has the property

$$\langle h| SQA |l\rangle = \frac{\langle h| QA |l\rangle}{E_l - E_h} = \frac{\langle h| A |l\rangle}{E_l - E_h} = \langle h| SA |l\rangle \tag{1.536}$$
$$\implies S(QA) = S(A)$$

The lowest order solutions are thus

$$\Lambda_1 = S(QVP) = S(VP) \tag{1.537}$$
$$\Lambda_2 = S(QV\Lambda_1) - S(\Lambda_1 VP) = S(VS(VP)) - S(S(VP)VP) \tag{1.538}$$

We can now expand the effective Hamiltonian in powers of V. From eq. 1.522, the interacting part of the effective Hamiltonian becomes

$$\begin{aligned}
H_{\text{eff}} - PH_0 P &= PV\Omega \\
&\approx PV(\Lambda_0 + \Lambda_1 + \Lambda_2) \\
&= PV\left[P + S(VP) + S(VS(VP)) - S(S(VP)VP) \right] \\
&= PVP + PVS(VP) + PVS(VS(VP)) - PVS(S(VP)VP)
\end{aligned} \tag{1.539}$$

Therefore,

$$H_{\text{eff}} = PHP + PVS(VP) + PVS(VS(VP)) - PVS(S(VP)VP) \tag{1.540}$$

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

$$PVSVP = PV \sum_l G_l VPP_l = PV \sum_l G_l V P_l \tag{1.541}$$

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

$$\begin{aligned}
PVSVSVP &= PVSV \sum_l G_l V P_l = PV \sum_l SVG_l V P_l \\
&= PV \sum_{l,l'} G_{l'} V G_l V P_l P_{l'} = PV \sum_l G_l V G_l V P_l
\end{aligned} \tag{1.542}$$

The fourth term is

$$\begin{aligned}
PVS(S(VP)VP) &= PVS(\sum_l G_l VPP_l VP) = PV \sum_{l,l'} G_{l'} G_l V P_l V PP_{l'} \\
&= PV \sum_{l'} G_{l'} \left(\sum_l G_l V P_l \right) V P_{l'}
\end{aligned} \tag{1.543}$$

The effective Hamiltonian up to third order in V is

$$\begin{aligned}
H_{\text{eff}} = PH_0 P + PV \sum_l G_l V P_l + PV \sum_l G_l V G_l V P_l \\
- PV \sum_{l,l'} G_{l'} G_l V P_l V P_{l'}
\end{aligned} \tag{1.544}$$

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:

$$|k_1\rangle \langle k_2| = c_{k_1}^\dagger c_{k_2} \tag{1.545}$$

$$P_k = |k, n_{d\sigma}\rangle \langle k, n_{d\sigma}| = c_k^\dagger c_k c_{d\sigma}^\dagger c_{d\sigma} = n_{k\sigma} n_{d\sigma} \tag{1.546}$$

The first term becomes

$$PH_0P = \sum_{k\sigma} \epsilon_{k\sigma} n_{k\sigma} + \epsilon_d n_d + \sum_{k\sigma} \left(V_{kd} c_{k\sigma}^\dagger c_{d\sigma} + \text{h.c.} \right) \tag{1.547}$$

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

$$PV \sum_l G_l V P_l = V \sum_{q\sigma} \left(\frac{V_q}{\epsilon_d - \epsilon_q} c_{q\sigma}^\dagger c_{d\sigma} + \frac{V_q^*}{\epsilon_q - \epsilon_d} c_{d\sigma}^\dagger c_{q\sigma} \right)$$

$$= \sum_{q\sigma}{}^+ \frac{|V_q|^2 c_{d\sigma}^\dagger c_{q\sigma} c_{q\sigma}^\dagger c_{d\sigma}}{\epsilon_d - \epsilon_q} + \sum_{q\sigma}{}^- \frac{|V_q|^2 c_{q\sigma}^\dagger c_{d\sigma} c_{d\sigma}^\dagger c_{q\sigma}}{\epsilon_q - \epsilon_d} \tag{1.548}$$

$$= \sum_{q\sigma}{}^+ \frac{|V_q|^2 n_{d\sigma} (1 - n_{q\sigma})}{\epsilon_d - \epsilon_q} + \sum_{q\sigma}{}^- \frac{|V_q|^2 n_{q\sigma} (1 - n_{d\sigma})}{\epsilon_q - \epsilon_d}$$

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

$$PV \sum_l G_l V P_l = \sum_q{}^+ \frac{|V_q|^2 n_{d\sigma}}{\epsilon_d - \epsilon_q} + \sum_q{}^- \frac{|V_q|^2 (1 - n_{d\sigma})}{\epsilon_q - \epsilon_d}$$

$$= n_d \left(\sum_q{}^+ \frac{|V_q|^2}{\epsilon_d - \epsilon_q} + 2 \sum_q{}^- \frac{|V_q|^2}{\epsilon_d - \epsilon_q} \right) \tag{1.549}$$

$$= n_d \delta \epsilon_d$$

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

$$|k, n_{d\sigma}\rangle \to \begin{cases} |q_e, n_d = 0\rangle \to \begin{cases} |q_e, n_d = 1\rangle \\ |q_e, q_h', n_d = 1\rangle \end{cases} \\ |q_h, n_d = 1\rangle \to \begin{cases} |q_h, q_e', n_d = 0\rangle \\ |q_h, n_d = 0\rangle \end{cases} \end{cases} \tag{1.550}$$

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

$$|k, n_d = 0\rangle \underbrace{\to |n_d = 1\rangle \to}_{\Delta E = \epsilon_k - \epsilon_q} |q_e, n_d = 0\rangle \underbrace{\to}_{\Delta E = \epsilon_q - \epsilon_d} |k', n_d = 1\rangle \tag{1.551}$$

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

$$|n_{d\sigma} = 1\rangle \underbrace{\to |k\sigma, n_d = 0\rangle \to}_{\Delta E = \epsilon_k - \epsilon_q} \begin{cases} |q_h \uparrow, n_{d\uparrow} = 1\rangle \\ |q_h \downarrow, n_{d\downarrow} = 1\rangle \end{cases} \underbrace{\to}_{\Delta E = \epsilon_q - \epsilon_d} |n_d = 0\rangle \tag{1.552}$$

Combining the two processes gives

$$\sum_q^+ \sum_{k\sigma} \frac{|V_q|^2 c_{d\sigma}^\dagger c_{q\sigma} c_{q\sigma}^\dagger c_{d\sigma} c_{d\sigma}^\dagger c_{k\sigma}}{(\epsilon_q - \epsilon_d)(\epsilon_k - \epsilon_q)} + \sum_{q\sigma'}^- \sum_{k\sigma} \frac{|V_q|^2 c_{q\sigma'}^\dagger c_{d\sigma'} c_{d\sigma'}^\dagger c_{q\sigma'} c_{k\sigma}^\dagger c_{d\sigma}}{(\epsilon_q - \epsilon_d)(\epsilon_k - \epsilon_q)}$$

$$= \sum_{k\sigma} \left(c_{k\sigma}^\dagger c_{d\sigma} \delta V_k^- + c_{d\sigma}^\dagger c_{k\sigma} \delta V_k^- \right) \tag{1.553}$$

where

$$\delta V^+ = \sum_q^+ \frac{|V_q|^2}{(\epsilon_q - \epsilon_d)(\epsilon_k - \epsilon_q)}$$

$$\delta V^- = \sum_q^- 2 \frac{|V_q|^2}{(\epsilon_q - \epsilon_d)(\epsilon_k - \epsilon_q)} \tag{1.554}$$

The total Hamiltonian can be written in the form

$$H_{\text{eff}} = \sum_{k\sigma} \epsilon_{k\sigma} n_{k\sigma} + (\epsilon_d + \delta\epsilon_d) n_d$$

$$+ \sum_{k\sigma} \left\{ \left(V_k^- + \delta V_k^- \right) c_{k\sigma}^\dagger c_{d\sigma} + \left(V_k^+ + \delta V_k^+ \right) c_{d\sigma}^\dagger c_{k\sigma} \right\} \tag{1.555}$$

We now evaluate the changes:

$$\delta\epsilon_d = \left(\sum_q^+ \frac{|V_q|^2}{\epsilon_d - \epsilon_q} + 2 \sum_q^- \frac{|V_q|^2}{\epsilon_d - \epsilon_q} \right)$$

$$\approx |V|^2 \rho |\delta D| \left(\frac{1}{\epsilon_d - D} + \frac{2}{\epsilon_d + D} \right) \tag{1.556}$$

$$= |V|^2 \rho |\delta D| \frac{D - 3\epsilon_d}{D^2 - \epsilon_d^2}$$

I used the approximation

$$\sum_{q=D-\delta D}^D f(q) = \int_{D-\delta D}^D dE \rho(E) f(E) \approx \rho f(D) \delta D \tag{1.557}$$

Also,

$$\delta V_k^+ = \sum_q^+ \frac{|V_q|^2}{(\epsilon_q - \epsilon_d)(\epsilon_k - \epsilon_q)}$$

$$\approx |V|^2 \rho |\delta D| \frac{1}{(D - \epsilon_d)(\epsilon_k - D)}$$

$$\delta V_k^- = 2 \sum_q^- \frac{|V_q|^2}{(\epsilon_q - \epsilon_d)(\epsilon_k - \epsilon_q)} \tag{1.558}$$

$$\approx -|V|^2 \rho |\delta D| \frac{2}{(D + \epsilon_d)(\epsilon_k + D)}$$

We now make the following assumptions:

- k is close to the Fermi level ($\epsilon_k \approx 0$)

- Because k is close to the Fermi surface, we assume the potential is independent of momenta: $V_k^+ \equiv v^+, V_k^- \equiv v^-$

- Since we truncated at third order, we need $D - |\epsilon_d| \gg v^\pm$. This gives us $D \gg |\epsilon_d|$.

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

2 URG Method

2.1 Formalism

This section is adapted from ref.[17]. 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'.

To begin, we choose an electron with a particular value of quantum numbers, which we label q. It might be the electron with the highest momentum or that at the first lattice site. The goal is to obtain a unitary transformation U_q that diagonalizes this Hamiltonian in this particular electron's basis. Once this is done, we can choose another electron (the next highest momentum or the second lattice site) and diagonalize the Hamiltonian in this electron's basis.

U_q is defined by

$$\tilde{\mathcal{H}} = U_q \mathcal{H} U_q^\dagger \text{ such that } \left[\tilde{\mathcal{H}}, n_q\right] = 0 \tag{2.1}$$

Another way to express the above problem is that, with the original Hamiltonian $\mathcal{H}$, the diagonal terms are not zero:

$$n_q \mathcal{H}(1 - n_q) \neq 0 \tag{2.2}$$

so we want to find a rotated Hamiltonian $\tilde{\mathcal{H}} = U_q \mathcal{H} U_q^\dagger$ such that the off-diagonal term is zero:

$$n_q \tilde{\mathcal{H}}(1 - n_q) = 0 \tag{2.3}$$

To make progress, we write the Hamiltonian $\mathcal{H}$ as

$$\mathcal{H} = \mathcal{H}^D + \mathcal{H}^I + \mathcal{H}^i \tag{2.4}$$

$\mathcal{H}^D$ is the diagonal part of the Hamiltonian, something of the form $\sum_k \epsilon_k n_k$. It also has the self energies that might arise from certain interactions. For example, if we have an interaction term of the form $J \sum_{k_1,k_2} c_{k_1}^\dagger c_{k_2}$, the term where both momenta are equal gives a diagonal term $J c_{k_1}^\dagger c_{k_1}$. Such terms are also included in $\mathcal{H}^D$.

$\mathcal{H}^I$ is the interaction between the current degree of freedom q and the remaining degrees of freedom k. It will consist of terms like $c_q^\dagger c_k$ or $c_k^\dagger c_q$ that scatter between the current degree of freedom and the other degrees of freedom.

Figure 4: Decomposition of Hamiltonian

The third term $\mathcal{H}^i$ has interactions between the remaining degrees of freedom. This term will also be diagonal in n_k because it doesn't involve scattering either from or into q states. It will involve terms like $c_{k_1}^\dagger c_{k_2}$.
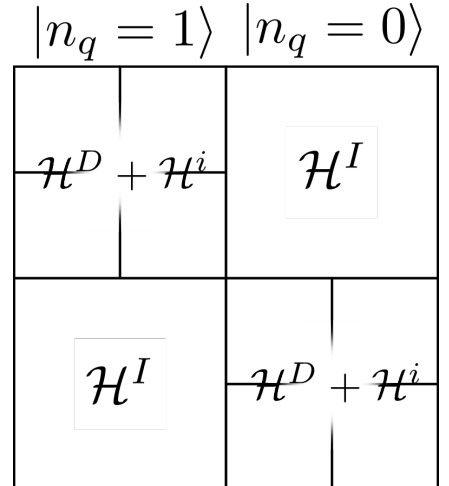
70

Let $\left\{ |\Psi\rangle_q \right\}$ be the set of states in which $\mathcal{H}$ assumes a diagonal form in the space of q. This diagonal form is of course also what we get when we apply the unitary transformation U_q on the Hamiltonian.

$$\mathcal{H} |\Psi\rangle_q = \tilde{\mathcal{H}} |\Psi\rangle_q \tag{2.5}$$

This is the equation we will use to find U_q. But first we will write ψ in the following fashion:

$$|\Psi\rangle = a_1 |1, \Psi_1\rangle + a_0 |0, \Psi_0\rangle \tag{2.6}$$

In the kets $|1, \Psi_1\rangle$ and $|0, \Psi_0\rangle$, the first entry $(0/1)$ signifies whether the degree of freedom q is occupied or not, and the second entry is the wavefunction of the remaining degrees of freedom. This is just a resolution of the total wavefunction in the two-dimensional Hilbert space of q. Substituting the decomposition of $|\Psi\rangle$ and $\mathcal{H}$ into eq. 2.5 gives

$$\tilde{\mathcal{H}} \left(a_1 |1, \Psi_1\rangle + a_0 |0, \Psi_0\rangle \right) = \left[\mathcal{H}^D + \mathcal{H}^I + \mathcal{H}^i \right] \left(a_1 |1, \Psi_1\rangle + a_0 |0, \Psi_0\rangle \right) \tag{2.7}$$

To get expressions from this, note that on the left hand side, $\tilde{\mathcal{H}}$ does not scatter q, so it will not change the left entry in the kets; it can only change the right entries. Similarly, on the right hand side, $\mathcal{H}^D$ and $\mathcal{H}^i$ will not change the occupation of the k degree of freedom. $\mathcal{H}^I$ however *will* change it. Matching the states with $|0\rangle$ gives

$$\tilde{\mathcal{H}} a_0 |0, \Psi_0\rangle = \left(\mathcal{H}^D + \mathcal{H}^i \right) a_0 |0, \Psi_0\rangle + \mathcal{H}^I a_1 |1, \Psi_1\rangle \tag{2.8}$$

We can simplify this equation by noting that

$$\mathcal{H}^D = \operatorname{Tr} \left[\mathcal{H}^D \hat{n}_q \right] \hat{n}_q + \operatorname{Tr} \left[\mathcal{H}^D (1 - \hat{n}_q) \right] (1 - \hat{n}_q) \tag{2.9}$$
$$\implies \mathcal{H}^D |0, \psi_0\rangle = \operatorname{Tr} \left[\mathcal{H}^D (1 - \hat{n}_q) \right] (1 - \hat{n}_q) |0, \psi_0\rangle \tag{2.10}$$

and

$$\mathcal{H}^I = \operatorname{Tr} \left[c_q^\dagger \mathcal{H} \right] c_q + c_q^\dagger \operatorname{Tr} \left[\mathcal{H} c_q \right] \implies \mathcal{H}^I |1, \psi_1\rangle = \operatorname{Tr} \left[c_q^\dagger \mathcal{H} \right] c_q |1, \psi_1\rangle \tag{2.11}$$

Substituting these in the equation gives

$$\tilde{\mathcal{H}} a_0 |0, \Psi_0\rangle = \left\{ \operatorname{Tr} \left[\mathcal{H}^D (1 - \hat{n}_q) \right] (1 - \hat{n}_q) + \mathcal{H}^i \right\} a_0 |0, \Psi_0\rangle + \operatorname{Tr} \left[c_q^\dagger \mathcal{H} \right] c_q a_1 |1, \Psi_1\rangle \tag{2.12}$$
$$\implies \left\{ \tilde{\mathcal{H}} - \mathcal{H}^i - \operatorname{Tr} \left[\mathcal{H}^D (1 - \hat{n}_q) \right] (1 - \hat{n}_q) \right\} a_0 |0, \Psi_0\rangle = \operatorname{Tr} \left[c_q^\dagger \mathcal{H} \right] c_q a_1 |1, \Psi_1\rangle \tag{2.13}$$

Defining $\hat{\omega} = \tilde{\mathcal{H}} - \mathcal{H}^i$, we get the result

$$a_0 |0, \Psi_0\rangle = \left[\hat{\omega} - \operatorname{Tr} \left[\mathcal{H}^D (1 - \hat{n}_q) \right] (1 - \hat{n}_q) \right]^{-1} \operatorname{Tr} \left[c_q^\dagger \mathcal{H} \right] c_q a_1 |1, \Psi_1\rangle \tag{2.14}$$

We define

$$\eta_q \equiv \frac{1}{\hat{\omega} - \operatorname{Tr} \left[\mathcal{H}^D (1 - \hat{n}_q) \right] (1 - \hat{n}_q)} \operatorname{Tr} \left[c_q^\dagger \mathcal{H} \right] c_q \tag{2.15}$$

which gives the equation a compact form

$$a_0 |0, \Psi_0\rangle = \eta_q a_1 |1, \Psi_1\rangle \tag{2.16}$$

The equation obtained by matching the states $|1\rangle$ is

$$\begin{aligned} a_1 \overline{\mathcal{H}} |1, \Psi_1\rangle &= \left(\mathcal{H}^D + \mathcal{H}^i \right) a_1 |1, \Psi_1\rangle + \mathcal{H}^I a_0 |0, \Psi_0\rangle \\ &= \left(\operatorname{Tr} \left[\mathcal{H}^D \hat{n}_q \right] \hat{n}_q + \mathcal{H}^i \right) a_1 |1, \Psi_1\rangle + c_q^\dagger \operatorname{Tr} \left[\mathcal{H} c_q \right] a_0 |0, \Psi_0\rangle \\ \implies a_1 |\Psi_1\rangle &= \left(\overline{\mathcal{H}} - \mathcal{H}^i - \operatorname{Tr} \left[\mathcal{H}^D \hat{n}_q \right] \hat{n}_q \right)^{-1} c_q^\dagger \operatorname{Tr} \left[\mathcal{H} c_q \right] a_0 |0, \Psi_0\rangle \\ &= \mu_q a_0 |0, \Psi_0\rangle \end{aligned} \tag{2.17}$$

where

$$\mu_q = \frac{1}{\hat{\omega} - \text{Tr}\left[\mathcal{H}^D \hat{n}_q\right] \hat{n}_q} c_q^\dagger \, \text{Tr}\left[\mathcal{H} c_q\right] \tag{2.18}$$

We thus get the following two equations:

$$a_0 \left|0, \Psi_0\right\rangle = \eta_q a_1 \left|1, \Psi_1\right\rangle \tag{2.19}$$

$$a_1 \left|1, \Psi_1\right\rangle = \mu_q a_0 \left|0, \Psi_0\right\rangle \tag{2.20}$$

Combining eqs. 2.19 and 2.20, we get

$$a_0 \left|0, \Psi_0\right\rangle = \eta_q a_1 \left|1, \Psi_1\right\rangle = \eta_q \mu_q a_0 \left|0, \Psi_0\right\rangle \tag{2.21}$$

Combining this with the fact that μ_q should have a $c_q^\dagger$ and hence should give $\mu_q \left|1, \Psi_1\right\rangle$, we get

$$\eta_q \mu_q = 1 - \hat{n}_q \tag{2.22}$$

Similarly, combining the equations the other way round gives

$$\mu_q \eta_q = \hat{n}_q \tag{2.23}$$

As a consequence,

$$\{\eta_q, \mu_q\} = 1$$
$$[\eta_q, \mu_q] = 1 - 2\hat{n}_q \tag{2.24}$$

Other properties include

$$\eta_q^2 = (\mu_q)^2 = 0 \tag{2.25}$$

$$\hat{n}_q \eta_q = (1 - \hat{n}_q)\mu_q = 0 \tag{2.26}$$

$$\eta_q \hat{n}_q = \eta_q \tag{2.27}$$

$$\mu_q(1 - \hat{n}_q) = \mu_q \tag{2.28}$$

We now need to find the unitary operation U_q that disentangles the state $\left|1, \Psi_1\right\rangle$ from the state $\left|\Psi\right\rangle$. For the sake of unitarity, we restrict $\mu_q = \eta_q^\dagger$. This restriction is transferred to the values of $\hat{\omega}$. Using eq. 2.19,

$$\left|\Psi\right\rangle = a_1 \left|1, \Psi_1\right\rangle + a_0 \left|0, \Psi_0\right\rangle = a_1 \left|1, \Psi_1\right\rangle + \eta_q a_1 \left|1, \Psi_1\right\rangle = (1 + \eta_q) \left|1, \Psi_1\right\rangle \tag{2.29}$$

This means that the operator U_q for going from $\left|, \Psi_1\right\rangle$ to $\left|\Psi\right\rangle$ is described by

$$U_q^{-1} = \mathcal{C} \left(1 + \eta_q + \mathcal{O}\right) \tag{2.30}$$

where $\mathcal{O}$ is some operator function of η_q and $\eta_q^\dagger$ such that

$$(1 + \eta_q + \mathcal{O}) \left|1, \Psi_1\right\rangle = (1 + \eta_q) \left|1, \Psi_1\right\rangle \implies \mathcal{O} \left|1, \Psi_1\right\rangle = 0 \tag{2.31}$$

and $\mathcal{C}$ is a real scalar. To find $\mathcal{O}$, note that we can write U_q^{-1} as

$$U_q^{-1} = \mathcal{C} \exp\left(\eta_q + \mathcal{O}\right) \tag{2.32}$$

This is because $\eta_q^2 = 0$ and since $\mathcal{O}$ is made up of η_q and $\eta_q^\dagger$ is has the same property. This exponential form allows us to write

$$U_q = \mathcal{C} \exp\left(-\eta_q - \mathcal{O}\right) = \mathcal{C} \left(1 - \eta_q - \mathcal{O}\right) \tag{2.33}$$

But, since U_q is required to be unitary, we can write, from eq. 2.30,

$$U_q^\dagger = U_q^{-1} = \mathcal{C} \left(1 + \eta_q + \mathcal{O}\right) \implies U_q^\dagger = \mathcal{C} \left(1 + \eta_q^\dagger + \mathcal{O}^\dagger\right) \tag{2.34}$$

Comparing the two expression of U_q in eqs. 2.33 and 2.34,

$$1 - \eta_q - \mathcal{O} = 1 + \eta_q^\dagger + \mathcal{O}^\dagger \implies -\eta_q = \mathcal{O}^\dagger \implies \mathcal{O} = -\eta_q^\dagger \tag{2.35}$$

This improves eq. 2.33:

$$U_q = \mathcal{C} \left(1 + \eta_q^\dagger - \eta_q \right) \tag{2.36}$$

To find $\mathcal{C}$, we can use the unitarity of U_q:

$$1 = U_q^\dagger U_q = \mathcal{C}^2 \left(1 + \{\eta_q^\dagger, \eta_q\} \right) = \mathcal{C}^2 \times 2 \implies \mathcal{C} = \frac{1}{\sqrt{2}} \tag{2.37}$$

The unitary operator that transforms the entangled eigenstate $|\Psi\rangle$ to the eigenstate with good quantum number n_q, $|1, \Psi_1\rangle$ is thus

$$U_q = \frac{1}{\sqrt{2}} \left(1 + \eta_q^\dagger - \eta_q \right) \tag{2.38}$$

The form of the rotated Hamiltonian can now be written down.

$$
\begin{aligned}
\widetilde{\mathcal{H}} &= U_q \mathcal{H} U_q^\dagger \\
&= \frac{1}{2} \left(1 + \eta_q^\dagger - \eta_q \right) \mathcal{H} \left(1 + \eta_q - \eta_q^\dagger \right) \\
&= \frac{1}{2} \left(1 + \eta_q^\dagger - \eta_q \right) \left(\mathcal{H} + \mathcal{H}\eta - \mathcal{H}\eta_q^\dagger \right) \\
&= \frac{1}{2} \left(\mathcal{H} + \mathcal{H}\eta - \mathcal{H}\eta_q^\dagger + \eta_q^\dagger \mathcal{H} + \eta_q^\dagger \mathcal{H}\eta_q - \eta_q^\dagger \mathcal{H}\eta_q^\dagger - \eta_q \mathcal{H} - \eta_q \mathcal{H}\eta_q + \eta_q \mathcal{H}\eta_q^\dagger \right) \\
&= \frac{1}{2} \left(\mathcal{H}^D + \mathcal{H}^i + \mathcal{H}^I + \mathcal{H}\eta - \mathcal{H}\eta_q^\dagger + \eta_q^\dagger \mathcal{H} + \eta_q^\dagger \mathcal{H}\eta_q - \eta_q^\dagger \mathcal{H}\eta_q^\dagger - \eta_q \mathcal{H} - \eta_q \mathcal{H}\eta_q + \eta_q \mathcal{H}\eta_q^\dagger \right) \\
&= \frac{1}{2} \left(\mathcal{H}^D + \mathcal{H}^i + \mathcal{H}^I + [\eta_q^\dagger - \eta, \mathcal{H}] + \eta_q^\dagger \mathcal{H}\eta_q - \eta_q^\dagger \mathcal{H}\eta_q^\dagger - \eta_q \mathcal{H}\eta_q + \eta_q \mathcal{H}\eta_q^\dagger \right)
\end{aligned} \tag{2.39}
$$

In the last step I split $\mathcal{H}$ using eq. 2.4. For reasons that will become apparent later, we will split the terms into two groups:

$$\widetilde{\mathcal{H}} = \frac{1}{2} \left(\underbrace{\mathcal{H}^D + \mathcal{H}^i + [\eta_q^\dagger - \eta, \mathcal{H}] + \eta_q^\dagger \mathcal{H}\eta_q + \eta_q \mathcal{H}\eta_q^\dagger}_{\text{group 1}} + \overbrace{\mathcal{H}^I - \eta_q^\dagger \mathcal{H}\eta_q^\dagger - \eta_q \mathcal{H}\eta_q}^{\text{group 2}} \right) \tag{2.40}$$

Group 2 consists of purely off-diagonal terms; they amount to 0. To see how, note that terms that have two η_k or two $\eta_q^\dagger$ can only be nonzero if the intervening $\mathcal{H}$ has a creation or destruction operator. We resolve the Hamiltonian in the basis of q in the following form:

$$
\begin{aligned}
\mathcal{H} &= \mathrm{Tr}\left[\mathcal{H}\hat{n}_q\right] \hat{n}_q + \mathrm{Tr}\left[\mathcal{H}(1 - \hat{n}_q)\right](1 - \hat{n}_q) + c_q^\dagger \mathrm{Tr}\left[\mathcal{H}c_q\right] + \mathrm{Tr}\left[c_q^\dagger \mathcal{H}\right] c_q \\
&= H_e \hat{n}_q + H_h (1 - \hat{n}_q) + c_q^\dagger T + T^\dagger c_q
\end{aligned} \tag{2.41}
$$

Using this form, we can write

$$\eta_q \mathcal{H}\eta_q = \eta_q c_q^\dagger T \eta_q \tag{2.42}$$

and

$$\eta_q^\dagger \mathcal{H}\eta_q^\dagger = \eta_q^\dagger T^\dagger c_q \eta_q^\dagger \tag{2.43}$$

We can also write the off-diagonal part as

$$\mathcal{H}^I = c_q^\dagger T + T^\dagger c_q \tag{2.44}$$

Group 2 becomes

$$\text{group } 2 = c_q^\dagger T + T^\dagger c_q - \eta_q^\dagger T^\dagger c_q \eta_q^\dagger - \eta_q c_q^\dagger T \eta_q \tag{2.45}$$

To simplify this, we use the definition of $\eta_q^\dagger$, eq. 2.18, to write η_q:

$$\eta_q = \left(\eta_q^\dagger\right)^\dagger = \ \text{Tr}\left[c_q^\dagger \mathcal{H}\right] c_q \frac{1}{\hat{\omega} - \ \text{Tr}\left[\mathcal{H}^D \hat{n}_q\right]\hat{n}_q} = T^\dagger c_q \frac{1}{\hat{\omega} - H_e \hat{n}_q} \tag{2.46}$$

Using this, we can write

$$\begin{aligned}
\eta_q c_q^\dagger T \eta_q &= T^\dagger c_q \frac{1}{\hat{\omega} - H_e \hat{n}_q} c_q^\dagger T \eta_q \\
&= T^\dagger c_q \left(\frac{1}{\hat{\omega} - H_e \hat{n}_q} c_q^\dagger T\right) \eta_q \tag{2.47} \\
&= T^\dagger c_q \eta_q^\dagger \eta_q \qquad \text{[eq. 2.18]} \\
&= T^\dagger c_q \hat{n}_q \qquad \text{[eq. 2.23]}
\end{aligned}$$

which gives

$$\eta_q c_q^\dagger T \eta_q = T^\dagger c_q \tag{2.48}$$

Similarly, we can express $\eta_q^\dagger$ by taking Hermitian conjugate of η_q:

$$\eta_q^\dagger = \frac{1}{\hat{\omega} - H_h\left(1 - \hat{n}_q\right)} T^\dagger c_q \tag{2.49}$$

which gives

$$\eta_q^\dagger T^\dagger c_q \eta_q^\dagger = c_q^\dagger T \tag{2.50}$$

Substituting the expressions 2.48 and 2.50, we get group $2 = 0$. Substituting this in the rotated Hamiltonian gives

$$\widetilde{\mathcal{H}} = \frac{1}{2}\left(\mathcal{H}^D + \mathcal{H}^i + \mathcal{H}\eta - \mathcal{H}\eta_q^\dagger + \eta_q^\dagger \mathcal{H} + \eta_q^\dagger \mathcal{H}\eta_q - \eta_q \mathcal{H} + \eta_q \mathcal{H}\eta_q^\dagger\right) \tag{2.51}$$

To simplify the last 6 terms, we note the following:

$$\eta_q^\dagger = \frac{1}{\omega - H_e \hat{n}_q} c_q^\dagger T, \qquad \eta_q = \frac{1}{\omega - H_h(1 - \hat{n}_q)} T^\dagger c_q \tag{2.52}$$

Then,

$$\begin{aligned}
&\Longrightarrow \frac{1}{\omega - H_e \hat{n}_q} c_q^\dagger T = c_q^\dagger T \frac{1}{\omega - H_h(1 - \hat{n}_q)} \\
&\Longrightarrow c_q^\dagger T H_h(1 - \hat{n}_q) = H_e \hat{n}_q c_q^\dagger T \\
&\Longrightarrow \frac{1}{\omega - H_e \hat{n}_q} c_q^\dagger T H_h(1 - \hat{n}_q) = \frac{1}{\omega - H_e \hat{n}_q} H_e \hat{n}_q c_q^\dagger T \\
&\Longrightarrow \eta_q^\dagger H_h(1 - \hat{n}_q) = H_e \hat{n}_q \frac{1}{\omega - H_e \hat{n}_q} c_q^\dagger T \\
&\Longrightarrow \eta_q^\dagger H_h(1 - \hat{n}_q) = H_e \hat{n}_q \eta_q^\dagger \\
&\Longrightarrow \eta_q^\dagger H_h = H_e \hat{\eta}_q^\dagger
\end{aligned} \tag{2.53}$$

Using this identity and its conjugate ($\eta_q H_e = H_h \hat{\eta}_q$), the expression for $\eta_q \mathcal{H}\eta_q^\dagger$ can be simplified:

$$\begin{aligned}
\eta_q \mathcal{H}\eta_q^\dagger &= \eta_q H_e \hat{n}_q \eta_q^\dagger \\
&= H_h \eta_q \eta_q^\dagger \tag{2.54} \\
&= H_h(1 - \hat{n}_q)
\end{aligned}$$

74

Similarly,

$$\eta_q^\dagger \mathcal{H} \eta_q = \eta_q^\dagger H_h \eta_q$$
$$= H_e \eta_q^\dagger \eta_q \tag{2.55}$$
$$= H_e \hat{n}_q$$

Also,

$$\mathcal{H}\eta - \mathcal{H}\eta_q^\dagger + \eta_q^\dagger \mathcal{H} - \eta_q \mathcal{H} = \left(\eta_q^\dagger H_h - H_e \eta_q^\dagger\right) + (H_h \eta - \eta H_e) + \eta_q^\dagger T^\dagger c_q - \eta_q c_q^\dagger T + \\ c_q^\dagger T \eta_q - T^\dagger c_q \eta_q^\dagger \tag{2.56}$$

By virtue of eq. 2.53 and its conjugate, the first two terms will vanish.

$$\mathcal{H}\eta - \mathcal{H}\eta_q^\dagger + \eta_q^\dagger \mathcal{H} - \eta_q \mathcal{H} = \eta_q^\dagger T^\dagger c_q - \eta_q c_q^\dagger T + c_q^\dagger T \eta_q - T^\dagger c_q \eta_q^\dagger \tag{2.57}$$

From eqs. 2.48 and 2.50,

$$\eta_q^\dagger T^\dagger c_q = \eta_q^\dagger \eta_q c_q^\dagger T \eta_q = \hat{n}_q c_q^\dagger T \eta_q = c_q^\dagger T \eta_q \tag{2.58}$$
$$T^\dagger c_q \eta_q^\dagger = \eta_q c_q^\dagger T \eta_q \eta_q^\dagger = \eta_q c_q^\dagger T (1 - \hat{n}_q) = \eta_q c_q^\dagger T \tag{2.59}$$
$$\tag{2.60}$$

Eq. 2.57 becomes

$$\mathcal{H}\eta - \mathcal{H}\eta_q^\dagger + \eta_q^\dagger \mathcal{H} - \eta_q \mathcal{H} = c_q^\dagger T \eta_q - \eta_q c_q^\dagger T + c_q^\dagger T \eta_q - \eta_q c_q^\dagger T \;\; = 2\left[c_q^\dagger T, \eta_q\right] \tag{2.61}$$

Putting it all together,

$$\widetilde{\mathcal{H}} = \frac{1}{2}\left(\mathcal{H}^D + \mathcal{H}^i + \mathcal{H}\eta - \mathcal{H}\eta_q^\dagger + \eta_q^\dagger \mathcal{H} + \eta_q^\dagger \mathcal{H} \eta_q - \eta_q \mathcal{H} + \eta_q \mathcal{H}\eta_q^\dagger\right)$$
$$= \frac{1}{2}\left(\mathcal{H}^D + \mathcal{H}^i\right) + \left[c_q^\dagger T, \eta_q\right] + \frac{1}{2}\left[H_e \hat{n}_q + H_h(1 - \hat{n}_q)\right] \tag{2.62}$$

One further simplification is possible. The last two terms constitute the total diagonal part of the Hamiltonian, but so do the first two terms:

$$\mathcal{H}^D + \mathcal{H}^i = H_e \hat{n}_q + H_h (1 - \hat{n}_q) \tag{2.63}$$

Hence,

$$\widetilde{\mathcal{H}} = \frac{1}{2}\left(\mathcal{H}^D + \mathcal{H}^i + \mathcal{H}\eta - \mathcal{H}\eta_q^\dagger + \eta_q^\dagger \mathcal{H} + \eta_q^\dagger \mathcal{H} \eta_q - \eta_q \mathcal{H} + \eta_q \mathcal{H}\eta_q^\dagger\right)$$
$$= H_e \hat{n}_q + H_h(1 - \hat{n}_q) + \left[c_q^\dagger T, \eta_q\right] \tag{2.64}$$
$$= \mathrm{Tr}\left[\mathcal{H}\hat{n}_q\right]\hat{n}_q + \mathrm{Tr}\left[\mathcal{H}\hat{(1 - n_q)}\right](1 - \hat{n}_q) + \left[c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right), \eta_q\right]$$

The two terms at the front can be written in a slightly different fashion.

$$\mathrm{Tr}\left[\mathcal{H}\hat{n}_q\right]\hat{n}_q + \mathrm{Tr}\left[\mathcal{H}(1 - \hat{n}_q)\right](1 - \hat{n}_q) = \mathrm{Tr}\left[\mathcal{H}\hat{n}_q\right]\hat{n}_q + \mathrm{Tr}\left[\mathcal{H}(\hat{n}_q - 1)\right](\hat{n}_q - 1)$$
$$= \mathrm{Tr}\left[\mathcal{H}\hat{n}_q\right]\hat{n}_q + \mathrm{Tr}\left[\mathcal{H}(\hat{n}_q - 1)\right]n_q - \mathrm{Tr}\left[\mathcal{H}\hat{(n_q - 1)}\right]$$
$$= \mathrm{Tr}\left[\mathcal{H}(2\hat{n}_q - 1)\right]\hat{n}_q - \mathrm{Tr}\left[\mathcal{H}(\hat{n}_q - 1)\right]$$
$$= \mathrm{Tr}\left[\mathcal{H}\left(\hat{n}_q - \frac{1}{2}\right)\right]2\hat{n}_q - \mathrm{Tr}\left[\mathcal{H}(\hat{n}_q - \frac{1}{2})\right] + \frac{1}{2}\mathrm{Tr}\left[\mathcal{H}\right] \tag{2.65}$$
$$= \mathrm{Tr}\left[\mathcal{H}\left(\hat{n}_q - \frac{1}{2}\right)\right](2\hat{n}_q - 1) + \frac{1}{2}\mathrm{Tr}\left[\mathcal{H}\right]$$
$$= \mathrm{Tr}\left[\mathcal{H}\tau_q\right]2\tau_q + \frac{1}{2}\mathrm{Tr}\left[\mathcal{H}\right]$$

The last term can be written as:

$$\left[c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right), \eta_q\right] = c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right)\eta_q - \eta_q c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right)$$
$$= \left(2\hat{n}_q - 1\right)c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right)\eta_q - \left(1 - 2\hat{n}_q\right)\eta_q c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right) \tag{2.66}$$

I used $\hat{n}_q c_q^\dagger = c_q^\dagger$ and $\hat{n}_q \eta_q = 0$. Then,

$$\left[c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right), \eta_q\right] = 2\tau_q\left\{c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right), \eta_q\right\} \tag{2.67}$$

The final form of the rotated Hamiltonian is

$$\widetilde{\mathcal{H}} = U_q \mathcal{H} U_q^\dagger = \mathrm{Tr}\left[\mathcal{H}\hat{n}_q\right]\hat{n}_q + \mathrm{Tr}\left[\mathcal{H}(1 - \hat{n}_q)\right]\left(1 - \hat{n}_q\right) + 2\tau_q\left\{c_q^\dagger \mathrm{Tr}\left(\mathcal{H}c_q\right), \eta_q\right\} \tag{2.68}$$

To check that this indeed commutes with $\hat{n}_q$,

$$\begin{aligned}
\left[\widetilde{\mathcal{H}}, \hat{n}_q\right] &= \left[\left[c_q^\dagger T, \eta_q\right], \hat{n}_q\right] \\
&= \left[c_q^\dagger T \eta_q, \hat{n}_q\right] - \left[\eta_q c_q^\dagger T, \hat{n}_q\right] \\
&= c_q^\dagger T \eta_q \hat{n}_q - \hat{n}_q c_q^\dagger T \eta_q \qquad \left[2^{\mathrm{nd}}\ [\ .\ ]\ \text{is } 0,\ \because c_q^\dagger \hat{n}_q = \hat{n}_q \eta_q = 0\right] \\
&= c_q^\dagger T \eta_q - c_q^\dagger T \eta_q \\
&= 0
\end{aligned} \tag{2.69}$$

The fixed point is reached when the denominator of the RG equation vanishes. This is equivalent to the condition:

$$\hat{\omega} - H_e \hat{n} = 0$$
$$\implies \omega_e = H_e$$

or

$$\hat{\omega} - H_h\left(1 - \hat{n}\right) = 0$$
$$\implies \omega_h = H_h$$

In either case, we see that the eigenvalue of $\hat{\omega}$ matches the eigenvalue of one of the blocks. This also leads to the vanishing of the off-diagonal block. To see how,

$$\begin{aligned}
&\eta^\dagger \eta\left|1, \Psi_1\right\rangle = \left|1, \Psi_1\right\rangle \qquad\qquad \left[\eta^\dagger \eta = \hat{n}\right] \\
\implies\ &\frac{1}{\hat{\omega} - \hat{H}_e}c^\dagger T \eta = \left|1, \Psi_1\right\rangle \\
\implies\ &c^\dagger T \eta = \left(\hat{\omega} - \hat{H}_e\right)\left|1, \Psi_1\right\rangle \\
&\qquad\quad = \left(\omega_e - H_e\right)\left|1, \Psi_1\right\rangle
\end{aligned} \tag{2.70}$$

If $\omega_e = H_e$, we will have $c^\dagger T = 0$. This implies $T^\dagger c = 0$ and hence $\mathcal{H}^I = 0$.

2.2   Prescription

Given a Hamiltonian

$$\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_0 + c^\dagger T + T^\dagger c \tag{2.71}$$

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. 2.68, 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

$$\Delta \mathcal{H}_{q\beta} = 2\tau_{q\beta} \left\{ c_{q\beta}^{\dagger} \text{Tr} \left(\mathcal{H} c_{q\beta} \right), \eta_{q\beta} \right\} \tag{2.72}$$

Decoupling the entire shell gives

$$\Delta \mathcal{H} = \sum_{q\beta} 2\tau_{q\beta} \left\{ c_{q\beta}^{\dagger} \text{Tr} \left(\mathcal{H} c_{q\beta} \right), \eta_{q\beta} \right\} \tag{2.73}$$

One can look at the particle and hole sectors separately. The particle sector involves those processes which create a particle with high energy in the intermediate state. The hole sector consists of those processes that destroy a deep-lying electron in the intermediate state. It is clear that the first term of the anticommutator, one that starts with $c^{\dagger}$ and ends with η will destroy an electron in the intermediate state. That gives the hole sector contribution:

$$\begin{aligned} \Delta^{-}\mathcal{H} &= \sum_{q\beta} c_{q\beta}^{\dagger} \text{Tr} \left(\mathcal{H} c_{q\beta} \right) \eta_{q\beta} \\ &= \sum_{q\beta} c_{q\beta}^{\dagger} \text{Tr} \left(\mathcal{H} c_{q\beta} \right) \frac{1}{\omega_h - \mathcal{H}^D} \text{Tr} \left(c_{q\beta}^{\dagger} \mathcal{H} \right) c_{q\beta} \end{aligned} \tag{2.74}$$

where we have replaced $\hat{\omega}$ by its eigenvalue ω_h and $H_h = \text{Tr} \left(\mathcal{H} \left(1 - \hat{n}_{q\beta} \right) \right)$. The other term in the commutator gives the particle sector contribution:

$$\begin{aligned} \Delta^{+}\mathcal{H} &= \sum_{q\beta} \eta_{q\beta} c_{q\beta}^{\dagger} \text{Tr} \left(\mathcal{H} c_{q\beta} \right) \\ &= \sum_{q\beta} \text{Tr} \left(c_{q\beta}^{\dagger} \mathcal{H} \right) c_{q\beta} \frac{1}{\omega_e - \mathcal{H}^D} c_{q\beta}^{\dagger} \text{Tr} \left(\mathcal{H} c_{q\beta} \right) \end{aligned} \tag{2.75}$$

where we used $2\tau\eta = -\eta$ and $H_e = \text{Tr} \left(\mathcal{H} \hat{n}_{q\beta} \right)$. 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 employ is that H_e and H_h will, in general, have the energies of all the electrons. But we consider only the energy of the on-shell electrons in the denominator. After integrating out these electrons, we can rearrange the remaining operators to determine which term in the Hamiltonian it renormalizes and what is the renormalization.

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

3 Star Graph URG

The star graph problem consists of N spin-like degrees of freedom (lablled 1 through N) individually talking to a spin at the center (labelled 0). Each spin i ($\in [0, N]$) has an on-site energy ϵ_i. The coupling strength

between 0 and i ($\in [1, N]$) is J_i. We choose the on-site energies such that $\epsilon_{i+1} > \epsilon_i, i \in [N-1, 1]$. In this way, ϵ_1 is the infrared limit and ϵ_N is the ultraviolet limit.

$$\mathcal{H} = \sum_{i=0}^{N} \epsilon_i S_i^z + \sum_{i=1}^{N} J_i \vec{S}_0 \cdot \vec{S}_i \tag{3.1}$$

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

$$\mathcal{H} = \sum_{i=0}^{N} \epsilon_i S_i^z + \sum_{i=1}^{N} J_i \left[S_0^z S_i^z + \frac{1}{2} \left(S_0^+ S_i^- + S_0^- S_i^+ \right) \right] \tag{3.2}$$

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

$$\mathcal{H}^D = \sum_{i=0}^{N} \epsilon_i S_i^z + \sum_{i=1}^{N} J_i S_0^z S_i^z \tag{3.3}$$

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

The RG involves decoupling the nodes N through 1, and looking at the resultant renormalization in ϵ_i and J_i. As a simplification, we will ignore the lower nodes in the denominator and keep only the node currently being decoupled, ie node N. Since node 0 is connected to node N, we will keep node 0 in the denominator as well. Making this simplification gives

$$\mathcal{H}^D = \epsilon_0 S_0^z + \epsilon_N S_N^z + J_N S_0^z S_N^z \tag{3.4}$$

3.1 Particle sector

This sector consists of the renormalization caused due to particle excitations in the intermediate state. In the spin language, this translates to looking at those terms where the node that is being decoupled, N, is upwards in the excited state.

$$\Delta^+ \mathcal{H} = \frac{1}{2} J_N S_0^+ S_N^- \frac{1}{\hat{\omega} - \mathcal{H}^D} \frac{1}{2} J_N S_0^- S_N^+ \tag{3.5}$$

Note that we have chosen those particle scattering term because the S_N^+ on the right will create an up spin in the intermediate state, hence justifying the particle sector. The next order of business is to evaluate the $\mathcal{H}^D$ in the propagator. Since the propagator has an $S_0^- S_N^+$ in front, we can substitute $S_0^z = -\frac{1}{2}$ and $S_N^z = \frac{1}{2}$ in $\mathcal{H}^D$. Any other value would be annihilated by the operator at the front ($S^+ |\frac{1}{2}\rangle = S^- |-\frac{1}{2}\rangle = 0$). Therefore, from eq. 3.4.

$$\mathcal{H}^D = -\frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N - \frac{1}{4} J_N \tag{3.6}$$

Substituting this in $\Delta^+ \mathcal{H}$ gives

$$\Delta^+ \mathcal{H} = \frac{1}{2} J_N S_0^+ S_N^- \frac{1}{\hat{\omega} + \frac{1}{2}\epsilon_0 - \frac{1}{2}\epsilon_N + \frac{1}{4} J_N} \frac{1}{2} J_N S_0^- S_N^+ \tag{3.7}$$

At this point we make another simplification, we replace $\hat{\omega}$ by its eigenvalue ω^+. The $+$ in the superscript indicates that it is from hte particle sector.

$$\begin{aligned} \Delta^+ \mathcal{H} &= \frac{1}{2} J_N S_0^+ S_N^- \frac{1}{\omega^+ + \frac{1}{2}\epsilon_0 - \frac{1}{2}\epsilon_N + \frac{1}{4} J_N} \frac{1}{2} J_N S_0^- S_N^+ \\ &= \frac{1}{4} J_N^2 S_0^+ S_N^- S_0^- S_N^+ \frac{1}{\omega^+ + \frac{1}{2}\epsilon_0 - \frac{1}{2}\epsilon_N + \frac{1}{4} J_N} \\ &= \frac{1}{4} J_N^2 S_0^+ S_0^- S_N^- S_N^+ \frac{1}{\omega^+ + \frac{1}{2}\epsilon_0 - \frac{1}{2}\epsilon_N + \frac{1}{4} J_N} \end{aligned} \tag{3.8}$$

Here we used the fact that the spins commute. We can now use the identities $S^+ S^- = \left(\frac{1}{2} + S^z\right)$ and $S^- S^+ = \left(\frac{1}{2} - S^z\right)$ to write

$$S_0^+ S_0^- S_N^- S_N^+ = \left(\frac{1}{2} + S_0^z\right)\left(\frac{1}{2} - S_N^z\right) \tag{3.9}$$

Since we want a particle in the intermediate state, we must have a hole in the initial state. Hence, we can substitute $S_N^z = -\frac{1}{2}$ in the last equation:

$$S_0^+ S_0^- S_N^- S_N^+ = \left(\frac{1}{2} + S_0^z\right) \tag{3.10}$$

This gives

$$\Delta^+ \mathcal{H} = \frac{1}{4} J_N^2 \left(\frac{1}{2} + S_0^z\right) \frac{1}{\omega^+ + \frac{1}{2}\epsilon_0 - \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \tag{3.11}$$

This is the final form and we can now read off the renormalizations. The term with S_0^z will renormalize the term in the Hamiltonian that comes with S_0^z, which is the term with ϵ_0.

$$\Delta^+ \epsilon_0 = \frac{1}{4} J_N^2 \frac{1}{\omega^+ + \frac{1}{2}\epsilon_0 - \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \tag{3.12}$$

The remaining part is operator less and will hence renormalize the on-site energy of the term that was just decoupled, that is N:

$$\Delta^+ \epsilon_N = \frac{1}{8} J_N^2 \frac{1}{\omega^+ + \frac{1}{2}\epsilon_0 - \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \tag{3.13}$$

3.2 Hole sector

This sector consists of the renormalization caused due to hole excitations in the intermediate state. In the spin language, this translates to looking at those terms where the node that is being decoupled, N, is downwards in the excited state.

$$\Delta^- \mathcal{H} = \frac{1}{2} J_N S_0^- S_N^+ \frac{1}{\hat{\omega} - \mathcal{H}^D} \frac{1}{2} J_N S_0^+ S_N^- \tag{3.14}$$

Note that we have chosen those particle scattering term because the S_N^- on the right will create a down spin in the intermediate state, hence justifying the hole sector. The next order of business is to evaluate the $\mathcal{H}^D$ in the propagator. Since the propagator has an $S_0^+ S_N^-$ in front, we can substitute $S_0^z = \frac{1}{2}$ and $S_N^z = -\frac{1}{2}$ in $\mathcal{H}^D$. Any other value would be annihilated by the operator at the front ($S^+ |\frac{1}{2}\rangle = S^- |-\frac{1}{2}\rangle = 0$). Therefore, from eq. 3.4.

$$\mathcal{H}^D = \frac{1}{2}\epsilon_0 - \frac{1}{2}\epsilon_N - \frac{1}{4}J_N \tag{3.15}$$

Substituting this in $\Delta^- \mathcal{H}$ gives

$$\Delta^- \mathcal{H} = \frac{1}{2} J_N S_0^- S_N^+ \frac{1}{\hat{\omega} - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \frac{1}{2} J_N S_0^+ S_N^- \tag{3.16}$$

At this point we make another simplification, we replace $\hat{\omega}$ by its eigenvalue ω^-.

$$\begin{aligned}
\Delta^- \mathcal{H} &= \frac{1}{2} J_N S_0^- S_N^+ \frac{1}{\omega^- - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \frac{1}{2} J_N S_0^+ S_N^- \\
&= \frac{1}{4} J_N^2 S_0^- S_N^+ S_0^+ S_N^- \frac{1}{\omega^- - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \\
&= \frac{1}{4} J_N^2 S_0^- S_0^+ S_N^+ S_N^- \frac{1}{\omega^- - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N}
\end{aligned} \tag{3.17}$$

Here we used the fact that the spins commute. We can now use the identities $S^+S^- = \left(\frac{1}{2} + S^z\right)$ and $S^-S^+ = \left(\frac{1}{2} - S^z\right)$ to write

$$S_0^- S_0^+ S_N^+ S_N^- = \left(\frac{1}{2} - S_0^z\right)\left(\frac{1}{2} + S_N^z\right) \tag{3.18}$$

Since we want a hole in the intermediate state, we must have a particle in the initial state. Hence, we can substitute $S_N^z = \frac{1}{2}$ in the last equation:

$$S_0^- S_0^+ S_N^+ S_N^- = \left(\frac{1}{2} - S_0^z\right) \tag{3.19}$$

This gives

$$\Delta^- \mathcal{H} = \frac{1}{4}J_N^2\left(\frac{1}{2} - S_0^z\right)\frac{1}{\omega^- - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \tag{3.20}$$

This is the final form and we can now read off the renormalizations. The term with S_0^z will renormalize the term in the Hamiltonian that comes with S_0^z, which is the term with ϵ_0.

$$\Delta^- \epsilon_0 = -\frac{1}{4}J_N^2\frac{1}{\omega^- - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \tag{3.21}$$

The remaining part is operator less and will hence renormalize the on-site energy of the term that was just decoupled, that is N:

$$\Delta^- \epsilon_N = \frac{1}{8}J_N^2\frac{1}{\omega^- - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \tag{3.22}$$

3.3 Summary

These are the scaling equations for the couplings ϵ_0 and ϵ_N on decoupling the Nth node. Further calculations will involve checking where the couplings are relevant, what fixed point conditions exist and form of the effective Hamiltonians at the fixed points. If we consider the RG equations for ϵ_0 for the time being,

$$\begin{aligned}
\Delta^+ \epsilon_0 &= \frac{1}{4}J_N^2\frac{1}{\omega^+ + \frac{1}{2}\epsilon_0 - \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \\
\Delta^- \epsilon_0 &= -\frac{1}{4}J_N^2\frac{1}{\omega^- - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N}
\end{aligned} \tag{3.23}$$

Since J_N does not renormalize and ϵ_N is the unrenormalized guy, we can absorb them into the ω to make matters simpler: $\omega_N^+ = \omega^+ + \frac{1}{4}J_N - \frac{1}{2}\epsilon_N$, $\omega_N^- = \omega^- + \frac{1}{4}J_N + \frac{1}{2}\epsilon_N$.

$$\begin{aligned}
\Delta^+ \epsilon_0 &= \frac{1}{4}J_N^2\frac{1}{\omega_N^+ + \frac{1}{2}\epsilon_0} \\
\Delta^- \epsilon_0 &= -\frac{1}{4}J_N^2\frac{1}{\omega_N^- - \frac{1}{2}\epsilon_0}
\end{aligned} \tag{3.24}$$

$\omega^{\pm}$ are numbers that remain fixed during renormalization. In general they also renormalize, but we haven't kept track of that in this simplified calculation. Note the property of ω_N^+ that it grows as we go on decoupling the nodes, because $\epsilon_N > \epsilon_{N-1}$. In contrast, ω_N^- shrinks as we go on decoupling nodes, for the same reason.

We can now look for nature of flow ((ir)relevance) and fixed points. From the URG prescription, we know that **a fixed point is reached when the denominator vanishes**.

For the hole sector, $\Delta^- \epsilon_0$ is positive when $\omega_N^- - \frac{1}{2}\epsilon_0 < 0$ and negative otherwise.

- For $\omega_N^- - \frac{1}{2}\epsilon_0 > 0$, ϵ_0 is irrelevant. This will lead to a runaway denominator, where ϵ_0 goes on decreasing and ω_N^- goes on increasing such that the denominator goes on increasing and there is no way of making it 0.

- For $\omega_N^- - \frac{1}{2}\epsilon_0 < 0$, ϵ_0 is relevant, so ϵ_0 will increase and ω_N^- will decrease, so the denominator will go on decreasing and never be zero.

For the particle sector, $\Delta^+\epsilon_0$ is positive when $\omega_N^+ + \frac{1}{2}\epsilon_0 > 0$ and negative otherwise. Hence, ϵ_0 will grow in the former regime and shrink in the latter. Lets consider the two cases separately:

- When $\omega_N^+ + \frac{1}{2}\epsilon_0 > 0$, ϵ_0 will grow. Since ω_N^+ also grows, the expression $\omega_N^+ + \frac{1}{2}\epsilon_0$ will become more and more positive as the RG progresses and there is no possibility of the denominator becoming zero. We cannot reach a fixed point in this regime, so ignore this regime.

- When $\omega_N^+ + \frac{1}{2}\epsilon_0 < 0$, ϵ_0 will shrink. Here it is possible to reach a fixed point, but in this case, both ϵ_i as well as ϵ_0 are decreasing, so this is like an overall scaling of the Hamiltonian. It is unlikely that it contains interesting physics, so we ignore this case as well and move on to the hole sector.

4 Kondo Model URG

$$\mathcal{H} = \sum_{k\alpha} \epsilon_k \hat{n}_{k\alpha} + \frac{J_z}{2} \sum_{k,k'} S_d^z \left(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow} \right) + \frac{J_t}{2} \sum_{k,k'} \left(S_d^+ c_{k\downarrow}^\dagger c_{k'\uparrow} + S_d^- c_{k\uparrow}^\dagger c_{k'\downarrow} \right) \tag{4.1}$$

We take an electron $q\uparrow$ on the shell. The diagonal part of the Hamiltonian is

$$\mathcal{H}^D = \epsilon_q \hat{n}_{q\uparrow} + \frac{1}{2} J_z S_d^z \hat{n}_{q\uparrow} \tag{4.2}$$

This is the piece 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 $\tau_{q\beta} = \hat{n}_{q\beta} - \frac{1}{2}$.

$$\mathcal{H}^D = \epsilon_q \tau_{q\uparrow} + \frac{1}{2} J_z S_d^z \tau_{q\uparrow} \tag{4.3}$$

A constant $\frac{1}{2}\epsilon_q$ has been dropped while transforming the first term. The second term transforms exactly because we can just 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

$$\mathcal{H}^I = \frac{1}{2} J_z \sum_{kq} S_d^z \left(c_{k\uparrow}^\dagger c_{q\uparrow} + c_{q\uparrow}^\dagger c_{k\uparrow} \right) + \frac{1}{2} J_t \sum_{kq} \left(S_d^+ c_{k\downarrow}^\dagger c_{q\uparrow} + S_d^- c_{q\uparrow}^\dagger c_{k\downarrow} \right) \tag{4.4}$$

These are the terms that come in the numerator.

4.1 Particle sector

The renormalization in the particle sector is

$$\Delta^+\mathcal{H} = \sum_{kk'q} \frac{1}{2} \left(J_z S_d^z c_{k\uparrow}^\dagger c_{q\uparrow} + J_t S_d^+ c_{k\downarrow}^\dagger c_{q\uparrow} \right) \frac{1}{\omega^+ - \mathcal{H}^D} \frac{1}{2} \left(J_z S_d^z c_{q\uparrow}^\dagger c_{k'\uparrow} + J_t S_d^- c_{q\uparrow}^\dagger c_{k'\downarrow} \right) \tag{4.5}$$

ω^+ represents the quantum fluctuation scale for the particle sector. Notice that all the operators on the left of the propagator have a $c_{q\uparrow}$ and those on the right have a $c_{q\uparrow}^\dagger$. This combination produces a particle

in the intermediate state. In this intermediate state, since we have $\tau_{q\uparrow} = \frac{1}{2}$, we can evaluate the diagonal part from eq. 4.3:

$$\mathcal{H}^D = \frac{1}{2}\epsilon_q + \frac{1}{4}J_z S_d^z \tag{4.6}$$

There are two terms in each bracket, so in total there are four terms. The first term has two S^z.

$$
\begin{aligned}
\Delta_1^+ \mathcal{H} &= \sum_{kk'q} \frac{1}{4} J_z^2 S_d^z c_{k\uparrow}^\dagger c_{q\uparrow} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{4}J_z S_d^z} S_d^z c_{q\uparrow}^\dagger c_{k'\uparrow} \\
&= \sum_{kk'q} \frac{1}{4} J_z^2 c_{k\uparrow}^\dagger c_{q\uparrow} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{4}J_z S_d^z} S_d^z S_d^z c_{q\uparrow}^\dagger c_{k'\uparrow} \\
&= \sum_{kk'q} \frac{1}{16} J_z^2 c_{k\uparrow}^\dagger c_{q\uparrow} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{4}J_z S_d^z} c_{q\uparrow}^\dagger c_{k'\uparrow} \\
&= \frac{1}{16} J_z^2 \sum_{kk'q} c_{k\uparrow}^\dagger c_{q\uparrow} c_{q\uparrow}^\dagger c_{k'\uparrow} \left[\frac{\frac{1}{2} + S_d^z}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{8}J_z} + \frac{\frac{1}{2} - S_d^z}{\omega^+ - \frac{1}{2}\epsilon_q + \frac{1}{8}J_z} \right] \\
&= \frac{1}{32} J_z^2 \sum_{kk'q} c_{k\uparrow}^\dagger c_{k'\uparrow} \left[\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{8}J_z} + \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q + \frac{1}{8}J_z} \right] \\
&+ \frac{1}{16} J_z^2 \sum_{kk'q} S_d^z c_{k\uparrow}^\dagger c_{k'\uparrow} \left[\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{8}J_z} - \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q + \frac{1}{8}J_z} \right]
\end{aligned} \tag{4.7}
$$

The first term is a potential scattering term; the second term renormalizes the up spin part of the S_d^z term, that is, J_z.

The second term gives

$$\Delta_2^+ \mathcal{H} = \sum_{kk'q} \frac{1}{4} J_z J_t S_d^z c_{k\uparrow}^\dagger c_{q\uparrow} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{8}J_z S_d^z} S_d^- c_{q\uparrow}^\dagger c_{k'\downarrow} \tag{4.8}$$

The S_d^- in the numerator on the right means we must have $S_d^z = -\frac{1}{2}$ in the denominator.

$$
\begin{aligned}
\Delta_2^+ \mathcal{H} &= \frac{1}{4} J_z J_t \sum_{kk'q} S_d^z c_{k\uparrow}^\dagger c_{q\uparrow} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q + \frac{1}{8}J_z} S_d^- c_{q\uparrow}^\dagger c_{k'\downarrow} \\
&= \frac{1}{4} J_z J_t \sum_{kk'q} S_d^z S_d^- c_{k\uparrow}^\dagger c_{q\uparrow} c_{q\uparrow}^\dagger c_{k'\downarrow} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q + \frac{1}{8}J_z} \\
&= -\frac{1}{8} J_z J_t \sum_{kk'q} S_d^- c_{k\uparrow}^\dagger c_{k'\downarrow} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q + \frac{1}{8}J_z}
\end{aligned} \tag{4.9}
$$

There we used $S_d^z S_d^- = -\frac{1}{2} S_d^-$. This renormalizes J_t.

The third term gives

$$\Delta_3^+ \mathcal{H} = \sum_{kk'q} \frac{1}{4} J_z J_t S_d^+ c_{k\downarrow}^\dagger c_{q\uparrow} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{4}J_z S_d^z} S_d^z c_{q\uparrow}^\dagger c_{k'\uparrow} \tag{4.10}$$

The S_d^+ in the numerator on the left means we must have $S_d^z = -\frac{1}{2}$ in the denominator.

$$\Delta_3^+ \mathcal{H} = \frac{1}{4} J_z J_t \sum_{kk'q} S_d^+ c_{k\downarrow}^\dagger c_{q\uparrow} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q + \frac{1}{8}J_z} S_d^z c_{q\uparrow}^\dagger c_{k'\uparrow}$$
$$= \frac{1}{4} J_z J_t \sum_{kk'q} S_d^+ S_d^z c_{k\downarrow}^\dagger c_{q\uparrow} c_{q\uparrow}^\dagger c_{k'\uparrow} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q + \frac{1}{8}J_z} \tag{4.11}$$
$$= -\frac{1}{8} J_z J_t \sum_{kk'q} S_d^+ c_{k\downarrow}^\dagger c_{k'\uparrow} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q + \frac{1}{8}J_z}$$

There we used $S_d^+ S_d^z = -\frac{1}{2} S_d^+$. This renormalizes J_t.

The fourth term gives

$$\Delta_4^+ \mathcal{H} = \sum_{kk'q} \frac{1}{4} J_t^2 S_d^+ c_{k\downarrow}^\dagger c_{q\uparrow} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{4}J_z S_d^z} S_d^- c_{q\uparrow}^\dagger c_{k'\downarrow} \tag{4.12}$$

The S_d^+ in the numerator on the left means we must have $S_d^z = -\frac{1}{2}$ in the denominator.

$$\Delta_4^+ \mathcal{H} = \frac{1}{4} J_t^2 \sum_{kk'q} S_d^+ c_{k\downarrow}^\dagger c_{q\uparrow} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q + \frac{1}{8}J_z} S_d^- c_{q\uparrow}^\dagger c_{k'\downarrow}$$
$$= \frac{1}{4} J_t^2 \sum_{kk'q} S_d^+ S_d^- c_{k\downarrow}^\dagger c_{q\uparrow} c_{q\uparrow}^\dagger c_{k'\downarrow} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q + \frac{1}{8}J_z} \tag{4.13}$$
$$= \frac{1}{4} J_t^2 \sum_{kk'q} \left(\frac{1}{2} + S_d^z \right) c_{k\downarrow}^\dagger c_{k'\downarrow} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q + \frac{1}{8}J_z}$$

There we used $S_d^+ S_d^- = \left(\frac{1}{2} + S_d^z \right)$. The first term produces a potential scattering and the second term renormalizes J_z.

4.2 Hole sector

The renormalization in the hole sector is

$$\Delta^- \mathcal{H} = \sum_{kk'q} \frac{1}{2} \left(J_z S_d^z c_{q\uparrow}^\dagger c_{k'\uparrow} + J_t S_d^- c_{q\uparrow}^\dagger c_{k'\downarrow} \right) \frac{1}{\omega^- - \mathcal{H}^D} \frac{1}{2} \left(J_z S_d^z c_{k\uparrow}^\dagger c_{q\uparrow} + J_t S_d^+ c_{k\downarrow}^\dagger c_{q\uparrow} \right) \tag{4.14}$$

The ω^- represents the quantum fluctuation energy scale for the hole sector. In this intermediate state, since we have $\tau_{q\uparrow} = -\frac{1}{2}$, we can evaluate the diagonal part from eq. 4.3:

$$\mathcal{H}^D = -\frac{1}{2}\epsilon_q - \frac{1}{4} J_z S_d^z \tag{4.15}$$

The first term has two S^z.

$$
\begin{aligned}
\Delta_1^- \mathcal{H} &= \sum_{kk'q} S_d^z c_{q\uparrow}^\dagger c_{k'\uparrow} \frac{1}{4} J_z^2 \frac{1}{\omega^- - \mathcal{H}^D} S_d^z c_{k\uparrow}^\dagger c_{q\uparrow} \\
&= \frac{1}{16} J_z^2 \sum_{kk'q} c_{k'\uparrow} c_{k\uparrow}^\dagger \frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{4} J_z S_d^z} \\
&= \frac{1}{16} J_z^2 \sum_{kk'q} c_{k'\uparrow} c_{k\uparrow}^\dagger \left[\frac{\frac{1}{2} + S_d^z}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{8} J_z} + \frac{\frac{1}{2} - S_d^z}{\omega^- + \frac{1}{2}\epsilon_q - \frac{1}{8} J_z} \right] \\
&= -\frac{1}{32} J_z^2 \sum_{kk'q} c_{k\uparrow}^\dagger c_{k'\uparrow} \left[\frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{8} J_z} + \frac{1}{\omega^- + \frac{1}{2}\epsilon_q - \frac{1}{8} J_z} \right] \\
&\quad - \frac{1}{16} J_z^2 \sum_{kk'q} c_{k\uparrow}^\dagger c_{k'\uparrow} S_d^z \left[\frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{8} J_z} - \frac{1}{\omega^- + \frac{1}{2}\epsilon_q - \frac{1}{8} J_z} \right]
\end{aligned}
\tag{4.16}
$$

In the last step, we dropped a constant term which came from the commutator of $c_k^\dagger$ and $c_{k'}$. Note that this term exactly cancels the first term in the particle sector.

The second term gives

$$
\Delta_2^- \mathcal{H} = \sum_{kk'q} \frac{1}{4} J_z J_t S_d^- c_{q\uparrow}^\dagger c_{k'\downarrow} \frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{4} J_z S_d^z} S_d^z c_{k\uparrow}^\dagger c_{q\uparrow}
\tag{4.17}
$$

The S_d^- in the numerator on the left means we must have $S_d^z = \frac{1}{2}$ in the denominator.

$$
\begin{aligned}
\Delta_2^- \mathcal{H} &= \frac{1}{4} J_z J_t \sum_{kk'q} S_d^- S_d^z c_{q\uparrow}^\dagger c_{k'\downarrow} c_{k\uparrow}^\dagger c_{q\uparrow} \frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{8} J_z} \\
&= \frac{1}{8} J_z J_t \sum_{kk'q} S_d^- c_{k'\downarrow} c_{k\uparrow}^\dagger \frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{8} J_z} \\
&= -\frac{1}{8} J_z J_t \sum_{kk'q} S_d^- c_{k\uparrow}^\dagger c_{k'\downarrow} \frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{8} J_z}
\end{aligned}
\tag{4.18}
$$

There we used $S_d^- S_d^z = \frac{1}{2} S_d^-$. This renormalizes J_t.

The third term gives

$$
\Delta_3^- \mathcal{H} = \sum_{kk'q} \frac{1}{4} J_z J_t S_d^z c_{q\uparrow}^\dagger c_{k'\uparrow} \frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{4} J_z S_d^z} S_d^+ c_{k\downarrow}^\dagger c_{q\uparrow}
\tag{4.19}
$$

The S_d^+ in the numerator on the right means we must have $S_d^z = \frac{1}{2}$ in the denominator.

$$
\begin{aligned}
\Delta_3^- \mathcal{H} &= \frac{1}{4} J_z J_t \sum_{kk'q} S_d^z S_d^+ c_{q\uparrow}^\dagger c_{k'\uparrow} c_{k\downarrow}^\dagger c_{q\uparrow} \frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{8} J_z} \\
&= \frac{1}{4} J_z J_t \sum_{kk'q} S_d^+ c_{k\downarrow}^\dagger c_{k'\uparrow} \frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{8} J_z} \\
&= -\frac{1}{8} J_z J_t \sum_{kk'q} S_d^+ c_{k\downarrow}^\dagger c_{k'\uparrow} \frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{8} J_z}
\end{aligned}
\tag{4.20}
$$

There we used $S_d^z S_d^+ = \frac{1}{2} S_d^+$. This renormalizes J_t.

The fourth term gives

$$\Delta_4^- \mathcal{H} = \sum_{kk'q} \frac{1}{4} J_t^2 S_d^- c_{q\uparrow}^\dagger c_{k'\downarrow} \frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{4}J_z S_d^z} S_d^+ c_{k\downarrow}^\dagger c_{q\uparrow} \tag{4.21}$$

The S_d^+ in the numerator on the right means we must have $S_d^z = \frac{1}{2}$ in the denominator.

$$\begin{aligned}
\Delta_4^- \mathcal{H} &= \frac{1}{4} J_t^2 \sum_{kk'q} S_d^- S_d^+ c_{q\uparrow}^\dagger c_{k'\downarrow} c_{k\downarrow}^\dagger c_{q\uparrow} \frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{8}J_z} \\
&= \frac{1}{4} J_t^2 \sum_{kk'q} \left(\frac{1}{2} - S_d^z\right) c_{k'\downarrow} c_{k\downarrow}^\dagger \frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{8}J_z} \\
&= -\frac{1}{4} J_t^2 \sum_{kk'q} \left(\frac{1}{2} - S_d^z\right) c_{k\downarrow}^\dagger c_{k'\downarrow} \frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{8}J_z}
\end{aligned} \tag{4.22}$$

There we used $S_d^- S_d^+ = \left(\frac{1}{2} - S_d^z\right)$.

4.3   Scaling equations

Focusing on the first terms of each sector, we can see that

$$\begin{aligned}
\Delta_1^+ \mathcal{H} &= \frac{1}{16} J_z^2 \sum_{kk'q} c_{k\uparrow}^\dagger c_{k'\uparrow} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{4}J_z S_d^z} \\
\Delta_1^- \mathcal{H} &= -\frac{1}{16} J_z^2 \sum_{kk'q} c_{k\uparrow}^\dagger c_{k'\uparrow} \frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{4}J_z S_d^z}
\end{aligned} \tag{4.23}$$

To connect the two ω, we can use $\eta = \eta^{\dagger\dagger}$. If we choose the scattering term $c^\dagger T = \sum_k S_d^z c_{q\uparrow}^\dagger c_{k\uparrow}$, then

$$\eta = \frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{4}J_z S_d^z} \sum_k S_d^z c_{k\uparrow}^\dagger c_{q\uparrow} \tag{4.24}$$

and

$$\begin{aligned}
\eta^\dagger &= \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{4}J_z S_d^z} \sum_k S_d^z c_{q\uparrow}^\dagger c_{k\uparrow} \\
\implies \left(\eta^\dagger\right)^\dagger &= \sum_k S_d^z c_{k\uparrow}^\dagger c_{q\uparrow} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{4}J_z S_d^z} \\
&= \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{4}J_z S_d^z} \sum_k S_d^z c_{k\uparrow}^\dagger c_{q\uparrow}
\end{aligned} \tag{4.25}$$

Comparing η and $\left(\eta^\dagger\right)^\dagger$, we can write

$$\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \frac{1}{4}J_z S_d^z} = \frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{4}J_z S_d^z} \tag{4.26}$$

Using this on eq. 4.23 gives

$$\Delta_1 \mathcal{H} \equiv \Delta_1^+ \mathcal{H} + \Delta_1^- \mathcal{H} = 0 \tag{4.27}$$

This means there is no net renormalization from the first terms in each sector. Doing similar things for the other terms gives

$$\begin{aligned}
\Delta_2^+ + \Delta_3^+ &= \Delta_2^- + \Delta_3^- \\
\implies \Delta_2 \mathcal{H} + \Delta_3 \mathcal{H} &= 2\Delta_2^+ + 2\Delta_3^+
\end{aligned} \tag{4.28}$$

Adding the terms that renormalize S_d^+ from both sectors gives the renormalization

$$-\frac{1}{2}J_z J_t \sum_q \frac{1}{\omega - \epsilon_q + \frac{1}{4}J_z} \tag{4.29}$$

Note that the term is actually $\frac{1}{2}S_d^+$ and not just S_d^+, so that has to be taken into account while reading off the renormalization. Performing the calculation with the spin down term gives an equal renormalization, so

$$\Delta J_t = -J_z J_t \sum_q \frac{1}{\omega - \epsilon_q + \frac{1}{4}J_z} \tag{4.30}$$

Similarly, adding the term 4 from both sectors gives a renormalization in $-\frac{1}{2}S_d^z c_{k\downarrow}^\dagger c_{k'\downarrow}^\dagger$:

$$-\frac{1}{2}J_t^2 \sum_q \frac{1}{\omega - \epsilon_q + \frac{1}{4}J_z} \tag{4.31}$$

Doing the calculation with the down spin should produce the other term, $\frac{1}{2}S_d^z c_{k\uparrow}^\dagger c_{k'\uparrow}$, but that does not add to the previous renormalization, so there is no multiplication by 2 here:

$$\Delta J_z = -J_t^2 \sum_q \frac{1}{\omega - \epsilon_q + \frac{1}{4}J_z} \tag{4.32}$$

For the symmetric model ($J_z = J_t = J$, we get the equation

$$\Delta J = -J^2 \sum_q \frac{1}{\omega - \epsilon_q + \frac{1}{4}J} \tag{4.33}$$

To obtain the familiar Kondo model one-loop form, we need to take low energy excitations ($\omega \ll \epsilon_q$, expand the denominator and take only $O(J^0)$ and assume isotropic dispersion $\epsilon_q = D$.

$$\delta J = J^2 \rho |\delta D| \frac{1}{D} \tag{4.34}$$

4.4   Renormalized Hamiltonian

The renormalized Hamiltonian after disentangling the shell at Λ_N is

$$\mathcal{H}_{N-1} = \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{k,k'<\Lambda_N} \left[\frac{J_z^{N-1}}{2} S_d^z \left(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow} \right) + \frac{J_t^{N-1}}{2} \left(S_d^+ c_{k\downarrow}^\dagger c_{k'\uparrow} + S_d^- c_{k\uparrow}^\dagger c_{k'\downarrow} \right) \right]$$
$$+ \frac{J_z^N}{2} \sum_{q=\Lambda_N} S_d^z \left(\hat{n}_{q\uparrow} - \hat{n}_{q\downarrow} \right) \tag{4.35}$$

where $J^i = J^{i+1} + \Delta J^{i+1}$.

5   Anderson Model URG

5.1   Without spin-spin interaction

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

$$\mathcal{H} = \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{k\sigma} \left(V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right) + \epsilon_d \sum_\sigma \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \tag{5.1}$$

At first order, the rotated Hamiltonian is

$$\mathcal{H}_{j-1} = 2^{-n_j} \text{Tr}_{1,2,\dots,n_j} \mathcal{H}_j + \sum_{q\beta} \tau_{q\beta} \left\{ c_{q\beta}^\dagger \text{Tr}_{q\beta} \left(\mathcal{H} c_{q\beta} \right), \eta_{q\beta} \right\} \tag{5.2}$$

n_j is the number of states on the shell Λ_j. We take the full Hamiltonian as our $\mathcal{H}_j$. Since this is the first step of the RG, the shell being decoupled is the highest one, which we call Λ_N.

Particle Sector

The particle sector involves only particle excitations. The state $q\beta$ is occupied in the intermediate (excited) state. This contribution will be given by the first term in the anticommutator of eq. 5.2.

Calculation of first term The first term, the initial trace, is a sequential trace over all the states on the shell being disentangled. At each trace, we consider only electrons on the current degree of freedom and on shells below the current shell:

$$\frac{1}{2} \text{Tr}_{q\uparrow} \mathcal{H}_j = \sum_{k<\Lambda_N,\sigma} \epsilon_k \hat{n}_{k\sigma} + \epsilon_d \sum_\sigma \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \frac{1}{2} \text{Tr}_{q\uparrow} \left\{ \epsilon_k \hat{n}_{q\uparrow} \right\}$$

$$= \sum_{k<\Lambda_N,\sigma} \epsilon_k \hat{n}_{k\sigma} + \epsilon_d \sum_\sigma \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \frac{1}{2} \epsilon_q \tag{5.3}$$

$$\frac{1}{2} \text{Tr}_{q\downarrow} \frac{1}{2} \text{Tr}_{q\uparrow} \mathcal{H}_j = \sum_{k<\Lambda_N,\sigma} \epsilon_k \hat{n}_{k\sigma} + \epsilon_d \sum_\sigma \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \epsilon_q$$

$$\implies 2^{-n_j} \text{Tr}_{1,2,\dots,n_j} \mathcal{H}_j = \sum_{k<\Lambda_N,\sigma} \epsilon_k \hat{n}_{k\sigma} + \epsilon_d \sum_\sigma \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \sum_{|q|=\Lambda_N} \epsilon_q \tag{5.4}$$

Calculation of second term The second term involves some other traces:

$$\text{Tr}_{q\beta} \left(\mathcal{H} c_{q\beta} \right) = \sum_{k\sigma} V_k \text{Tr}_{q\beta} \left(c_{k\sigma}^\dagger c_{d\sigma} c_{q\beta} \right)$$

$$= \sum_{k\sigma} V_k c_{d\sigma} \delta_{\sigma\beta} \delta_{kq} \tag{5.5}$$

$$= V_q c_{d\beta}$$

$$\text{Tr}_{q\beta} \left(c_{q\beta}^\dagger \mathcal{H} \right) = V_q^* c_{d\beta}^\dagger$$

$$\mathcal{H}^D = \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \epsilon_d \sum_\sigma \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow}$$

$$\text{Tr}_{q\beta} \left(\mathcal{H}^D \hat{n}_{q\beta} \right) = \sum_{k<\Lambda_N,\sigma} \epsilon_k \hat{n}_{k\sigma} + \epsilon_d \sum_\sigma \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \epsilon_q \tag{5.6}$$

There is a more straightforward way of getting these expressions. Some thought reveals that $c_{q\beta}^\dagger \text{Tr}_{q\beta} \left(\mathcal{H} c_{q\beta} \right)$ is, by definition, the part of the Hamiltonian that scatters from electrons *not at* $q\beta$ to $q\beta$. In other words, **it is that off-diagonal part of the Hamiltonian that involves a $c_{q\beta}^\dagger$**. That part is, of course, $V_q c_{q\beta}^\dagger c_{d\beta}$. Similarly, $\text{Tr}_{q\beta} \left(c_{q\beta}^\dagger \mathcal{H} \right) c_{q\beta}$ is the off-diagonal part that has a $c_{q\beta}$, $V_q^* c_{d\beta}^\dagger c_{q\beta}$. Finally, the term in the denominator of η is simply the diagonal part of the Hamiltonian, which in our case is the kinetic

energies of all the electrons and the impurity diagonal part. The point of this paragraph is that one can write down these terms simply by looking at the Hamiltonian and without carrying out any trace.

$$\eta_{q\beta} = \mathrm{Tr}_{q\beta}\left(c^\dagger_{q\beta}\mathcal{H}\right)c_{q\beta}\frac{1}{\hat{\omega} - \mathrm{Tr}_{q\beta}\left(\mathcal{H}^D\hat{n}_{q\beta}\right)\hat{n}_{q\beta}}$$

$$= V^*_q c^\dagger_{d\beta}c_{q\beta}\frac{1}{\hat{\omega} - \left(\sum_{k<\Lambda_N,\sigma}\epsilon_k\hat{n}_{k\sigma} + \epsilon_d\sum_\sigma\hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} - \epsilon_q\right)\hat{n}_{q\beta}} \tag{5.7}$$

$$= V^*_q c^\dagger_{d\beta}c_{q\beta}\frac{1}{\omega\tau_{q\beta} - \left(\epsilon_d\sum_\sigma\hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + \epsilon_q\right)\tau_{q\beta}}$$

At the last step, I replaced $\hat{\omega} - \sum_{k<\Lambda_N,\sigma}\epsilon_k\hat{n}_{k\sigma}\hat{n}_{q\beta} - \frac{1}{2}\left(\epsilon_d\sum_\sigma\hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} + \epsilon_q\right)$ with $\omega\tau_{q\beta}$. Note that since this term has a $c^\dagger_{d\beta}$, it will not vanish only when acting on a state with $\hat{n}_{d\beta} = 0$. Hence we can drop the terms $\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}$ and $\epsilon_{d\beta}\hat{n}_{d\beta}$ in the denominator. Also, since it has a $c_{q\beta}$, we can set the $\tau_{q\beta}$ in the denominator to $\frac{1}{2}$. Putting together the individual pieces, we can now write the second term:

$$\sum_{q\beta}\tau_{q\beta}\left\{c^\dagger_{q\beta}\mathrm{Tr}_{q\beta}\left(\mathcal{H}c_{q\beta}\right),\eta_{q\beta}\right\} = \sum_{q\beta}\tau_{q\beta}\left\{V_q c^\dagger_{q\beta}c_{d\beta}, V^*_q c^\dagger_{d\beta}c_{q\beta}\frac{1}{\frac{1}{2}\left(\omega - \epsilon_q - \epsilon_d\hat{n}_{d\bar{\beta}}\right)}\right\}$$

$$= \sum_{q\beta}2\tau_{q\beta}\left\{V_q c^\dagger_{q\beta}c_{d\beta}, V^*_q c^\dagger_{d\beta}c_{q\beta}\frac{1}{\omega - \epsilon_q - \epsilon_d\hat{n}_{d\bar{\beta}}}\right\} \tag{5.8}$$

We now note that the factor with ω can be written as follows:

$$\frac{1}{\omega - \epsilon_q - \epsilon_d\hat{n}_{d\bar{\beta}}} = \frac{\hat{n}_{d\bar{\beta}}}{\omega - \epsilon_q - \epsilon_d} + \frac{1 - \hat{n}_{d\bar{\beta}}}{\omega - \epsilon_q}$$

$$= \hat{n}_{d\bar{\beta}}\frac{\epsilon_d}{\left(\omega - \epsilon_q - \epsilon_d\right)\left(\omega - \epsilon_q\right)} + \frac{1}{\omega - \epsilon_q} \tag{5.9}$$

Since these terms commute with the other terms, they can be taken out of the anticommutator; what's left is

$$\left\{V_q c^\dagger_{q\beta}c_{d\beta}, V^*_q c^\dagger_{d\beta}c_{q\beta}\right\} = |V_q|^2\left[\hat{n}_{q\beta}\left(1 - \hat{n}_{d\beta}\right) + \hat{n}_{d\beta}\left(1 - \hat{n}_{q\beta}\right)\right] \tag{5.10}$$

The τ and the $\hat{n}$ can be multiplied:

$$2\tau_{q\beta}\left(1 - \hat{n}_{q\beta}\right) = \left(\hat{n}_{q\beta} - 1\right) \tag{5.11}$$

$$2\tau_{q\beta}\hat{n}_{q\beta} = \hat{n}_{q\beta} \tag{5.12}$$

The total thing becomes

$$\sum_{q\beta}|V_q|^2\left[\hat{n}_{d\beta}\left(\hat{n}_{q\beta} - 1\right) + \hat{n}_{q\beta}\left(1 - \hat{n}_{d\beta}\right)\right]\left[\hat{n}_{d\bar{\beta}}\frac{\epsilon_d}{\left(\omega - \epsilon_q - \epsilon_d\right)\left(\omega - \epsilon_q\right)} + \frac{1}{\omega - \epsilon_q}\right]$$

$$= \sum_{q\beta}|V_q|^2\left[\hat{n}_{q\beta} - \hat{n}_{d\beta}\right]\left[\hat{n}_{d\bar{\beta}}\frac{\epsilon_d}{\left(\omega - \epsilon_q - \epsilon_d\right)\left(\omega - \epsilon_q\right)} + \frac{1}{\omega - \epsilon_q}\right] \tag{5.13}$$

Putting $\hat{n}_{q\beta} = 1$, and dropping the non-operator terms, we get

$$\sum_\beta\hat{n}_{d\beta}\sum_q|V_q|^2\frac{\epsilon_q - \omega + 2\epsilon_d}{\left(\omega - \epsilon_q\right)\left(\omega - \epsilon_q - \epsilon_d\right)} - \hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\sum_{q\beta}|V_q|^2\frac{\epsilon_d}{\left(\omega - \epsilon_q\right)\left(\omega - \epsilon_q - \epsilon_d\right)} \tag{5.14}$$

The first term is the renormalization in on-site energy, $\sum_\beta\hat{n}_{d\beta}\Delta\epsilon_{d\beta}$, and the second term is the renormalization in the onsite repulsion, $\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\Delta U$.

Renormalized Hamiltonian Combining eqs. 5.4 and 5.14, we get

$$\mathcal{H}_{N-1} = \sum_{k<\Lambda_N,\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{|q|=\Lambda_N} \epsilon_q + \sum_\sigma (\epsilon_{d\sigma} + \Delta\epsilon_{d\sigma})\,\hat{n}_{d\sigma} + (U + \Delta U)\,\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} \tag{5.15}$$

The second term is the renormalization in the kinetic energy of the disentangled electrons, the third term is the renormalized impurity site energy and the fourth term is the renormalized onsite repulsion.

$$\Delta\epsilon_d^N \equiv \epsilon_d\big|_{N-1} - \epsilon_d\big|_N = \sum_q |V_q|^2 \frac{\epsilon_q - \omega + 2\epsilon_d}{(\omega - \epsilon_q)(\omega - \epsilon_q - \epsilon_d)} \tag{5.16}$$

According to Hewson eq. 3.62 (page 68),

$$\frac{\mathrm{d}\epsilon_d}{\mathrm{d}\ln D} = -\frac{\Delta}{\pi} + O(V^3) = -\rho_0|V|^2 + O(V^3) \tag{5.17}$$

in the limit of $U + \epsilon_d \gg D$ and $|\epsilon_d| \ll D$, under the assumptions that V_k is independent of k and the conduction band is flat ($\rho(\epsilon) = \rho_0$ for $\epsilon \in [-D, D]$).

Assuming that we integrate out a ring at energy D and of thickness $-|\delta D|$, such that $\epsilon_q = D$ everywhere on the ring, the number of available states is

$$\delta n = \frac{\mathrm{d}n}{\mathrm{d}E} \times \delta E = \rho(D) \times |\delta D| \tag{5.18}$$

We can then replace the summation in eq. 5.16 by δn:

$$\delta\epsilon_d(D) = |V|^2\rho(D)|\delta D|\frac{D - \omega + 2\epsilon_d}{(\omega - D)(\omega - D - \epsilon_d)} \tag{5.19}$$

where $\rho(D)$ is the number of single-spin states on the shell D. This can be compared to eq. 5.17. In two dimensions, the energy density of states is independent of energy. Setting $\omega = 0$, we get

$$\begin{aligned}
\delta\epsilon_d(D) &= |V|^2\rho(D)|\delta D|\frac{D + 2\epsilon_d}{D(D + \epsilon_d)} \\
&= |V|^2\rho(D)\frac{|\delta D|}{D}\frac{D + 2\epsilon_d}{D + \epsilon_d}
\end{aligned} \tag{5.20}$$

I used $\delta D = -|\delta D|$. Changing to continuum equation,

$$\frac{\mathrm{d}\epsilon_d}{\mathrm{d}\ln D} = -\frac{\Delta}{\pi}\frac{D + 2\epsilon_d}{D + \epsilon_d} \tag{5.21}$$

In the regime where the single-occupied impurity level is comfortably inside the conduction band ($D \gg |\epsilon_d|$), we can approximate both the numerator and denominator as simply D. Then,

$$\frac{\mathrm{d}\epsilon_d}{\mathrm{d}\ln D} = -\frac{\Delta}{\pi} \tag{5.22}$$

$$\implies \epsilon_d + \frac{\Delta}{\pi}\log D = \text{constant} \tag{5.23}$$

Turning to the general equation 5.16, under the assumption of momentum-independent scattering, the continuum equation is

$$\begin{aligned}
\frac{\mathrm{d}\epsilon_d}{\mathrm{d}\ln D} &= |V|^2 n(D)\frac{\omega - D - 2\epsilon_d}{(\omega - D)(\omega - D - \epsilon_d)} \\
&= |V|^2 n(D)\left(\frac{2}{\omega - D} - \frac{1}{\omega - D - \epsilon_d}\right)
\end{aligned} \tag{5.24}$$

$n(D)$ is not the density of states, but the total number of states on the shell at energy D. Similarly, the renormalization in U is

$$
\begin{aligned}
\delta U &= -\sum_{q\beta} |V_q|^2 \frac{\epsilon_d}{(\omega - \epsilon_q)(\omega - \epsilon_q - \epsilon_d)} \\
&= -|V|^2 n(D) \sum_{\beta} \frac{\epsilon_d}{(\omega - D)(\omega - D - \epsilon_d)} \\
&= -2|V|^2 n(D) \frac{\epsilon_d}{(\omega - D)(\omega - D - \epsilon_d)} \\
\implies \frac{\mathrm{d}U}{\mathrm{d}\ln D} &= 2|V|^2 n(D) \frac{\epsilon_d}{(\omega - D)(\omega - D - \epsilon_d)} \\
&= 2|V|^2 n(D) \left(\frac{1}{\omega - D - \epsilon_d} - \frac{1}{\omega - D} \right)
\end{aligned}
\tag{5.25}
$$

In the penultimate step, I used the fact that since the onsite energy for either spin is same, the summation just returns a factor of 2. Putting $\omega = 0$,

$$
\begin{aligned}
\frac{\mathrm{d}\epsilon_d}{\mathrm{d}\ln D} &= |V|^2 n(D) \left(\frac{1}{D + \epsilon_d} - \frac{2}{D} \right) \\
\frac{\mathrm{d}U}{\mathrm{d}\ln D} &= 2|V|^2 n(D) \left(\frac{1}{D} - \frac{1}{D + \epsilon_d} \right)
\end{aligned}
\tag{5.26}
$$

5.2 With Kondo-like interaction

The four-Fermi interaction we are considering is of the form

$$
\mathcal{H}_I = \sum_{k,k',\sigma_i} u c_{d\sigma_2}^\dagger c_{d\sigma_4} c_{k'\sigma_3} c_{k\sigma_1}^\dagger \delta_{(\sigma_1 + \sigma_2 = \sigma_3 + \sigma_4)}
\tag{5.27}
$$

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

$$
\mathcal{H}_I = \underbrace{\sum_{k,k',\sigma,\sigma'} u_1 \hat{n}_{d\sigma'} c_{k\sigma}^\dagger c_{k'\sigma}}_{\text{spin-preserving scattering}} + \overbrace{\sum_{k,k',\sigma} u_2 c_{d\overline{\sigma}}^\dagger c_{d\sigma} c_{k\sigma}^\dagger c_{k'\overline{\sigma}}}^{\text{spin-flip scattering}}
\tag{5.28}
$$

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 ($k\sigma \to k'\sigma, d\sigma' \to d\sigma'$). We label this coupling as u_P. The other coupling involves a spin-flip scattering, so we label that as u_A.

$$
\mathcal{H}_{I,N} = \sum_{k,k',\sigma,\sigma'} u_P \hat{n}_{d\sigma'} c_{k\sigma}^\dagger c_{k'\sigma} + \sum_{k,k',\sigma} u_A c_{d\overline{\sigma}}^\dagger c_{d\sigma} c_{k\sigma}^\dagger c_{k'\overline{\sigma}}
\tag{5.29}
$$

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

$$
u_{\uparrow\uparrow} \hat{n}_{d\uparrow} c_{k\uparrow}^\dagger c_{k'\uparrow} + u_{\downarrow\downarrow} \hat{n}_{d\downarrow} c_{k\downarrow}^\dagger c_{k'\uparrow} + u_{\uparrow\downarrow} \hat{n}_{d\uparrow} c_{k\downarrow}^\dagger c_{k'\downarrow} + u_{\downarrow\uparrow} \hat{n}_{d\downarrow} c_{k\uparrow}^\dagger c_{k'\uparrow}
\tag{5.30}
$$

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

$$
\begin{aligned}
\mathcal{H}_I &= J_z \frac{\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow}}{2} \sum_{kk'} \left(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow} \right) + J_t \sum_{kk'} \left[c_{d\uparrow}^\dagger c_{d\downarrow} c_{k\downarrow}^\dagger c_{k'\uparrow} + c_{d\downarrow}^\dagger c_{d\uparrow} c_{k\uparrow}^\dagger c_{k'\downarrow} \right] \\
&= 2 J_z S_d^z s^z + J_t \left(S_d^+ s^- + S_d^- s^+ \right)
\end{aligned}
\tag{5.31}
$$

The spin-like operators are defined as

$$S_d^z \equiv \frac{1}{2} \left(\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow} \right) \qquad\qquad S_d^+ \equiv c_{d\uparrow}^\dagger c_{d\downarrow} \qquad S_d^- \equiv c_{d\downarrow}^\dagger c_{d\uparrow}$$

$$s_{kk'}^z \equiv \frac{1}{2} \left(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow} \right) \qquad\qquad s_{kk'}^+ \equiv c_{k\uparrow}^\dagger c_{k'\downarrow} \qquad s_{kk'}^- \equiv c_{k\downarrow}^\dagger c_{k'\uparrow} \qquad (5.32)$$

$$s^a \equiv \sum_{kk'} s_{kk'}^a$$

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

$$\mathcal{H} = \sum_{k\sigma} \left(\epsilon_k \hat{n}_{k\sigma} + V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right) + \epsilon_d \sum_\sigma \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + 2 J_z S_d^z s^z + J_t \left(S_d^+ s^- + S_d^- s^+ \right) \qquad (5.33)$$

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

$$\mathcal{H}_I = J \left[S_d^z s^z + \frac{1}{2} \left(S_d^+ s^- + S_d^- s^+ \right) \right] = J \mathbf{S_d} \cdot \mathbf{s} \qquad (5.34)$$

The Hamiltonian for a single electron $q\beta$ on the Nth shell is

$$\mathcal{H}_N = H_{N-1} + H_{\text{imp}} + \left(\epsilon_q + \beta J_z S_d^z \right) \hat{n}_{q\beta} + V_q c_{q\beta}^\dagger c_{d\beta} + h.c. + \sum_{k<\Lambda_N} \left[J_z S_d^z \beta \left(c_{k\beta}^\dagger c_{q\beta} + c_{q\beta}^\dagger c_{k\beta} \right) \right.$$

$$\left. + J_t \left(c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{q\beta} + c_{d\overline{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\overline{\beta}} \right) \right] \qquad (5.35)$$

where H_{imp} is the impurity-diagonal part of the Hamiltonian $(\epsilon_d \hat{n}_d + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow})$ and

$$H_{N-1} = \sum_{k<\Lambda_N,\sigma} \left[\left(\epsilon_k + \sigma J_z S_d^z \right) \hat{n}_{k\sigma} + V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right] + H_{I,N-1} \qquad (5.36)$$

The diagonal part (the part that appears in the denominator of the URG equations) is

$$\mathcal{H}_D = \sum_{k<\Lambda_N,\sigma} \left(\epsilon_k + \sigma J_z S_d^z \right) \hat{n}_{k\sigma} + \epsilon_q \hat{n}_{q\beta} + \beta J_z S_d^z \hat{n}_{q\beta} + H_{imp} \qquad (5.37)$$

As a simplification, we will ignore the terms that pertain to the lower electrons $(k < q)$ in $\mathcal{H}_D$.

$$\mathcal{H}_D^+ = \epsilon_q \hat{n}_{q\beta} + \beta J_z S_d^z \hat{n}_{q\beta} + H_{imp} \qquad (5.38)$$

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

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

$$J_z S_d^z \sum_k \left(\hat{n}_{k\uparrow} - \hat{n}_{k\downarrow} \right) = J_z S_d^z \sum_k \left(\hat{\tau}_{k\uparrow} - \hat{\tau}_{k\downarrow} \right) \qquad (5.39)$$

where $\tau \equiv \hat{n} - \frac{1}{2}$ and $\mathcal{C}$ is non-dynamic and will hence be dropped. This transforms the diagonal part $\mathcal{H}^D$. Eq. 5.38 becomes

$$\mathcal{H}_D^+ = \epsilon_q \hat{\tau}_{q\beta} + \beta J_z S_d^z \hat{\tau}_{q\beta} + H_{imp} \qquad (5.40)$$

5.2.1 Particle sector

The renormalization in the Hamiltonian in the particle sector is

$$\Delta^+ \mathcal{H}_N = \sum_{q\beta} \left[V_q^* c_{d\beta}^\dagger c_{q\beta} + J_z \beta S_d^z \sum_k c_{k\beta}^\dagger c_{q\beta} + J_t \sum_k c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{q\beta} \right] \times \frac{1}{\hat{\omega}^+ - \mathcal{H}_D}$$

$$\times \left[V_q c_{q\beta}^\dagger c_{d\beta} + J_z \beta S_d^z \sum_k c_{q\beta}^\dagger c_{k\beta} + J_t \sum_k c_{d\overline{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\overline{\beta}} \right] \tag{5.41}$$

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. Since this state is characterized by a particle in the intermediate state, the diagonal part can be evaluated by substituting $\tau_{q\beta} = \frac{1}{2}$ in eq. 5.38:

$$\mathcal{H}_D^+ = \epsilon_q \frac{1}{2} + \frac{1}{2} \beta J_z S_d^z + H_{imp} \tag{5.42}$$

1.

$$\Delta_1^+ \mathcal{H}_N = \sum_{q\beta} |V_q|^2 c_{d\beta}^\dagger c_{q\beta} \frac{1}{\hat{\omega}^+ - \mathcal{H}_D^+} c_{q\beta}^\dagger c_{d\beta} \tag{5.43}$$

The intermediate state is characterized by $\hat{n}_{d\beta} = 0, \hat{n}_{q\beta} = 1$. Therefore, at the propagator, we have

$$H_1 = \mathcal{H}_D^+ = \epsilon_q \frac{1}{2} + \frac{1}{2} \beta J_z S_d^z + H_{imp}$$

$$= \epsilon_q \frac{1}{2} - \frac{1}{4} J_z \hat{n}_{d\overline{\beta}} + \epsilon_d \hat{n}_{d\overline{\beta}} \tag{5.44}$$

H_1 is the intermediate state Hamiltonian. As a simplification, we replace $\hat{\omega}^+$ with its eigenvalue $2\omega^+ \tau^+ = \omega^+$.

$$\Delta_1^+ \mathcal{H}_N = \sum_{q\beta} |V_q|^2 c_{d\beta}^\dagger c_{q\beta} \frac{1}{\hat{\omega}^+ - H_1} c_{q\beta}^\dagger c_{d\beta}$$

$$= \sum_{q\beta} |V_q|^2 c_{d\beta}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{d\beta} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d \hat{n}_{d\overline{\beta}} + \frac{1}{4} J_z \hat{n}_{d\overline{\beta}}} \tag{5.45}$$

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,

$$\Delta_1^+ \mathcal{H}_N = \sum_{q\beta} |V_q|^2 \hat{n}_{d\beta} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q + \left(\frac{J_z}{2} - \epsilon_d\right) \hat{n}_{d\overline{\beta}}}$$

$$= \sum_{q\beta} |V(q)|^2 \hat{n}_{d\beta} \left[\frac{\hat{n}_{d\overline{\beta}}}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4} J_z} + \frac{\left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega^+ - \frac{1}{2}\epsilon_q} \right] \tag{5.46}$$

$$= \sum_{q\beta} |V(q)|^2 \hat{n}_{d\beta} \left[\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q} + \hat{n}_{d\overline{\beta}} \left(\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4} J_z} - \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q} \right) \right]$$

2.

$$\Delta_2^+ \mathcal{H}_N = \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_z \beta S_d^z c_{q\beta}^\dagger c_{k\beta} \tag{5.47}$$

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

$$c_{d\beta}^\dagger J_z \beta S_d^z = c_{d\beta}^\dagger \frac{1}{2} \left(-J_z\right) \hat{n}_{d\overline{\beta}} \tag{5.48}$$

The expression simplifies to

$$\Delta_2^+ \mathcal{H}_N = \frac{1}{2}\left(-J_z\right)\sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{q\beta} \hat{n}_{d\bar{\beta}} \frac{1}{\omega^+ - \mathcal{H}_D^+} c_{q\beta}^\dagger c_{k\beta} \tag{5.49}$$

Intermediate $(\hat{n}_{q\beta} = 1, \hat{n}_{d\bar{\beta}} = 1, \hat{n}_{d\beta} = 0)$ energy is

$$H_1 = \mathcal{H}_D^+ = \frac{1}{2}\epsilon_q + \frac{1}{4}J_z\beta S_d^z + \epsilon_d = \frac{1}{2}\epsilon_q - \frac{1}{4}J_z + \epsilon_d \tag{5.50}$$

The first term $\frac{1}{2}\epsilon_q + \frac{1}{4}J_z\beta S_d^z$ 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.

$$\Delta_2^+ \mathcal{H}_N = -\frac{1}{2}J_z \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{q\beta} \hat{n}_{d\bar{\beta}} c_{q\beta}^\dagger c_{k\beta} \frac{1}{\omega^+ - H_1}$$

$$= -\frac{1}{2}J_z \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{k\beta} \frac{\hat{n}_{d\bar{\beta}}}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \tag{5.51}$$

3.

$$\Delta_3^+ \mathcal{H}_N = \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_t c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\bar{\beta}} \tag{5.52}$$

Intermediate $(\hat{n}_{d\beta} = 0, \hat{n}_{q\beta} = \hat{n}_{d\bar{\beta}} = 1)$ energy is

$$H_1 = \frac{1}{2}\epsilon_q - \frac{1}{4}J_z + \epsilon_d \tag{5.53}$$

$$\Delta_3^+ \mathcal{H}_N = \sum_{q\beta k} J_t V_q^* c_{d\beta}^\dagger c_{q\beta} c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\bar{\beta}} \frac{1}{\omega^+ - H_1}$$

$$= -J_t \sum_{q\beta k} V_q^* \hat{n}_{d\beta} \left(1 - \hat{n}_{q\beta}\right) c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}} \frac{1}{\omega^+ - H_1} \tag{5.54}$$

$$= -J_t \sum_{q\beta k} V_q^* c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}} \frac{\hat{n}_{d\bar{\beta}}}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}$$

4.

$$\Delta_4^+ \mathcal{H}_N = \sum_{q\beta k\sigma} J_z\beta S_d^z c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} V_q c_{q\beta}^\dagger c_{d\beta} \tag{5.55}$$

The first step is a simplification:

$$J_z\beta S_d^z c_{d\beta} = \frac{1}{2}\left(-J_z\right)\hat{n}_{d\bar{\beta}} c_{d\beta} \tag{5.56}$$

Intermediate $(\hat{n}_{d\beta} = 0, \hat{n}_{q\beta} = \hat{n}_{d\bar{\beta}} = 1)$ energy is

$$H_1 = \frac{1}{2}\epsilon_q - \frac{1}{4}J_z + \epsilon_d \tag{5.57}$$

$$\Delta_4^+ \mathcal{H}_N = -\frac{1}{2}J_z \sum_{q\beta k} V_q \hat{n}_{d\bar{\beta}} c_{k\beta}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{d\beta} \frac{1}{\omega^+ - H_1}$$

$$= \sum_{q\beta k} -\frac{1}{2}J_z V_q \hat{n}_{d\bar{\beta}} \left(1 - \hat{n}_{q\beta}\right) c_{k\beta}^\dagger c_{d\beta} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \tag{5.58}$$

$$= -\frac{1}{2}J_z \sum_{q\beta k} V_q c_{k\beta}^\dagger c_{d\beta} \frac{\hat{n}_{d\bar{\beta}}}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}$$

5.

$$\Delta_5^+ \mathcal{H}_N = \sum_{q\beta k\sigma} J_t c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} V_q c_{q\beta}^\dagger c_{d\beta} \tag{5.59}$$

Intermediate $(\hat{n}_{d\beta} = 0, \hat{n}_{q\beta} = \hat{n}_{d\overline{\beta}} = 1)$ energy is

$$H_1 = \frac{1}{2}\epsilon_q - \frac{1}{4}J_z + \epsilon_d \tag{5.60}$$

$$\begin{aligned}
\Delta_5^+ \mathcal{H}_N &= \sum_{q\beta k} J_t V_q c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{d\beta} \frac{1}{\omega^+ - H_1} \\
&= -\sum_{q\beta k} J_t V_q \left(1 - \hat{n}_{q\beta}\right) \hat{n}_{d\beta} c_{k\overline{\beta}}^\dagger c_{d\overline{\beta}} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \\
&= -J_t \sum_{q\beta k} V_q c_{k\beta}^\dagger c_{d\beta} \frac{\hat{n}_{d\overline{\beta}}}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}
\end{aligned} \tag{5.61}$$

6.

$$\Delta_6^+ \mathcal{H}_N = \sum_{k'q\beta k} J_z S_d^z \beta c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_z S_d^z \beta c_{q\beta}^\dagger c_{k'\beta} \tag{5.62}$$

The first step is a simplification:

$$\left(\beta S_d^z\right)^2 = \frac{1}{4}\left(\hat{n}_{d\beta} - \hat{n}_{d\overline{\beta}}\right)^2 = \frac{1}{4}\left(\hat{n}_{d\beta} + \hat{n}_{d\overline{\beta}} - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right) = \frac{1}{4}\left(\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right) \tag{5.63}$$

Note that this term projects onto the singly-occupied subspace; both the doubly- and zero-occupied states will give zero for this term. Intermediate $(\hat{n}_{q\beta} = 1)$ energy is

$$H_1 = \frac{1}{2}\epsilon_q + \frac{1}{2}\beta J_z S_d^z + H_{imp} \tag{5.64}$$

Since the $(S^z)^2$ term filters out only the single-occupied subspace, we can write $H_{imp} = \epsilon_d$.

$$\begin{aligned}
\Delta_6^+ \mathcal{H}_N &= \frac{1}{4}J_z^2 \sum_{k'q\beta k} \left(\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right) c_{k\beta}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{k'\beta} \frac{1}{\omega^+ - H_1} \\
&= \frac{1}{4}J_z^2 \sum_{k'q\beta k} \left(\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right)\left(1 - \hat{n}_{q\beta}\right) c_{k\beta}^\dagger c_{k'\beta} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - H_{imp} - \frac{1}{2}\beta J_z S_d^z} \\
&= \frac{1}{4}J_z^2 \sum_{k'q\beta k} c_{k\beta}^\dagger c_{k'\beta} \frac{\left(\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right)}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d - \frac{1}{2}\beta J_z S_d^z} \\
&= \frac{1}{4}J_z^2 \sum_{k'q\beta k} c_{k\beta}^\dagger c_{k'\beta} \left[\frac{\hat{n}_{d\beta}\left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d - \frac{1}{4}J_z} + \frac{\hat{n}_{d\overline{\beta}}\left(1 - \hat{n}_{d\beta}\right)}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}\right]
\end{aligned} \tag{5.65}$$

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 $\hat{n}_\uparrow\left(1 - \hat{n}_\downarrow\right) + \hat{n}_\downarrow\left(1 - \hat{n}_\uparrow\right)$.

7.

$$\Delta_7^+ \mathcal{H}_N = \sum_{q\beta kk'} \beta J_z S_d^z c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_t c_{d\overline{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\overline{\beta}} \tag{5.66}$$

The first step is a simplification:

$$\beta S_d^z c_{d\overline{\beta}}^\dagger c_{d\beta} = \beta S_d^z S_{d\overline{\beta}}^+ = \beta \frac{1}{2}\overline{\beta} S_{d\overline{\beta}}^+ = -\frac{1}{2} c_{d\overline{\beta}}^\dagger c_{d\beta} \tag{5.67}$$

Intermediate ($\hat{n}_{d\beta} = 0, \hat{n}_{q\beta} = \hat{n}_{d\overline{\beta}} = 1$) energy is

$$H_1 = \frac{1}{2}\epsilon_q + \beta J_z S_d^z + \epsilon_d = \frac{1}{2}\epsilon_q - \frac{1}{4}J_z + \epsilon_d \tag{5.68}$$

$$\begin{aligned}
\Delta_7^+ \mathcal{H}_N &= \sum_{q\beta kk'} \frac{1}{2} J_z J_t c_{k\beta}^\dagger c_{q\beta} c_{d\overline{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\overline{\beta}} \frac{-1}{\omega^+ - H_1} \\
&= -\frac{1}{2} J_z J_t \sum_{q\beta kk'} (1 - \hat{n}_{q\beta}) c_{d\overline{\beta}}^\dagger c_{d\beta} c_{k\beta}^\dagger c_{k'\overline{\beta}} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \\
&= -\frac{1}{2} J_z J_t \sum_{q\beta kk'} c_{d\overline{\beta}}^\dagger c_{d\beta} c_{k\beta}^\dagger c_{k'\overline{\beta}} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}
\end{aligned} \tag{5.69}$$

8.

$$\Delta_8^+ \mathcal{H}_N = \sum_{q\beta kk'} J_t c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_z \beta S_d^z c_{q\beta}^\dagger c_{k'\beta} \tag{5.70}$$

The first step is a simplification:

$$c_{d\beta}^\dagger c_{d\overline{\beta}} \beta S_d^z = S_{d\beta}^+ \beta S_d^z = \beta \frac{1}{2}\overline{\beta} S_{d\overline{\beta}}^+ = -\frac{1}{2} c_{d\beta}^\dagger c_{d\overline{\beta}} \tag{5.71}$$

Intermediate ($\hat{n}_{d\beta} = 0, \hat{n}_{q\beta} = \hat{n}_{d\overline{\beta}} = 1$) energy is

$$H_1 = \frac{1}{2}\epsilon_q + \beta J_z S_d^z + \epsilon_d = \frac{1}{2}\epsilon_q - \frac{1}{4}J_z + \epsilon_d \tag{5.72}$$

$$\begin{aligned}
\Delta_8^+ \mathcal{H}_N &= -\sum_{q\beta kk'} \frac{1}{2} J_z J_t c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{q\beta} c_{q\beta}^\dagger c_{k'\beta} \frac{1}{\omega^+ - H_1} \\
&= -\frac{1}{2} J_z J_t \sum_{q\beta kk'} (1 - \hat{n}_{q\beta}) c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{k'\beta} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \\
&= -\frac{1}{2} J_z J_t \sum_{q\beta kk'} c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{k'\beta} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}
\end{aligned} \tag{5.73}$$

9.

$$\Delta_9^+ \mathcal{H}_N = \sum_{q\beta kk\prime} J_t c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{q\beta} \frac{1}{\omega^+ - \mathcal{H}_D^+} J_t c_{d\overline{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\overline{\beta}} \tag{5.74}$$

Intermediate ($\hat{n}_{d\beta} = 0, \hat{n}_{q\beta} = \hat{n}_{d\overline{\beta}} = 1$) energy is

$$H_1 = \frac{1}{2}\epsilon_q - \frac{1}{4}J_z + \epsilon_d \tag{5.75}$$

$$\begin{aligned}
\Delta_9^+ \mathcal{H}_N &= \sum_{q\beta kk\prime} J_t^2 c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{q\beta} c_{d\overline{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\overline{\beta}} \frac{1}{\omega^+ - H_1} \\
&= J_t^2 \sum_{q\beta kk\prime} (1 - \hat{n}_{q\beta}) \hat{n}_{d\beta} (1 - \hat{n}_{d\overline{\beta}}) c_{k\overline{\beta}}^\dagger c_{k'\overline{\beta}} \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \\
&= J_t^2 \sum_{q\beta kk\prime} c_{k\overline{\beta}}^\dagger c_{k'\beta} \frac{\hat{n}_{d\overline{\beta}} (1 - \hat{n}_{d\beta})}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}
\end{aligned} \tag{5.76}$$

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 $\sum_\beta \hat{n}_{d\beta}\hat{n}_{d\overline{\beta}} = 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}$. 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 $V\hat{n}_{d\overline{\beta}}$, not strictly of V. In other words, if we split V as $V = V\left[\hat{n}_{d\overline{\beta}} + \left(1 - \hat{n}_{d\overline{\beta}}\right)\right] = V^1 \hat{n}_{d\overline{\beta}} + V^0\left(1 - \hat{n}_{d\overline{\beta}}\right)$, then these terms will renormalize V^1. However, we do not make this distinction here because in the particle sector, we will get the renormalization in V^0, and they will turn out to be the same, so we can just talk about the renormalization in V instead of splitting it. Terms 7 and * renormalize J_t and 9 renormalizes the anti-parallel part of J_z, that is, the part in which the conduction electron has spin $\overline{\beta}$. 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 5.3 just under eq. 5.127. Otherwise it will renormalize J_z.

$$\Delta^+ \epsilon_d = \sum_q |V(q)|^2 \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q} \tag{5.77}$$

$$\Delta^+ U = \sum_q 2|V(q)|^2 \left(\frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} - \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q} \right) \tag{5.78}$$

$$\Delta^+ V = -\left(\frac{1}{2}J_z + J_t\right) \sum_q V_q \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \tag{5.79}$$

$$\Delta^+ J_t = -J_z J_t \sum_q \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \tag{5.80}$$

$$\Delta^+ J_z = -J_t^2 \sum_q \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \tag{5.81}$$

5.2.2 Hole sector

The renormalization in the Hamiltonian in the hole sector is

$$\Delta^- \mathcal{H}_N = \sum_{q\beta} \left[V_q c_{q\beta}^\dagger c_{d\beta} + J_z \beta S_d^z \sum_{k\sigma} \hat{n}_{d\sigma} c_{k\beta} c_{q\beta}^\dagger + J_t \sum_{k\sigma} c_{d\overline{\beta}}^\dagger c_{q\beta}^\dagger c_{d\beta} c_{k\overline{\beta}} \right] \times \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-}$$

$$\times \left[V_q^* c_{d\beta}^\dagger c_{q\beta} + J_z \beta S_d^z \sum_{k\sigma} \hat{n}_{d\sigma} c_{q\beta} c_{k\beta}^\dagger + J_t \sum_{k\sigma} c_{d\beta}^\dagger c_{k\overline{\beta}}^\dagger c_{d\overline{\beta}} c_{q\beta} \right] \tag{5.82}$$

$\mathcal{H}_D^-$ is the energy of the hole state. Since the hole state consists of a missing electron, the diagonal part can be evaluated by substituting $\tau_{q\beta} = -\frac{1}{2}$ in eq. 5.38.

$$\mathcal{H}_D^- = -\frac{1}{2}\epsilon_q - \frac{1}{2}\beta J_z S_d^z + H_{\text{imp}} \tag{5.83}$$

1.

$$\Delta_1^- \mathcal{H}_N = \sum_{q\beta} |V_q|^2 c_{q\beta}^\dagger c_{d\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} c_{d\beta}^\dagger c_{q\beta} \tag{5.84}$$

The intermediate $(\hat{n}_{q\beta} = 0, \hat{n}_{d\beta} = 1)$ energy is

$$H_1 = \epsilon_d + (\epsilon_d + U)\hat{n}_{d\overline{\beta}} - \frac{1}{2}\epsilon_q - \frac{1}{2}\beta J_z S_d^z = -\frac{1}{2}\epsilon_q - \frac{1}{4}J_z\left(1 - \hat{n}_{d\overline{\beta}}\right) + \epsilon_d + (\epsilon_d + U)\hat{n}_{d\overline{\beta}} \tag{5.85}$$

$$\Delta_1^- \mathcal{H}_N = \sum_{q\beta} |V_q|^2 \hat{n}_{q\beta} \left(1 - \hat{n}_{d\beta}\right) \frac{1}{\omega^- - H_1} \tag{5.86}$$

For hole excitations, the initial state must be filled, so we can set $\hat{n}_{q\beta} = 1$.

$$
\begin{aligned}
\Delta_1^- \mathcal{H}_N &= \sum_{q\beta} |V_q|^2 \hat{n}_{q\beta} \left(1 - \hat{n}_{d\beta}\right) \frac{1}{\omega^- + \frac{1}{2}\epsilon_q + \frac{1}{4}J_z \left(1 - \hat{n}_{d\overline{\beta}}\right) - \epsilon_d - (\epsilon_d + U)\,\hat{n}_{d\overline{\beta}}} \\
&= \sum_{q\beta} |V_q|^2 \left(1 - \hat{n}_{d\beta}\right) \left[\frac{\hat{n}_{d\overline{\beta}}}{\omega^- + \frac{1}{2}\epsilon_q - 2\epsilon_d - U} + \frac{1 - \hat{n}_{d\overline{\beta}}}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \right] \\
&= \sum_{q\beta} |V(q)|^2 \left[\hat{n}_{d\overline{\beta}} \left(\frac{1}{\omega^- + \frac{1}{2}\epsilon_q - 2\epsilon_d - U} - \frac{2}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \right) \right. \\
&\qquad \left. + \hat{n}_{d\uparrow}\hat{n}_{d\downarrow} \left(\frac{1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} - \frac{1}{\omega^- + \frac{1}{2}\epsilon_q - 2\epsilon_d - U} \right) \right]
\end{aligned}
\tag{5.87}
$$

2.

$$\Delta_2^- \mathcal{H}_N = \sum_{q\beta k} V_q c_{q\beta}^\dagger c_{d\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_z \beta S_d^z c_{k\beta}^\dagger c_{q\beta} \tag{5.88}$$

The first step is a simplification:

$$c_{d\beta} J_z \beta S_d^z = c_{d\beta} \frac{1}{2} J_z \left(1 - \hat{n}_{d\overline{\beta}}\right) \tag{5.89}$$

The intermediate $(\hat{n}_{q\beta} = 0, \hat{n}_{d\beta} = 1)$ energy is

$$H_1 = -\frac{1}{2}\epsilon_q + \epsilon_d + (\epsilon_d + U)\,\hat{n}_{d\overline{\beta}} - \frac{1}{4}J_z \left(1 - \hat{n}_{d\overline{\beta}}\right) \tag{5.90}$$

$$
\begin{aligned}
\Delta_2^- \mathcal{H}_N &= \sum_{q\beta k} \frac{1}{2} J_z \left(1 - \hat{n}_{d\overline{\beta}}\right) V_q c_{q\beta}^\dagger c_{d\beta} \left(1 - \hat{n}_{d\overline{\beta}}\right) c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega^- - H_1} \\
&= -\sum_{q\beta k} \hat{n}_{q\beta} c_{k\beta}^\dagger c_{d\beta} \frac{V_q \frac{1}{2} J_z \left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d - (\epsilon_d + U)\,\hat{n}_{d\overline{\beta}} + \frac{1}{4}J_z \left(1 - \hat{n}_{d\overline{\beta}}\right)} \\
&= -\frac{1}{2} J_z \sum_{q\beta k} V_q \hat{n}_{q\beta} c_{k\beta}^\dagger c_{d\beta} \frac{\left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}
\end{aligned}
\tag{5.91}
$$

3.

$$\Delta_3^- \mathcal{H}_N = \sum_{q\beta k} V_q c_{q\beta}^\dagger c_{d\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_t c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{q\beta} \tag{5.92}$$

The intermediate $(\hat{n}_{q\beta} = \hat{n}_{d\overline{\beta}} = 0, \hat{n}_{d\beta} = 1)$ energy is

$$H_1 = \epsilon_d - \frac{1}{2}\epsilon_q - \frac{1}{2}J_z \beta S_d^z = \epsilon_d - \frac{1}{2}\epsilon_q - \frac{1}{4}J_z \tag{5.93}$$

$$
\begin{aligned}
\Delta_3^- \mathcal{H}_N &= \sum_{q\beta k} J_t V_q c_{q\beta}^\dagger c_{d\beta} c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{q\beta} \frac{1}{\omega^- - H_1} \\
&= \sum_{q\beta k} J_t V_q \hat{n}_{q\beta} \left(1 - \hat{n}_{d\beta}\right) c_{k\overline{\beta}}^\dagger c_{d\overline{\beta}} \frac{-1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \\
&= -J_t \sum_{q\beta k} V_q c_{k\overline{\beta}}^\dagger c_{d\beta} \frac{1 - \hat{n}_{d\overline{\beta}}}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}
\end{aligned}
\tag{5.94}
$$

4.

$$\Delta_4^- \mathcal{H}_N = \sum_{q\beta k} \frac{1}{2} J_z \beta S_d^z c_{q\beta}^\dagger c_{k\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} V_q^* c_{d\beta}^\dagger c_{q\beta} \tag{5.95}$$

There is a simplification:

$$\frac{1}{2} J_z \beta S_d^z c_{d\beta}^\dagger = \frac{1}{2} J_z \left(1 - \hat{n}_{d\bar{\beta}}\right) c_{d\beta}^\dagger \tag{5.96}$$

The intermediate $(\hat{n}_{q\beta} = 0, \hat{n}_{d\beta} = 1)$ energy is

$$H_1 = -\frac{1}{2}\epsilon_q + \epsilon_d + (\epsilon_d + U)\hat{n}_{d\bar{\beta}} - \frac{1}{4}J_z \left(1 - \hat{n}_{d\bar{\beta}}\right) \tag{5.97}$$

$$
\begin{aligned}
\Delta_4^- \mathcal{H}_N &= \sum_{q\beta k} V_q^* c_{q\beta}^\dagger c_{k\beta} c_{d\beta}^\dagger c_{q\beta} \frac{\frac{1}{2}J_z \left(1 - \hat{n}_{d\bar{\beta}}\right)}{\omega^- - H_1} \\
&= \sum_{q\beta k} \hat{n}_{q\beta} V_q^* c_{k\beta} c_{d\beta}^\dagger \frac{\frac{1}{2}J_z \left(1 - \hat{n}_{d\bar{\beta}}\right)}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d - (\epsilon_d + U)\hat{n}_{d\bar{\beta}} + \frac{1}{4}J_z \left(1 - \hat{n}_{d\bar{\beta}}\right)} \\
&= -\frac{1}{2}J_z \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{k\beta} \frac{1 - \hat{n}_{d\bar{\beta}}}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}
\end{aligned}
\tag{5.98}
$$

5.

$$\Delta_5^- \mathcal{H}_N = \sum_{q\beta k} J_t c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\bar{\beta}} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} V_q^* c_{d\beta}^\dagger c_{q\beta} \tag{5.99}$$

The intermediate $(\hat{n}_{q\beta} = \hat{n}_{d\bar{\beta}} = 0, \hat{n}_{d\beta} = 1)$ energy is

$$H_1 = -\frac{1}{2}\epsilon_q + \epsilon_d - \frac{1}{4}J_z \tag{5.100}$$

$$
\begin{aligned}
\Delta_5^- \mathcal{H}_N &= \sum_{q\beta k} J_t V_q^* c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\bar{\beta}} c_{d\beta}^\dagger c_{q\beta} \frac{1}{\hat{\omega}^- - H_1} \\
&= -J_t \sum_{q\beta k} V_q^* \hat{n}_{q\beta} \left(1 - \hat{n}_{d\beta}\right) c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}} \frac{1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \\
&= -J_t \sum_{q\beta k} V_q^* c_{d\beta}^\dagger c_{k\beta} \frac{1 - \hat{n}_{d\bar{\beta}}}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}
\end{aligned}
\tag{5.101}
$$

6.

$$\Delta_6^- \mathcal{H}_N = \sum_{q\beta k k'} J_z \beta S_d^z c_{q\beta}^\dagger c_{k'\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_z \beta S_d^z c_{k\beta}^\dagger c_{q\beta} \tag{5.102}$$

From eq. 5.63,

$$\left(\beta S_d^z\right)^2 = \frac{1}{4}\left(\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right) \tag{5.103}$$

The intermediate $(\hat{n}_{q\beta} = 0)$ energy is

$$H_1 = H_{\text{imp}} - \frac{1}{2}\epsilon_q - \frac{1}{2}\beta J_z S_d^z \tag{5.104}$$

$$\Delta_6^- \mathcal{H}_N = \sum_{q\beta kk'} \frac{J_z^2}{4} \left(\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right) c_{q\beta}^\dagger c_{k'\beta} c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega^- - H_1}$$

$$= \frac{J_z^2}{4} \sum_{q\beta kk'} \hat{n}_{q\beta} \left(\hat{n}_d - 2\hat{n}_{d\uparrow}\hat{n}_{d\downarrow}\right) c_{k'\beta} c_{k\beta}^\dagger \frac{1}{\omega^- + \frac{1}{2}\epsilon_q - H_{\text{imp}} + \frac{1}{2}\beta J_z S_d^z}$$

$$= -\frac{J_z^2}{4} \sum_{q\beta kk'} c_{k\beta}^\dagger c_{k'\beta} \left[\frac{\hat{n}_{d\beta}\left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} + \frac{\hat{n}_{d\overline{\beta}}\left(1 - \hat{n}_{d\beta}\right)}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d - \frac{1}{4}J_z} \right]$$

$$+ \frac{J_z^2}{4} \sum_{q\beta k} \left[\frac{\hat{n}_{d\beta}\left(1 - \hat{n}_{d\overline{\beta}}\right)}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} + \frac{\hat{n}_{d\overline{\beta}}\left(1 - \hat{n}_{d\beta}\right)}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d - \frac{1}{4}J_z} \right] \tag{5.105}$$

7.

$$\Delta_7^- \mathcal{H}_N = \sum_{q\beta kk'} J_z \beta S_d^z c_{q\beta}^\dagger c_{k'\beta} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_t c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{q\beta} \tag{5.106}$$

Simplification:

$$\beta S_d^z c_{d\beta}^\dagger c_{d\overline{\beta}} = \beta S_d^z S_{d\beta}^+ = \beta \frac{1}{2}\beta S_{d\beta}^+ = \frac{1}{2} c_{d\beta}^\dagger c_{d\overline{\beta}} \tag{5.107}$$

The intermediate $(\hat{n}_{q\beta} = \hat{n}_{d\overline{\beta}} = 0, \hat{n}_{d\beta} = 1)$ energy is

$$H_1 = \epsilon_d - \frac{1}{2}\epsilon_q - \frac{1}{4}J_z \tag{5.108}$$

$$\Delta_7^- \mathcal{H}_N = \sum_{q\beta kk'} \frac{1}{2} J_z J_t c_{q\beta}^\dagger c_{k'\beta} c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{q\beta} \frac{1}{\omega^- - H_1}$$

$$= \sum_{q\beta kk'} \frac{1}{2} J_z J_t \hat{n}_{q\beta} c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{k'\beta} \frac{-1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}$$

$$= -\frac{1}{2} J_z J_t \sum_{q\beta kk'} c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{k'\beta} \frac{1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}$$

$$= -\frac{1}{2} J_z J_t \sum_{q\beta kk'} c_{d\overline{\beta}}^\dagger c_{d\beta} c_{k\beta}^\dagger c_{k'\overline{\beta}} \frac{1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \tag{5.109}$$

8.

$$\Delta_8^- \mathcal{H}_N = \sum_{q\beta kk'} J_t c_{d\overline{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\overline{\beta}} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_z \beta S_d^z c_{k\beta}^\dagger c_{q\beta} \tag{5.110}$$

Simplification:

$$c_{d\overline{\beta}}^\dagger c_{d\beta} \beta S_d^z = S_{d\overline{\beta}}^+ S_d^z \beta = \beta \frac{1}{2} S_{d\overline{\beta}}^+ \beta = \frac{1}{2} c_{d\overline{\beta}}^\dagger c_{d\beta} \tag{5.111}$$

The intermediate $(\hat{n}_{q\beta} = \hat{n}_{d\overline{\beta}} = 0, \hat{n}_{d\beta} = 1)$ energy is

$$H_1 = -\frac{1}{2}\epsilon_q - \frac{1}{4}J_z + \epsilon_d \tag{5.112}$$

$$\Delta_8^- \mathcal{H}_N = \sum_{q\beta kk'} \frac{1}{2} J_z J_t c_{d\overline{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\overline{\beta}} c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega^- - H_1}$$

$$= \sum_{q\beta kk'} \frac{1}{2} J_z J_t \hat{n}_{q\beta} c_{d\overline{\beta}}^\dagger c_{d\beta} c_{k\beta}^\dagger c_{k'\overline{\beta}} \frac{-1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d - \frac{1}{4}J_z}$$

$$= -\frac{1}{2} J_z J_t \sum_{q\beta kk'} c_{d\overline{\beta}}^\dagger c_{d\beta} c_{k\beta}^\dagger c_{k'\overline{\beta}} \frac{1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \tag{5.113}$$

9.

$$\Delta_9^- \mathcal{H}_N = \sum_{q\beta kk'} J_t c_{d\overline{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\overline{\beta}} \frac{1}{\hat{\omega}^- - \mathcal{H}_D^-} J_t c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{q\beta} \tag{5.114}$$

The intermediate $(\hat{n}_{q\beta} = \hat{n}_{d\overline{\beta}} = 0, \hat{n}_{d\beta} = 1)$ energy is

$$H_1 = -\frac{1}{2}\epsilon_q - \frac{1}{4}J_z + \epsilon_d \tag{5.115}$$

$$\begin{aligned}
\Delta_9^- \mathcal{H}_N &= \sum_{q\beta kk'} J_t^2 c_{d\overline{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k'\overline{\beta}} c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger c_{q\beta} \frac{1}{\omega^- - H_1} \\
&= \sum_{q\beta kk'} J_t^2 \hat{n}_{q\beta} c_{d\overline{\beta}}^\dagger c_{d\beta} c_{k'\overline{\beta}} c_{d\beta}^\dagger c_{d\overline{\beta}} c_{k\overline{\beta}}^\dagger \frac{1}{\omega^- - H_1} \\
&= -\sum_{q\beta kk'} J_t^2 \hat{n}_{q\beta} \hat{n}_{d\overline{\beta}} c_{d\beta} c_{k'\overline{\beta}} c_{d\beta}^\dagger c_{k\overline{\beta}}^\dagger \frac{1}{\omega^- - H_1} \\
&= \sum_{q\beta kk'} J_t^2 \hat{n}_{q\beta} \hat{n}_{d\overline{\beta}} (1 - \hat{n}_{d\beta}) c_{k'\overline{\beta}} c_{k\overline{\beta}}^\dagger \frac{1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \\
&= -J_t^2 \sum_{q\beta kk'} c_{k\beta}^\dagger c_{k'\beta} \frac{\hat{n}_{d\beta}(1 - \hat{n}_{d\overline{\beta}})}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} + J_t^2 \sum_{qk\beta} \frac{\hat{n}_{d\overline{\beta}}(1 - \hat{n}_{d\beta})}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}
\end{aligned} \tag{5.116}$$

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.

$$\begin{aligned}
\Delta^- \epsilon_d &= \sum_q |V(q)|^2 \left(\frac{1}{\omega^- + \frac{1}{2}\epsilon_q - 2\epsilon_d - U} - \frac{2}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \right) + \\
&\quad \sum_{qk} \left[\frac{\frac{1}{4}J_z^2 + J_t^2}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} + \frac{\frac{1}{4}J_z^2}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d - \frac{1}{4}J_z} \right]
\end{aligned}$$

$$\begin{aligned}
\Delta^- U &= 2\sum_q |V(q)|^2 \left(\frac{1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} - \frac{1}{\omega^- + \frac{1}{2}\epsilon_q - 2\epsilon_d - U} \right) - \\
&\quad 2\sum_{qk} \left[\frac{\frac{1}{4}J_z^2 + J_t^2}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} + \frac{\frac{1}{4}J_z^2}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d - \frac{1}{4}J_z} \right]
\end{aligned}$$

$$\Delta^- V = -\left(\frac{1}{4}J_z + J_t \right) \sum_q V_q \frac{1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}$$

$$\Delta^- J_t = -J_z J_t \sum_q \frac{1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}$$

$$\Delta^- J_z = -J_t^2 \sum_q \frac{1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}$$

5.3 Particle-Hole symmetry

The Anderson model Hamiltonian, eq. 5.33, has an impurity particle-hole symmetry for a certain condition of the couplings. To see this, we apply the particle-hole transformation $c_k \to c_k^\dagger, c_d \to -c_d^\dagger$ 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

$$\epsilon_d \sum_\sigma \hat{n}_{d\sigma} \to 2\epsilon_d - \epsilon_d \sum_\sigma \hat{n}_{d\sigma} \tag{5.117}$$

$$U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} \to U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} - U \sum_\sigma \hat{n}_{d\sigma} + U \tag{5.118}$$

$$\sum_{k\sigma} V(k)c_{k\sigma}^\dagger c_{d\sigma} + hc \to \sum_{k\sigma} -V(k)c_{k\sigma}c_{d\sigma}^\dagger + hc = \sum_{k\sigma} V^*(k)c_{k\sigma}^\dagger c_{d\sigma} + hc \tag{5.119}$$

$$S^z \sum_{kq} s_{kq}^z \to (-S^z) \sum_{kq} \left(-s_{kq}^z\right) = S^z \sum_{kq} s_{kq}^z \tag{5.120}$$

$$S^\pm \sum_{kq} s_{kq}^\mp \to \left(-S^\pm\right) \sum_{kq} \left(-s_{kq}^\mp\right) = S^\pm \sum_{kq} s_{kq}^\mp \tag{5.121}$$

The transformation of the spin terms, eqs. 5.120 and 5.121, 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: $\hat{S} = \hat{n} - \frac{1}{2} \to \frac{1}{2} - \hat{n} = -\hat{S}$. The spin terms are thus invariant under the particle-hole transformation. The impurity-bath hopping term can be made symmetric by making $V(k)$ real; then we would have, from eq. 5.119,

$$V(k)\left(c_{k\sigma}^\dagger c_{d\sigma} + c_{d\sigma}^\dagger c_{k\sigma}\right) \to V(k)\left(c_{d\sigma}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger c_{d\sigma}\right) \tag{5.122}$$

The impurity diagonal terms, ϵ_d and U, require a specific condition. Combining eqs. 5.117 and 5.118,

$$\epsilon_d \hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} \to (-\epsilon_d - U)\hat{n}_{d\sigma} + U\hat{n}_{d\uparrow}\hat{n}_{d\downarrow} \tag{5.123}$$

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

$$\epsilon_d = -\epsilon_d - U \implies \epsilon_d + \frac{1}{2}U = 0 \tag{5.124}$$

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. If we measure the energies with w.r.t this singly occupied state, the energy of the particle state is $E_p = 2\epsilon_d + U - \epsilon_d = \epsilon_d + U$ and that of the hole state is $E_h = 0 - \epsilon_d = -\epsilon_d$. Particle-hole symmetry then requires the particle and hole levels to be degenerate, which means $E_p = E_h$, and we recover the condition eq. 5.124.
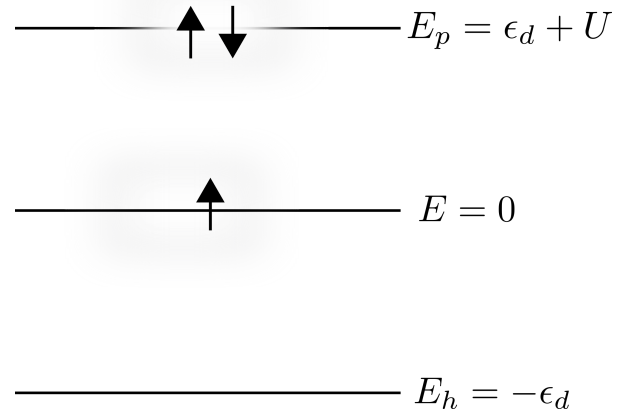

Figure 5: Particle and hole excitations of the impurity

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

$$\Delta \left(\epsilon_d + \frac{1}{2}U \right) = 0 \tag{5.125}$$

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 both the particle and hole equations, we can find the RG equation for the asymmetry parameter

$$\Delta^+ \gamma \equiv \Delta^+ \left(\epsilon_d + \frac{1}{2}U \right) = \sum_q |V(q)|^2 \frac{1}{\omega^+ - \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z}$$
$$\Delta^- \gamma \equiv \Delta^- \left(\epsilon_d + \frac{1}{2}U \right) = -\sum_q |V(q)|^2 \frac{1}{\omega^- + \frac{1}{2}\epsilon_q - \epsilon_d + \frac{1}{4}J_z} \tag{5.126}$$

At this point, we must note that ω^+ and ω^-, the quantum fluctuation energy scales, for the particle and hole sectors are not entirely independent. Recall that if we require the RG to be unitary, we must have $\eta(\omega^-) = \left(\eta^\dagger(\omega^+) \right)^\dagger$. This condition constrains the relation between $\omega^\pm$. To see what the relation is, we can demand $\Delta\gamma \equiv \Delta^+\gamma + \Delta^-\gamma = 0$. That gives

$$\omega^+ - \frac{1}{2}\epsilon_q = \omega^- + \frac{1}{2}\epsilon_q \tag{5.127}$$

If we apply this condition to the term 6 in hole sector, we see that it cancels the term 6 in particle sector.

5.4 "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,

$$\delta\epsilon_d = -\sum_q \frac{|V_q|^2}{\omega^+ - \epsilon_q} \tag{5.128}$$

If we assume an isotropic dispersion ($\epsilon_q = D$), where D is the current(running) bandwidth and a momentum-independent hopping potential V,

$$\delta\epsilon_d = -\frac{1}{\omega^+ - D} \sum_q |V_q|^2 = -\frac{1}{\omega^+ - D}\rho(D)|\delta D||V|^2$$

There we used

$$\sum_q = \sum_{\epsilon_q \in [D-|\delta D|, D]} = \rho(D)|\delta D| \tag{5.129}$$

where $\rho(D)$ is the single-spin density of states at the energy D and $|\Delta D|$ is the thickness of the band that we disentangled at this step. In the literature, we usually define a quantity that denotes the amount of hybridisation between the impurity and the bath: $\Delta \equiv \pi\rho(D)|V|^2$. In terms of this Δ, we get

$$\delta\epsilon_d = -\frac{\Delta|\delta D|}{\omega^+ - D} \tag{5.130}$$

For low energy excitations, we can use $\omega^+ \ll D$. Further, since we have defined $\delta\epsilon_d = \epsilon_d(D-|\delta D|)-\epsilon_d(D)$, we must have $\delta D = D - |\delta D| - D = -|\delta D|$.

$$\frac{d\epsilon_d}{dD} = -\frac{\Delta}{D} \tag{5.131}$$

This is the form obtained from Poor Man's scaling of the asymmetric Anderson model.

5.5 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:

$$2\Delta J_z = 2\Delta J_t = \Delta J = -J^2 \sum_q \frac{1}{\omega^+ - \epsilon_q - \epsilon_d + \frac{1}{4}J} \tag{5.132}$$

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 $\omega^+ - \epsilon_d \to \tilde{\omega}^+$.

$$2\Delta J_z = 2\Delta J_t = \Delta J = -J^2 \sum_q \frac{1}{\tilde{\omega}^+ - \epsilon_q + \frac{1}{4}J} \tag{5.133}$$

If we now consider low energy excitations $(\tilde{\omega}^+ - \epsilon_q \approx -\epsilon_q)$ and expand the denominator in powers of J and keep only the lowest order, we get

$$\Delta J = -J^2 \sum_q \frac{1}{-\epsilon_q} \tag{5.134}$$

For an isotropic dispersion, we can use $\epsilon_q = D$. The sum can then be evaluated as

$$\sum_q = \rho(D)\Delta D \tag{5.135}$$

The flow equation of J becomes

$$\Delta J = J^2 \rho(D) \frac{|\Delta D|}{D} \tag{5.136}$$

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,

$$\frac{\mathrm{d}J}{\mathrm{d}\ln D} = -J^2 \rho(D) \tag{5.137}$$

5.6 Connection with Kondo URG result

Recall eq. 5.133.

$$\Delta J = -J^2 \sum_q \frac{1}{\tilde{\omega}^+ - \epsilon_q + \frac{1}{4}J} \tag{5.138}$$

For $\tilde{\omega}^+ = \frac{1}{2}D$, we get

$$\Delta J = 2J^2 \sum_q \frac{1}{D - \frac{1}{2}J} \tag{5.139}$$

This has the same fixed point structure as the Kondo URG scaling equation.

5.7 Fixed points for the symmetric Anderson model with $J_z = J_t$

We first consider the simpler case where $\epsilon_d + \frac{1}{2}U = 0$ and $J_z = J_t = \frac{1}{2}J$. We also assume an isotropic dispersion $\epsilon_q = D$ and momentum independent potential $V(q) \equiv V$. For convenience, we define $n(D) =$
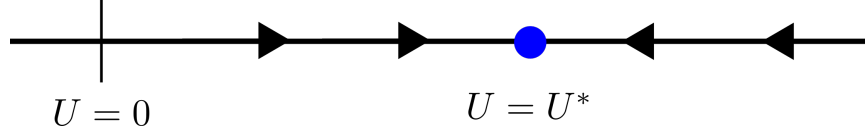
Figure 6: Flows towards local moment for $J = 0$

$\sum_{\epsilon_q = D}$ and $\mathcal{V}(D) = \sum_{\epsilon_k < D}$. The former is the number of states on the energy shell at D, while the latter is the number of states inside the energy shell D. The scaling equations for the hole sector become:

$$\Delta U = \frac{|V|^2 \left(U + \frac{1}{2}J\right) n(D)}{\left(\omega^- - D\right)\left(\omega^- - D - \frac{1}{2}U - \frac{1}{4}J\right)} - \frac{1}{8}\frac{J^2 n(D)\mathcal{V}(D)\left[6\left(\omega^- - D\right) - 3U - J\right]}{\left(\omega^- - \epsilon_q - \frac{1}{2}U\right)^2 - \frac{1}{16}J^2}$$

$$\Delta V = -\frac{3}{4}JVn(D)\frac{1}{\omega^- - D - \frac{1}{2}U - \frac{1}{4}J}$$

$$\Delta J = -\frac{1}{2}J^2 n(D)\frac{1}{\omega^- - D - \frac{1}{2}U - \frac{1}{4}J}$$

In absence of Kondo-type interaction ($J = 0$)

We first consider the case where $J = 0$. The only relevant equation is then that of U, because V and J will then not flow.

$$\Delta U = \frac{|V|^2 U n(D)}{\left(\omega^- - D\right)\left(\omega^- - D - \frac{1}{2}U\right)} \tag{5.140}$$

To get a feel for this equation, we look at a specific value of $\omega^- = \frac{1}{2}U$. For this value,

$$\Delta U = \frac{|V|^2 U n(D)}{D\left(D - \frac{1}{2}U\right)} \tag{5.141}$$

If we start with bare values U and D such that $U < 2D$, then U is relevant, and it will increase. Meanwhile, the bandwidth will decrease as we go to lower energies. The fixed point is achieved when the denominator becomes zero.

$$U^* = 2D^* \tag{5.142}$$

The opposite thing happens if we start with bare values such that $U > 2D$. Then, U is irrelevant and it will decrease until it reaches the same fixed point condition. This fixed point, characterized by $U^* = 2D^*$ and $J = 0$, is the *local moment fixed point*. It is stable along both directions in the $U-$axis. It is however unstable to perturbations in J, as we will see later.

There is another fixed point in this picture, the free orbital fixed point at $U = V = 0$. It is unstable in all directions. The two fixed points and the flows are schematically shown in fig. 6. One specific flow line for $J = 0$ is shown in fig. 7.

With the Kondo-type interaction ($J > 0$)

In this case, all three equations will come into play. Using the value $\omega^- = \frac{1}{2}U + \frac{1}{2}J$, the equations become

$$\Delta U = \frac{|V|^2 \left(U + \frac{1}{2}J\right) n(D)}{\left(D - \frac{1}{4}J\right)\left(D - \frac{1}{2}U - \frac{1}{2}J\right)} + \frac{1}{8}\frac{J^2 n(D)\mathcal{V}(D)\left[6D - 2J\right]}{\left(D - \frac{1}{4}J\right)\left(D - \frac{3}{4}J\right)}$$

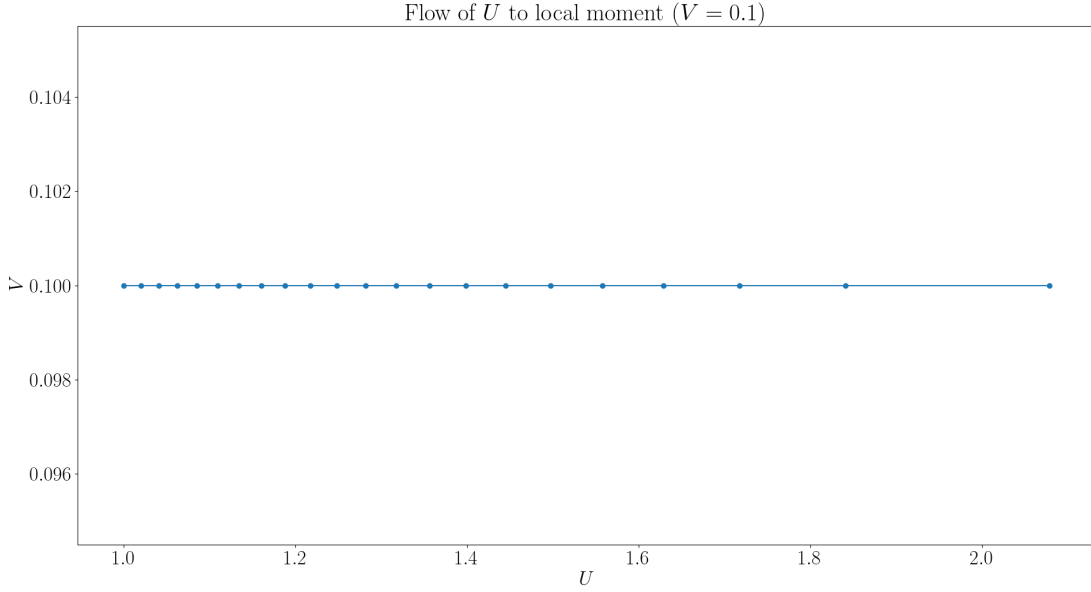$$\Delta V = \frac{3}{4}Jn(D)V\frac{1}{D - \frac{1}{4}J}$$

104

Figure 7: Plot of a particular flow from free orbital (leftmost) to local moment (rightmost) for $J = 0$

$$\Delta J = \frac{1}{2} J^2 n(D) \frac{1}{D - \frac{1}{4}J}$$

We can now see how the couplings will flow if we start at the local moment fixed point and add a small perturbation J. Because of the condition for the local moment fixed point, we know that $D^* - \frac{1}{2}U^* = 0$. Also, close to the local moment, J is small so we can ignore the J^2 term. The equations thus become

$$\Delta U = -2 \frac{|V|^2 \left(U^* + \frac{1}{2}J\right) n(D)}{\left(D^* - \frac{1}{4}J\right) J} < 0$$

$$\Delta V = \frac{3}{4} J n(D) V \frac{1}{D^* - \frac{1}{4}J} > 0$$

$$\Delta J = \frac{1}{2} J^2 n(D) \frac{1}{D^* - \frac{1}{4}J} > 0$$

The U is irrelevant and will flow down. The J on the other hand is relevant and will flow to some large value. This fixed point, characterized by a large positive J is the strong-coupling fixed point.

A similar flow happens if we start from the free orbital fixed point. There, U is 0, and the equations look like

$$\Delta U = \frac{1}{2} \frac{|V|^2 J n(D)}{\left(D - \frac{1}{4}J\right)\left(D - \frac{1}{2}J\right)} > 0$$

$$\Delta V = \frac{3}{4} J n(D) V \frac{1}{D - \frac{1}{4}J} > 0$$

$$\Delta J = \frac{1}{2} J^2 n(D) \frac{1}{D - \frac{1}{4}J} > 0$$

Here both U and J are relevant and they flow up to the strong-coupling fixed point. A schematic flow diagram is shown in fig. 8.
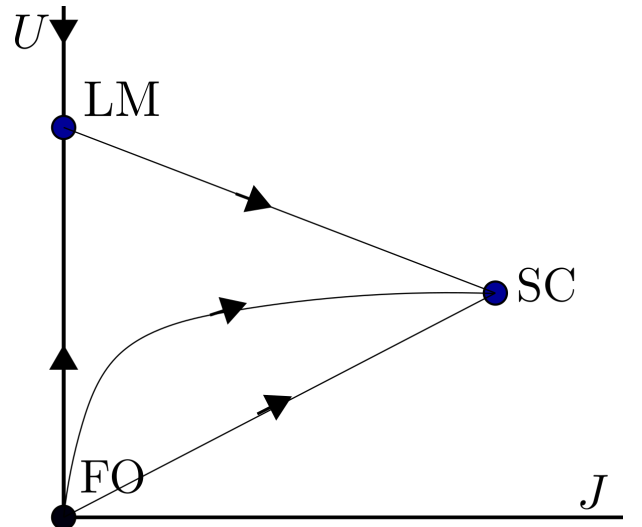

Figure 8: Schematic flows from local moment and free orbital to strong-coupling

6 Connection between Unitary Renormalization Group and Poor Man's Scaling

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

$$\mathcal{H}\left|\Psi\right\rangle = E\left|\Psi\right\rangle \tag{6.1}$$

$\mathcal{H}$ is the total Hamiltonian and $\left|\Psi\right\rangle$ and E are the exact eigenstate and eigenvalue of $\mathcal{H}$. The problems we deal with typically have a bath of mobile electrons, with energies spanning from $-D$ to D. We are interested in finding effective Hamiltonians after "removing" the highest shell in the conduction bath. This will give us a Hamiltonian to which we can again apply the same procedure.

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

$$\left|\Psi\right\rangle = \left|\Psi_0\right\rangle + \left|\Psi_1\right\rangle \tag{6.2}$$

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

$$\mathcal{H} = \mathcal{H}^d + V_0 + V_+ + V_- \tag{6.3}$$

$\mathcal{H}^d$ 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. 6.3 and 6.2 in eq. 6.1 gives

$$\left(\mathcal{H}^d + V_0 + V_+ + V_-\right)\left(\left|\Psi_0\right\rangle + \left|\Psi_1\right\rangle\right) = E\left(\left|\Psi_0\right\rangle + \left|\Psi_1\right\rangle\right) \tag{6.4}$$

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

$$\begin{aligned}
\left(\mathcal{H}_0^d + V_0\right)\left|\Psi_0\right\rangle + V_-\left|\Psi_1\right\rangle &= E\left|\Psi_0\right\rangle \\
\left(\mathcal{H}_1^d + V_0\right)\left|\Psi_1\right\rangle + V_+\left|\Psi_0\right\rangle &= E\left|\Psi_1\right\rangle
\end{aligned} \tag{6.5}$$

Eliminating $\left|\Psi_1\right\rangle$ from the two equations gives

$$\left(\mathcal{H}_0^d + V_0 + V_- \frac{1}{E - \mathcal{H}_1^d - V_0} V_+\right)\left|\Psi_0\right\rangle = E\left|\Psi_0\right\rangle \tag{6.6}$$

This new Hamiltonian,

$$\tilde{\mathcal{H}}_0 = \mathcal{H}_0^d + V_0 + V_- \frac{1}{E - \mathcal{H}_1^d - V_0} V_+ \tag{6.7}$$

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

$$\Delta V_0\big|_{PMS} = V_- \frac{1}{E - \mathcal{H}_1^d - V_0} V_+ \tag{6.8}$$

We can write down the renormalized Schrodinger equation in the low energy subspace, from eq. 6.6,

$$\tilde{\mathcal{H}}_0\left|\Psi_0\right\rangle = E\left|\Psi_0\right\rangle \tag{6.9}$$

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. 6.1.

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

$$\mathcal{H} |\Phi\rangle = \mathcal{H}' |\Phi\rangle \tag{6.10}$$

This definition of $\mathcal{H}'$ is the very minimum that we must have in order to fulfill our goal (decouple q). The final expression for the renormalization can be written directly from the PMS expression simply by replacing E with $\mathcal{H}'$.

$$\Delta V_0 \big|_{URG} = V_- \frac{1}{\mathcal{H}_1' - \mathcal{H}_1^d - V_0} V_+ \tag{6.11}$$

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

$$U |\Phi\rangle = |\Phi_0\rangle \quad \text{and} \quad \left[\hat{n}_q, \tilde{\mathcal{H}} \right] = 0 \tag{6.12}$$

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 me 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.

In the context of URG, we define a quantum fluctuation energy scale $\hat{\omega}$:

$$\hat{\omega} = \mathcal{H}_1' - V_0 \tag{6.13}$$

This allows us to write

$$\Delta V_0 \big|_{URG} = V_- \frac{1}{\hat{\omega} - \mathcal{H}_1^d} V_+ \tag{6.14}$$

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

$$\left(\hat{\omega} - \mathcal{H}_1^d \right) V_+ |\Psi_0\rangle \quad \text{or} \quad \left(\hat{\omega} - \mathcal{H}_1^d \right) V_- |\Psi_1\rangle \tag{6.15}$$

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.
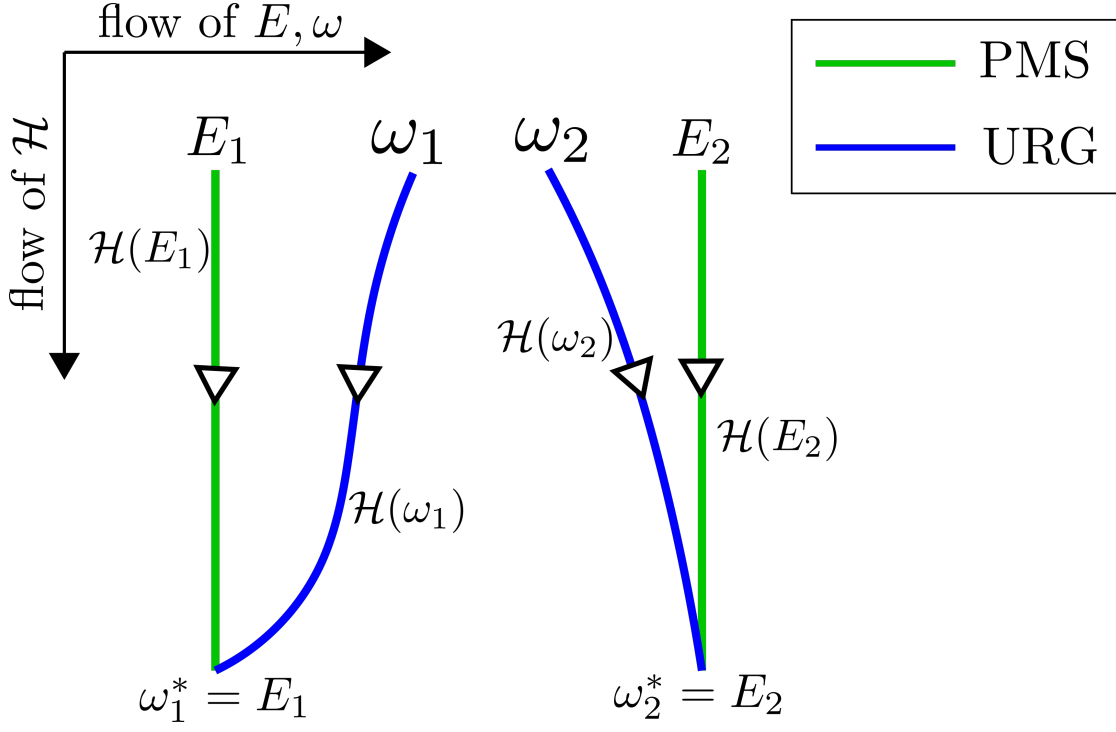
Figure 9: Flows of PMS(green) and URG(blue)

To make matters more clear, we can look at a specific term. For the SIAM, we will consider the scattering $V = c_{q\uparrow}^\dagger c_{d\uparrow}$. $q \uparrow$ is a state in the high energy subspace.

$$\Delta V_P = c_{d\uparrow}^\dagger c_{q\uparrow} \frac{1}{E - \hat{\mathcal{H}}_0} c_{q\uparrow}^\dagger c_{d\uparrow} \tag{6.16}$$

The intermediate energy (at the propagator) is

$$E_1 = \epsilon_d \hat{n}_{d\bar\beta} + \epsilon_q \tag{6.17}$$

which gives

$$\begin{aligned}
\Delta V_P &= c_{d\uparrow}^\dagger c_{q\uparrow} \frac{1}{E - \epsilon_q - \epsilon_d \hat{n}_{d\bar\beta}} c_{q\uparrow}^\dagger c_{d\uparrow} \\
&= \frac{1}{E - \epsilon_q - \epsilon_d \hat{n}_{d\bar\beta}} c_{d\uparrow}^\dagger c_{q\uparrow} c_{q\uparrow}^\dagger c_{d\uparrow} \\
&= \left(\frac{\hat{n}_{d\bar\beta}}{E^a - \epsilon_q - \epsilon_d} + \frac{1 - \hat{n}_{d\bar\beta}}{E^b - \epsilon_q} \right) c_{d\uparrow}^\dagger c_{q\uparrow} c_{q\uparrow}^\dagger c_{d\uparrow}
\end{aligned} \tag{6.18}$$

There are two terms. The two terms differ in their initial states; one starts from $n_{d\bar\beta} = 1$ (corresponding to E^a) and the other starts from $n_{d\bar\beta} = 0$ (corresponding to E^b). From the definition of the $T-$matrix we can see that different initial states will give rise to different final eigenstates. To treat the various energies E^a and E^b on an equal footing, we need to subtract off the initial energies:

$$\begin{aligned}
E_0 &= \epsilon_d + (\epsilon_d + U)\, \hat{n}_{d\bar\beta} \\
\implies E_0^a &= 2\epsilon_d + U \\
E_0^b &= \epsilon_d
\end{aligned} \tag{6.19}$$

Defining $\xi = E - E_0$, We can then write

$$\begin{aligned}
\Delta V_P &= \left(\frac{\hat{n}_{d\bar\beta}}{\xi + E_0^a - \epsilon_q - \epsilon_d} + \frac{1 - \hat{n}_{d\bar\beta}}{\xi + E_0^b - \epsilon_q} \right) c_{d\uparrow}^\dagger c_{q\uparrow} c_{q\uparrow}^\dagger c_{d\uparrow} \\
&= \left(\frac{\hat{n}_{d\bar\beta}}{\xi - \epsilon_q + \epsilon_d + U} + \frac{1 - \hat{n}_{d\bar\beta}}{\xi - \epsilon_q + \epsilon_d} \right) c_{d\uparrow}^\dagger c_{q\uparrow} c_{q\uparrow}^\dagger c_{d\uparrow}
\end{aligned} \tag{6.20}$$

The quantity ξ now represents the energy of the many-body eigenstate above the non-interacting state. We typically take that to be very small and ignore it w.r.t the bandwidth ϵ_q. This gives the ground state of the total Hamiltonian.

$$\Delta V_P = -\left(\frac{\hat{n}_{d\bar{\beta}}}{\epsilon_q - \epsilon_d - U} + \frac{1 - \hat{n}_{d\bar{\beta}}}{\epsilon_q - \epsilon_d}\right) c_{d\uparrow}^\dagger c_{q\uparrow} c_{q\uparrow}^\dagger c_{d\uparrow} \tag{6.21}$$

The URG calculation proceeds similarly with the ω replacing the E.

$$\Delta V_U = \left(\frac{\hat{n}_{d\bar{\beta}}}{\omega - \epsilon_q + \epsilon_d + U} + \frac{1 - \hat{n}_{d\bar{\beta}}}{\omega - \epsilon_q + \epsilon_d}\right) c_{d\uparrow}^\dagger c_{q\uparrow} c_{q\uparrow}^\dagger c_{d\uparrow} \tag{6.22}$$

Setting $\omega = 0$ gives us the lowest energy scale renormalization and reproduces the PMS result, while tuning the value of ω allows us to access high energy states as well. The η in URG can be written for PMS as well:

$$\eta_p = \frac{1}{E - \hat{\mathcal{H}}_0} V, \eta_p^\dagger = \frac{1}{E - \hat{\mathcal{H}}_0} V^\dagger \tag{6.23}$$

Here V destroys a high energy electron and $V^\dagger$ creates one.[3]

References

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