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1 Preliminaries

1.1 T -matrix and S -matrix

It is defined as

$$V\psi = T\phi \quad (1.1)$$

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

$$H_0\phi = E\phi \quad (1.2)$$

$$(H_0 + V)\psi = E\psi \quad (1.3)$$

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

$$\psi = \phi + G_0V\psi \quad (1.4)$$

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

$$\begin{aligned} \psi &= \phi + G_0T\phi \\ \implies \psi &= (1 + G_0T)\phi \end{aligned} \quad (1.5)$$

Eq. 1.4 can also be written as

$$\psi = (1 - G_0V)^{-1}\phi \quad (1.6)$$

Comparing the last two equations gives

$$\begin{aligned} 1 &= (1 - G_0V)(1 + G_0T) \\ \implies T &= V + VG_0T \end{aligned} \quad (1.7)$$

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

$$T = V + VG_0V + VG_0VG_0V + \dots \quad (1.8)$$

From scattering theory, we can write

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

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

$$f(k', k) \sim \langle k' | T | k \rangle \quad (1.10)$$

By definition, the S -matrix is

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

Also,

$$S = 1 - 2i\pi\rho T \quad (1.12)$$

Therefore,

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

1.2 An identity

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

$$HA = A(\lambda + H) \quad (1.14)$$

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

$$(E - H)A = AE - A(\lambda + H) = A(E - \lambda - H) \quad (1.15)$$

$$\implies A(E - \lambda - H)^{-1} = (E - H)^{-1}A \quad (1.16)$$

1.3 Landau's theory of Fermi liquid

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

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

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.

$$\Psi^* \xrightarrow{\text{turn interactions off}} \Phi \quad (1.18)$$

$$\Phi^* \xrightarrow{\text{turn interactions off}} \Psi \quad (1.19)$$

If some state Γ^* , instead of flowing into an ideal excited state, gets lost while the interactions are being turned off, then we aren't considering that system. All excited states must flow into some ideal state and vice-versa. This means that the interacting excited states can be labelled by the same good quantum numbers \vec{k} and σ . That is, if some eigenstate of the interacting system flows into the ideal eigenstate $\{n_{k\sigma}\}$, we can just as well use the distribution $\{n_{k\sigma}\}$ to label the interacting eigenstate. *The particle and hole excitations of the ideal system might flow into some very complicated state of the interacting system, which we call a quasiparticle(hole).* In other words, a system (ideal ground state + particle

of momentum k) goes to (interacting ground state + quasip of momentum k). If an interacting eigenstate corresponds to the state $\{n_{k\sigma}\}$, then $\{n_{k\sigma}\}$ is said to be the quasiparticle distribution function for that interacting state. Just as we denote eigenstates of the total ideal system using the collection of particles and holes, similarly we use the quasiparticle and quasiholes to describe eigenstates of the interacting system. Let $k_+ > k_F$ and $k_- < k_F$. Then,

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

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

$$(1.22)$$

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

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

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

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

$$\delta n_k = n_k - n_k^0 \quad (1.25)$$

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.

$$\mathcal{E}^0[n_k] = \sum_k n_k \epsilon_k \quad (1.26)$$

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

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

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

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

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

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

Then, up to first order,

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

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

$$\xi_k = \xi_k^0 + \sum_q \frac{\partial \xi_k}{\partial n_q} \delta n_q \quad (1.31)$$

Eq. 1.28 then becomes

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

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 ,

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

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

A temperature-dependent free energy can be concocted using

$$F[\delta n_k] = \delta \mathcal{E}[\delta n_k] - TS[\delta n_k] \quad (1.34)$$

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

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

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

$$\left. \frac{dF}{d\delta n_q} \right|_{\delta n_q = \langle \delta n_q \rangle} = 0 \quad (1.36)$$

1.4 The model

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

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 allow the up and down spins to fluctuate on the d-site, leading to zero average magnetization.
- $\Delta \gg U \gg \epsilon_d$: Hybridisation now fluctuates the up and down spins, leading to zero average magnetization.

1.5 Atomic limit ($t = 0$)

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

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

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

For a magnetic solution, we need

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

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

$$\epsilon_d > -U \quad (1.41)$$

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

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

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

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

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

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

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

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

Now,

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

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

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

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

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

Therefore,

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

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

$$\rho_d^0(E) = -\frac{1}{\pi} \text{Im} [G_f^0] = -\frac{1}{\pi} \lim_{\eta \rightarrow 0} \frac{1}{E - \epsilon_d + i\eta} = \delta(E - \epsilon_d) \quad (1.51)$$

$$\rho_d(E) = -\frac{1}{\pi} \text{Im} [G_f] = -\frac{1}{\pi} \lim_{\eta \rightarrow 0} \frac{1}{E - \epsilon_d + i(\eta + \Delta)} = \frac{1}{\pi} \frac{\Delta}{(E - \epsilon_d)^2 + \Delta^2} \quad (1.52)$$

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:

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

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

T -matrix is defined by

$$T = V + VGT \quad (1.54)$$

We also have

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

The conduction electron Green's function can be calculated as

$$\begin{aligned} G_c(k, k', E) &= \delta_{k,k'} G_c^0(k, E) + G_c^0(k) t G_f^0 t G_c^0(k') + \\ &G_c^0(k) t G_f^0 t \sum_q G_c^0(q) t G_f^0 t G_c^0(k') + \dots \end{aligned} \quad (1.56)$$

Noting that

$$t \sum_q G_c^0(q) t = \Sigma_c, \quad (1.57)$$

we have

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

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

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

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

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

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

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

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

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

Comparing with eq. 1.59, we can write

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

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,

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

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

A quantum dot is a set of electrons that are localised in a sufficiently small region so that their spectrum is quantised. The localization means that double occupation will come at a cost of U .

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

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.

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

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

$$\Delta E = UN + \epsilon_N - eV \quad (1.67)$$

Tuning the voltage can make these two levels degenerate.

$$eV^* = UN + \epsilon_N \quad (1.68)$$

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,

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

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

1.7 Total Hamiltonian: Mean field treatment

$$n_{d\uparrow}n_{d\downarrow} \approx n_{d\uparrow}\langle n_{d\downarrow} \rangle + n_{d\downarrow}\langle n_{d\uparrow} \rangle + \text{constant} \quad (1.70)$$

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

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

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

An alternative way of writing that is

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

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

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

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

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

we get

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

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,

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

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

$$1 = U_c \rho_d(E=0) \quad (1.78)$$

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

$$U_c = \pi \Delta \quad (1.79)$$

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

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

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

$$\epsilon_{d\sigma} = \epsilon_d + U \langle n_{d\sigma} \rangle = \epsilon_d + \frac{U}{2} \pm \frac{U}{2} m = \pm \frac{U}{2} m \quad (1.82)$$

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

We get two Lorentzian peaks at $E = \pm \frac{U m}{2}$, 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 $T \rightarrow 0$. Thus, the singlet phase shift at ϵ_F approaches $\frac{\pi}{2}$ as $T \rightarrow 0$.

1.9 Derivation of the Kondo Hamiltonian:

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

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

$$H = H_0 + V = \begin{matrix} & \text{low} & \text{high} \\ \text{low} & \begin{pmatrix} H^L & v^\dagger \end{pmatrix} \\ \text{high} & \begin{pmatrix} v & H^H \end{pmatrix} \end{matrix} \quad (1.85)$$

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

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

$$\bar{H} = e^{-S} H e^S = H_0 + (V + [H_0, S]) + \frac{1}{2} ([V, S] + [[H_0, S], S]) \quad (1.87)$$

Defining S such that the first order term vanishes,

$$V = [S, H_0] \quad (1.88)$$

$$\bar{H} = H_0 + \frac{1}{2} [V, S] \quad (1.89)$$

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

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

Comparing with the definition of V , we can write

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

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

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

$$[V, S] = \begin{pmatrix} 0 & v^\dagger \\ v & 0 \end{pmatrix} \begin{pmatrix} 0 & -s^\dagger \\ s & 0 \end{pmatrix} - \begin{pmatrix} 0 & -s^\dagger \\ s & 0 \end{pmatrix} \begin{pmatrix} 0 & v^\dagger \\ v & 0 \end{pmatrix} = \begin{pmatrix} v^\dagger s + s^\dagger v & 0 \\ 0 & -v s^\dagger - s v^\dagger \end{pmatrix} \quad (1.93)$$

Hence,

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

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

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

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

$$\begin{aligned} \Delta H &= \frac{1}{2}(v^\dagger s + s^\dagger v) = \frac{1}{2} \left(v^\dagger \sum_{HL} s_{HL} |H\rangle \langle L| + \text{h.c.} \right) \\ &= \frac{1}{2} \sum_{HL} \left[v^\dagger |H\rangle \langle L| \frac{v_{HL}}{E_L - E_H} + |L\rangle \langle H| \frac{v_{LH}^\dagger}{E_L - E_H} v \right] \end{aligned} \quad (1.96)$$

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

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

This can also be written as

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

where

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

$T(E)$, 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

$$\begin{aligned} \Delta H_{ll'} &= \sum_H v_{lH}^\dagger v_{Hl'} \frac{1}{E_L - E_H} \\ \Rightarrow \Delta H &= V \left(\sum_H \frac{1}{\Delta_{LH}} |H\rangle \langle H| \right) V \end{aligned} \quad (1.100)$$

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,

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

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,

$$\begin{aligned} \Delta H &= V \frac{|0\rangle \langle 0|}{\epsilon_d} V - V \frac{|\uparrow\downarrow\rangle \langle \uparrow\downarrow|}{\epsilon_d + U} V \\ &= \sum_{k_1, k_2, \sigma_1, \sigma_2} V(k_1) V^*(k_2) \left[\frac{c_{d\sigma_2}^\dagger c_{k_2\sigma_2} |0\rangle \langle 0| c_{k_1\sigma_1}^\dagger c_{d\sigma_1}}{\epsilon_d} - \frac{c_{k_1\sigma_1}^\dagger c_{d\sigma_1} |\uparrow\downarrow\rangle \langle \uparrow\downarrow| c_{d\sigma_2}^\dagger c_{k_2\sigma_2}}{\epsilon_d + U} \right] \\ &= \sum_{k_1, k_2, \sigma_1, \sigma_2} V(k_1) V^*(k_2) \frac{c_{d\sigma_2}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_1} |d\sigma_1, h_{k_1\sigma_1}\rangle \langle d\sigma_1, h_{k_1\sigma_1}|}{\epsilon_d} \\ &\quad - \sum_{k_1, k_2, \sigma_1, \sigma_2} V(k_1) V^*(k_2) \frac{c_{k_1\sigma_1}^\dagger c_{d\sigma_1} c_{d\sigma_2}^\dagger c_{k_2\sigma_2} |d\bar{\sigma}_2, e_{k_2\sigma_2}\rangle \langle d\bar{\sigma}_2, e_{k_2\sigma_2}|}{\epsilon_d + U} \\ &= \sum_{k_1, k_2, \sigma_1, \sigma_2} V(k_1) V^*(k_2) \left[\frac{c_{d\sigma_2}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_1}}{\epsilon_d} - \frac{c_{k_1\sigma_1}^\dagger c_{d\sigma_1} c_{d\sigma_2}^\dagger c_{k_2\sigma_2}}{\epsilon_d + U} \right] P_{n_d=1} \end{aligned} \quad (1.102)$$

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

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

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 $n_d = 1$.

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

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

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

Similarly,

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

Finally, putting all this together,

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

where

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

Assuming $V(k) \equiv t$,

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

where

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

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

1.10 Obtaining the resistivity minimum and log-dependence

The model we are working with is

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

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

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

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

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

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

$$T = V + VG_0V \quad (1.115)$$

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

1.10.1 First order scattering

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

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

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

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

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

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

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

For spin-flip, the matrix element is

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

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

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

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

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

1.10.2 Second order scattering

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

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

The second order transition matrix contribution is of the form

$$T_{i \rightarrow j}^{(2)} = \langle j | V G_0 V | i \rangle = \sum_l \frac{\langle j | V | l \rangle \langle l | V | i \rangle}{E_i - E_l} \quad (1.122)$$

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:

$$\begin{aligned} T_{11}^{(2)} &= \sum_q \frac{\langle k'_{\uparrow} d_{\sigma} | V | q_{\uparrow} d_{\sigma} \rangle \langle q_{\uparrow} d_{\sigma} | V | k_{\uparrow} d_{\sigma} \rangle}{\epsilon_k - \epsilon_q} \\ &= (Jm_d)^2 \sum_q \frac{1 - P(q)}{\epsilon_k - \epsilon_q} = J^2 m_d^2 \sum_q \frac{1 - P(q)}{\epsilon_k - \epsilon_q} \end{aligned} \quad (1.123)$$

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,

$$T_{12}^{(2)} = \sum_q \frac{\langle q_{\uparrow} k'_{\uparrow} d_{\sigma} | V | k'_{\uparrow} k_{\uparrow} d_{\sigma} \rangle \langle k'_{\uparrow} k_{\uparrow} d_{\sigma} | V | q_{\uparrow} k_{\uparrow} d_{\sigma} \rangle}{\epsilon_q - \epsilon_{k'}} P(q) \quad (1.124)$$

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

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

For the third process,

$$T_{13}^{(2)} = \sum_q \frac{\langle k'_{\uparrow} d_{\downarrow} | V | q_{\downarrow} d_{\uparrow} \rangle \langle q_{\downarrow} d_{\uparrow} | V | k_{\uparrow} d_{\downarrow} \rangle}{\epsilon_k - \epsilon_q} \quad (1.126)$$

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

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

For the fourth process,

$$\begin{aligned}
T_{14}^{(2)} &= \sum_q \frac{\langle q_{\downarrow} k'_{\uparrow} d_{\uparrow} | V | k'_{\uparrow} k_{\uparrow} d_{\downarrow} \rangle \langle k'_{\uparrow} k_{\uparrow} d_{\downarrow} | V | q_{\downarrow} k_{\uparrow} d_{\uparrow} \rangle}{\epsilon_q - \epsilon'_k} \\
&= -\lambda_-^2 J^2 \sum_q \frac{P(q)}{\epsilon_q - \epsilon_k} \\
&= \lambda_-^2 J^2 \sum_q \frac{P(q)}{\epsilon_k - \epsilon_q}
\end{aligned} \tag{1.128}$$

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

$$\begin{aligned}
T_{\text{nonflip}}^{(2)} &= \sum_{i=1}^4 T_{1i}^{(2)} = J^2 \sum_q \frac{m_d^2 + \lambda_+^2 - P(q) (\lambda_+^2 - \lambda_-^2)}{\epsilon_k - \epsilon_q} \\
&= J^2 \sum_q \frac{s(s+1) - m_d + 2m_d P(q)}{\epsilon_k - \epsilon_q} \\
&= J^2 [s(s+1) - m_d] (\alpha + \gamma) + 2J^2 m_d \gamma
\end{aligned} \tag{1.129}$$

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

$$\begin{aligned}
T_{\text{nonflip}}^{(2)} &= 2J^2 m_d \gamma \\
&= 2J^2 m_d \int d\epsilon N(\epsilon) \frac{P(\epsilon)}{\epsilon_k - \epsilon} = \frac{\sqrt{2} J^2 m_d m^{\frac{3}{2}}}{\pi^2 \hbar^3} \int d\epsilon \frac{\sqrt{\epsilon} P(\epsilon)}{\epsilon_k - \epsilon}
\end{aligned} \tag{1.130}$$

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

$$\begin{aligned}
T_{\text{nonflip}}^{(2)} &= \frac{\sqrt{2} J^2 m_d m^{\frac{3}{2}}}{\pi^2 \hbar^3} \sqrt{\epsilon_k} \ln \left| \frac{\sqrt{\epsilon_k} + \sqrt{\epsilon_F}}{\sqrt{\epsilon_k} - \sqrt{\epsilon_F}} \right| \\
&= \frac{\sqrt{2} J^2 m_d m^{\frac{3}{2}}}{\pi^2 \hbar^3} \sqrt{\epsilon_k} \ln \left| \frac{\epsilon_k + \epsilon_F + 2\sqrt{\epsilon_k \epsilon_F}}{\epsilon_k - \epsilon_F} \right|
\end{aligned} \tag{1.131}$$

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

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

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

$$\begin{aligned} T_{21}^{(2)} &= -J^2(m_d + 1)\lambda_+ \sum_q \frac{1 - P_q}{\epsilon_k - \epsilon_q} \\ T_{23}^{(2)} &= J^2m_d\lambda_+ \sum_q \frac{1 - P_q}{\epsilon_k - \epsilon_q} \\ T_{22}^{(2)} &= J^2(m_d + 1)\lambda_+ \sum_q \frac{P(q)}{\epsilon_k - \epsilon_q} \\ T_{24}^{(2)} &= -\lambda_+m_dJ^2 \sum_q \frac{P(q)}{\epsilon_k - \epsilon_q} \end{aligned} \quad (1.135)$$

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

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

$$\begin{aligned} T_{\text{flip}}^{(2)} &= 2J^2\lambda_+ \sum_q \frac{P(q)}{\epsilon_k - \epsilon_q} \\ &= 2J^2\lambda_+ N(\epsilon_F) \ln \left| \frac{T_F}{T} \right| \end{aligned} \quad (1.137)$$

Adding the first order contribution,

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

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

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

1.11 The Kondo resonance

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

$$T_{a \rightarrow b} = \sum_{s, m_s} |\langle s, m_s | a \rangle|^2 T_s \quad (1.140)$$

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

$$T_{|k\uparrow, d_\uparrow\rangle \rightarrow |k'\uparrow d_\uparrow\rangle} = T_1 \quad (1.141)$$

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

$$T_{|k\uparrow, d_\downarrow\rangle \rightarrow |k'\uparrow d_\downarrow\rangle} = \frac{T_1 + T_0}{2} \quad (1.142)$$

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

$$T_{|k\uparrow, d_\downarrow\rangle \rightarrow |k'\downarrow d_\uparrow\rangle} = \frac{T_1 - T_0}{2} \quad (1.143)$$

Therefore,

$$\begin{aligned} T_1 &= T_{|k\uparrow, d_\downarrow\rangle \rightarrow |k'\uparrow d_\downarrow\rangle} + T_{|k\uparrow, d_\downarrow\rangle \rightarrow |k'\downarrow d_\uparrow\rangle} = T_{\text{nonflip}} + T_{\text{flip}} \\ T_0 &= T_{|k\uparrow, d_\downarrow\rangle \rightarrow |k'\uparrow d_\downarrow\rangle} - T_{|k\uparrow, d_\downarrow\rangle \rightarrow |k'\downarrow d_\uparrow\rangle} = T_{\text{nonflip}} - T_{\text{flip}} \end{aligned} \quad (1.144)$$

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

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

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

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

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

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

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

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

$$T = V(1 + TG) \quad (1.149)$$

For the singlet and triplet T -matrices, it becomes

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

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

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

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

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

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

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

$$|T_s| \leq \frac{1}{\pi N_0} \quad (1.154)$$

From eq. 1.13, we can write

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

Eq. 1.60 allows us to write

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

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,

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

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

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

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

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

$$\begin{aligned} T_1 &= \frac{1}{\frac{2}{J_{\text{eff}}} - (\alpha + \gamma)} \\ T_0 &= \frac{-1}{\frac{2}{3J_{\text{eff}}} + \alpha + \gamma} \end{aligned} \quad (1.160)$$

$\alpha + \gamma$ can be calculated as

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

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

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

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

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

Since

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

we can write

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

Similarly,

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

giving

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

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

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

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,

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

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 $E = 0$:

$$\Sigma(E) = \Sigma(0) + E \left. \frac{d\Sigma}{dE} \right|_{E=0} + O(E^2) \quad (1.170)$$

Defining

$$Z^{-1} \equiv 1 - \left. \frac{d\Sigma}{dE} \right|_{E=0} \quad (1.171)$$

we can write

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

The interacting Green's function for the impurity becomes

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

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

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

Defining the renormalised parameters

$$\epsilon_d^* = Z(\epsilon_d + \Sigma(0)) \quad (1.175)$$

$$\Delta^* = Z\Delta \quad (1.176)$$

we have

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

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

$$Z = 1, \Sigma = 0 \implies \epsilon_d^* = \epsilon_d, \Delta^* = \Delta \quad (1.178)$$

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:

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

Similarly, the renormalised version of eq. 1.52 is

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

Using eq. 1.179 gives

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

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,

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

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

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

Hence the total wavefunction of singlet+Fermi-sea is

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

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

$$a_q = \langle \Phi | \langle S_q | \sum_k a_k |S_k\rangle | \Phi \rangle = \langle \Phi | b_q | \Psi \rangle \quad (1.185)$$

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

$$\begin{aligned}
E|\Psi\rangle &= H_K|\Psi\rangle = |\Phi\rangle \otimes H_k \sum_{k>k_F} a_k |S_k\rangle \\
&= |\Phi\rangle \otimes \sum_{k>k_F} a_k \left(\epsilon_k |S_k\rangle - \frac{3J}{2} \sum_{k'>k_F} |S_{k'}\rangle \right) \\
&= \sum_{k>k_F} a_k \left(\epsilon_k b_k^\dagger - \frac{3J}{2} \sum_{k'>k_F} b_{k'}^\dagger \right) |\Phi\rangle
\end{aligned} \tag{1.186}$$

Multiplying b_q from left gives

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

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

$$\begin{aligned}
E\langle\Phi|b_q|\Psi\rangle &= Ea_q = a_q \epsilon_q - \frac{3J}{2} \sum_k a_k \\
\implies a_q &= \frac{3J/2}{\epsilon_q - E} \sum_k a_k \\
\implies \sum_q a_q &= \sum_q \frac{3J/2}{\epsilon_q - E} \sum_k a_k
\end{aligned} \tag{1.188}$$

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

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

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

$$\begin{aligned}
\frac{2}{3JN(0)} &= \ln \left| \frac{D - E}{\epsilon_F - E} \right| \approx \ln \left| \frac{D}{\epsilon_F - E} \right| \\
\implies E &= \epsilon_F - D e^{-\frac{2}{3N(0)J}}
\end{aligned} \tag{1.191}$$

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

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

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

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

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

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

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

$$k \uparrow, d \downarrow \rightarrow q \downarrow, d \uparrow \rightarrow k' \uparrow, d \downarrow \quad (1.196)$$

The T -matrix term is

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

Using eq. 1.16, we can write

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

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

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

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

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

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

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

N is the density of states. Also,

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

Putting it all together,

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

For the second possible scattering,

$$q \downarrow k \uparrow d \uparrow \rightarrow k' \uparrow k \uparrow d \downarrow \rightarrow k' \uparrow q \downarrow d \uparrow \quad (1.204)$$

we get

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

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

$$\begin{aligned} T_2 &= J_T^2 \left(\frac{1}{2} + S_d^z \right) N|\delta D| c_{k\uparrow} c_{k'\uparrow}^\dagger \frac{1}{E - D - \epsilon_{k'}} \\ &= -J_T^2 \left(\frac{1}{2} + S_d^z \right) N|\delta D| c_{k'\uparrow}^\dagger c_{k\uparrow} \frac{1}{E - D - \epsilon_{k'}} \end{aligned} \quad (1.206)$$

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 :

$$k \downarrow, d \uparrow \rightarrow q \uparrow d \downarrow \rightarrow k' \downarrow d \uparrow \quad (1.207)$$

$$q \uparrow k \downarrow d \downarrow \rightarrow k' \downarrow k \downarrow d \uparrow \rightarrow k' \downarrow q \uparrow d \downarrow \quad (1.208)$$

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

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

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

The total second order contribution is

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

Comparing this with the S_d^z term in the Hamiltonian

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

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

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

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

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

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

1.14.2 Renormalization of J_T

Consider the scattering

$$k \uparrow d \downarrow \rightarrow q \downarrow d \uparrow \rightarrow k' \downarrow d \uparrow \quad (1.215)$$

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

The minus sign at the front comes from the term

$$-S_d^z c_{k'\downarrow}^\dagger c_{q\downarrow} \quad (1.217)$$

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

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

The second process is

$$q \uparrow k \uparrow d \downarrow \rightarrow k' \downarrow k \uparrow d \uparrow \rightarrow q \uparrow k' \downarrow d \uparrow \quad (1.219)$$

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

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

$$+S_d^z c_{k'\uparrow}^\dagger c_{q\uparrow} \quad (1.221)$$

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

$$-S_d^z c_{k'\downarrow}^\dagger c_{q\downarrow} \quad (1.222)$$

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 process.

$$T_3 = T_1 \quad (1.223)$$

$$T_4 = T_2 \quad (1.224)$$

The total contribution is

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

Comparing with the S_d^+ term in the Hamiltonian

$$J_T S_d^+ c_{k'\downarrow}^\dagger c_{k\uparrow} \quad (1.226)$$

we can write

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

Again neglecting the terms in the denominator, we get

$$\frac{dJ_T}{dD} = -J_T J_z N \frac{2}{D} \quad (1.228)$$

This is the scaling equation for J_T .

1.14.3 Flow of the couplings

Switching to the dimensionless couplings

$$g_1 = NJ_z, g_2 = NJ_T \quad (1.229)$$

the equations become

$$\frac{dg_1}{dD} = -\frac{2g_2^2}{D} \quad (1.230)$$

$$\frac{dg_2}{dD} = -\frac{2g_1g_2}{D} \quad (1.231)$$

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

$$\frac{dg_1}{dg_2} = \frac{g_2}{g_1} \implies g_1^2 - g_2^2 = \text{constant} \quad (1.232)$$

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 $g_2 \rightarrow -g_2$, analyzing the upper half ($g_2 > 0$) suffices. The antiferromagnetic case is easy. $g_1 > 0$ means g_1 will always increase the RG flow. The only solution is that both g_1 and g_2 flow to infinity. For the ferromagnetic case, if $|g_1| > g_2$, g_1 will increase and the representative point will reach the x-axis ($g_2 = 0$). At this point, both the couplings will stop changing because both the derivatives involve g_2 . So the fixed point in this case is $g_2 = 0$ and g_1 is some negative value. However, if $|g_1| < g_2$, the representative point will reach the positive y-axis. Since $g_2 \neq 0$ here, g_1 will continue to grow and become positive at some point. From there, it becomes the antiferromagnetic case.

Setting $g_1 = g_2 = g > 0$ and integrating either of the scaling equations gives

$$\begin{aligned} g(D') &= \frac{g_0}{1 - 2g_0 \ln \frac{D}{D'}} \\ \implies 2g(D') &= \frac{1}{\ln \frac{D'}{T_K}} \end{aligned} \quad (1.233)$$

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.

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

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

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

where the transition matrix T is

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

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

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

The first process is

$$k\alpha \xrightarrow{\sigma^b} q\lambda \xrightarrow{\sigma^a} k'\beta \quad (1.238)$$

$$d\sigma \xrightarrow{S_d^b} d\sigma'' \xrightarrow{S_d^a} d\sigma' \quad (1.239)$$

The transition matrix element is

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

The second process is

$$k\alpha \longrightarrow k\alpha \xrightarrow{\sigma^a} q\lambda \quad (1.241)$$

$$q\lambda \xrightarrow{\sigma^b} k'\beta \longrightarrow k'\beta \quad (1.242)$$

$$d\sigma \xrightarrow{S_d^b} d\sigma'' \xrightarrow{S_d^a} d\sigma' \quad (1.243)$$

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

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

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

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

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

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

Therefore,

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

The correction to the coupling J can be read off:

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

This gives the same scaling equations we found earlier.

1.15 Universality

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

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

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

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

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

$$\begin{aligned} \ln \frac{k_B T_K}{D} &= - \int_{g_0}^1 \frac{dg}{2g^2} (1+g) = -\frac{1}{2g_0} + \frac{1}{2} \ln g_0 + O(1) \\ &= -\frac{1}{2g_0} + \frac{1}{2} \ln 2g_0 + O(1) \end{aligned} \quad (1.251)$$

This gives a better estimate of the Kondo temperature

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

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

$$k_B T_K = D y(g) \quad (1.253)$$

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

$$\frac{dT_K}{dD} = 0 \quad (1.254)$$

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

$$\begin{aligned} y(g) + D \frac{dy(g)}{dD} &= 0 \\ \implies y + D \frac{dy}{dg} \frac{dg}{dD} &= 0 \\ \implies y - 2g^2 \frac{dy}{dg} &= 0 \\ \implies y &= e^{-\frac{1}{2g}} \end{aligned} \quad (1.255)$$

This gives almost the same solution as eq. 1.252:

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

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

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

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

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

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. For example,

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

Similarly,

$$\begin{aligned} S^x &= \frac{1}{2} (c_\uparrow^\dagger c_\downarrow + c_\downarrow^\dagger c_\uparrow) \\ S^y &= \frac{-i}{2} (c_\uparrow^\dagger c_\downarrow - c_\downarrow^\dagger c_\uparrow) \end{aligned} \quad (1.260)$$

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

$$|\uparrow\rangle = c_\uparrow^\dagger |0\rangle \quad (1.261)$$

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

$$\mu = -i \frac{\pi}{2} k_B T \quad (1.262)$$

The new Hamiltonian is

$$\tilde{H} = H - \mu(n_d - 1) \quad (1.263)$$

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

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

The modified partition function is

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

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

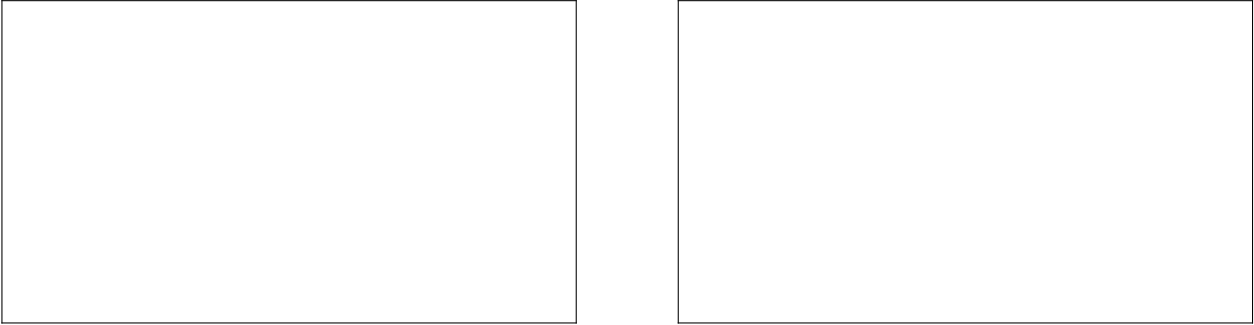
$$Z \Big|_{n_d=0} = Z \Big|_{n_d=0} \quad (1.266)$$

Hence,

$$\tilde{Z} = Z \quad (1.267)$$

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

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

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

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

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,

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

The second diagram gives

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

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

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

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

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

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

$$C_V = \gamma T \quad (1.278)$$

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

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

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,

$$\frac{|0_\uparrow, d_\downarrow\rangle - |0_\downarrow, d_\uparrow\rangle}{\sqrt{2}} \quad (1.280)$$

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

$$E_1 = -\frac{3}{2}J + \frac{3}{2}J = 0 \quad (1.281)$$

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

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

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.

$$n = \sum_{\sigma} \frac{\delta}{\pi} \implies 1 = \frac{2\delta}{\pi} \implies \delta = \frac{\pi}{2} \quad (1.283)$$

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 $\Delta r = a$:

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

where the formula for k_F was used.

In a Fermi gas, the energy levels are separated by

$$\Delta\epsilon = \frac{\partial\epsilon}{\partial k} \Delta k \quad (1.285)$$

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

$$\Delta\epsilon = \frac{\partial\epsilon}{\partial k} \frac{\pi}{L} \quad (1.286)$$

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

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

The energy becomes

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

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

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

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 ,

$$\begin{aligned} \tilde{\epsilon}_p = & \underbrace{\epsilon_F}_{\text{Fermi gas}} + \underbrace{\frac{p_F^*}{m} (p - p_F)}_{\text{linear contribution for } p \text{ close to } p_F} \\ & + \underbrace{\sum_{q\sigma} f(p, q) (n_q - n_q^0)}_{\text{interacting between two quasiparticles at momenta } p \text{ and } q} \end{aligned} \quad (1.290)$$

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

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

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

$$\alpha = \frac{d\delta_\sigma}{dE} \quad (1.292)$$

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

$$\delta_\sigma(\tilde{\epsilon}, \{n_{q,\sigma}\}) = \delta_\sigma(\tilde{\epsilon} = \epsilon_F, n_k = n_k^0) + \alpha (\tilde{\epsilon} - \epsilon_F) + \Phi \sum_q \delta n_{q,-\sigma} \quad (1.293)$$

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,

$$\delta_\uparrow^0 = \frac{\pi}{2} + \Phi \sum_q \delta n_{q\downarrow}^0 \quad (1.294)$$

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

$$\delta_\uparrow^0 = \frac{\pi}{2} \quad (1.295)$$

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

$$N(\mu = 0) = N^0 \quad (1.296)$$

$$N(E' = E + \mu) = N(E' = E) + \frac{dN}{dE'} (E' - E) = N^0 + \rho\Delta\mu \quad (1.297)$$

$$\implies \sum_q \delta n_q = N - N^0 = \rho\Delta\mu \quad (1.298)$$

Hence, from eq. 1.293,

$$\begin{aligned} \delta_\uparrow &= \frac{\pi}{2} + \alpha(\epsilon'_F - \epsilon_F) + \Phi \sum_q \delta n_{q\downarrow} \\ &= \delta_\uparrow^0 + \alpha\Delta\mu + \Phi\rho\Delta\mu \end{aligned} \quad (1.299)$$

Hence the change in the phase is

$$0 = \Delta\delta_\uparrow = \Delta\mu(\alpha + \Phi\rho) \implies \alpha = -\Phi\rho \quad (1.300)$$

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

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

Hence,

$$\begin{aligned} \rho &= \frac{dn_\sigma}{dE} = \rho^0 + \frac{1}{\pi} \frac{d\delta_\sigma}{dE} \\ \implies \rho &= \rho^0 + \frac{1}{\pi} \alpha \end{aligned} \quad (1.302)$$

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

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

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

$$\begin{aligned} C_v &= \frac{\pi^2 k_B^2}{3} (\rho_\uparrow + \rho_\downarrow) T \\ &= \frac{2\alpha}{\pi} \frac{\pi^2 k_B^2}{3} T \end{aligned} \quad (1.304)$$

In presence of a magnetic field B , the magnetization is

$$m = \delta n \times \mu \quad (1.305)$$

where μ is the magnetic moment

$$\mu = -\frac{g}{2}\mu_B \quad (1.306)$$

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

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

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

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

Hence,

$$\sum_k \delta n_{k\sigma} = N_\sigma(E_\sigma^B) - N(E) = \frac{dN}{dE^B} (E^B - E) = -\rho \frac{g\mu_B}{2} \sigma B \quad (1.309)$$

This modifies the phase shift at the Fermi surface,

$$\begin{aligned} \delta_\sigma(\epsilon_F) &= \frac{\pi}{2} + \alpha \left(\epsilon_F - \frac{g\mu_B}{2} \sigma B - \epsilon_F \right) + \Phi \sum_q \delta n_{q,-\sigma} \\ &= \frac{\pi}{2} - \sigma \frac{g\mu_B}{2} \alpha B + \Phi \rho \frac{g\mu_B}{2} \sigma B \\ &= \frac{\pi}{2} - 2\alpha \frac{g\mu_B}{2} \sigma B \end{aligned} \quad (1.310)$$

Hence,

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

The susceptibility is

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

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

$$\mu = -\frac{g}{2}\mu_B \quad (1.313)$$

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

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

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

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

The magnetic susceptibility comes out to be

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

The Wilson ratio R can now be computed,

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

1.18 Numerical renormalization group calculation

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

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

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

$$|1\rangle = (\lambda_1 H_c |0\rangle + \lambda_2 |0\rangle) \quad (1.319)$$

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:

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

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

$$\lambda = -\langle 0|H_c|0\rangle \quad (1.321)$$

Therefore,

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

The general state can be shown to be

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

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

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

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

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

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

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

Taking the complex conjugate of this gives

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

Defining

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

we can write

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

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

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

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

$$d_n = \Lambda^{-n} (1 - \Lambda^{-1}) \quad (1.331)$$

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

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

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

$$a_{m,n}^\dagger = \sum_k \psi_m(k) c_k^\dagger \quad (1.333)$$

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

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

$$b_{m,n}^\dagger = \sum_k \phi_m(k) c_k^\dagger \quad (1.335)$$

Then,

$$a_{m,n}^\dagger + b_{m,n}^\dagger = \frac{2}{\sqrt{d_n}} \sum_{\pm k \in []} \cos\left(\frac{2\pi m k}{d_n}\right) c_k^\dagger \quad (1.336)$$

Summing over n involves summing over all momenta.

$$\begin{aligned} \sum_n (a_{m,n}^\dagger + b_{m,n}^\dagger) &= \frac{2}{\sqrt{d_n}} \sum_k \cos\left(\frac{2\pi m k}{d_n}\right) c_k^\dagger \\ \Rightarrow \sum_n (a_{0,n}^\dagger + b_{0,n}^\dagger) &= \frac{2}{\sqrt{d_n}} \sum_k c_k^\dagger \end{aligned} \quad (1.337)$$

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

$$\sum_{k,q} c_k^\dagger c_q = \sum_k c_k^\dagger \sum_q c_q \quad (1.338)$$

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

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

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

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

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

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

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

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

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

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

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

$$H = \lim_{N \rightarrow \infty} H_N = \lim_{N \rightarrow \infty} D' \Lambda^{\frac{1-N}{2}} \overline{H}_N \quad (1.344)$$

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

$$\overline{H}_N = \sum_m E_m |m\rangle \langle m| \quad (1.345)$$

The next Hamiltonian is then

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

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 are found to represent interacting Fermi liquids. The effective Hamiltonian can be shown to resemble the Anderson model, but with modified parameters,

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

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

Under mean-field,

$$\begin{aligned} n_{d\uparrow} n_{d\downarrow} &\approx n_{d\uparrow} \langle n_{d\downarrow} \rangle + \langle n_{d\uparrow} \rangle n_{d\downarrow} - \langle n_{d\uparrow} \rangle \langle n_{d\downarrow} \rangle \\ \implies \langle n_{d\uparrow} n_{d\downarrow} \rangle &= \langle n_{d\uparrow} \rangle \langle n_{d\downarrow} \rangle \\ &= \sum_{k,q} \langle n_{k\sigma} \rangle \langle n_{q,-\sigma} \rangle \end{aligned} \quad (1.348)$$

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:

$$\langle n_q^> \rangle = \langle \psi^> | c_k^\dagger c_k | \psi^> \rangle = n_k^p \quad (1.349)$$

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

$$\langle n_q^< \rangle = \langle \psi^< | c_k^\dagger c_k | \psi^< \rangle = -\langle \psi^< | c_k c_k^\dagger | \psi^< \rangle = -n_k^h \quad (1.350)$$

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

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

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

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

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

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

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

1.19.2 Calculation of C_v

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

$$\frac{d\langle E \rangle}{dT} = \sum_{k,\sigma} \epsilon_{k\sigma} \frac{d\langle \delta n_{k\sigma} \rangle}{dT} \quad (1.354)$$

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

$$\begin{aligned} \langle \delta n_{k\sigma} \rangle(T) &= \frac{1}{e^{\beta\epsilon_{k\sigma}} + 1} \\ \Rightarrow \frac{d\langle \delta n_{k\sigma} \rangle}{dT} &= \frac{e^{\beta\epsilon_{k\sigma}}}{(e^{\beta\epsilon_{k\sigma}} + 1)^2} \left[\frac{1}{k_B T^2} \epsilon_{k\sigma} - \frac{1}{k_B T} (2\epsilon_{k\sigma} - \epsilon_k) \frac{d\langle \delta n_{k\sigma} \rangle}{dT} \right] \end{aligned} \quad (1.355)$$

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

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

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

$$\begin{aligned}
\frac{d\langle E \rangle}{dT} &= \frac{1}{k_B T^2} \sum_{\sigma} \rho_{\sigma}(0) \int_{-\infty}^{\infty} d\epsilon_{\sigma} \epsilon_{\sigma}^2 \frac{e^{\beta\epsilon_{k\sigma}}}{(e^{\beta\epsilon_{k\sigma}}+1)^2} \\
&= -\frac{1}{T} \sum_{\sigma} \rho_{\sigma}(0) \int_{-\infty}^{\infty} d\epsilon_{\sigma} \epsilon_{\sigma}^2 f'(\epsilon_{\sigma}) \\
&= -\frac{1}{T} \sum_{\sigma} \rho_{\sigma}(0) \int_1^0 df \epsilon_{\sigma}^2
\end{aligned} \tag{1.357}$$

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

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

Therefore,

$$\frac{d\langle E \rangle}{dT} = -k_B^2 T \sum_{\sigma} \rho_{\sigma}(0) \int_1^0 df [\ln(f^{-1} - 1)]^2 \tag{1.359}$$

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

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

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 , $\epsilon_{k\sigma} \rightarrow \epsilon_{k\sigma} + \sigma h$. where $h = \frac{1}{2}gB\mu_B$. The magnetisation is

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

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

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

The susceptibility is

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

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

The Wilson ratio is

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

1.19.4 Relation between the density of states and scattering phase shift

The Green's function is of the general form

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

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:

$$\begin{aligned} \Sigma(\omega) &= \Sigma(0, 0) + \omega \Sigma'(0) + O(i\omega^2) \\ &\equiv \Sigma(0) + (1 - Z^{-1}) \omega \end{aligned} \quad (1.369)$$

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

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

The density of states at the Fermi surface is given by

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

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

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

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

$$G = G_0 + G_0 T G_0 \quad (1.373)$$

we can write

$$T = V^2 G_d \quad (1.374)$$

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

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

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

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

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

$$\begin{aligned} \delta(\omega) &= \tan^{-1} \frac{\Delta^*}{\omega - \epsilon_d^*} \\ \implies \epsilon_d^* &= -\Delta^* \cot \delta(0) \end{aligned} \quad (1.377)$$

Substituting this in the density of states expression gives

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

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

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

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

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

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

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

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 Δn_\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 rule¹, we can relate the phase shift $\delta(0)$ due to scattering (at the Fermi surface) off a local impurity to the number of electrons bound in the potential well produced by that impurity:

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

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 write²

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

¹JS Langer and V Ambegaokar. Friedel sum rule for a system of interacting electrons

²Mukherjee and Lal-Holographic unitary renormalization group for correlated electrons - I: A tensor network approach-
<https://doi.org/10.1016/j.nuclphysb.2020.115170>

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

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

From the work of Seki and Yunoki³, we know that this quantity is essentially the winding number of the curve $\Gamma(D)$ in the complex plane spanned by the real and imaginary parts of D , and is equal to the change in Luttinger's volume V_L at $T = 0$.

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

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

$$\begin{aligned}
\tilde{N} &= \frac{1}{\pi} \sum_{\sigma} \delta_{\sigma}(0) \\
\implies \delta(0) &= \frac{\pi}{2} \tilde{N} = -\frac{\pi}{2} \Delta V_L
\end{aligned} \tag{1.389}$$

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

³Topological interpretation of the luttinger theorem. Physical Review B, 96(8):085124, 2017

1.20 Microscopic approach

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

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

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

$$\gamma_{\text{imp}} = \frac{2\pi k_B^2}{3} \frac{\tilde{\Delta}}{\tilde{\epsilon}_d^2 + \tilde{\Delta}^2} \quad (1.392)$$

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

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

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

where

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

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

1.21 Renormalized perturbation theory

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

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

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

Including the self energy gives

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

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

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

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

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

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

$$\tilde{G}_d = \frac{1}{E - \tilde{\epsilon}_d + i\tilde{\Delta}} \quad (1.401)$$

The Anderson hamiltonian

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

can be written in the form

$$H = \tilde{H}_{qp} - \tilde{H}_c \quad (1.403)$$

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

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

$$\tilde{H}_{qp}^I = \tilde{U} \tilde{n}_{d\uparrow} \tilde{n}_{d\downarrow} \quad (1.405)$$

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

$$\tilde{c}_d^\dagger = \sqrt{z} c_d^\dagger \quad (1.406)$$

$$\tilde{c}_d = \sqrt{z} c_d \quad (1.407)$$

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

$$\tilde{H}_c = \lambda_1 \tilde{n}_d + \lambda_2 \tilde{n}_{d\uparrow} \tilde{n}_{d\downarrow} \quad (1.408)$$

where

$$\lambda_1 = z \Sigma(0, 0) \quad (1.409)$$

$$\lambda_2 = z^2 [\Gamma_{\uparrow\downarrow}(0, 0) - U] \quad (1.410)$$

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

$$\begin{aligned} \tilde{\Sigma}(0) &= 0 \\ \tilde{\Sigma}'(0) &= 0 \end{aligned} \quad (1.411)$$

Close to the Fermi surface, we also have

$$\tilde{\Gamma}_{\uparrow\downarrow}(0) = \tilde{U} \quad (1.412)$$

$$\tilde{\Gamma}_{\sigma\sigma}(0) = 0 \quad (1.413)$$

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

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

$$\lambda_i = \sum_n \lambda_i^{(n)} \tilde{U}^n \quad (1.415)$$

$$z = \sum_n z^{(n)} \tilde{U}^n \quad (1.416)$$

$$(1.417)$$

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

$$G^0 = \frac{1}{E - \tilde{\epsilon}_d + i\tilde{\Delta}} \quad (1.418)$$

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

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

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

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

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

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

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

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

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

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

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

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

We can recognize that

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

Therefore,

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

Up to first order, we can write

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

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

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

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

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

Substituting in to the parent equation, we get

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

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.

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

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

Multiplying both equations throughout by Z , we get

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

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

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

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

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

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

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

$$\tilde{\gamma} \sim \tilde{\rho}_d(0) \quad (1.437)$$

The susceptibilities are given by

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

Substituting from eq. 1.436,

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

Similarly,

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

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

$$\rho_{d\sigma} = \frac{-1}{\pi} \text{Im} [G_d] \quad (1.441)$$

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

Luttinger proved that

$$\int_{-\infty}^0 \Sigma' G dE = 0 \quad (1.443)$$

In order to use this, note that

$$\begin{aligned} \ln G_d^{-1} &= \ln (E - \epsilon_d + i\Delta - \Sigma) \\ \implies \frac{d \ln G_d^{-1}}{dE} &= \frac{1}{E - \epsilon_d + i\Delta - \Sigma} (1 - \Sigma') = G_d - \Sigma' G_d \\ \implies G_d &= \Sigma' G_d - \frac{d \ln G_d}{dE} \end{aligned} \quad (1.444)$$

Substituting this expression for G_d in eq. 1.442,

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

The first integral is zero, courtesy Luttinger. We get

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

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

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

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 far outside the bandwidth, as shown in fig. 1. The maximum energy scale at which scattering with conduction electrons can take place is of the order of the bandwidth D . Since the impurity energies are much higher than the bandwidth, no charge fluctuation can take place. The impurity state will be fixed at ϵ_d . The only remaining degree of freedom will be the spin fluctuations, and we can then do the S-W transformation.

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

$U + \epsilon_d \gg D \gg |\epsilon_d|, \Delta$. The total Hamiltonian is

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

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 impossible.

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

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

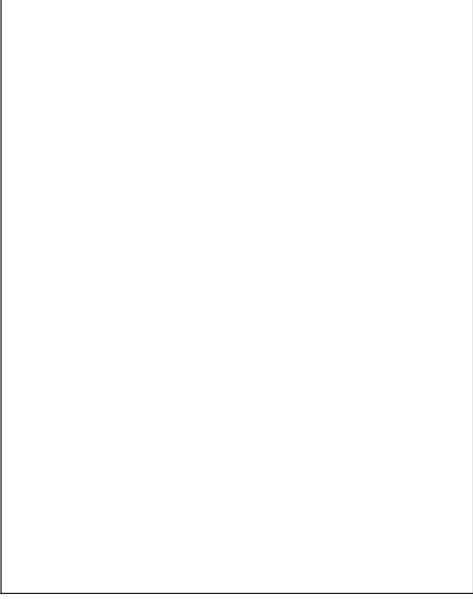


Figure 1: Impurity levels outside

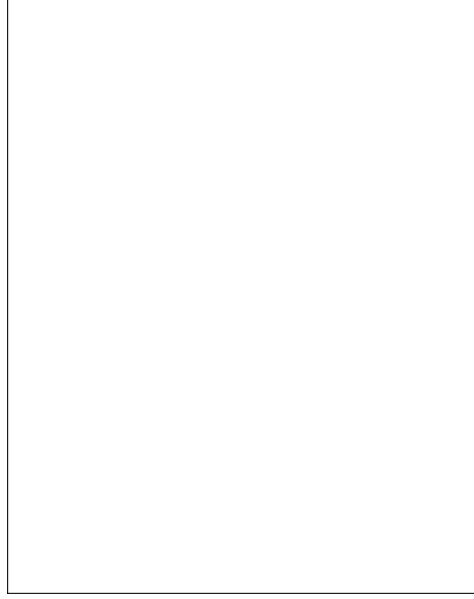


Figure 2: Impurity levels inside

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

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

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} .

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

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

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

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

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

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

$$H^{(1)} = \sum_{k^+, \sigma} \alpha_{k\sigma} T_{k\sigma}^+ + \sum_{k^-, \sigma} \beta_{k\sigma} T_{k\sigma}^- \quad (1.454)$$

$T^{+,-}$ 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

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

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

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

The change in ϵ_0 is

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

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

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

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

$$\frac{d\epsilon_d}{d \ln D} = -\frac{\Delta}{\pi} \quad (1.459)$$

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:

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

$-(U + \epsilon_d)$ 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

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

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.

$$H^{(2)} = \sum_{k^+, q, \sigma} \alpha_{k\sigma} T_{k\sigma}^+ \gamma_{q,k,\sigma} c_{d\sigma}^\dagger c_{q\sigma} + \sum_{k^-, q, \sigma} \beta_{k\sigma} T_{k\sigma}^- \gamma_{q,k,\sigma} c_{d\sigma} c_{q\sigma}^\dagger \quad (1.462)$$

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

$$\begin{aligned} \alpha_{k\sigma} \gamma_{q,k,\sigma} &= \frac{\langle 1_{d\sigma} | V_{kd}^* c_{d\sigma}^\dagger c_{k\sigma} | k\sigma \rangle \langle k\sigma | V_{kd} c_{k\sigma}^\dagger c_{d\sigma} | 1_{d\sigma} \rangle \langle 1_{d\sigma} | V_{kd} c_{q\sigma} c_{d\sigma}^\dagger | q\sigma \rangle}{(E_{1_{d\sigma}} - E_{k\sigma})(E_q - E_k)} \\ &= \alpha_{k\sigma} \frac{V_{kd}}{\epsilon_q - \epsilon_k} \end{aligned} \quad (1.463)$$

The renormalization in V_{kd} is therefore

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

Close to the band edge, we get

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

Therefore,

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

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

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

Defining the constant as

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

we get

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

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

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

$$\tilde{J} = -\frac{|V|^2}{\tilde{\epsilon}_d} = \frac{a|V|^2}{D} \quad (1.471)$$

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

$$\begin{aligned} T_K &\sim D \sqrt{\tilde{J}N(0)^2} \exp\left(-\frac{1}{2\tilde{J}N(0)^2}\right) = \sqrt{\Delta D} \exp\left(-\frac{D}{2\Delta}\right) \\ &\sim D \sqrt{\frac{\Delta}{D}} \exp\left(\frac{\epsilon_d}{2\Delta}\right) \end{aligned} \quad (1.472)$$

A different result is obtained if one is in the regime of $\epsilon_d < -D$. This is the situation mentioned at the very beginning of the discussion, fig. 1. Assuming $U \rightarrow \infty$ and ϵ_d outside the conduction band, we can do a SWT and the T_K obtained is q. 1.252,

$$J = -\frac{V^2}{\epsilon_d} \quad (1.473)$$

$$g = J\rho = -\frac{\Delta}{\epsilon_d} \quad (1.474)$$

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

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

For $\epsilon_d^* \gg \Delta$, the renormalization will stop at $D \sim \epsilon_d$. Note that we had assumed $D \gg \epsilon_d$. That was the starting condition, that is, ϵ_d deep inside the Fermi surface. During the renormalization, D will keep on decreasing and ϵ_d will continuously increase. At some value of D , they will become equal and the impurity level will go outside the Fermi surface. At this point, none of the impurity levels can renormalize any more, because the relevant energy scales are greater than the cutoff. Hence the renormalization stops at this point.

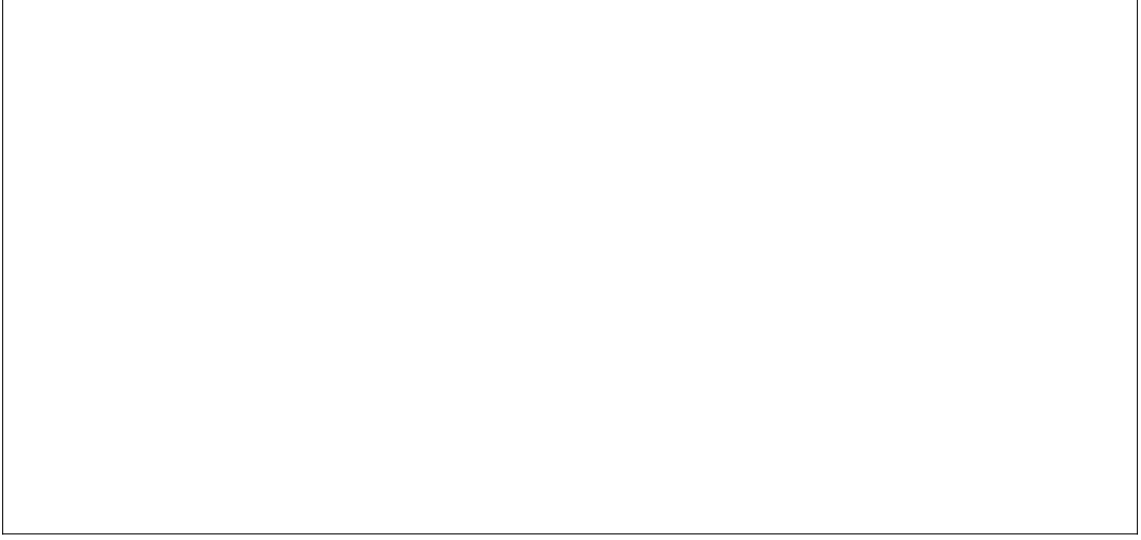


Figure 3: Renormalization in the energy levels when $\epsilon_d^* \gg \Delta$

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

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

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

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

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

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

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

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

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:

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

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

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

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

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

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.

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

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

$$x_1 + \ln x_1 = x_2 \quad (1.484)$$

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

$$O(x_1) = O(x_2) \quad (1.485)$$

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

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

$$(1.488)$$

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

$$\epsilon_d^* \gg \Delta \implies \bar{\epsilon}_d \gg \Delta \quad (1.489)$$

Applying this to eq. 1.482 means

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

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,

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

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

$$Z = 1 + \exp(\beta h) + \exp(-\beta h) + 1 = 2(1 + \cosh \beta h) \quad (1.492)$$

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

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

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

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

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

$$\chi T = \frac{1}{2\mathcal{D}} \quad (1.496)$$

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,

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

where

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

Therefore,

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

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

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

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

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

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

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

Differentiating with B gives

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

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

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

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

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

$$\implies \chi T \propto T \quad (1.506)$$

We can now visualize the various phases as the temperature is changed. For $T \gg U, \epsilon_d$, all the four states $|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |2\rangle$ are degenerate ($\mathcal{D} = 4$), the average occupancy is $\langle n_d \rangle = \frac{0+1+1+2}{4} = 1$ and the effective Curie constant is $\frac{1}{2\mathcal{D}} = \frac{1}{8}$. At lower temperatures $U \gg T \gg T^*$, the level $|2\rangle$ is disconnected from the conduction band and the three remaining states are now degenerate ($\mathcal{D} = 3$). The average occupancy becomes $\frac{0+1+1}{3} = \frac{2}{3}$ and the effective Curie constant is now $\frac{1}{2 \times 3} = \frac{1}{6}$. At still lower temperatures $T^* \gg T$, the singly-occupied levels become disconnected and the impurity occupancy becomes 0. The effective Curie constant in this regime is linear in T .

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

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

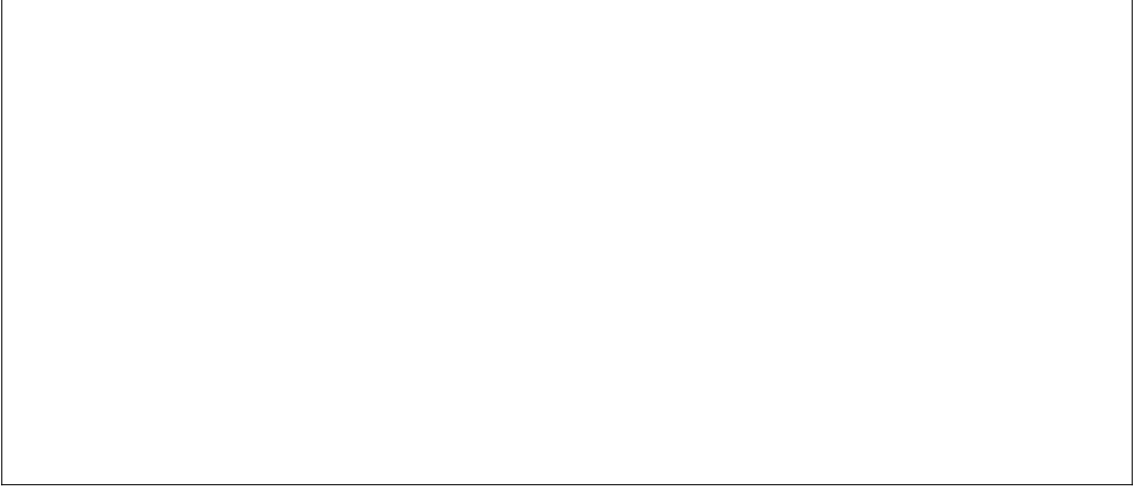


Figure 4: Renormalization in energy levels when $|\epsilon_d^*| \lesssim \Delta$

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

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

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

$$\sim \frac{k_B T}{\epsilon_d} \quad (1.508)$$

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.

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

For $\epsilon_d^* \ll -\Delta$, the scaling will stop when the impurity level again goes out of the Fermi surface. But this time, it goes out from below. This again decouples the singly-occupied state from the conduction band and the scaling stops. This happens at say $\tilde{D} = -\tilde{\epsilon}_d = \tilde{T}$. Since the singly-occupied impurity level is now well below $-D$, we have $\langle n_d \rangle = 1$ and we are comfortably in the Kondo limit and the SWT and a consequent poor man's scaling can be performed, which will give eqs. 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; there is no charge fluctuation. At high temperatures $T \gg T_K$, the impurity is essentially decoupled and we get a susceptibility of the form eq. 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.

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

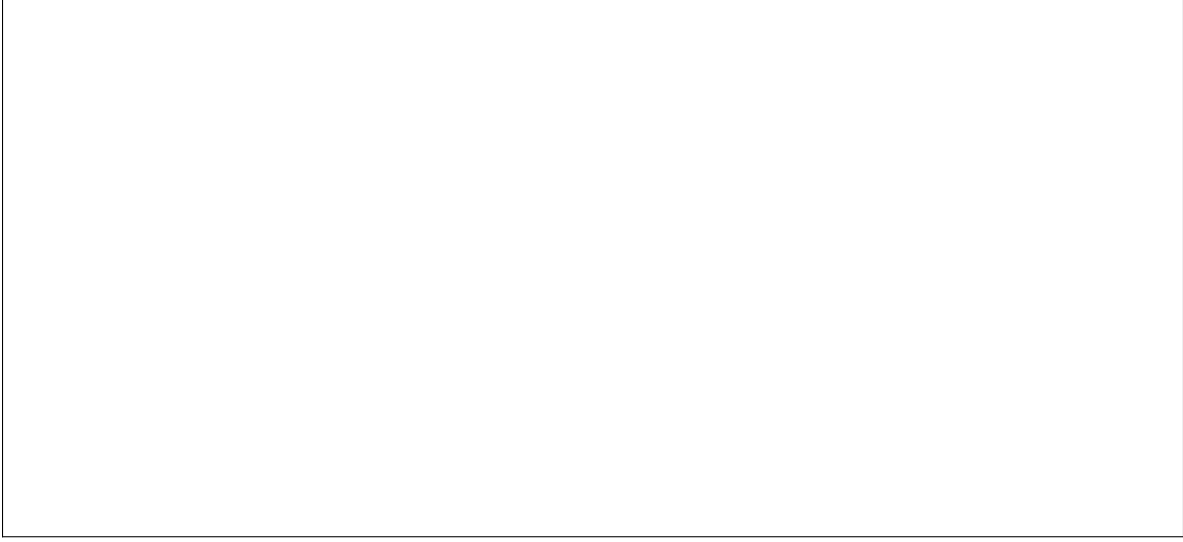


Figure 5: Renormalization in energy levels when $\epsilon_d^* \ll -\Delta$

Jefferson's calculation

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

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

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

$$H\psi = E\psi \quad (1.510)$$

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

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

Its orthogonal subspace has a projection operator

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

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

$$P\{\psi\}_d = \{\phi\} \quad (1.513)$$

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

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

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:

$$\Omega\{\phi\} = \{\psi\} \quad (1.515)$$

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

$$\Omega\{\phi\}^\perp = 0 \quad (1.516)$$

This allows us to write

$$\Omega P\phi = \Omega\phi \quad (1.517)$$

$$\Omega P\phi^\perp = \Omega \times 0 = 0 = \Omega\phi^\perp \quad (1.518)$$

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

$$\Omega P = \Omega \quad (1.519)$$

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

$$H\Omega\phi = E\Omega\phi \quad (1.520)$$

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

$$PH\Omega\phi = EP\Omega\phi = E\phi \quad (1.521)$$

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

$$H_{\text{eff}} = PH\Omega = PH_0P + PV\Omega = PH_0P + PV\Omega \quad (1.522)$$

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

$$\Omega V\psi = (E\Omega P - \Omega PH_0)\psi \quad (1.523)$$

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

$$\Omega V\psi = (E - \Omega H_0 P)\psi \quad (1.524)$$

Subtracting the Schrodinger 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

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

The second order equation is

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

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.

$$A_1 = -QVP \tag{1.530}$$

$$A_2 = -QV \Lambda_1 + \Lambda_1 V P \tag{1.531}$$

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

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

The lowest order solutions are thus

$$\Lambda_1 = S(QVP) = S(VP) \tag{1.537}$$

$$\Lambda_2 = S(QV\Lambda_1) - S(\Lambda_1VP) = S(VS(VP)) - S(S(VP)VP) \tag{1.538}$$

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

$$\begin{aligned}
H_{\text{eff}} - PH_0P &= PV\Omega \\
&\approx PV(\Lambda_0 + \Lambda_1 + \Lambda_2) \\
&= PV[P + S(VP) + S(VS(VP)) - S(S(VP)VP)] \\
&= PVP + PVS(VP) + PVS(VS(VP)) - PVS(S(VP)VP)
\end{aligned} \tag{1.539}$$

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

$$PVSVP = PV \sum_l G_l V P P_l = PV \sum_l G_l V P_l \tag{1.541}$$

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

$$\begin{aligned} PVS SVSP &= PVS V \sum_l G_l V P_l = PV \sum_l SV G_l V P_l \\ &= PV \sum_{l,l'} G_{l'} V G_l V P_l P_{l'} = PV \sum_l G_l V G_l V P_l \end{aligned} \quad (1.542)$$

The fourth term is

$$\begin{aligned} PVS(S(VP)VP) &= PVS\left(\sum_l G_l V P P_l V P\right) = PV \sum_{l,l'} G_{l'} G_l V P_l V P P_{l'} \\ &= PV \sum_{l'} G_{l'} \left(\sum_l G_l V P_l\right) V P_{l'} \end{aligned} \quad (1.543)$$

The effective Hamiltonian up to third order in V is

$$\begin{aligned} H_{\text{eff}} &= PH_0P + PV \sum_l G_l V P_l + PV \sum_l G_l V G_l V P_l \\ &\quad - PV \sum_{l,l'} G_{l'} G_l V P_l V P_{l'} \end{aligned} \quad (1.544)$$

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:

$$|k_1\rangle \langle k_2| = c_{k_1}^\dagger c_{k_2} \quad (1.545)$$

$$P_k = |k, n_{d\sigma}\rangle \langle k, n_{d\sigma}| = c_k^\dagger c_k c_{d\sigma}^\dagger c_{d\sigma} = n_{k\sigma} n_{d\sigma} \quad (1.546)$$

The first term becomes

$$PH_0P = \sum_{k\sigma} \epsilon_{k\sigma} n_{k\sigma} + \epsilon_d n_d + \sum_{k\sigma} \left(V_{kd} c_{k\sigma}^\dagger c_{d\sigma} + \text{h.c.} \right) \quad (1.547)$$

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

$$\begin{aligned} PV \sum_l G_l V P_l &= V \sum_{q\sigma} \left(\frac{V_q}{\epsilon_d - \epsilon_q} c_{q\sigma}^\dagger c_{d\sigma} + \frac{V_q^*}{\epsilon_q - \epsilon_d} c_{d\sigma}^\dagger c_{q\sigma} \right) \\ &= \sum_{q\sigma}^+ \frac{|V_q|^2 c_{d\sigma}^\dagger c_{q\sigma} c_{q\sigma}^\dagger c_{d\sigma}}{\epsilon_d - \epsilon_q} + \sum_{q\sigma}^- \frac{|V_q|^2 c_{q\sigma}^\dagger c_{d\sigma} c_{d\sigma}^\dagger c_{q\sigma}}{\epsilon_q - \epsilon_d} \\ &= \sum_{q\sigma}^+ \frac{|V_q|^2 n_{d\sigma} (1 - n_{q\sigma})}{\epsilon_d - \epsilon_q} + \sum_{q\sigma}^- \frac{|V_q|^2 n_{q\sigma} (1 - n_{d\sigma})}{\epsilon_q - \epsilon_d} \end{aligned} \quad (1.548)$$

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

$$\begin{aligned}
PV \sum_l G_l V P_l &= \sum_q^+ \frac{|V_q|^2 n_{d\sigma}}{\epsilon_d - \epsilon_q} + \sum_q^- \frac{|V_q|^2 (1 - n_{d\sigma})}{\epsilon_q - \epsilon_d} \\
&= n_d \left(\sum_q^+ \frac{|V_q|^2}{\epsilon_d - \epsilon_q} + 2 \sum_q^- \frac{|V_q|^2}{\epsilon_d - \epsilon_q} \right) \\
&= n_d \delta \epsilon_d
\end{aligned} \tag{1.549}$$

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

$$|k, n_{d\sigma}\rangle \rightarrow \begin{cases} |q_e, n_d = 0\rangle \rightarrow \begin{cases} |q_e, n_d = 1\rangle \\ |q_e, q'_h, n_d = 1\rangle \end{cases} \\ |q_h, n_d = 1\rangle \rightarrow \begin{cases} |q_h, q'_e, n_d = 0\rangle \\ |q_h, n_d = 0\rangle \end{cases} \end{cases} \tag{1.550}$$

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

$$|k, n_d = 0\rangle \xrightarrow[\Delta E = \epsilon_k - \epsilon_q]{|n_d = 1\rangle} |q_e, n_d = 0\rangle \xrightarrow[\Delta E = \epsilon_q - \epsilon_d]{|k', n_d = 1\rangle} \tag{1.551}$$

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

$$|n_{d\sigma} = 1\rangle \xrightarrow[\Delta E = \epsilon_k - \epsilon_q]{|k\sigma, n_d = 0\rangle} \begin{cases} |q_h \uparrow, n_{d\uparrow} = 1\rangle \\ |q_h \downarrow, n_{d\downarrow} = 1\rangle \end{cases} \xrightarrow[\Delta E = \epsilon_q - \epsilon_d]{|n_d = 0\rangle} \tag{1.552}$$

Combining the two processes gives

$$\begin{aligned}
\sum_q^+ \sum_{k\sigma} \frac{|V_q|^2 c_{d\sigma}^\dagger c_{q\sigma} c_{q\sigma}^\dagger c_{d\sigma} c_{d\sigma}^\dagger c_{k\sigma}}{(\epsilon_q - \epsilon_d)(\epsilon_k - \epsilon_q)} + \sum_{q\sigma'}^- \sum_{k\sigma} \frac{|V_q|^2 c_{q\sigma'}^\dagger c_{d\sigma'} c_{d\sigma'}^\dagger c_{q\sigma'} c_{k\sigma}^\dagger c_{d\sigma}}{(\epsilon_q - \epsilon_d)(\epsilon_k - \epsilon_q)} \\
= \sum_{k\sigma} \left(c_{k\sigma}^\dagger c_{d\sigma} \delta V_k^- + c_{d\sigma}^\dagger c_{k\sigma} \delta V_k^- \right)
\end{aligned} \tag{1.553}$$

where

$$\begin{aligned}
\delta V^+ &= \sum_q^+ \frac{|V_q|^2}{(\epsilon_q - \epsilon_d)(\epsilon_k - \epsilon_q)} \\
\delta V^- &= \sum_q^- 2 \frac{|V_q|^2}{(\epsilon_q - \epsilon_d)(\epsilon_k - \epsilon_q)}
\end{aligned} \tag{1.554}$$

The total Hamiltonian can be written in the form

$$H_{\text{eff}} = \sum_{k\sigma} \epsilon_{k\sigma} n_{k\sigma} + (\epsilon_d + \delta\epsilon_d) n_d + \sum_{k\sigma} \left\{ (V_k^- + \delta V_k^-) c_{k\sigma}^\dagger c_{d\sigma} + (V_k^+ + \delta V_k^+) c_{d\sigma}^\dagger c_{k\sigma} \right\} \quad (1.555)$$

We now evaluate the changes:

$$\begin{aligned} \delta\epsilon_d &= \left(\sum_q^+ \frac{|V_q|^2}{\epsilon_d - \epsilon_q} + 2 \sum_q^- \frac{|V_q|^2}{\epsilon_d - \epsilon_q} \right) \\ &\approx |V|^2 \rho |\delta D| \left(\frac{1}{\epsilon_d - D} + \frac{2}{\epsilon_d + D} \right) \\ &= |V|^2 \rho |\delta D| \frac{D - 3\epsilon_d}{D^2 - \epsilon_d^2} \end{aligned} \quad (1.556)$$

I used the approximation

$$\sum_{q=D-\delta D}^D f(q) = \int_{D-\delta D}^D dE \rho(E) f(E) \approx \rho f(D) \delta D \quad (1.557)$$

Also,

$$\begin{aligned} \delta V_k^+ &= \sum_q^+ \frac{|V_q|^2}{(\epsilon_q - \epsilon_d)(\epsilon_k - \epsilon_q)} \\ &\approx |V|^2 \rho |\delta D| \frac{1}{(D - \epsilon_d)(\epsilon_k - D)} \\ \delta V_k^- &= 2 \sum_q^- \frac{|V_q|^2}{(\epsilon_q - \epsilon_d)(\epsilon_k - \epsilon_q)} \\ &\approx -|V|^2 \rho |\delta D| \frac{2}{(D + \epsilon_d)(\epsilon_k + D)} \end{aligned} \quad (1.558)$$

We now make the following assumptions:

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

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

2 URG Formalism

We are given a Hamiltonian \mathcal{H} which is not diagonal in a particular occupation number basis of the electrons, \hat{n}_k : $[\mathcal{H}, n_k] \neq 0$. The goal is to obtain the unitary transformation U_k that diagonalizes this Hamiltonian in this particular basis:

$$\tilde{\mathcal{H}} = U_k \mathcal{H} U_k^\dagger \text{ such that } [\tilde{\mathcal{H}}, n_k] = 0 \quad (2.1)$$

Another way to express the above problem is that, with the original Hamiltonian \mathcal{H} , the diagonal terms are not zero:

$$n_k \mathcal{H} (1 - n_k) \neq 0 \quad (2.2)$$

so we want to find a rotated Hamiltonian $\tilde{\mathcal{H}} = U_k \mathcal{H} U_k^\dagger$ such that the off-diagonal term is zero:

$$n_k \tilde{\mathcal{H}} (1 - n_k) = 0 \quad (2.3)$$

To find the form for U_k , we define a few things. First,

$$P_k = U_k^\dagger n_k U_k \quad (2.4)$$

To get a feel for what P_k is, note that

$$[\mathcal{H}, P_k] = [U_k^\dagger U_k \mathcal{H}, U_k^\dagger n_k U_k] = U_k^\dagger [\tilde{\mathcal{H}}, n_k] U_k = 0 \quad (2.5)$$

P_k is hence those degrees of freedom in which the given Hamiltonian \mathcal{H} is diagonal. Hence it is natural that they are obtained by rotating the n_k . If we were to go to the eigenbasis of \mathcal{H} , the form for $\tilde{\mathcal{H}}$ will be

$$\begin{pmatrix} E_1 & \\ & E_2 \end{pmatrix} \quad (2.6)$$

while the form for P_k will be

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad (2.7)$$

It is obvious that

$$P_k^2 = P_k \quad (2.8)$$

Another thing that we will define is

$$\overline{\mathcal{H}} = P_k \mathcal{H} P_k \quad (2.9)$$

$\overline{\mathcal{H}}$ is a matrix that, in the eigenbasis of \mathcal{H} , has only the upper diagonal block of \mathcal{H} . That is, you first form a matrix by keeping only the upper diagonal block of $\tilde{\mathcal{H}}$ and then rotating to the basis of n_k . Finally, let ψ be a wavefunction such that

$$P\psi = \psi \quad (2.10)$$

This means that ψ is an eigenvector of P_k and hence also of \mathcal{H} since P_k and \mathcal{H} commute.

Combining $P_k \mathcal{H} = \mathcal{H} P_k$ and the idempotence of P_k gives

$$\mathcal{H} P_k = P_k \mathcal{H} = P_k \mathcal{H} P_k = \overline{\mathcal{H}} \quad (2.11)$$

Operating this equation on ψ gives

$$\mathcal{H} \psi = \overline{\mathcal{H}} \psi \quad (2.12)$$

This is the equation we will use to find U_k . But first we will write ψ in the following fashion:

$$|\psi\rangle = a_1 |1, \psi_1\rangle + a_0 |0, \psi_0\rangle \quad (2.13)$$

The first entry signifies whether the degree of freedom k 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 k .

We will also write the Hamiltonian \mathcal{H} as

$$\mathcal{H} = \mathcal{H}^D + \mathcal{H}^I + \mathcal{H}^i \quad (2.14)$$

\mathcal{H}^D is the diagonal part of the Hamiltonian, something of the form $\epsilon_k n_k$. \mathcal{H}^I is the interaction between the current degree of freedom k and the remaining degrees of freedom. It will consist of terms like $c_q^\dagger c_k$ or $c_k^\dagger c_q$. 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 of k states. It will involve terms like $c_{q_1}^\dagger c_{q_2}$.

Substituting the decomposition of $|\psi\rangle$ and \mathcal{H} into eq. 2.12 gives

$$\overline{\mathcal{H}} (a_1 |1, \psi_1\rangle + a_0 |0, \psi_0\rangle) = [\mathcal{H}^D + \mathcal{H}^I + \mathcal{H}^i] (a_1 |1, \psi_1\rangle + a_0 |0, \psi_0\rangle) \quad (2.15)$$

To get expressions from this, note that on the left hand side, $\overline{\mathcal{H}}$ does not scatter k , so it will not change 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

$$\overline{\mathcal{H}} a_0 |0, \psi_0\rangle = (\mathcal{H}^D + \mathcal{H}^i) a_0 |0, \psi_0\rangle + \mathcal{H}^I a_1 |1, \psi_1\rangle \quad (2.16)$$

We can simplify this equation by noting that

$$\mathcal{H}^D = \text{Tr} [\mathcal{H}^D \hat{n}_k] \hat{n}_k + \text{Tr} [\mathcal{H}^D (1 - \hat{n}_k)] (1 - \hat{n}_k) \quad (2.17)$$

$$\implies \mathcal{H}^D |0, \psi_0\rangle = \text{Tr} [\mathcal{H}^D (1 - \hat{n}_k)] (1 - \hat{n}_k) |0, \psi_0\rangle \quad (2.18)$$

and

$$\mathcal{H}^I = \text{Tr} [c_k^\dagger \mathcal{H}] c_k + c_k^\dagger \text{Tr} [\mathcal{H} c_k] \implies \mathcal{H}^I |1, \psi_1\rangle = \text{Tr} [c_k^\dagger \mathcal{H}] c_k |1, \psi_1\rangle \quad (2.19)$$

Substituting these in the equation gives

$$\overline{\mathcal{H}}a_0|0, \psi_0\rangle = \{ \text{Tr} [\mathcal{H}^D(1 - \hat{n}_k)] (1 - \hat{n}_k) + \mathcal{H}^i \} a_0|0, \psi_0\rangle + \text{Tr} [c_k^\dagger \mathcal{H}] c_k a_1|1, \psi_1\rangle \quad (2.20)$$

$$\implies \{ \overline{\mathcal{H}} - \mathcal{H}^i - \text{Tr} [\mathcal{H}^D(1 - \hat{n}_k)] (1 - \hat{n}_k) \} a_0|0, \psi_0\rangle = \text{Tr} [c_k^\dagger \mathcal{H}] c_k a_1|1, \psi_1\rangle \quad (2.21)$$

Defining $\hat{\omega} = \overline{\mathcal{H}} - \mathcal{H}^i$, we get the result

$$a_0|0, \psi_0\rangle = [\hat{\omega} - \text{Tr} [\mathcal{H}^D(1 - \hat{n}_k)] (1 - \hat{n}_k)]^{-1} \text{Tr} [c_k^\dagger \mathcal{H}] c_k a_1|1, \psi_1\rangle \quad (2.22)$$

We define

$$\eta_k \equiv \frac{1}{\hat{\omega} - \text{Tr} [\mathcal{H}^D(1 - \hat{n}_k)] (1 - \hat{n}_k)} \text{Tr} [c_k^\dagger \mathcal{H}] c_k \quad (2.23)$$

which gives the equation a compact form

$$a_0|0, \psi_0\rangle = \eta_k a_1|1, \psi_1\rangle \quad (2.24)$$

The equation obtained by matching the states $|1\rangle$ is

$$\begin{aligned} a_1 \overline{\mathcal{H}}|1, \psi_1\rangle &= (\mathcal{H}^D + \mathcal{H}^i) a_1|1, \psi_1\rangle + \mathcal{H}^I a_0|0, \psi_0\rangle \\ &= (\text{Tr} [\mathcal{H}^D \hat{n}_k] \hat{n}_k + \mathcal{H}^i) a_1|1, \psi_1\rangle + c_k^\dagger \text{Tr} [\mathcal{H} c_k] a_0|0, \psi_0\rangle \\ \implies a_1|1, \psi_1\rangle &= (\overline{\mathcal{H}} - \mathcal{H}^i - \text{Tr} [\mathcal{H}^D \hat{n}_k] \hat{n}_k)^{-1} c_k^\dagger \text{Tr} [\mathcal{H} c_k] a_0|0, \psi_0\rangle \\ &= \eta_k^\dagger a_0|0, \psi_0\rangle \end{aligned} \quad (2.25)$$

where

$$\eta_k^\dagger = \frac{1}{\hat{\omega} - \text{Tr} [\mathcal{H}^D \hat{n}_k] \hat{n}_k} c_k^\dagger \text{Tr} [\mathcal{H} c_k] \quad (2.26)$$

We thus get the following two equations:

$$a_0|0, \psi_0\rangle = \eta_k a_1|1, \psi_1\rangle \quad (2.27)$$

$$a_1|1, \psi_1\rangle = \eta_k^\dagger a_0|0, \psi_0\rangle \quad (2.28)$$

Combining eqs. 2.27 and 2.28, we get

$$a_0|0, \psi_0\rangle = \eta_k a_1|1, \psi_1\rangle = \eta_k \eta_k^\dagger a_0|0, \psi_0\rangle \quad (2.29)$$

Combining this with the fact that η_k^\dagger should have a c_k^\dagger and hence should give $\eta_k^\dagger|1, \psi_1\rangle$, we get

$$\eta_k \eta_k^\dagger = 1 - \hat{n}_k \quad (2.30)$$

Similarly, combining the equations the other way round gives

$$\eta_k^\dagger \eta_k = \hat{n}_k \quad (2.31)$$

As a consequence,

$$\begin{aligned}\left\{\eta_k, \eta_k^\dagger\right\} &= 1 \\ \left[\eta_k, \eta_k^\dagger\right] &= 1 - 2\hat{n}_k\end{aligned}\tag{2.32}$$

Other properties include

$$\eta_k^2 = \left(\eta_k^\dagger\right)^2 = 0\tag{2.33}$$

$$\hat{n}_k \eta_k = (1 - \hat{n}_k) \eta_k^\dagger = 0\tag{2.34}$$

$$\eta_k \hat{n}_k = \eta_k\tag{2.35}$$

$$\eta^\dagger (1 - \hat{n}_k) = \eta_k^\dagger\tag{2.36}$$

We now need to find the unitary operation U_k that disentangles the state $|1, \psi_1\rangle$ from the state $|psi\rangle$. Using eq. 2.27,

$$|\psi\rangle = a_1 |1, \psi_1\rangle + a_0 |0, \psi_0\rangle = a_1 |1, \psi_1\rangle + \eta_k a_1 |1, \psi_1\rangle = (1 + \eta_k) |1, \psi_1\rangle\tag{2.37}$$

This means that the operator U_k for going from $|, \psi_1\rangle$ to $|\psi\rangle$ is described by

$$U_k^{-1} = \mathcal{C} (1 + \eta_k + \mathcal{O})\tag{2.38}$$

where \mathcal{O} is some operator function of η_k and η_k^\dagger such that

$$(1 + \eta_k + \mathcal{O}) |1, \psi_1\rangle = (1 + \eta_k) |1, \psi_1\rangle \implies \mathcal{O} |1, \psi_1\rangle = 0\tag{2.39}$$

and \mathcal{C} is a real scalar. To find \mathcal{O} , note that we can write U_k^{-1} as

$$U_k^{-1} = \mathcal{C} \exp(\eta_k + \mathcal{O})\tag{2.40}$$

This is because $\eta_k^2 = 0$ and since \mathcal{O} is made up of η_k and η_k^\dagger it has the same property. This exponential form allows us to write

$$U_k = \mathcal{C} \exp(-\eta_k - \mathcal{O}) = \mathcal{C} (1 - \eta_k - \mathcal{O})\tag{2.41}$$

But, since U_k is required to be unitary, we can write, from eq. 2.38,

$$U_k^\dagger = U_k^{-1} = \mathcal{C} (1 + \eta_k + \mathcal{O}) \implies U_k = \mathcal{C} \left(1 + \eta_k^\dagger + \mathcal{O}^\dagger\right)\tag{2.42}$$

Comparing the two expressions of U_k in eqs. 2.41 and 2.42,

$$1 - \eta_k - \mathcal{O} = 1 + \eta_k^\dagger + \mathcal{O}^\dagger \implies -\eta_k = \mathcal{O}^\dagger \implies \mathcal{O} = -\eta_k^\dagger\tag{2.43}$$

This improves eq. 2.41:

$$U_k = \mathcal{C} \left(1 + \eta_k^\dagger - \eta_k\right)\tag{2.44}$$

To find \mathcal{C} , we can use the unitarity of U_k :

$$1 = U_k^\dagger U_k = \mathcal{C}^2 \left(1 + \left\{ \eta_k^\dagger, \eta_k \right\} \right) = \mathcal{C}^2 \times 2 \implies \mathcal{C} = \frac{1}{\sqrt{2}} \quad (2.45)$$

The unitary operator that transforms the entangled eigenstate $|\psi\rangle$ to the eigenstate with good quantum number n_k , $|1, \psi_1\rangle$ is thus

$$U_k = \frac{1}{\sqrt{2}} \left(1 + \eta_k^\dagger - \eta_k \right) \quad (2.46)$$

The form of the rotated Hamiltonian can now be written down.

$$\begin{aligned} \tilde{\mathcal{H}} &= U_k \mathcal{H} U_k^\dagger \\ &= \frac{1}{2} \left(1 + \eta_k^\dagger - \eta_k \right) \mathcal{H} \left(1 + \eta_k - \eta_k^\dagger \right) \\ &= \frac{1}{2} \left(1 + \eta_k^\dagger - \eta_k \right) \left(\mathcal{H} + \mathcal{H}\eta - \mathcal{H}\eta_k^\dagger \right) \\ &= \frac{1}{2} \left(\mathcal{H} + \mathcal{H}\eta - \mathcal{H}\eta_k^\dagger + \eta_k^\dagger \mathcal{H} + \eta_k^\dagger \mathcal{H}\eta_k - \eta_k^\dagger \mathcal{H}\eta_k^\dagger - \eta_k \mathcal{H} - \eta_k \mathcal{H}\eta_k + \eta_k \mathcal{H}\eta_k^\dagger \right) \\ &= \frac{1}{2} \left(\mathcal{H}^D + \mathcal{H}^i + \mathcal{H}^I + \mathcal{H}\eta - \mathcal{H}\eta_k^\dagger + \eta_k^\dagger \mathcal{H} + \eta_k^\dagger \mathcal{H}\eta_k - \eta_k^\dagger \mathcal{H}\eta_k^\dagger - \eta_k \mathcal{H} - \eta_k \mathcal{H}\eta_k + \eta_k \mathcal{H}\eta_k^\dagger \right) \end{aligned} \quad (2.47)$$

In the last step I split \mathcal{H} using eq. 2.14. At this stage, note that terms that have two η_k or two η_k^\dagger can only be nonzero if the intervening \mathcal{H} has a creation or destruction operator. If we resolve the Hamiltonian in the basis of k in the following form:

$$\begin{aligned} \mathcal{H} &= \text{Tr} [\mathcal{H} \hat{n}_k] \hat{n}_k + \text{Tr} [\mathcal{H} (1 - \hat{n}_k)] (1 - \hat{n}_k) + c_k^\dagger \text{Tr} [\mathcal{H} c_k] + \text{Tr} [c_k^\dagger \mathcal{H}] c_k \\ &= H_e \hat{n}_k + H_h (1 - \hat{n}_k) + c_k^\dagger T + T^\dagger c_k \end{aligned} \quad (2.48)$$

Using this form, we can write

$$\eta_k \mathcal{H} \eta_k = \eta_k c_k^\dagger T \eta_k \quad (2.49)$$

and

$$\eta_k^\dagger \mathcal{H} \eta_k^\dagger = \eta_k^\dagger T^\dagger c_k \eta_k^\dagger \quad (2.50)$$

To simplify this, note the following relation:

$$\eta_k c_k^\dagger T \eta_k = T^\dagger c_k \quad (2.51)$$

To prove this, we will use eqs. 2.23 and 2.26.

$$\eta_k^\dagger = \frac{1}{\hat{\omega} - \text{Tr} [\mathcal{H}^D \hat{n}_k] \hat{n}_k} c_k^\dagger T \quad (2.52)$$

$$\implies (\hat{\omega} - \text{Tr} [\mathcal{H}^D \hat{n}_k] \hat{n}_k) \eta_k^\dagger = c_k^\dagger T \quad (2.53)$$

$$(2.54)$$

Taking the Hermitian conjugate gives

$$\eta_k (\hat{\omega} - \text{Tr} [\mathcal{H}^D \hat{n}_k] \hat{n}_k) = T^\dagger c_k \quad (2.55)$$

While taking the conjugate, I used the fact that $\hat{\omega}$ is Hermitian:

$$\begin{aligned} \hat{\omega} &= \overline{\mathcal{H}} - \mathcal{H}^i \\ &= P_k \mathcal{H} P_k - [H_e \hat{n} + H_h (1 - \hat{n}) - \text{Tr} [\mathcal{H} \hat{n}_1 \hat{n}_2 \dots \hat{n}_N] \hat{n}_1 \hat{n}_2 \dots \hat{n}_N] \end{aligned} \quad (2.56)$$

From eq. 2.31, we get

$$\eta_k^\dagger \eta_k = \hat{n} \quad (2.57)$$

$$\implies \frac{1}{\hat{\omega} - \text{Tr} [\mathcal{H}^D \hat{n}_k] \hat{n}_k} c_k^\dagger T \eta_k = \hat{n} \quad (2.58)$$

$$\implies c_k^\dagger T \eta_k = (\hat{\omega} - \text{Tr} [\mathcal{H}^D \hat{n}_k] \hat{n}_k) \hat{n} \quad (2.59)$$

$$(2.60)$$

Multiplying with η_k from left and then using eq. 2.55 gives

$$\eta_k c_k^\dagger T \eta_k = T^\dagger c_k \quad (2.61)$$

This proves eq. 2.51. The Hermitian conjugate of the equation is

$$\eta_k^\dagger T^\dagger c_k \eta_k^\dagger = c_k^\dagger T \quad (2.62)$$

Substituting eqs. 2.51 and 2.62 in eqs. 2.49 and 2.50 gives

$$\eta_k \mathcal{H} \eta_k + \eta_k^\dagger \mathcal{H} \eta_k^\dagger = c_k^\dagger T + T^\dagger c_k \quad (2.63)$$

Since \mathcal{H}^I is the part of the Hamiltonian that causes scattering between $|n_k = 0\rangle$ and $|n_k = 1\rangle$, we can write, from eq. 2.48,

$$\mathcal{H}^I = c_k^\dagger T + T^\dagger c_k \quad (2.64)$$

Comparing eqs. 2.63 and 2.64, we get

$$\mathcal{H}^I - \eta_k \mathcal{H} \eta_k - \eta_k^\dagger \mathcal{H} \eta_k^\dagger = 0 \quad (2.65)$$

Substituting this in the rotated Hamiltonian gives

$$\tilde{\mathcal{H}} = \frac{1}{2} \left(\mathcal{H}^D + \mathcal{H}^i + \mathcal{H} \eta - \mathcal{H} \eta_k^\dagger + \eta_k^\dagger \mathcal{H} + \eta_k^\dagger \mathcal{H} \eta_k - \eta_k \mathcal{H} + \eta_k \mathcal{H} \eta_k^\dagger \right) \quad (2.66)$$

To simplify the last 6 terms, we note the following:

$$\eta_k^\dagger = \frac{1}{\overline{H} - H_e \hat{n}_k} c_k^\dagger T, \quad \eta_k = \frac{1}{\overline{H} - H_h (1 - \hat{n}_k)} T^\dagger c_k \quad (2.67)$$

Then,

$$\begin{aligned}
&\implies \frac{1}{\overline{H} - H_e \hat{n}_k} c_k^\dagger T = c_k^\dagger T \frac{1}{\overline{H} - H_h (1 - \hat{n}_k)} \\
&\implies c_k^\dagger T H_h (1 - \hat{n}_k) = H_e \hat{n}_k c_k^\dagger T \\
&\implies \frac{1}{\overline{H} - H_e \hat{n}_k} c_k^\dagger T H_h (1 - \hat{n}_k) = \frac{1}{\overline{H} - H_e \hat{n}_k} H_e \hat{n}_k c_k^\dagger T \\
&\implies \eta_k^\dagger H_h (1 - \hat{n}_k) = H_e \hat{n}_k \frac{1}{\overline{H} - H_e \hat{n}_k} c_k^\dagger T \\
&\implies \eta_k^\dagger H_h (1 - \hat{n}_k) = H_e \hat{n}_k \eta_k^\dagger \\
&\implies \eta_k^\dagger H_h = H_e \hat{\eta}_k^\dagger
\end{aligned} \tag{2.68}$$

Using this identity and its conjugate ($\eta_k H_e = H_h \hat{\eta}_k$), the expression for $\eta_k H \eta_k^\dagger$ can be simplified:

$$\begin{aligned}
\eta_k \mathcal{H} \eta_k^\dagger &= \eta_k H_e \hat{n}_k \eta_k^\dagger \\
&= H_h \eta_k \eta_k^\dagger \\
&= H_h (1 - \hat{n}_k)
\end{aligned} \tag{2.69}$$

Similarly,

$$\begin{aligned}
\eta_k^\dagger \mathcal{H} \eta_k &= \eta_k^\dagger H_h \eta_k \\
&= H_e \eta_k^\dagger \eta_k \\
&= H_e \hat{n}_k
\end{aligned} \tag{2.70}$$

Also,

$$\begin{aligned}
\mathcal{H} \eta - \mathcal{H} \eta_k^\dagger + \eta_k^\dagger \mathcal{H} - \eta_k \mathcal{H} &= \left(\eta_k^\dagger H_h - H_e \eta_k^\dagger \right) + (H_h \eta - \eta H_e) + \eta_k^\dagger T^\dagger c_k - \eta_k c_k^\dagger T + \\
&\quad c_k^\dagger T \eta_k - T^\dagger c_k \eta_k^\dagger
\end{aligned} \tag{2.71}$$

By virtue of eq. 2.68 and its conjugate, the first two terms will vanish.

$$\mathcal{H} \eta - \mathcal{H} \eta_k^\dagger + \eta_k^\dagger \mathcal{H} - \eta_k \mathcal{H} = \eta_k^\dagger T^\dagger c_k - \eta_k c_k^\dagger T + c_k^\dagger T \eta_k - T^\dagger c_k \eta_k^\dagger \tag{2.72}$$

From eq. 2.51,

$$\eta_k^\dagger T^\dagger c_k = \eta_k^\dagger \eta_k c_k^\dagger T \eta_k = \hat{n}_k c_k^\dagger T \eta_k = c_k^\dagger T \eta_k \tag{2.73}$$

$$T^\dagger c_k \eta_k^\dagger = \eta_k c_k^\dagger T \eta_k \eta_k^\dagger = \eta_k c_k^\dagger T (1 - \hat{n}_k) = \eta_k c_k^\dagger T \tag{2.74}$$

$$\tag{2.75}$$

Eq. 2.72 becomes

$$\mathcal{H} \eta - \mathcal{H} \eta_k^\dagger + \eta_k^\dagger \mathcal{H} - \eta_k \mathcal{H} = c_k^\dagger T \eta_k - \eta_k c_k^\dagger T + c_k^\dagger T \eta_k - \eta_k c_k^\dagger T = 2 \left[c_k^\dagger T, \eta_k \right] \tag{2.76}$$

Putting it all together,

$$\begin{aligned}\tilde{\mathcal{H}} &= \frac{1}{2} \left(\mathcal{H}^D + \mathcal{H}^i + \mathcal{H}\eta - \mathcal{H}\eta_k^\dagger + \eta_k^\dagger \mathcal{H} + \eta_k^\dagger \mathcal{H}\eta_k - \eta_k \mathcal{H} + \eta_k \mathcal{H}\eta_k^\dagger \right) \\ &= \frac{1}{2} (\mathcal{H}^D + \mathcal{H}^i) + \left[c_k^\dagger T, \eta_k \right] + \frac{1}{2} [H_e \hat{n}_k + H_h (1 - \hat{n}_k)]\end{aligned}\quad (2.77)$$

One further simplification is possible. The last two terms constitute the total diagonal part of the Hamiltonian, but so do the first two terms:

$$\mathcal{H}^D + \mathcal{H}^i = H_e \hat{n}_k + H_h (1 - \hat{n}_k) \quad (2.78)$$

Hence,

$$\begin{aligned}\tilde{\mathcal{H}} &= \frac{1}{2} \left(\mathcal{H}^D + \mathcal{H}^i + \mathcal{H}\eta - \mathcal{H}\eta_k^\dagger + \eta_k^\dagger \mathcal{H} + \eta_k^\dagger \mathcal{H}\eta_k - \eta_k \mathcal{H} + \eta_k \mathcal{H}\eta_k^\dagger \right) \\ &= H_e \hat{n}_k + H_h (1 - \hat{n}_k) + \left[c_k^\dagger T, \eta_k \right] \\ &= \text{Tr} [\mathcal{H} \hat{n}_k] \hat{n}_k + \text{Tr} [\mathcal{H} (1 - \hat{n}_k)] (1 - \hat{n}_k) + \left[c_k^\dagger \text{Tr} (\mathcal{H} c_k), \eta_k \right]\end{aligned}\quad (2.79)$$

The two terms at the front can be written in a slightly different fashion.

$$\begin{aligned}\text{Tr} [\mathcal{H} \hat{n}_k] \hat{n}_k + \text{Tr} [\mathcal{H} (1 - \hat{n}_k)] (1 - \hat{n}_k) &= \text{Tr} [\mathcal{H} \hat{n}_k] \hat{n}_k + \text{Tr} [\mathcal{H} (\hat{n}_k - 1)] (\hat{n}_k - 1) \\ &= \text{Tr} [\mathcal{H} \hat{n}_k] \hat{n}_k + \text{Tr} [\mathcal{H} (\hat{n}_k - 1)] n_k - \text{Tr} [\mathcal{H} (\hat{n}_k - 1)] \\ &= \text{Tr} [\mathcal{H} (2\hat{n}_k - 1)] \hat{n}_k - \text{Tr} [\mathcal{H} (\hat{n}_k - 1)] \\ &= \text{Tr} \left[\mathcal{H} \left(\hat{n}_k - \frac{1}{2} \right) \right] 2\hat{n}_k - \text{Tr} \left[\mathcal{H} \left(\hat{n}_k - \frac{1}{2} \right) \right] + \frac{1}{2} \text{Tr} [\mathcal{H}] \\ &= \text{Tr} \left[\mathcal{H} \left(\hat{n}_k - \frac{1}{2} \right) \right] (2\hat{n}_k - 1) + \frac{1}{2} \text{Tr} [\mathcal{H}] \\ &= \text{Tr} [\mathcal{H} \tau_k] 2\tau_k + \frac{1}{2} \text{Tr} [\mathcal{H}]\end{aligned}\quad (2.80)$$

The last term can be written as:

$$\begin{aligned}\left[c_k^\dagger \text{Tr} (\mathcal{H} c_k), \eta_k \right] &= c_k^\dagger \text{Tr} (\mathcal{H} c_k) \eta_k - \eta_k c_k^\dagger \text{Tr} (\mathcal{H} c_k) \\ &= (2\hat{n}_k - 1) c_k^\dagger \text{Tr} (\mathcal{H} c_k) \eta_k - (1 - 2\hat{n}_k) \eta_k c_k^\dagger \text{Tr} (\mathcal{H} c_k)\end{aligned}\quad (2.81)$$

I used $\hat{n}_k c_k^\dagger = c_k^\dagger$ and $\hat{n}_k \eta_k = 0$. Then,

$$\left[c_k^\dagger \text{Tr} (\mathcal{H} c_k), \eta_k \right] = 2\tau_k \left\{ c_k^\dagger \text{Tr} (\mathcal{H} c_k), \eta_k \right\} \quad (2.82)$$

The final form of the rotated Hamiltonian is

$$\tilde{\mathcal{H}} = U_k \mathcal{H} U_k^\dagger = \frac{1}{2} \text{Tr} [\mathcal{H}] + 2\tau_k \text{Tr} [\mathcal{H} \tau_k] + 2\tau_k \left\{ c_k^\dagger \text{Tr} (\mathcal{H} c_k), \eta_k \right\} \quad (2.83)$$

To check that this indeed commutes with \hat{n}_k ,

$$\begin{aligned}
\left[\widetilde{\mathcal{H}}, \hat{n}_k \right] &= \left[\left[c_k^\dagger T, \eta_k \right], \hat{n}_k \right] \\
&= \left[c_k^\dagger T \eta_k, \hat{n}_k \right] - \left[\eta_k c_k^\dagger T, \hat{n}_k \right] \\
&= c_k^\dagger T \eta_k \hat{n}_k - \hat{n}_k c_k^\dagger T \eta_k \quad \left[2^{\text{nd}} [\cdot] \text{ is } 0, \because c_k^\dagger \hat{n}_k = \hat{n}_k \eta_k = 0 \right] \\
&= c_k^\dagger T \eta_k - c_k^\dagger T \eta_k \\
&= 0
\end{aligned} \tag{2.84}$$

3 Kondo Model URG

3.1 Calculation of renormalized Hamiltonian

$$\mathcal{H} = \sum_{k\alpha} \epsilon_k \hat{n}_{k\alpha} + \frac{J}{2} \sum_{k,k',\alpha,\alpha'} \mathbf{S} \cdot \sigma_{\alpha\alpha'} c_{k\alpha}^\dagger c_{k'\alpha'} \quad (3.1)$$

The effective Hamiltonian after one step of the RG on the Hamiltonian \mathcal{H}_j is

$$\mathcal{H}_{j,1} = \frac{1}{2} \text{Tr}_1 [\mathcal{H}_j] + \tau_1 \text{Tr}_1 [\mathcal{H}_j \tau_1] + \tau_1 \left\{ c_1^\dagger \text{Tr}_1 (\mathcal{H}_j c_1), \eta_1 \right\} \quad (3.2)$$

The second term is of order τ^2 , so we drop it because they will vanish in thermodynamic limit:

$$\mathcal{H}_{j,1} = \frac{1}{2} \text{Tr}_1 [\mathcal{H}_j] + \tau_1 \left\{ c_1^\dagger \text{Tr}_1 (\mathcal{H}_j c_1), \eta_1 \right\} \quad (3.3)$$

We will keep dropping terms of second order from now on. Also, we will assume at each The second run gives

$$\begin{aligned} \mathcal{H}_{j,2} &= \frac{1}{2} \text{Tr}_2 [\mathcal{H}_{j,1}] + \tau_2 \left\{ c_2^\dagger \text{Tr}_2 (\mathcal{H}_{j,1} c_2), \eta_2 \right\} \\ \frac{1}{2} \text{Tr}_2 [\mathcal{H}_{j,1}] &= \frac{1}{2} \text{Tr}_2 \left[\frac{1}{2} \text{Tr}_1 [\mathcal{H}_j] + \tau_1 \left\{ c_1^\dagger \text{Tr}_1 (\mathcal{H}_j c_1), \eta_1 \right\} \right] \\ &= \frac{1}{2^2} \text{Tr}_{1,2} [\mathcal{H}_j] + \frac{1}{2} \tau_1 \text{Tr}_2 \left\{ c_1^\dagger \text{Tr}_1 (\mathcal{H}_j c_1), \eta_1 \right\} \\ \text{Tr}_2 [\mathcal{H}_{j,1} c_2] &= \text{Tr}_2 \left[\frac{1}{2} \text{Tr}_1 [\mathcal{H}_j] c_2 + \tau_1 \left\{ c_1^\dagger \text{Tr}_1 (\mathcal{H}_j c_1), \eta_1 \right\} c_2 \right] \\ &= \frac{1}{2} \text{Tr}_2 [(\text{Tr}_1 \mathcal{H}_j) c_2] + \tau_1 \text{Tr}_2 \left[\left\{ c_1^\dagger \text{Tr}_1 (\mathcal{H}_j c_1), \eta_1 \right\} c_2 \right] \\ \implies \tau_2 \left\{ c_2^\dagger \text{Tr}_2 (\mathcal{H}_{j,1} c_2), \eta_2 \right\} &= \frac{1}{2} \tau_2 \left\{ c_2^\dagger \text{Tr}_2 [(\text{Tr}_1 \mathcal{H}_j) c_2], \eta_2 \right\} \end{aligned} \quad (3.4)$$

Therefore,

$$\mathcal{H}_{j,2} = \frac{1}{2^2} \text{Tr}_{1,2} [\mathcal{H}_j] + \frac{1}{2} \tau_1 \text{Tr}_2 \left\{ c_1^\dagger \text{Tr}_1 (\mathcal{H}_j c_1), \eta_1 \right\} + \frac{1}{2} \tau_2 \left\{ c_2^\dagger \text{Tr}_2 [(\text{Tr}_1 \mathcal{H}_j) c_2], \eta_2 \right\} \quad (3.5)$$

As part of keeping only the first order quantum fluctuations, we consider only one electron on the shell at a time. That is, in the second term, \mathcal{H}_j will have only 1 electron on the j^{th} shell and that electron will have the index 1. Similarly, in the third term, the only electron on the shell will have index 2. That means that the Tr_2 and Tr_1 are redundant in second and third terms respectively. These redundant traces will cancel the half factors in front, giving us

$$\begin{aligned} \mathcal{H}_{j,2} &= \frac{1}{2^2} \text{Tr}_{1,2} [\mathcal{H}_j] + \tau_1 \left\{ c_1^\dagger \text{Tr}_1 (\mathcal{H}_j c_1), \eta_1 \right\} + \tau_2 \left\{ c_2^\dagger \text{Tr}_2 [(\mathcal{H}_j) c_2], \eta_2 \right\} \\ &= \frac{1}{2^2} \text{Tr}_{1,2} [\mathcal{H}_j] + \sum_{l=1}^2 \tau_l \left\{ c_l^\dagger \text{Tr}_l (\mathcal{H}_j c_l), \eta_l \right\} \end{aligned} \quad (3.6)$$

Proceeding similarly, the effective Hamiltonian obtained after disentangling all (N_j) momentum+spin states on the shell Λ_j is

$$\mathcal{H}_{j-1} = 2^{-N_j} \text{Tr}_{1,2,\dots,N_j} \mathcal{H}_j + \sum_{l=1}^{N_j} \tau_l \left\{ c_l^\dagger \text{Tr}_l [\mathcal{H}_j c_l], \eta_l \right\} \quad (3.7)$$

Here, l and the indices $1, 2, \dots, N$ refer to fermionic degrees of freedom on the shell Λ_j . That is, they are a placeholder for (\mathbf{q}, β) where $|\mathbf{q}| = \Lambda_j$ and $\beta \in \{\uparrow, \downarrow\}$. More explicitly, the index 1 designates $(\mathbf{k}_{1,\uparrow})$, the index 2 means $(\mathbf{k}_{1,\downarrow})$, the index 3 means $(\mathbf{k}_{2,\uparrow})$ and so on.

Let $j = j_{\max}$. That is, this is the first decoupling. Then, $\mathcal{H}_j = \mathcal{H}$. The first term in eq. 3.7 is

$$\frac{1}{2^{N_j}} \text{Tr}_{1,2,\dots,N_j} \mathcal{H} \quad (3.8)$$

As discussed before, in order to consider just the leading order quantum fluctuations, we will make the following simplification: While evaluating the first trace, say Tr_1 , we will assume the only electron on the j^{th} shell has that index. Therefore,

$$\begin{aligned} \frac{1}{2} \text{Tr}_{k_1\sigma} \mathcal{H} &= \frac{1}{2} \text{Tr}_{k_1\sigma} \left[\sum_{\substack{k < \Lambda_j \\ \alpha}} \epsilon_k \hat{n}_{k\alpha} + \frac{J}{2} \sum_{\substack{k, k' < \Lambda_j \\ \alpha, \alpha'}} \mathbf{S} \cdot \sigma_{\alpha\alpha'} c_{k\alpha}^\dagger c_{k'\alpha'} + \epsilon_{k_1} \hat{n}_{k_1\sigma} + \frac{J}{2} S^z \sigma_\sigma^z \hat{n}_{k_1\sigma} \right] \\ &= \sum_{\substack{k < \Lambda_j \\ \alpha}} \epsilon_k \hat{n}_{k\alpha} + \frac{J}{2} \sum_{\substack{k, k' < \Lambda_j \\ \alpha, \alpha'}} \mathbf{S} \cdot \sigma_{\alpha\alpha'} c_{k\alpha}^\dagger c_{k'\alpha'} + \frac{\epsilon_{k_1}}{2} + \frac{J}{2} S^z \frac{\sigma}{2} \\ &\equiv H_{j-1} + \frac{\epsilon_{k_1}}{2} + \frac{J}{2} S^z \frac{\sigma}{2} \end{aligned} \quad (3.9)$$

The H_{j-1} part will not change. To take the next partial trace $k_1\bar{\sigma}$, we add an electron in this state to the previous Hamiltonian:

$$\begin{aligned} \frac{1}{2} \text{Tr}_{k_1\bar{\sigma}} \left[\frac{1}{2} \text{Tr}_{k_1\sigma} \mathcal{H} \right] &= \frac{1}{2} \text{Tr}_{k_1\bar{\sigma}} \left[H_{j-1} + \frac{\epsilon_{k_1}}{2} + \frac{J}{2} S^z \frac{\sigma}{2} + \epsilon_{k_1} \hat{n}_{k_1\bar{\sigma}} + \frac{J}{2} S^z \sigma_\sigma^z \hat{n}_{k_1\bar{\sigma}} \right] \\ &= H_{j-1} + \frac{\epsilon_{k_1}}{2} + \frac{J}{2} S^z \frac{\sigma}{2} + \frac{1}{2} \text{Tr}_{k_1\bar{\sigma}} \left[\epsilon_{k_1} \hat{n}_{k_1\bar{\sigma}} + \frac{J}{2} S^z \sigma_\sigma^z \hat{n}_{k_1\bar{\sigma}} \right] \\ &= H_{j-1} + \frac{\epsilon_{k_1}}{2} + \frac{J}{2} S^z \frac{\sigma}{2} + \frac{\epsilon_{k_1}}{2} + \frac{J}{2} S^z \frac{\bar{\sigma}}{2} \\ &= H_{j-1} + \epsilon_{k_1} \end{aligned} \quad (3.10)$$

Tracing over all the states will then give

$$\frac{1}{2^{N_j}} \text{Tr}_{1,2,\dots,N_j} \mathcal{H} = H_{j-1} + \sum_{|k|=\Lambda_j} \epsilon_k \quad (3.11)$$

Now I need to compute the second term. That term involves another trace, $\text{Tr}_l [\mathcal{H}c_l]$. The kinetic energy term will not survive this. The only terms that will survive are those that have exactly one $c_{q\beta}^\dagger$.

$$\langle n_{q\beta} | c_{k\alpha}^\dagger c_{k\alpha} c_{q\beta} | n_{q\beta} \rangle = \begin{cases} c_{k\alpha}^\dagger c_{k\alpha} \langle n_{q\beta} | c_{q\beta} | n_{q\beta} \rangle = 0 & \text{if } k\alpha \neq q\beta \\ \langle n_{q\beta} | c_{q\beta}^\dagger c_{q\beta}^2 | n_{q\beta} \rangle = 0 & \text{if } k\alpha = q\beta \end{cases} \quad (3.12)$$

$$\langle n_{q\beta} | c_{k\alpha}^\dagger c_{k'\alpha'} c_{q\beta} | n_{q\beta} \rangle = \begin{cases} c_{k\alpha}^\dagger c_{k'\alpha'} \langle n_{q\beta} | c_{q\beta} | n_{q\beta} \rangle = 0 & \text{if } k\alpha \neq q\beta \neq k'\alpha' \\ \langle n_{q\beta} | c_{q\beta}^\dagger c_{q\beta}^2 | n_{q\beta} \rangle = 0 & \text{if } k\alpha = q\beta = k'\alpha' \\ \langle n_{q\beta} | c_{q\beta}^\dagger c_{k'\alpha'} c_{q\beta} | n_{q\beta} \rangle = c_{k'\alpha'} & \text{if } k\alpha = q\beta \neq k'\alpha' \end{cases} \quad (3.13)$$

Therefore, the trace becomes

$$\text{Tr} [\mathcal{H}c_{q\beta}] = \frac{J}{2} \sum_{k\alpha \neq q\beta} \mathbf{S} \cdot \sigma_{\beta\alpha} c_{k\alpha} \quad (3.14)$$

In line with our intention of keeping just the leading order quantum fluctuations and placing just one electron on the current shell, we will assume the $k\alpha$ degree of freedom lies on lower shells ($k < \Lambda^*$).

$$\text{Tr} [\mathcal{H}c_{q\beta}] = \frac{J}{2} \sum_{k < \Lambda^*, \alpha} \mathbf{S} \cdot \sigma_{\beta\alpha} c_{k\alpha} \quad (3.15)$$

Its conjugate is

$$\text{Tr} [c_{q\beta}^\dagger \mathcal{H}] = \frac{J}{2} \sum_{k < \Lambda^*, \alpha} \mathbf{S} \cdot \sigma_{\alpha\beta} c_{k\alpha}^\dagger \quad (3.16)$$

We also compute another trace: $\text{Tr}_{q\beta} (\mathcal{H}^D \hat{n}_{q\beta})$, where

$$\begin{aligned} \mathcal{H}^D \hat{n}_{q\beta} &= \mathcal{H}_{j-1}^D \hat{n}_{q\beta} + \epsilon_q \hat{n}_{q\beta}^2 + \frac{J}{2} S^z \sigma_{\beta\beta}^z \hat{n}_{q\beta}^2 \\ &= \left[\mathcal{H}_{j-1}^D + \epsilon_q + \frac{J}{2} S^z \sigma_{\beta\beta}^z \right] \hat{n}_{q\beta} \end{aligned} \quad (3.17)$$

Therefore,

$$\text{Tr}_{q\beta} (\mathcal{H}^D \hat{n}_{q\beta}) = \mathcal{H}_{j-1}^D + \epsilon_q + \frac{J}{2} S^z \sigma_{\beta\beta}^z \quad (3.18)$$

This allows us to write the $\eta_{q\beta}$:

$$\begin{aligned} \eta_{q\beta} &= \left[\eta_{q\beta}^\dagger \right]^\dagger = \left[\frac{1}{\hat{\omega} - \text{Tr} (\mathcal{H}^D \hat{n}_{q\beta}) \hat{n}_{q\beta}} c_{q\beta}^\dagger T \right]^\dagger \\ &= \text{Tr} \left[c_{q\beta}^\dagger \mathcal{H} \right] c_{q\beta} \frac{1}{\hat{\omega} - \text{Tr} (\mathcal{H}^D \hat{n}_{q\beta}) \hat{n}_{q\beta}} \\ &= \frac{J}{2} \sum_{k < \Lambda^*, \alpha} \mathbf{S} \cdot \sigma_{\alpha\beta} c_{k\alpha}^\dagger c_{q\beta} \frac{1}{\hat{\omega} - \left(\mathcal{H}_{j-1}^D + \epsilon_q + \frac{J}{2} S^z \sigma_{\beta\beta}^z \right) \hat{n}_{q\beta}} \end{aligned} \quad (3.19)$$

Since $\hat{\omega}$ is diagonal in $\hat{n}_{q\beta}$ by definition, we can absorb the diagonal piece $\mathcal{H}_{j-1}^D \hat{n}_{q\beta}$ and a constant ϵ_q and redefine $\hat{\omega}$.

$$\begin{aligned}\eta_{q\beta} &= \frac{J}{2} \sum_{k < \Lambda^*, \alpha} \mathbf{S} \cdot \sigma_{\alpha\beta} c_{k\alpha}^\dagger c_{q\beta} \frac{1}{\hat{\omega} - \epsilon_q \tau_{q\beta} - \frac{J}{2} S^z \sigma_{\beta\beta}^z \hat{n}_{q\beta}} \\ &= \frac{J}{2} \sum_{k < \Lambda^*, \alpha} \mathbf{S} \cdot \sigma_{\alpha\beta} c_{k\alpha}^\dagger c_{q\beta} \frac{1}{\hat{\omega} - \epsilon_q \tau_{q\beta} - \frac{J}{2} S^z \sigma_{\beta\beta}^z \hat{n}_{q\beta}}\end{aligned}\quad (3.20)$$

Define $\mathcal{X}_{q\beta} = \sum_{k < \Lambda^*, \alpha} \mathbf{S} \cdot \sigma_{\alpha\beta} c_{k\alpha}^\dagger c_{q\beta}$. The second term in the effective Hamiltonian \mathcal{H}_{j-1} can then be written as

$$\sum_{q\beta} \tau_{q\beta} \left\{ c_{q\beta}^\dagger \text{Tr}_{q\beta} [\mathcal{H}_j c_{q\beta}], \eta_{q\beta} \right\} = \sum_{\substack{|q|=\Lambda_j, \\ \beta=\uparrow, \downarrow}} \tau_{q\beta} \left\{ \frac{J}{2} \mathcal{X}_{q\beta}^\dagger, \frac{J}{2} \mathcal{X}_{q\beta} \frac{1}{\hat{\omega} - \epsilon_q \tau_{q\beta} - \frac{J}{2} S^z \sigma_{\beta\beta}^z \hat{n}_{q\beta}} \right\}\quad (3.21)$$

Substituting $\hat{\omega} = 2\omega \tau_{q\beta}$,

$$\sum_{q\beta} \tau_{q\beta} \left\{ c_{q\beta}^\dagger \text{Tr}_{q\beta} [\mathcal{H}_j c_{q\beta}], \eta_{q\beta} \right\} = \left(\frac{J}{2} \right)^2 \sum_{\substack{|q|=\Lambda_j, \\ \beta=\uparrow, \downarrow}} \tau_{q\beta} \left\{ \mathcal{X}_{q\beta}^\dagger, \mathcal{X}_{q\beta} \frac{1}{2\omega \tau_{q\beta} - \epsilon_q \tau_{q\beta} - \frac{J}{2} S^z \sigma_{\beta\beta}^z \hat{n}_{q\beta}} \right\}\quad (3.22)$$

Assuming the factor with ω commutes, we can write this as

$$\sum_{q\beta} \tau_{q\beta} \left\{ c_{q\beta}^\dagger \text{Tr}_{q\beta} [\mathcal{H}_j c_{q\beta}], \eta_{q\beta} \right\} = \left(\frac{J}{2} \right)^2 \sum_{\substack{|q|=\Lambda_j, \\ \beta=\uparrow, \downarrow}} \tau_{q\beta} \frac{1}{2\omega \tau_{q\beta} - \epsilon_q \tau_{q\beta} - \frac{J}{2} S^z \sigma_{\beta\beta}^z \hat{n}_{q\beta}} \left\{ \mathcal{X}_{q\beta}^\dagger, \mathcal{X}_{q\beta} \right\}\quad (3.23)$$

The anticommutator can now be evaluated:

$$\begin{aligned}\left\{ \mathcal{X}_{q\beta}^\dagger, \mathcal{X}_{q\beta} \right\} &= \sum_{k, k' < \Lambda^*, \alpha\gamma} \left\{ \mathbf{S} \cdot \sigma_{\beta\gamma} c_{q\beta}^\dagger c_{k'\gamma}, \mathbf{S} \cdot \sigma_{\alpha\beta} c_{k\alpha}^\dagger c_{q\beta} \right\} \\ &= \sum_{a,b} \sum_{\substack{k, k' < \Lambda^* \\ \alpha\gamma}} \left\{ S^a \sigma_{\beta\gamma}^a c_{q\beta}^\dagger c_{k'\gamma}, S^b \sigma_{\alpha\beta}^b c_{k\alpha}^\dagger c_{q\beta} \right\} \\ &= \sum_{a,b} \sum_{\substack{k, k' < \Lambda^* \\ \alpha\gamma}} \left[S^a S^b \sigma_{\beta\gamma}^a \sigma_{\alpha\beta}^b \hat{n}_{q\beta} c_{k'\gamma} c_{k\alpha}^\dagger + S^b S^a \sigma_{\alpha\beta}^b \sigma_{\beta\gamma}^a (1 - \hat{n}_{q\beta}) c_{k\alpha}^\dagger c_{k'\gamma} \right]\end{aligned}\quad (3.24)$$

Since we will replace $\hat{\omega}$ with some function of τ_l , the fraction with ω will commute with all the operators. Therefore,

$$\begin{aligned}
\sum_{l=1}^N \tau_l \left\{ c_l^\dagger \text{Tr}_l [\mathcal{H}_j c_l], \eta_l \right\} &= \sum_{\substack{|q|=\Lambda_j, \\ \beta=\uparrow, \downarrow}} \frac{J^2 \tau_{q\beta}}{4 (\hat{\omega} - \xi_{q\beta} \tau_{q\beta})} \sum_{\substack{k\alpha \neq q\beta \\ k'\alpha' \neq q\beta}} \left\{ \mathbf{S} \cdot \sigma_{\beta\alpha} c_{q\beta}^\dagger c_{k\alpha}, \mathbf{S} \cdot \sigma_{\alpha'\beta} c_{k'\alpha'}^\dagger c_{q\beta} \right\} \\
&= \frac{J}{2} \sum_{l=1}^N \frac{J \tau_{q\beta}}{2 (\hat{\omega} - \xi_{q\beta} \tau_{q\beta})} \sum_{m \neq l \neq m'} \mathcal{C}_{m,m',l}
\end{aligned} \tag{3.25}$$

where $m \equiv k\alpha, m' \equiv k'\alpha'$ and $\mathcal{C}_{lmm'}$ is the anticommutator $\left\{ \mathbf{S} \cdot \sigma_{\beta\alpha} c_{q\beta}^\dagger c_{k\alpha}, \mathbf{S} \cdot \sigma_{\alpha'\beta} c_{k'\alpha'}^\dagger c_{q\beta} \right\}$. Denote the prefactor in eq. 3.25 as $\Gamma_{q\beta}$. The sum $\sum_{m \neq l \neq m'}$ is over all points m, m' except the point $m = m' = l$. Split the sum in the following way:

$$\sum_{m \neq l \neq m'} = \sum_{\substack{|k|, |k'| < \Lambda_j \\ \alpha, \alpha'}} + \sum_{\substack{k=k'=q \\ \alpha=\alpha' \neq \beta}} + \text{other terms} \tag{3.26}$$

The second term gives

$$\begin{aligned}
\sum_{\substack{k=k'=q \\ \alpha=\alpha' \neq \beta}} \left\{ \mathbf{S} \cdot \sigma_{\beta\alpha} c_{q\beta}^\dagger c_{q\alpha}, \mathbf{S} \cdot \sigma_{\alpha'\beta} c_{k'\alpha'}^\dagger c_{q\beta} \right\} &= \sum_{\alpha \neq \beta} \left\{ \mathbf{S} \cdot \sigma_{\beta\alpha} c_{q\beta}^\dagger c_{q\alpha}, \mathbf{S} \cdot \sigma_{\alpha\beta} c_{q\alpha}^\dagger c_{q\beta} \right\} \\
&= \sum_{\alpha \neq \beta} (\mathbf{S} \cdot \sigma_{\beta\alpha}) (\mathbf{S} \cdot \sigma_{\alpha\beta}) \hat{n}_{q\beta} (1 - \hat{n}_{q\alpha}) + \alpha \leftrightarrow \beta
\end{aligned} \tag{3.27}$$

Keeping in mind that $\alpha \neq \beta$ and hence only those $\sigma_{\beta\alpha}$ that have off-diagonal terms can survive, the scalar products evaluate to

$$(\mathbf{S} \cdot \sigma_{\beta\alpha}) (\mathbf{S} \cdot \sigma_{\alpha\beta}) = \left(S^x \sigma_{\beta\alpha}^x + S^y \sigma_{\beta\alpha}^y \right) \left(S^x \sigma_{\alpha\beta}^x + S^y \sigma_{\alpha\beta}^y \right) \tag{3.28}$$

Now, we use the following identities:

$$(S^a)^2 = \frac{1}{4} \tag{3.29}$$

$$S^x S^y = -S^y S^x = \frac{i}{2} S^z \tag{3.30}$$

$$\sigma_{\alpha\beta}^x = \sigma_{\beta\alpha}^x \tag{3.31}$$

$$\sigma_{\alpha\beta}^y = -\sigma_{\beta\alpha}^y \tag{3.32}$$

For the special case $\alpha \neq \beta$, we have

$$\sigma_{\alpha\beta}^x = \sigma_{\beta\alpha}^x = 1 \tag{3.33}$$

$$\sigma_{\alpha\beta}^y = -\sigma_{\beta\alpha}^y = -i\sigma_{\alpha\alpha}^z = i\sigma_{\beta\beta}^z \tag{3.34}$$

Using these identities, the scalar product becomes

$$\begin{aligned}
(\mathbf{S} \cdot \sigma_{\beta\alpha}) (\mathbf{S} \cdot \sigma_{\alpha\beta}) &= (S^x - S^y \sigma_{\alpha\beta}^y) (S^x + S^y \sigma_{\alpha\beta}^y) \\
&= \frac{1}{4} + [S^x, S^y] \sigma_{\alpha\beta}^y - \frac{1}{4} (\sigma_{\alpha\beta}^y)^2 \\
&= \frac{1}{2} + i S^z \sigma_{\alpha\beta}^y \\
&= \frac{1}{2} - S^z \sigma_{\beta\beta}^z
\end{aligned} \tag{3.35}$$

The second term then gives

$$\begin{aligned}
\sum_{\substack{k=k'=q \\ \alpha=\alpha' \neq \beta}} \left\{ \mathbf{S} \cdot \sigma_{\beta\alpha} c_{q\beta}^\dagger c_{q\alpha}, \mathbf{S} \cdot \sigma_{\alpha'\beta} c_{k'\alpha'q\beta}^\dagger \right\} &= \sum_{\alpha \neq \beta} \hat{n}_{q\beta} (1 - \hat{n}_{q\alpha}) \left(\frac{1}{2} - S^z \sigma_{\beta\beta}^z \right) + \alpha \leftrightarrow \beta \\
&= \left[\frac{(n_{q\beta} - n_{q\bar{\beta}})^2}{2} - S^z \sigma_{\beta\beta}^z 2 \frac{n_{q\beta} - n_{q\bar{\beta}}}{2} \right]
\end{aligned} \tag{3.36}$$

The term with S^z can be simplified:

$$\sigma_{\beta\beta}^z \frac{n_{q\beta} - n_{q\bar{\beta}}}{2} = \begin{cases} \frac{n_{q\uparrow} - n_{q\downarrow}}{2} & \text{when } \beta = \uparrow \\ -\frac{n_{q\downarrow} - n_{q\uparrow}}{2} & \text{when } \beta = \downarrow \end{cases} = \frac{n_{q\uparrow} - n_{q\downarrow}}{2} \equiv s_q^z \tag{3.37}$$

The second term thus becomes

$$\sum_{\substack{k=k'=q \\ \alpha=\alpha' \neq \beta}} \left\{ \mathbf{S} \cdot \sigma_{\beta\alpha} c_{q\beta}^\dagger c_{q\alpha}, \mathbf{S} \cdot \sigma_{\alpha'\beta} c_{k'\alpha'q\beta}^\dagger \right\} = \left[\frac{(n_{q\beta} - n_{q\bar{\beta}})^2}{2} - 2S^z s_q^z \right] \tag{3.38}$$

We drop the first term because it does not have S^z and hence does not renormalize the Ising term. Joining with the $\Gamma_{q\beta}$ prefactor, we get

$$\frac{J}{2} \sum_{l=1}^N \Gamma_{q\beta} \sum_{\substack{k=k'=q \\ \alpha=\alpha' \neq \beta}} \mathcal{C}_{m,m',l} = \frac{J}{2} \sum_{l=1}^N \frac{J\tau_{q\beta}}{2(\hat{\omega} - \xi_{q\beta}\tau_{q\beta})} (-2S^z s_q^z) \tag{3.39}$$

We replace $\hat{\omega}$ with $2\omega\tau_{q\beta}$. This gives

$$\frac{J}{2} \sum_{l=1}^N \Gamma_{q\beta} \sum_{\substack{k=k'=q \\ \alpha=\alpha' \neq \beta}} \mathcal{C}_{m,m',l} = -\frac{J^2}{2} \sum_{|q|=\Lambda_j} S^z s_q^z \sum_{\beta} \frac{\tau_{q\beta}}{(2\omega\tau_{q\beta} - \xi_{q\beta}\tau_{q\beta})} \tag{3.40}$$

By setting $\tau_{q\beta} = \frac{\beta}{2}$, we can perform the sum over β :

$$\sum_{\beta} \frac{\tau_{q\beta}}{(2\omega\tau_{q\beta} - \xi_{q\beta}\tau_{q\beta})} = \frac{1}{2} \left[\frac{1}{\omega - \frac{\epsilon_q}{2} - \frac{1}{2} \frac{J}{2} S^z \sigma_{\uparrow\uparrow}^z} - \frac{1}{-\omega + \frac{\epsilon_q}{2} + \frac{1}{2} \frac{J}{2} S^z \sigma_{\downarrow\downarrow}^z} \right] = \frac{\omega - \frac{\epsilon_q}{2}}{(\omega - \frac{\epsilon_q}{2})^2 - \frac{J^2}{64}} \tag{3.41}$$

In total, we get

$$-\frac{J^2}{2} \frac{\omega - \frac{\epsilon_j}{2}}{\left(\omega - \frac{\epsilon_j}{2}\right)^2 - \frac{J^2}{64}} \sum_{|q|=\Lambda_j} S^z s_q^z \quad (3.42)$$

The first term gives

$$\begin{aligned} \sum_{\substack{|k|, |k'| < \Lambda_j \\ \alpha, \alpha'}} \mathcal{C}_{m, m', l} &= \sum_{\substack{|k|, |k'| < \Lambda_j \\ \alpha, \alpha'}} \left\{ \mathbf{S} \cdot \sigma_{\beta\alpha'} c_{q\beta}^\dagger c_{k'\alpha'}, \mathbf{S} \cdot \sigma_{\alpha\beta} c_{k\alpha}^\dagger c_{q\beta} \right\} \\ &= (1 - \hat{n}_{q\beta}) \sum_{\substack{|k|, |k'| < \Lambda_j \\ \alpha, \alpha'}} c_{k\alpha}^\dagger c_{k'\alpha'} (\mathbf{S} \cdot \sigma_{\alpha\beta}) (\mathbf{S} \cdot \sigma_{\beta\alpha'}) \\ &\quad + \hat{n}_{q\beta} \sum_{\substack{|k|, |k'| < \Lambda_j \\ \alpha, \alpha'}} c_{k'\alpha'} c_{k\alpha}^\dagger (\mathbf{S} \cdot \sigma_{\beta\alpha'}) (\mathbf{S} \cdot \sigma_{\alpha\beta}) \end{aligned} \quad (3.43)$$

Taking the term with $1 - \hat{n}_{q\beta}$ as the renormalizing term, the renormalization becomes

$$\begin{aligned} \frac{J}{2} \sum_{l=1}^N \Gamma_{q\beta} \sum_{\substack{|k|, |k'| < \Lambda_j \\ \alpha, \alpha'}} \mathcal{C}_{m, m', l} &= \frac{J^2}{4} \sum_{\substack{|k|, |k'| < \Lambda_j \\ \alpha, \alpha'}} \sum_{|q|=\Lambda_j, \beta} \frac{\tau_{q\beta}}{(2\omega\tau_{q\beta} - \xi_{q\beta}\tau_{q\beta})} c_{k\alpha}^\dagger c_{k'\alpha'} (\mathbf{S} \cdot \sigma_{\alpha\beta}) (\mathbf{S} \cdot \sigma_{\beta\alpha'}) \\ &= \frac{J^2}{4} \sum_{\substack{|k|, |k'| < \Lambda_j \\ \alpha, \alpha'}} c_{k\alpha}^\dagger c_{k'\alpha'} \sum_{|q|=\Lambda_j, \beta} \frac{\tau_{q\beta}}{(2\omega\tau_{q\beta} - \xi_{q\beta}\tau_{q\beta})} (\mathbf{S} \cdot \sigma_{\alpha\beta}) (\mathbf{S} \cdot \sigma_{\beta\alpha'}) \end{aligned} \quad (3.44)$$

Combining eqs. 3.11, 3.42 and 3.44, the renormalized Hamiltonian is

$$\begin{aligned} \mathcal{H}_{j-1} &= \sum_{\substack{k, k' \\ \alpha, \alpha'}}^< \left(\epsilon_k \hat{n}_{k\alpha} + \frac{J}{2} \mathbf{S} \cdot \sigma_{\alpha\alpha'} c_{k\alpha}^\dagger c_{k'\alpha'} \right) + n_j \epsilon_j - \frac{J^2}{2} \frac{\omega - \frac{\epsilon_j}{2}}{\left(\omega - \frac{\epsilon_j}{2}\right)^2 - \frac{J^2}{64}} \sum_{|q|=\Lambda_j} S^z s_q^z \\ &\quad + \frac{J^2}{4} \sum_{\substack{|k|, |k'| < \Lambda_j \\ \alpha, \alpha'}} c_{k\alpha}^\dagger c_{k'\alpha'} \sum_{|q|=\Lambda_j, \beta} \frac{\tau_{q\beta}}{(2\omega\tau_{q\beta} - \xi_{q\beta}\tau_{q\beta})} (\mathbf{S} \cdot \sigma_{\alpha\beta}) (\mathbf{S} \cdot \sigma_{\beta\alpha'}) \end{aligned} \quad (3.45)$$

3.2 Fixed-point Hamiltonian

The RG starts from $j = N$ and runs down to $j^* < N$. As a result, integrating out the j^{th} Hamiltonian gives the $(j-1)^{\text{th}}$ Hamiltonian. Λ_N is the highest momentum being integrated out and is thus the Brillouin zone edge. From eq. 3.45, we can write

$$\begin{aligned} J^{j-1} &= J^j + \frac{n_j J_j^2 \left(\omega - \frac{\hbar v_F}{2} \Lambda^j \right)}{\left(\omega - \frac{\hbar v_F}{2} \Lambda^j \right)^2 - \frac{1}{16} J_j^2} \\ \implies \Delta J^j &\equiv J^{j-1} - J^j = \frac{n_j J_j^2 \left(\omega - \frac{\hbar v_F}{2} \Lambda^j \right)}{\left(\omega - \frac{\hbar v_F}{2} \Lambda^j \right)^2 - \frac{1}{16} J_j^2} \end{aligned} \quad (3.46)$$

Parameterizing the momenta as $\Lambda_j = \Lambda_N e^{j-N}$, we can write

$$-\Delta \log \Lambda_j \equiv -(\log \Lambda_{j-1} - \log \Lambda_j) = \log \frac{\Lambda_j}{\Lambda_{j-1}} = \log \frac{e^{j-N}}{e^{j-N-1}} = 1 \quad (3.47)$$

We can then write the difference equation, eq. 3.46, as

$$-\frac{\Delta J_j}{\Delta \Lambda_j} = \frac{n_j J_j^2 \left(\omega - \frac{\hbar v_F}{2} \Lambda_j \right)}{\left(\omega - \frac{\hbar v_F}{2} \Lambda_j \right)^2 - \frac{1}{16} J_j^2} \quad (3.48)$$

Changing this to a continuum equation gives

$$\frac{dJ}{d\tilde{\Lambda}} = -\frac{n}{\Lambda} \frac{\left(\omega - \tilde{\Lambda} \right)}{\left(\frac{\omega - \tilde{\Lambda}}{J} \right)^2 - \frac{1}{16}} \quad (3.49)$$

where $\tilde{\Lambda} = \frac{\hbar v_F}{2} \Lambda$. Define a dimensionless coupling

$$K = \frac{J}{\omega - \tilde{\Lambda}} \quad (3.50)$$

Therefore,

$$\frac{dJ}{d\tilde{\Lambda}} = \frac{d \left[K \left(\omega - \tilde{\Lambda} \right) \right]}{d\tilde{\Lambda}} = \left(\omega - \tilde{\Lambda} \right) \frac{dK}{d\tilde{\Lambda}} - K \quad (3.51)$$

Rewriting the RG equation 3.49 in terms of K gives

$$\begin{aligned} \left(\omega - \tilde{\Lambda} \right) \frac{dK}{d\tilde{\Lambda}} - K &= -\frac{nK^2}{\Lambda} \frac{\left(\omega - \tilde{\Lambda} \right)}{1 - \frac{K^2}{16}} \\ \Rightarrow \tilde{\Lambda} \frac{dK}{d\tilde{\Lambda}} &= \frac{K}{\frac{\omega}{\tilde{\Lambda}} - 1} + \frac{nK^2}{\frac{K^2}{16} - 1} \end{aligned} \quad (3.52)$$

Close to the Fermi surface ($\tilde{\Lambda} \rightarrow 0$),

$$\frac{dK}{d \log \tilde{\Lambda}} = \frac{n(0)K^2}{\frac{K^2}{16} - 1} \equiv \beta(K) \quad (3.53)$$

where $n(0)$ is the DOS on FS. There are two fixed points, $K^* = 0$ and $K^* = 4$. At both these points, $\beta(K)$ changes sign. At $K = 0$, it changes between 0^+ and 0^- , while at $K = 4$, it switches between $\pm\infty$.

Integrating eq. 3.53 from Λ_N to Λ^* gives

$$\begin{aligned}
& \int_{K_N}^{K^*} dK \frac{1 - \frac{K^2}{16}}{K^2} = -n(0) \int_{\Lambda_N}^{\Lambda^*} d \log \tilde{\Lambda} \\
\Rightarrow & -n(0) \log \frac{\Lambda^*}{\Lambda_N} = \int_{K_N}^{K^*} dK \left(\frac{1}{K^2} - \frac{1}{16} \right) = \frac{1}{K_N} - \frac{1}{K^*} - \frac{K^* - K_N}{16} \\
\Rightarrow & \Lambda^* = \Lambda_N \exp \left[-\frac{1}{n(0)} \left(\frac{1}{K_N} + \frac{K_N}{16} - \frac{1}{2} \right) \right] \\
\Rightarrow & T_K = \frac{E(\Lambda^*)}{k_B} = \frac{\hbar v_F \Lambda^*}{k_B} = \frac{\hbar v_F \Lambda_N}{k_B} \exp \left[-\frac{1}{n(0)} \left(\frac{1}{K_N} + \frac{K_N}{16} - \frac{1}{2} \right) \right] \\
\Rightarrow & \xi_K = \frac{2\pi}{\Lambda^*} = \frac{2\pi}{\Lambda_N} \exp \left[\frac{1}{n(0)} \left(\frac{1}{K_N} + \frac{K_N}{16} - \frac{1}{2} \right) \right]
\end{aligned} \tag{3.54}$$

At the fixed point, the effective Hamiltonian is of the form

$$\begin{aligned}
\mathcal{H} &= \sum_{k < \Lambda^*, \sigma} \epsilon_k \hat{n}_{k\sigma} + \frac{J^*}{2} \sum_{\substack{k_1, k_2 < \Lambda^* \\ \alpha, \beta}} \mathbf{S} \cdot \sigma_{\alpha\beta} c_{k_1, \alpha}^\dagger c_{k_2, \beta} + \sum_{k > \Lambda^*} J_k S^z s_k^z \\
&\equiv \mathcal{H}_0^* + \frac{J^*}{2} \sum_{\substack{k_1, k_2 < \Lambda^* \\ \alpha, \beta}} \mathbf{S} \cdot \sigma_{\alpha\beta} c_{k_1, \alpha}^\dagger c_{k_2, \beta} + \sum_{k > \Lambda^*} J_k S^z s_k^z
\end{aligned} \tag{3.55}$$

\mathcal{H}_0^* is the kinetic energy of the Kondo cloud (electrons lying inside Λ^*). The zero-mode Hamiltonian is

$$\begin{aligned}
\mathcal{H}_{\text{coll}} &= \frac{J^*}{2} \sum_{\substack{k_1, k_2 < \Lambda^* \\ \alpha, \beta}} \mathbf{S} \cdot \sigma_{\alpha\beta} c_{k_1, \alpha}^\dagger c_{k_2, \beta} + \sum_{k > \Lambda^*} J_k S^z s_k^z \\
&= J^* \mathbf{S} \cdot \mathbf{s} + S^z \sum_{k > \Lambda^*} J_k s_k^z
\end{aligned} \tag{3.56}$$

where

$$\mathbf{s} = \sum_{k_1, k_2 < \Lambda^*} \mathbf{s}_{k_1, k_2} \equiv \sum_{\substack{k_1, k_2 < \Lambda^* \\ \alpha, \beta}} \frac{\vec{\sigma}_{\alpha\beta}}{2} c_{k_1, \alpha}^\dagger c_{k_2, \beta} \tag{3.57}$$

and (consequently),

$$s_{k,q}^z = \sum_{\alpha,\beta} \frac{\sigma_{\alpha\beta}^z}{2} c_{k,\alpha}^\dagger c_{q,\beta} = \frac{1}{2} (c_{k\uparrow}^\dagger c_{q\uparrow} + c_{k\downarrow}^\dagger c_{q\downarrow}) \quad (3.58)$$

$$s_{k,q}^x = \frac{1}{2} (c_{k\uparrow}^\dagger c_{q\downarrow} + c_{k\downarrow}^\dagger c_{q\uparrow}) \quad (3.59)$$

$$s_{k,q}^y = \frac{-i}{2} (c_{k\uparrow}^\dagger c_{q\downarrow} - c_{k\downarrow}^\dagger c_{q\uparrow}) \quad (3.60)$$

$$s_{k,q}^+ = c_{k\uparrow}^\dagger c_{q\downarrow} \quad (3.61)$$

$$s_{k,q}^- = c_{k\downarrow}^\dagger c_{q\uparrow} \quad (3.62)$$

$$s_k^z \equiv s_{k,k}^z = \sum_{\alpha,\beta} \frac{\sigma_{\alpha\beta}^z}{2} c_{k,\alpha}^\dagger c_{k,\beta} = \frac{1}{2} (\hat{n}_{k\uparrow} - \hat{n}_{k\downarrow}) \quad (3.63)$$

The ground state is

$$|\Psi^*\rangle = \frac{1}{\sqrt{2}} \sum_{|\mathbf{k}| < \Lambda^*} (|\uparrow_d\rangle |\downarrow_{\mathbf{k}}\rangle |\downarrow_{\mathbf{q}}\rangle - |\downarrow_d\rangle |\uparrow_{\mathbf{k}}\rangle |\uparrow_{\mathbf{q}}\rangle) \quad (3.64)$$

The ground state energy is obtained by acting the Hamiltonian on this state:

$$\begin{aligned} \mathcal{H}_{\text{coll}} |\Psi^*\rangle &= -\frac{3J^*}{2} |\Psi^*\rangle - \frac{J^q}{4} |\Psi^*\rangle \\ &= -\frac{1}{4} (6J^* + J^q) |\Psi^*\rangle \end{aligned} \quad (3.65)$$

The $-\frac{3J^*}{2}$ comes from the action of

$$\mathbf{S} \cdot \mathbf{s} = S_{\text{tot}} (S_{\text{tot}} + 1) - S^2 - s^2 = S_{\text{tot}} (S_{\text{tot}} + 1) - \frac{3}{2} \quad (3.66)$$

on the singlet state ($S_{\text{tot}} = 0$), \mathbf{S}_{tot} being $\mathbf{S} + \mathbf{s}$. The lowest value of the energy occurs when \mathbf{q} is placed on the shell Λ^* , because J^q falls rapidly with distance from the Kondo cloud. Therefore,

$$E_g = -\frac{7J^*}{4} \quad (3.67)$$

3.3 Some entanglement measures

We can represent the ground state wavefunction in a compact manner:

$$|\Psi^*\rangle = |\uparrow_d\rangle |\downarrow_{\mathbf{k}}\rangle |\downarrow_{\mathbf{q}}\rangle - |\downarrow_d\rangle |\uparrow_{\mathbf{k}}\rangle |\uparrow_{\mathbf{q}}\rangle \quad (3.68)$$

$|\uparrow_k\rangle$ represents $\sum_{k < \Lambda^*} |\uparrow_k\rangle$. We can label the states of the combined Hilbert space of Kondo cloud and impurity as 1, 2, 3 and 4, which represent $|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle$ respectively. The

ground state, in this notation, is $|\Psi^*\rangle = \frac{1}{\sqrt{2}} (|2\rangle |\downarrow\rangle - |3\rangle |\uparrow\rangle)$. First we compute the density matrix for this state:

$$\begin{aligned}\rho_{\text{all}} &= |\Psi^*\rangle \langle \Psi^*| \\ &= \frac{1}{2} [|2\rangle \langle 2| \otimes |\downarrow\rangle \langle \downarrow| - |2\rangle \langle 3| \otimes |\downarrow\rangle \langle \uparrow| - |3\rangle \langle 2| \otimes |\uparrow\rangle \langle \downarrow| + |3\rangle \langle 3| \otimes |\uparrow\rangle \langle \uparrow|]\end{aligned}\quad (3.69)$$

The reduced density matrix for the local Fermi liquid (LFL) is obtained by partial tracing over the cloud+impurity, that is, over the states $|1\rangle$ through $|4\rangle$.

$$\begin{aligned}\rho_{\text{LFL}} &= \text{Tr}_{\text{imp+cloud}} [\rho_{\text{all}}] \\ &= \sum_i \langle i| \rho_{\text{all}} |i\rangle \\ &= \frac{1}{2} (|\uparrow\rangle \langle \uparrow| + |\downarrow\rangle \langle \downarrow|)\end{aligned}\quad (3.70)$$

This is just $\frac{1}{2}$ times identity matrix in two dimensions, so the eigenvalues are both $\frac{1}{2}$. The von-Neumann entropy for a matrix ρ is defined as $S = -\sum_{\lambda} \lambda \ln \lambda$, where the sum is over the eigenvalues of the matrix.

$$S_{\text{LFL}} = -2 \times \frac{1}{2} \ln \frac{1}{2} = \ln 2 \quad (3.71)$$

Since von-Neumann entropy is independent of which partial system I trace over, it will be same if I had instead traced over the imp+cloud system. Still I will calculate the reduced density matrix because I will need it to trace over the cloud or the impurity.

$$\begin{aligned}\rho_{\text{imp+cloud}} &= \text{Tr}_{\text{LFL}} [\rho_{\text{all}}] \\ &= \sum_{m=\pm\uparrow,\downarrow} \langle m| \rho_{\text{all}} |m\rangle \\ &= \frac{1}{2} (|2\rangle \langle 2| + |3\rangle \langle 3|) \\ &= \frac{1}{2} \begin{pmatrix} 0 & & & \\ & 1 & & \\ & & 1 & \\ & & & 0 \end{pmatrix}\end{aligned}\quad (3.72)$$

As mentioned just before, the non-zero eigenvalues are again both $\frac{1}{2}$ so the von-Neumann entropy is the same as S_{LFL} :

$$S_{\text{imp+cloud}} = -2 \times \frac{1}{2} \ln \frac{1}{2} = \ln 2 \quad (3.73)$$

To find the von-Neumann entropy for just the impurity, we can partial trace over the cloud:

$$\begin{aligned}
\rho_{\text{imp}} &= \text{Tr}_{\text{cloud}} [\rho_{\text{imp+cloud}}] \\
&= \text{Tr}_{\text{cloud}} \left[\frac{1}{2} (|\uparrow\rangle \langle\uparrow| \otimes |\downarrow\rangle \langle\downarrow| + |\downarrow\rangle \langle\downarrow| \otimes |\uparrow\rangle \langle\uparrow|) \right] \\
&= \frac{1}{2} (|\uparrow\rangle \langle\uparrow| + |\downarrow\rangle \langle\downarrow|) \\
&= \frac{1}{2} \begin{pmatrix} 1 & \\ & 1 \end{pmatrix} \\
S_{\text{imp}} &= \ln 2
\end{aligned} \tag{3.74}$$

which also means

$$S_{\text{cloud}} = \ln 2 \tag{3.75}$$

We thus have the conclusion that all partial systems (imp, cloud, LFL, imp+cloud, cloud+LFL, imp+LFL) have an entropy of $\ln 2$ and are thus maximally entangled with their partners. We can also compute the mutual information between the LFL and imp+cloud systems. It is defined as $I(A, B) = S_A + S_B - S_{AB}$.

$$I(\text{imp+cloud}, \text{LFL}) = S_{\text{imp+cloud}} + S_{\text{LFL}} - S_{\text{all}} = 2 \ln 2 \tag{3.76}$$

where I used the fact that S_{all} is 0 because $|\Psi^*\rangle$ is a pure state.

3.4 Local Fermi liquid Hamiltonian

The effective Hamiltonian of the disentangled electrons is found by tracing out the impurity and cloud parts from the total density matrix of the low energy Hamiltonian $\mathcal{H}_{\text{coll}}$:

$$\begin{aligned}
\rho &= \exp [-\beta \mathcal{H}_{\text{coll}}] \\
&= \exp [-\beta (\mathcal{H}_0 + J^* \mathbf{S} \cdot \mathbf{s} + 2S^z h)]
\end{aligned} \tag{3.77}$$

where \mathcal{H}_0 is the kinetic energy of the disentangled electrons and $h = \frac{1}{2} \sum_{k>\Lambda^*} J_k s_k^z$.

$$\begin{aligned}
\rho &= \rho_0 \exp [-\beta (J^* \mathbf{S} \cdot \mathbf{s} + 2S^z h)] \\
\rho_{\text{eff}} &= \rho_0 \text{Tr}_{\text{imp+cloud}} \exp [-\beta (J^* \mathbf{S} \cdot \mathbf{s} + 2S^z h)]
\end{aligned} \tag{3.78}$$

To take the trace, we diagonalize the matrix:

$$\begin{aligned}
J^* \mathbf{S} \cdot \mathbf{s} + 2S^z h &= \begin{pmatrix} |\uparrow\uparrow\rangle & |\uparrow\downarrow\rangle & |\downarrow\uparrow\rangle & |\downarrow\downarrow\rangle \\ h + \frac{J^*}{4} & h - \frac{J^*}{4} & \frac{J^*}{2} & \\ & \frac{J^*}{2} & -h - \frac{J^*}{4} & \\ & & & -h + \frac{J^*}{4} \end{pmatrix} \\
&\rightarrow \begin{pmatrix} |\uparrow\uparrow\rangle & |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle & |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle & |\downarrow\downarrow\rangle \\ h + \frac{J^*}{4} & -\frac{J^*}{4} + A & & \\ & & -\frac{J^*}{4} - A & \\ & & & -h + \frac{J^*}{4} \end{pmatrix}
\end{aligned} \tag{3.79}$$

where $A = \sqrt{h^2 + \left(\frac{J^*}{2}\right)^2}$. We can now take the trace by exponentiating this matrix:

$$\begin{aligned}
\exp[-\beta(J^* \mathbf{S} \cdot \mathbf{s} + 2S^z h)] &= \begin{pmatrix} |\uparrow\uparrow\rangle & |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle & |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle & |\downarrow\downarrow\rangle \\ e^{-\beta(h + \frac{J^*}{4})} & e^{-\beta(-\frac{J^*}{4} + A)} & & \\ & & e^{-\beta(-\frac{J^*}{4} - A)} & \\ & & & e^{-\beta(-h + \frac{J^*}{4})} \end{pmatrix} \\
\Rightarrow \text{Tr} \left[e^{-\beta(J^* \mathbf{S} \cdot \mathbf{s} + 2S^z h)} \right] &= e^{-\beta \frac{J^*}{4}} 2 \cosh \beta h + e^{\beta \frac{J^*}{4}} 2 \cosh A\beta
\end{aligned} \tag{3.80}$$

In the limit of low temperature ($\beta \rightarrow \infty$), we have $e^{-\beta \frac{J^*}{4}} \rightarrow 0$ and $\cosh A\beta \rightarrow e^{A\beta}$. We can then write

$$\rho_{\text{eff}} = \rho_0 \text{Tr} \left[e^{-\beta(J^* \mathbf{S} \cdot \mathbf{s} + 2S^z h)} \right] = \exp \left(-\beta \left[\mathcal{H}_0 - \frac{J^*}{4} - A \right] \right) \equiv \exp(-\beta \mathcal{H}_{\text{eff}}) \tag{3.81}$$

The effective Hamiltonian for the disentangled electrons is thus

$$\begin{aligned}
\mathcal{H}_{\text{eff}} &= \mathcal{H}_0 - \frac{J^*}{4} - A = \mathcal{H}_0 - \frac{J^*}{4} - \sqrt{h^2 + \left(\frac{J^*}{2}\right)^2} \\
&= \mathcal{H}_0 - \frac{J^*}{4} - \frac{J^*}{2} \sqrt{1 + \left(\frac{2h}{J^*}\right)^2} \\
&= \mathcal{H}_0 - \frac{J^*}{4} - \frac{J^*}{2} - \frac{h^2}{J^*} + \dots \\
&\approx \sum_{k > \Lambda^*, \sigma} \epsilon_k \hat{n}_{k\sigma} - \frac{3J^*}{4} - \frac{h^2}{J^*} \\
&= \sum_{k > \Lambda^*, \sigma} \epsilon_k \hat{n}_{k\sigma} - \frac{3J^*}{4} - \frac{1}{J^*} \sum_{k, q > \Lambda^*} J^k J^q s_k^z s_q^z
\end{aligned} \tag{3.82}$$

Recognizing the constant negative energy as the Kondo singlet ground state energy and noting that since the Λ^k falls sharply as we move away from Λ^* , we can truncate the second sum at the first shell Λ^* , we obtain the Hamiltonian for the local Fermi liquid.

$$\mathcal{H}_{LFL} = \epsilon_* \sum_{k=\Lambda^*, \sigma} \hat{n}_{k\sigma} - J^* \sum_{k, q=\Lambda^*} s_k^z s_q^z \tag{3.83}$$

LFL stands for local Fermi liquid; it is the Hamiltonian closest to the cloud. We now consider quasiparticle excitations $\delta n_{k\sigma}$. The ground state energy is

$$\begin{aligned}
E_0 &= \epsilon_* \sum_{k=\Lambda^*, \sigma} n_{k\sigma} - J^* \sum_{k, q=\Lambda^*} s_k^z s_q^z \\
&= \epsilon_* \sum_{k=\Lambda^*, \sigma} n_{k\sigma} - \frac{J^*}{4} \sum_{k, q=\Lambda^*} (n_{k\uparrow} - n_{k\downarrow}) (n_{q\uparrow} - n_{q\downarrow}) \\
&= \epsilon_* \sum_{k=\Lambda^*, \sigma} n_{k\sigma} - \frac{J^*}{4} \sum_{k, q=\Lambda^*, \sigma} n_{k\sigma} (n_{q\sigma} - n_{q\bar{\sigma}})
\end{aligned} \tag{3.84}$$

The excited energy is

$$\begin{aligned}
E &= \epsilon_* \sum_{k=\Lambda^*, \sigma} (n_{k\sigma} + \delta n_{k\sigma}) - \frac{J^*}{4} \sum_{k, q=\Lambda^*} (n_{k\sigma} + \delta n_{k\sigma}) (n_{q\sigma} - n_{q\bar{\sigma}} + \delta n_{q\sigma} - \delta n_{q\bar{\sigma}}) \\
&= E_0 + \epsilon_* \sum_{k=\Lambda^*, \sigma} \delta n_{k\sigma} - \\
&\quad \frac{J^*}{4} \sum_{k, q=\Lambda^*} [n_{k\sigma} (\delta n_{q\sigma} - \delta n_{q\bar{\sigma}}) + \delta n_{k\sigma} (n_{q\sigma} - n_{q\bar{\sigma}}) + \delta n_{k\sigma} (\delta n_{q\sigma} - \delta n_{q\bar{\sigma}})] \\
&= E_0 + \epsilon_* \sum_{k=\Lambda^*, \sigma} \delta n_{k\sigma} - \frac{J^*}{4} \sum_{k, q=\Lambda^*} [2n_{k\sigma} (\delta n_{q\sigma} - \delta n_{q\bar{\sigma}}) + \delta n_{k\sigma} (\delta n_{q\sigma} - \delta n_{q\bar{\sigma}})]
\end{aligned} \tag{3.85}$$

Therefore, the energy of one quasiparticle is

$$\begin{aligned}\xi_{k\sigma} &= \frac{\delta E}{\delta n_{k\sigma}} = \epsilon_* - \frac{J^*}{4} \sum_{q=\Lambda^*} [2n_{q\sigma} - 2n_{q\bar{\sigma}} + \delta n_{q\sigma} - \delta n_{q\bar{\sigma}} + \delta n_{q\sigma} - \delta n_{q\bar{\sigma}}] \\ &= \epsilon_* - \frac{J^*}{2} \sum_{q=\Lambda^*} [n_{q\sigma} - n_{q\bar{\sigma}} + \delta n_{q\sigma} - \delta n_{q\bar{\sigma}}]\end{aligned}\quad (3.86)$$

Assuming that the Kondo cloud imparts an interaction of the form $Un_{\uparrow}n_{\downarrow}$ to the LFL, the self energy will have only antiferromagnetic terms:

$$\xi_{k\sigma} = \epsilon_* + \frac{J^*}{2} \sum_{q=\Lambda^*} [n_{q\bar{\sigma}} + \delta n_{q\bar{\sigma}}] \quad (3.87)$$

Due to scattering from impurity, the local Fermi liquid electrons suffer a phase shift $\delta_{k\sigma}$, such that their spherical wave wavefunctions are of the form

$$\psi(\mathbf{r}) \sim \frac{1}{r} \sin(\mathbf{k} \cdot \mathbf{r} + \delta_{k\sigma}) \quad (3.88)$$

Open boundary conditions ensure

$$\mathbf{k} \cdot \mathbf{R} + \delta_{k\sigma} = n\pi \implies k = \frac{n\pi - \delta_{k\sigma}}{R} \quad (3.89)$$

We thus see that as a result of the scattering, the momentum eigenvalues change by $\Delta k = -\frac{1}{R}\delta_{k\sigma}$. This will change E_k by

$$\Delta E_k = \frac{\partial E_k}{\partial k} \Delta k = -\frac{\delta_{k\sigma}}{R} \frac{\partial E_k}{\partial k} \quad (3.90)$$

The total energy in presence of scattering is thus

$$\xi_{k\sigma} = E_k - \frac{\delta_{k\sigma}}{R} \frac{\partial E_k}{\partial k} \quad (3.91)$$

Comparing with eq. 3.86 and noting that $E_k = \epsilon_*$ is the bare kinetic energy, we get

$$\frac{\delta_{k\sigma}}{R} \frac{\partial E_k}{\partial k} = -\frac{J^*}{2} \sum_{q=\Lambda^*} [n_{q\bar{\sigma}} + \delta n_{q\bar{\sigma}}] \quad (3.92)$$

The quantity $\frac{\partial E_k}{\partial k}$ is calculated as

$$\begin{aligned}dE_k &\equiv E_{\mathbf{k}+\mathbf{dk}} - E_k \\ &= -2t [\cos(k_x + dk) + \cos(k_y + dk)] + 2t [\cos(k_x) + \cos(k_y)] \\ &= 2tdk (\sin k_x + \sin k_y)\end{aligned}\quad (3.93)$$

Close to the Fermi surface, $(\sin k_x + \sin k_y) \approx k_{Fx} + k_{Fy}$. Therefore,

$$\frac{\partial E_k}{\partial k} = 2t (k_{Fx} + k_{Fy}) \quad (3.94)$$

Defining $\Delta\epsilon \equiv 2t (k_{Fx} + k_{Fy}) \frac{\pi}{R}$, we can write eq. 3.92 as

$$\begin{aligned} \frac{\delta_{k\sigma}}{\pi} \Delta\epsilon &= -\frac{J^*}{2} \sum_{q=\Lambda^*} [n_{q\bar{\sigma}} + \delta n_{q\bar{\sigma}}] \\ \implies \delta_{k\sigma} &= -\frac{\pi J^*}{2\Delta\epsilon} \sum_{q=\Lambda^*} [n_{q\bar{\sigma}} + \delta n_{q\bar{\sigma}}] \end{aligned} \quad (3.95)$$

We can expand the phase shift as a function of the quasiparticle energy and the quasiparticle distribution, around $n_{k\sigma} = n_{k\sigma}^{(0)}$ and $\epsilon_* = E_F$:

$$\begin{aligned} \delta_{k\sigma} &= \delta_{k\sigma}(n^{(0)}, E_F) + \frac{\partial \delta_{k\sigma}}{\partial \epsilon_*} (\epsilon_* - E_F) + \sum_q \frac{\partial \delta_{k\sigma}}{\partial n_{q\bar{\sigma}}} \delta n_{q\bar{\sigma}} \\ &= \frac{\pi}{2} + \alpha (\epsilon_* - E_F) + \Phi \sum_q \delta n_{q\bar{\sigma}} \end{aligned} \quad (3.96)$$

From here on, Nozières' calculation gives the value of Wilson ratio.

3.5 Calculation of susceptibility from partition function

The susceptibility can be calculated from the impurity partition function Z_{imp} , eq. 1.491:

$$\chi_{\text{imp}} = \lim_{B \rightarrow 0} \frac{1}{Z_{\text{imp}}^2 \beta} \left[Z_{\text{imp}} \frac{\partial^2 Z_{\text{imp}}}{\partial B^2} - \left(\frac{\partial Z_{\text{imp}}}{\partial B} \right)^2 \right] \quad (3.97)$$

To calculate Z_{imp} , we will use the Hamiltonian of the impurity+cloud:

$$\mathcal{H}_K = J^* \mathbf{S} \cdot \mathbf{s} + h S^z \quad (3.98)$$

In the presence of a magnetic field on the impurity, the Hamiltonian becomes

$$\begin{aligned} \mathcal{H}_K(B) &= J^* \mathbf{S} \cdot \mathbf{s} + h S^z + B S^z \\ &= J^* \mathbf{S} \cdot \mathbf{s} + B' S^z \end{aligned} \quad (3.99)$$

where $B = J^* \sum_k s_k^z$ and h is an external field. $B' = B + h$ is the total field on the impurity spin. We can write the expression for susceptibility in terms of this total field:

$$\chi_{\text{imp}} = \lim_{B' \rightarrow h} \frac{1}{Z_{\text{imp}}^2 \beta} \left[Z_{\text{imp}} \frac{\partial^2 Z_{\text{imp}}}{\partial B'^2} - \left(\frac{\partial Z_{\text{imp}}}{\partial B'} \right)^2 \right] \quad (3.100)$$

From eq. 3.99, we can write the partition function:

$$Z_{\text{imp}} = 2e^{\frac{\beta J^*}{4}} \left[\cosh \frac{\beta B'}{2} + \cosh \left(\frac{\beta}{2} \sqrt{B'^2 + J^2} \right) \right] \quad (3.101)$$

Since the $2e^{\frac{\beta J^*}{4}}$ factor in front will remain unaffected by the derivatives and will get canceled from numerator and denominator while calculating χ , I will drop that henceforth.

$$\begin{aligned} Z_{\text{imp}} &= \cosh \frac{\beta B'}{2} + \cosh \left(\frac{\beta}{2} \sqrt{B'^2 + J^2} \right) \\ Z_{\text{imp}}^2 &= \cosh^2 \frac{\beta B'}{2} + \cosh^2 \left(\frac{\beta}{2} \sqrt{B'^2 + J^2} \right) + 2 \cosh \frac{\beta B'}{2} \cosh \left(\frac{\beta}{2} \sqrt{B'^2 + J^2} \right) \\ \frac{\partial Z_{\text{imp}}}{\partial B'} &= \frac{\beta}{2} \left[\sinh \frac{\beta B'}{2} + \frac{B'}{\sqrt{B'^2 + J^2}} \sinh \left(\frac{\beta}{2} \sqrt{B'^2 + J^2} \right) \right] \end{aligned} \quad (3.102)$$

$$\begin{aligned} \left(\frac{\partial Z_{\text{imp}}}{\partial B'} \right)^2 &= \left(\frac{\beta}{2} \right)^2 \left\{ \sinh^2 \frac{\beta B'}{2} + \frac{B'^2}{B'^2 + J^2} \sinh^2 \left(\frac{\beta}{2} \sqrt{B'^2 + J^2} \right) \right. \\ &\quad \left. + 2 \sinh \frac{\beta B'}{2} \frac{B'}{\sqrt{B'^2 + J^2}} \sinh \left(\frac{\beta}{2} \sqrt{B'^2 + J^2} \right) \right\} \end{aligned} \quad (3.103)$$

$$\begin{aligned} \frac{\partial^2 Z_{\text{imp}}}{\partial B'^2} &= \left(\frac{\beta}{2} \right)^2 \left\{ \cosh \frac{\beta B'}{2} + \frac{B'^2}{B'^2 + J^2} \cosh \left(\frac{\beta}{2} \sqrt{B'^2 + J^2} \right) \right. \\ &\quad \left. + \frac{2}{\beta} \frac{J^2}{(J^2 + B'^2)^{\frac{3}{2}}} \sinh \left(\frac{\beta}{2} \sqrt{B'^2 + J^2} \right) \right\} \end{aligned} \quad (3.104)$$

$$\begin{aligned} Z_{\text{imp}} \frac{\partial^2 Z_{\text{imp}}}{\partial B'^2} &= \left(\frac{\beta}{2} \right)^2 \left\{ \cosh^2 \frac{\beta B'}{2} + \cosh \frac{\beta B'}{2} \cosh \left(\frac{\beta}{2} \sqrt{J^2 + B'^2} \right) \right. \\ &\quad \left. + Z_{\text{imp}} \frac{B'^2}{B'^2 + J^2} \cosh \left(\frac{\beta}{2} \sqrt{B'^2 + J^2} \right) \right. \\ &\quad \left. + Z_{\text{imp}} \frac{2}{\beta} \frac{J^2}{(J^2 + B'^2)^{\frac{3}{2}}} \sinh \left(\frac{\beta}{2} \sqrt{B'^2 + J^2} \right) \right\} \end{aligned} \quad (3.105)$$

The total expression is

$$\chi_{\text{imp}} = \frac{\beta \sigma_1 + \frac{2 \sinh \sigma_2}{\sqrt{\sigma_3}} + \frac{B^2 \beta \cosh \sigma_2}{\sigma_3} - \frac{2B^2 \sinh \sigma_2}{\sigma_3^{\frac{3}{2}}}}{4 (\cosh \sigma_2 + \sigma_1)} - \left[\frac{\frac{\sinh \frac{\beta B}{2}}{2} + \frac{B \sinh \sigma_2}{2\sqrt{\sigma_3}}}{\cosh \sigma_2 + \sigma_1} \right]^2 \quad (3.106)$$

$$\sigma_1 = \cosh \frac{\beta B}{2}, \sigma_3 = B^2 + J^{*2}, \sigma_2 = \frac{\beta \sqrt{\sigma_3}}{2} \quad (3.107)$$

In the absence of LFL magnetization, we can set $B = 0$. Then eq. 3.103 vanishes and what remains is

$$Z_{\text{imp}} = 1 + \cosh \frac{\beta J^*}{2} \quad (3.108)$$

$$\frac{\partial^2 Z_{\text{imp}}}{\partial B'^2} = \left(\frac{\beta}{2}\right)^2 \left[1 + \frac{2}{\beta J^*} \sinh \left(\frac{\beta J^*}{2}\right)\right] = \frac{\beta}{2} \left[\frac{\beta}{2} + \frac{1}{J^*} \sinh \left(\frac{\beta J^*}{2}\right)\right] \quad (3.109)$$

$$\chi_{\text{imp}} = \frac{1}{\beta Z_{\text{imp}}} \frac{\partial^2 Z_{\text{imp}}}{\partial B'^2} = \frac{\beta + \frac{2}{J^*} \sinh \left(\frac{\beta J^*}{2}\right)}{4 \left(1 + \cosh \frac{\beta J^*}{2}\right)} \quad (3.110)$$

The Wilson ratio is defined as $W \equiv 4T_K \chi(T=0)$. It turns out to be

$$\begin{aligned} W &= \lim_{\beta \rightarrow \infty} 4T_K \frac{\beta + \frac{2}{J^*} \exp \left(\frac{\beta J^*}{2}\right)}{4 \left(1 + \exp \left(\frac{\beta J^*}{2}\right)\right)} \\ &= \lim_{\beta \rightarrow \infty} 4T_K \frac{\frac{2}{J^*} \exp \left(\frac{\beta J^*}{2}\right)}{4 \exp \left(\frac{\beta J^*}{2}\right)} \\ &= \frac{2T_K}{J^*} \end{aligned} \quad (3.111)$$

The quantity $\frac{\chi}{\beta}$ saturates to a certain value at large temperature:

$$\begin{aligned} \frac{\chi}{\beta}(\beta \rightarrow 0) &= \lim_{\beta \rightarrow 0} \frac{1}{8} \left(1 + \frac{2}{J^*} \frac{\sinh \frac{\beta J^*}{2}}{\beta}\right) \\ &= \frac{1}{4} \end{aligned} \quad (3.112)$$

3.6 Effective Hamiltonian of Kondo cloud

To study the excitations of the Kondo cloud, we look at the Hamiltonian of impurity+cloud:

$$\mathcal{H}^* = \sum_{k < \Lambda^*, \sigma} \epsilon_k \hat{n}_{k\sigma} + J^* \mathbf{S} \cdot \mathbf{s} = \mathcal{H}_0^* + J^* \mathbf{S} \cdot \mathbf{s} \quad (3.113)$$

In order to separate the cloud from the impurity, take the groundstate wavefunction of \mathcal{H}^* :

$$|\Psi\rangle = a_{\downarrow} |\uparrow_{\text{imp}}\rangle |\downarrow\rangle + a_{\uparrow} |\downarrow_{\text{imp}}\rangle |\uparrow\rangle \quad (3.114)$$

Note that $|\uparrow\rangle, |\downarrow\rangle$ are many-electron states. The eigenvalue equation for this state is

$$\begin{aligned} \frac{1}{J^*} (E_0 - \mathcal{H}_0^*) |\Psi\rangle &= \left(S^z s^z + \frac{1}{2} S^+ s^- + \frac{1}{2} S^- s^+\right) (a_{\downarrow} |\uparrow_{\text{imp}}\rangle |\downarrow\rangle + a_{\uparrow} |\downarrow_{\text{imp}}\rangle |\uparrow\rangle) \\ &= \frac{s^z}{2} (a_{\downarrow} |\uparrow_{\text{imp}}\rangle |\downarrow\rangle - a_{\uparrow} |\downarrow_{\text{imp}}\rangle |\uparrow\rangle) + a_{\downarrow} |\downarrow_{\text{imp}}\rangle \frac{s^+}{2} |\downarrow\rangle + a_{\uparrow} |\uparrow_{\text{imp}}\rangle \frac{s^-}{2} |\uparrow\rangle \end{aligned} \quad (3.115)$$

Comparing the coefficients of $|\uparrow_{\text{imp}}\rangle$ and $|\downarrow_{\text{imp}}\rangle$, we get

$$\begin{aligned}\frac{1}{J^*} (E_0 - \mathcal{H}_0^*) a_{\downarrow} |\downarrow\rangle &= \frac{s^z}{2} a_{\downarrow} |\downarrow\rangle + a_{\uparrow} \frac{s^-}{2} |\uparrow\rangle \\ \frac{1}{J^*} (E_0 - \mathcal{H}_0^*) a_{\uparrow} |\uparrow\rangle &= -\frac{s^z}{2} a_{\uparrow} |\uparrow\rangle + a_{\downarrow} \frac{s^+}{2} |\downarrow\rangle\end{aligned}\quad (3.116)$$

From the first equation, we can isolate $|\downarrow\rangle$:

$$|\downarrow\rangle = \left[\frac{1}{J^*} (E_0 - \mathcal{H}_0^*) - \frac{s^z}{2} \right]^{-1} \frac{a_{\uparrow}}{a_{\downarrow}} s^- |\uparrow\rangle \quad (3.117)$$

Substituting this in the second equation gives

$$\begin{aligned}\frac{1}{J^*} (E_0 - \mathcal{H}_0^*) |\uparrow\rangle &= -\frac{s^z}{2} |\uparrow\rangle + \frac{1}{2} s^+ \left[\frac{1}{J^*} (E_0 - \mathcal{H}_0^*) - \frac{s^z}{2} \right]^{-1} s^- |\uparrow\rangle \\ (E_0 - \mathcal{H}_0^*) |\uparrow\rangle &= \left[-\frac{J^*}{2} s^z + \left(\frac{J^*}{2} \right)^2 s^+ \frac{1}{(E_0 - \mathcal{H}_0^*) - \frac{J^*}{2} s^z} s^- \right] |\uparrow\rangle \\ &\equiv \mathcal{H}_{\text{eff}} |\uparrow\rangle\end{aligned}\quad (3.118)$$

Now we can simplify the effective Hamiltonian for the Kondo cloud. First put $E_0 = 0$ and $s^z = \frac{1}{2}$. The latter is obvious from the fact that this is the effective Hamiltonian for the up-spin state. The justification for the former will be given later. Then,

$$\begin{aligned}H_{\text{eff}} &= -\frac{J^*}{4} - \left(\frac{J^*}{2} \right)^2 s^+ \frac{1}{\frac{J^*}{4} + \mathcal{H}_0^*} s^- \\ &= -\frac{J^*}{4} - J^* s^+ \frac{1}{1 + \frac{4\mathcal{H}_0^*}{J^*}} s^-\end{aligned}\quad (3.119)$$

We can expand the denominator in a power series:

$$\frac{1}{1 + \frac{4\mathcal{H}_0^*}{J^*}} = 1 - \frac{4\mathcal{H}_0^*}{J^*} + \frac{16}{J^{*2}} \mathcal{H}_0^{*2} \quad (3.120)$$

Substituting this gives

$$\begin{aligned}H_{\text{eff}} &= -\frac{J^*}{4} - J^* s^+ \left(1 - \frac{4\mathcal{H}_0^*}{J^*} + \frac{16}{J^{*2}} \mathcal{H}_0^{*2} \right) s^- \\ &= -\frac{J^*}{4} - J^* s^+ s^- + 4s^+ \mathcal{H}_0^* s^- - \frac{16}{J^*} s^+ \mathcal{H}_0^{*2} s^-\end{aligned}\quad (3.121)$$

Now we simplify the terms individually:

$$\begin{aligned}
s^+ s^- &= \frac{1}{2} + s^z = 1 \\
\Rightarrow -\frac{J^*}{4} - J^* s^+ s^- &= -\frac{J^*}{4} - J^* = -\frac{5J^*}{4} \\
4s^+ \mathcal{H}_0^* s^- &= 4s^+ s^- \mathcal{H}_0^* + 4s^+ [\mathcal{H}_0^*, s^-] = 4\mathcal{H}_0^* + 4s^+ [\mathcal{H}_0^*, s^-] \\
-\frac{16}{J^*} s^+ \mathcal{H}_0^{*2} s^- &= -\frac{16}{J^*} s^+ \mathcal{H}_0^* (s^- \mathcal{H}_0^* + [\mathcal{H}_0^*, s^-]) \\
&= -\frac{16}{J^*} (s^+ \mathcal{H}_0^* [\mathcal{H}_0^*, s^-] + \mathcal{H}_0^{*2} + s^+ [\mathcal{H}_0^*, s^-] \mathcal{H}_0^*) \\
&= -\frac{16}{J^*} (\mathcal{H}_0^{*2} + s^+ \{\mathcal{H}_0^*, [\mathcal{H}_0^*, s^-]\})
\end{aligned} \tag{3.122}$$

We can calculate the commutator by looking at the expression of s^- from eq. 3.62: $s^- = \sum_{k_1, k_2} c_{k_1\downarrow}^\dagger c_{k_2\uparrow}$. Using the identities

$$\begin{aligned}
[n_{k\sigma}, c_{k_1\downarrow}^\dagger] &= c_{k_1\downarrow}^\dagger \delta_{kk_1} \delta_{\sigma,\downarrow} \\
[n_{k\sigma}, c_{k_2\uparrow}] &= -c_{k_2\uparrow} \delta_{kk_2} \delta_{\sigma,\uparrow}
\end{aligned} \tag{3.123}$$

the commutator becomes

$$\begin{aligned}
[\mathcal{H}_0^*, s^-] &= \sum_{k, k_1, k_2, \sigma} \epsilon_k [n_{k\sigma}, c_{k_1\downarrow}^\dagger c_{k_2\uparrow}] \\
&= \sum_{k, k_1, k_2, \sigma} \epsilon_k \left\{ -c_{k_1\downarrow}^\dagger c_{k_2\uparrow} \delta_{kk_2} \delta_{\sigma,\uparrow} + c_{k_2\uparrow}^\dagger \delta_{kk_1} \delta_{\sigma,\downarrow} c_{k_2\uparrow} \right\} \\
&= \sum_{k_1 k_2} c_{k_1\downarrow}^\dagger c_{k_2\uparrow} (\epsilon_{k_1} - \epsilon_{k_2})
\end{aligned} \tag{3.124}$$

$$\begin{aligned}
4s^+ [\mathcal{H}_0^*, s^-] &= 4 \sum_{k_1 k_2 k_3 k_4} c_{k_3\uparrow}^\dagger c_{k_4\downarrow} c_{k_1\downarrow}^\dagger c_{k_2\uparrow} (\epsilon_{k_1} - \epsilon_{k_2}) \\
\{\mathcal{H}_0^*, [\mathcal{H}_0^*, s^-]\} &= \sum_{k, \sigma, k_1 k_2} \epsilon_k (\epsilon_{k_1} - \epsilon_{k_2}) \left\{ n_{k\sigma}, c_{k_1\downarrow}^\dagger c_{k_2\downarrow} \right\} \\
&= \sum_{k, \sigma, k_1 k_2} \epsilon_k (\epsilon_{k_1} - \epsilon_{k_2}) \left\{ n_{k\sigma}, c_{k_1\downarrow}^\dagger c_{k_2\downarrow} \right\}
\end{aligned} \tag{3.125}$$

To simplify this anticommutator, note

$$\begin{aligned}
c_{k_1\downarrow}^\dagger c_{k_2\uparrow} n_{k\sigma} &= c_{k_1\downarrow}^\dagger c_{k_2\uparrow} c_{k\sigma}^\dagger c_{k\sigma} \\
&= c_{k_1\downarrow}^\dagger \left(\delta_{kk_2} \delta_{\sigma\uparrow} - c_{k\sigma}^\dagger c_{k_2\uparrow} \right) c_{k\sigma} \\
&= \delta_{kk_2} \delta_{\sigma\uparrow} c_{k_1\downarrow}^\dagger c_{k\sigma} + c_{k\sigma}^\dagger c_{k_1\downarrow}^\dagger c_{k_2\uparrow} c_{k\sigma} \\
&= \delta_{kk_2} \delta_{\sigma\uparrow} c_{k_1\downarrow}^\dagger c_{k_2\uparrow} - c_{k\sigma}^\dagger c_{k_1\downarrow}^\dagger c_{k\sigma} c_{k_2\uparrow} \\
&= \delta_{kk_2} \delta_{\sigma\uparrow} c_{k_1\downarrow}^\dagger c_{k_2\uparrow} - c_{k\sigma}^\dagger \left(\delta_{kk_1} \delta_{\sigma\downarrow} - c_{k\sigma} c_{k_1\downarrow}^\dagger \right) c_{k_2\uparrow} \\
&= (\delta_{kk_2} \delta_{\sigma\uparrow} - \delta_{kk_1} \delta_{\sigma\downarrow}) c_{k_1\downarrow}^\dagger c_{k_2\uparrow} + n_{k\sigma} c_{k_1\downarrow}^\dagger c_{k_2\uparrow} \\
\Rightarrow \left\{ n_{k\sigma}, c_{k_1\downarrow}^\dagger c_{k_2\uparrow} \right\} &= [(\delta_{kk_2} \delta_{\sigma\uparrow} - \delta_{kk_1} \delta_{\sigma\downarrow}) + 2n_{k\sigma}] c_{k_1\downarrow}^\dagger c_{k_2\uparrow}
\end{aligned} \tag{3.126}$$

Therefore,

$$\begin{aligned}
\{\mathcal{H}_0^*, [\mathcal{H}_0^*, s^-]\} &= \sum_{k,\sigma,k_1k_2} \epsilon_k (\epsilon_{k_1} - \epsilon_{k_2}) [\delta_{kk_2} \delta_{\sigma\uparrow} - \delta_{kk_1} \delta_{\sigma\downarrow} + 2n_{k\sigma}] c_{k_1\downarrow}^\dagger c_{k_2\uparrow} \\
&= \sum_{k,k_1k_2} (\epsilon_{k_1} - \epsilon_{k_2}) \left[\delta_{kk_2} \epsilon_{k_2} - \delta_{kk_1} \epsilon_{k_1} + 2\epsilon_k \sum_{\sigma} n_{k\sigma} \right] c_{k_1\downarrow}^\dagger c_{k_2\uparrow} \\
&= \sum_{k_1k_2} (\epsilon_{k_1} - \epsilon_{k_2}) \left[\epsilon_{k_2} - \epsilon_{k_1} + 2 \sum_{k\sigma} \epsilon_k n_{k\sigma} \right] c_{k_1\downarrow}^\dagger c_{k_2\uparrow} \\
&\approx - \sum_{k_1k_2} (\epsilon_{k_1} - \epsilon_{k_2})^2 c_{k_1\downarrow}^\dagger c_{k_2\uparrow} \\
\Rightarrow s^+ \{\mathcal{H}_0^*, [\mathcal{H}_0^*, s^-]\} &= - \sum_{k_1k_2k_3k_4} (\epsilon_{k_1} - \epsilon_{k_2})^2 c_{k_3\uparrow}^\dagger c_{k_4\downarrow} c_{k_1\downarrow}^\dagger c_{k_2\uparrow}
\end{aligned} \tag{3.127}$$

These give

$$\begin{aligned}
4s^+ \mathcal{H}_0^* s^- &= 4\mathcal{H}_0^{*2} + 4 \sum_{k_1k_2k_3k_4} c_{k_3\uparrow}^\dagger c_{k_4\downarrow} c_{k_1\downarrow}^\dagger c_{k_2\uparrow} (\epsilon_{k_1} - \epsilon_{k_2}) \\
-\frac{16}{J^*} s^+ \mathcal{H}_0^{*2} s^- &= -\frac{16}{J^*} \mathcal{H}_0^{*2} + \frac{16}{J^*} \sum_{k_1k_2k_3k_4} (\epsilon_{k_1} - \epsilon_{k_2})^2 c_{k_3\uparrow}^\dagger c_{k_4\downarrow} c_{k_1\downarrow}^\dagger c_{k_2\uparrow}
\end{aligned} \tag{3.128}$$

The effective Hamiltonian eq. 3.121 is then

$$H_{\text{eff}} = -\frac{5J^*}{4} + 4\mathcal{H}_0^* - \frac{16}{J^*} \mathcal{H}_0^{*2} + \sum_{k_1k_2k_3k_4} \left[4(\epsilon_{k_1} - \epsilon_{k_2}) + \frac{16}{J^*} (\epsilon_{k_1} - \epsilon_{k_2})^2 \right] c_{k_3\uparrow}^\dagger c_{k_4\downarrow} c_{k_1\downarrow}^\dagger c_{k_2\uparrow} \tag{3.129}$$

This is the effective Kondo cloud Hamiltonian for the state $|\uparrow\uparrow\rangle$.

We can also evaluate the effective Hamiltonian for the orthogonal state $|\downarrow\rangle$. First we solve the coupled set of eqs. 3.116 to eliminate $|\uparrow\rangle$:

$$\begin{aligned} |\uparrow\rangle &= \left[\frac{1}{J^*} (E_0 - \mathcal{H}_0^*) + \frac{s^z}{2} \right]^{-1} \frac{a_{\downarrow}}{a_{\uparrow}} \frac{s^+}{2} |\downarrow\rangle \\ \implies (E_0 - \mathcal{H}_0^*) |\downarrow\rangle &= \left[\frac{J^*}{2} s^z + \left(\frac{J^*}{2} \right)^2 s^- \frac{1}{(E_0 - \mathcal{H}_0^*) + \frac{J^*}{2} s^z} s^+ \right] |\downarrow\rangle \end{aligned} \quad (3.130)$$

Again substituting $E = 0$ and $s^z = -\frac{1}{2}$ gives

$$\begin{aligned} H_{\text{eff}} &= -\frac{J^*}{4} - \left(\frac{J^*}{2} \right)^2 s^- \frac{1}{\mathcal{H}_0^* + \frac{J^*}{4}} s^+ \\ &= -\frac{J^*}{4} - J^* s^- \frac{1}{1 + \frac{4\mathcal{H}_0^*}{J^*}} s^+ \\ &= -\frac{J^*}{4} - J^* s^- \left(1 - \frac{4\mathcal{H}_0^*}{J^*} + \frac{16}{J^{*2}} \mathcal{H}_0^{*2} \right) s^+ \\ &= -\frac{J^*}{4} - J^* s^- s^+ + 4s^- \mathcal{H}_0^* s^+ - \frac{16}{J^*} s^- \mathcal{H}_0^{*2} s^+ \\ &= -\frac{J^*}{4} - J^* \left(\frac{1}{2} - s^z \right) + 4s^- \mathcal{H}_0^* s^+ - \frac{16}{J^*} s^- \mathcal{H}_0^{*2} s^+ \\ &= -\frac{5J^*}{4} + 4 \left[\mathcal{H}_0^* + \sum (\epsilon_{k_1} - \epsilon_{k_2}) c_{k_3\downarrow}^\dagger c_{k_4\uparrow} c_{k_1\uparrow}^\dagger c_{k_2\downarrow} \right] \\ &\quad - \frac{16}{J^*} \left[\mathcal{H}_0^{*2} + \sum (\epsilon_{k_1}^2 - \epsilon_{k_2}^2) c_{k_3\downarrow}^\dagger c_{k_4\uparrow} c_{k_1\uparrow}^\dagger c_{k_2\downarrow} \right] \\ &= -\frac{5J^*}{4} + 4\mathcal{H}_0^* - \frac{16}{J^*} \mathcal{H}_0^{*2} + \sum \left[4(\epsilon_{k_1} - \epsilon_{k_2}) + \frac{16}{J^*} (\epsilon_{k_2}^2 - \epsilon_{k_1}^2) \right] c_{k_3\downarrow}^\dagger c_{k_4\uparrow} c_{k_1\uparrow}^\dagger c_{k_2\downarrow} \end{aligned} \quad (3.131)$$

Justification for the choice $E = 0$

We want to look at the excitations of the Kondo model in the ground state of the cloud+impurity composite system. If we assume that a single localized impurity cannot destabilize the Fermi surface of the Kondo cloud electrons, the total energy of composite system must be greater than zero. Otherwise, the total system will come below the Fermi surface to form a bound system and the Fermi surface will get destabilized. Consequently, the minimum energy of the composite system has to be $E_0 = 0$.

The requirement that the total energy of the composite system be zero constrains the kinetic energy of the Kondo cloud. This is understood by noting that from eq. 3.55, the Hamiltonian of Kondo+impurity part is $\mathcal{H}_0^* + \mathbf{S} \cdot \mathbf{s}$. This should give an eigenvalue of 0

in the ground state. The second term in the Hamiltonian acting on the singlet state gives $-\frac{3J^*}{2}$. Therefore, we get

$$\mathcal{H}_0^* - \frac{3J^*}{2} = E_0 = 0 \quad (3.132)$$

$$\implies \mathcal{H}_0^s = \frac{3J^*}{2} \quad (3.133)$$

This is the minimum value of the kinetic energy for the Kondo cloud Hamiltonian; anything lower than this would lead to a total energy E_0 less than 0 and the destabilization of the Fermi surface. This tells us that just as one electron comes below the Fermi surface to form the singlet with the impurity spin, other electrons have to excite suitably above the Fermi surface (that is, become more energetic) in order to constrain the ground state energy at 0. Excitations of the cloud then involve higher values of $\mathcal{H}_0^* > \frac{3J^*}{2}$ and lead to excitations of the composite system as a whole ($E_0 > 0$). The spectrum of \mathcal{H}_0^* can then be thought to be gapped; the kinetic energy must start from a non-zero value. It is not possible to have a kinetic energy infinitesimally close to the Fermi surface.

4 Anderson Model URG

$$\mathcal{H} = \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{k\sigma} \left(V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right) + \sum_{\sigma} \epsilon_{d\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \quad (4.1)$$

One electron on shell

At first order, the rotated Hamiltonian is

$$\mathcal{H}_{j-1} = 2^{-n_j} \text{Tr}_{1,2,\dots,n_j} \mathcal{H}_j + \sum_{q\beta} \tau_{q\beta} \left\{ c_{q\beta}^\dagger \text{Tr}_{q\beta} (\mathcal{H} c_{q\beta}), \eta_{q\beta} \right\} \quad (4.2)$$

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 .

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:

$$\begin{aligned} \frac{1}{2} \text{Tr}_{q\uparrow} \mathcal{H}_j &= \sum_{k < \Lambda_N, \sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{\sigma} \epsilon_{d\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \frac{1}{2} \text{Tr}_{q\uparrow} \{ \epsilon_k \hat{n}_{q\uparrow} \} \\ &= \sum_{k < \Lambda_N, \sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{\sigma} \epsilon_{d\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \frac{1}{2} \epsilon_q \\ \frac{1}{2} \text{Tr}_{q\downarrow} \frac{1}{2} \text{Tr}_{q\uparrow} \mathcal{H}_j &= \sum_{k < \Lambda_N, \sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{\sigma} \epsilon_{d\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \epsilon_q \\ \implies 2^{-n_j} \text{Tr}_{1,2,\dots,n_j} \mathcal{H}_j &= \sum_{k < \Lambda_N, \sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{\sigma} \epsilon_{d\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \sum_{|q|=\Lambda_N} \epsilon_q \end{aligned} \quad (4.3)$$

$$\implies 2^{-n_j} \text{Tr}_{1,2,\dots,n_j} \mathcal{H}_j = \sum_{k < \Lambda_N, \sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{\sigma} \epsilon_{d\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \sum_{|q|=\Lambda_N} \epsilon_q \quad (4.4)$$

Calculation of second term The second term involves some other traces:

$$\begin{aligned} \text{Tr}_{q\beta} (\mathcal{H} c_{q\beta}) &= \sum_{k\sigma} V_k \text{Tr}_{q\beta} \left(c_{k\sigma}^\dagger c_{d\sigma} c_{q\beta} \right) \\ &= \sum_{k\sigma} V_k c_{d\sigma} \delta_{\sigma\beta} \delta_{kq} \\ &= V_q c_{d\beta} \end{aligned} \quad (4.5)$$

$$\text{Tr}_{q\beta} \left(c_{q\beta}^\dagger \mathcal{H} \right) = V_q^* c_{d\beta}^\dagger \quad (4.6)$$

$$\begin{aligned}
\mathcal{H}^D &= \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{\sigma} \epsilon_{d\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \\
\text{Tr}_{q\beta} (\mathcal{H}^D \hat{n}_{q\beta}) &= \sum_{k < \Lambda_N, \sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{\sigma} \epsilon_{d\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \epsilon_q \\
\eta_{q\beta} &= \text{Tr}_{q\beta} \left(c_{q\beta}^\dagger \mathcal{H} \right) c_{q\beta} \frac{1}{\hat{\omega} - \text{Tr}_{q\beta} (\mathcal{H}^D \hat{n}_{q\beta}) \hat{n}_{q\beta}} \\
&= V_q^* c_{d\beta}^\dagger c_{q\beta} \frac{1}{\hat{\omega} - \left(\sum_{k < \Lambda_N, \sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{\sigma} \epsilon_{d\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \right) \hat{n}_{q\beta} - \epsilon_q \hat{n}_{q\beta}} \\
&= V_q^* c_{d\beta}^\dagger c_{q\beta} \frac{1}{\omega \hat{n}_{q\beta} - \left(\sum_{\sigma} \epsilon_{d\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + \epsilon_q \right) \hat{n}_{q\beta}}
\end{aligned} \tag{4.7}$$

At the last step, **I replaced $\hat{\omega} - \sum_{k < \Lambda_N, \sigma} \epsilon_k \hat{n}_{k\sigma} \hat{n}_{q\beta}$ with $\omega \hat{n}_{q\beta}$** . Note that since this term has a $c_{d\beta}^\dagger$, 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 $\hat{n}_{q\beta}$ in the denominator to 1. Putting together the individual pieces, we can now write the second term:

$$\sum_{q\beta} \tau_{q\beta} \left\{ c_{q\beta}^\dagger \text{Tr}_{q\beta} (\mathcal{H} c_{q\beta}), \eta_{q\beta} \right\} = \sum_{q\beta} \tau_{q\beta} \left\{ V_q c_{q\beta}^\dagger c_{d\beta}, V_q^* c_{d\beta}^\dagger c_{q\beta} \frac{1}{\omega - \epsilon_q - \epsilon_{d\bar{\beta}} \hat{n}_{d\bar{\beta}}} \right\} \tag{4.8}$$

We now note that the factor with ω can be written as follows:

$$\frac{1}{\omega - \epsilon_q - \epsilon_{d\bar{\beta}} \hat{n}_{d\bar{\beta}}} = \frac{\hat{n}_{d\bar{\beta}}}{\omega - \epsilon_q - \epsilon_{d\bar{\beta}}} + \frac{1 - \hat{n}_{d\bar{\beta}}}{\omega - \epsilon_q} \tag{4.9}$$

Since these terms commute with the other terms, they can be taken out of the anticommutator; what's left is

$$\left\{ V_q c_{q\beta}^\dagger c_{d\beta}, V_q^* c_{d\beta}^\dagger c_{q\beta} \right\} = |V_q|^2 [\hat{n}_{q\beta} (1 - \hat{n}_{d\beta}) + \hat{n}_{d\beta} (1 - \hat{n}_{q\beta})] \tag{4.10}$$

The τ and the \hat{n} can be multiplied:

$$\tau_{q\beta} (1 - \hat{n}_{q\beta}) = \frac{1}{2} (\hat{n}_{q\beta} - 1) \tag{4.11}$$

$$\tau_{q\beta} \hat{n}_{q\beta} = \frac{1}{2} \hat{n}_{q\beta} \tag{4.12}$$

The total thing becomes

$$\begin{aligned}
&\sum_{q\beta} \frac{1}{2} |V_q|^2 [\hat{n}_{d\beta} (\hat{n}_{q\beta} - 1) + \hat{n}_{q\beta} (1 - \hat{n}_{d\beta})] \left[\frac{\hat{n}_{d\bar{\beta}}}{\omega - \epsilon_q - \epsilon_{d\bar{\beta}}} + \frac{1 - \hat{n}_{d\bar{\beta}}}{\omega - \epsilon_q} \right] \\
&= \sum_{q\beta} \frac{1}{2} |V_q|^2 [\hat{n}_{q\beta} - \hat{n}_{d\beta}] \left[\frac{\hat{n}_{d\bar{\beta}}}{\omega - \epsilon_q - \epsilon_{d\bar{\beta}}} + \frac{1 - \hat{n}_{d\bar{\beta}}}{\omega - \epsilon_q} \right]
\end{aligned} \tag{4.13}$$

Putting $\hat{n}_{q\beta} = 1$, and dropping the non-operator terms, we get

$$\sum_{\beta} \frac{1}{2} \hat{n}_{d\beta} \sum_q |V_q|^2 \frac{\epsilon_q - \omega + 2\epsilon_{d\beta}}{(\omega - \epsilon_q)(\omega - \epsilon_q - \epsilon_{d\beta})} - \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \sum_{q\beta} \frac{1}{2} |V_q|^2 \frac{\epsilon_{d\beta}}{(\omega - \epsilon_q)(\omega - \epsilon_q - \epsilon_{d\beta})} \quad (4.14)$$

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. 4.4 and 4.14, we get

$$\mathcal{H}_{N-1} = \sum_{k < \Lambda_N, \sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{|q|=\Lambda_N} \epsilon_q + \sum_{\sigma} (\epsilon_{d\sigma} + \Delta\epsilon_{d\sigma}) \hat{n}_{d\sigma} + (U + \Delta U) \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \quad (4.15)$$

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.

$$\Delta\epsilon_{d\beta}^N \equiv \epsilon_{d\beta}|_{N-1} - \epsilon_{d\beta}|_N = \frac{1}{2} \sum_q |V_q|^2 \frac{\epsilon_q - \omega + 2\epsilon_{d\beta}}{(\omega - \epsilon_q)(\omega - \epsilon_q - \epsilon_{d\beta})} \quad (4.16)$$

Since the equation is same for $\beta = \uparrow, \downarrow$, we can drop the β index. According to Hewson eq. 3.62 (page 68),

$$\frac{d\epsilon_d}{d \ln D} = -\frac{\Delta}{\pi} + O(V^3) = -\rho_0 |V|^2 + O(V^3) \quad (4.17)$$

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

$$\delta n = \frac{dn}{dE} \times \delta E = \rho(D) \times |\delta D| \quad (4.18)$$

We can then replace the summation in eq. 4.16 by δn :

$$\delta\epsilon_d(D) = \frac{1}{2} |V|^2 \rho(D) |\delta D| \frac{D - \omega + 2\epsilon_d}{(\omega - D)(\omega - D - \epsilon_d)} \quad (4.19)$$

where $\rho(D)$ is the number of single-spin states on the shell D . This can be compared to eq. 4.17. In two dimensions, the energy density of states is independent of energy. **Setting $\omega = 0$** , we get

$$\begin{aligned} \delta\epsilon_d(D) &= \frac{1}{2} |V|^2 \rho(D) \frac{|\delta D|}{D} \frac{D + 2\epsilon_d}{D + \epsilon_d} \\ &= -\frac{1}{2} |V|^2 \rho(D) \delta(\ln D) \frac{D + 2\epsilon_d}{D + \epsilon_d} \end{aligned} \quad (4.20)$$

I used $\delta D = -|\delta D|$. Changing to continuum equation,

$$\frac{d\epsilon_d}{d \ln D} = -\frac{\Delta}{2\pi} \frac{D + 2\epsilon_d}{D + \epsilon_d} \quad (4.21)$$

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,

$$\frac{d\epsilon_d}{d \ln D} = -\frac{\Delta}{2\pi} \quad (4.22)$$

$$\implies \epsilon_d + \frac{\Delta}{2\pi} \log D = \text{constant} \quad (4.23)$$

This differs from eq. 3.65 in Hewson by a factor 2π vs π .

Turning to the general equation 4.16, under the assumption of momentum-independent scattering, the continuum equation is

$$\frac{d\epsilon_d}{d \ln D} = \frac{1}{2} |V|^2 n(D) \frac{\omega - D - 2\epsilon_d}{(\omega - D)(\omega - D - \epsilon_d)} \quad (4.24)$$

$n(D)$ is not the density of states, but the total number of states on the shell at energy D . Similarly, the renormalization in U is

$$\begin{aligned} \delta U &= - \sum_{q\beta} \frac{1}{2} |V_q|^2 \frac{\epsilon_{d\beta}}{(\omega - \epsilon_q)(\omega - \epsilon_q - \epsilon_{d\beta})} \\ &= -\frac{1}{2} |V|^2 n(D) \sum_{\beta} \frac{\epsilon_{d\beta}}{(\omega - D)(\omega - D - \epsilon_{d\beta})} \\ &= -|V|^2 n(D) \frac{\epsilon_d}{(\omega - D)(\omega - D - \epsilon_d)} \\ \implies \frac{dU}{d \ln D} &= |V|^2 n(D) \frac{\epsilon_d}{(\omega - D)(\omega - D - \epsilon_d)} \end{aligned} \quad (4.25)$$

In the last step, I used the fact that since the onsite energy for either spin is same, the summation just returns a factor of 2.

Alternate

We will write the Hamiltonian in terms of $\tau = \hat{n} - \frac{1}{2}$:

$$\begin{aligned}
\mathcal{H} &= \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{k\sigma} \left(V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right) + \sum_{\sigma} \epsilon_{d\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \\
&= \sum_{k\sigma} \epsilon_k \left(\tau_{k\sigma} + \frac{1}{2} \right) + \sum_{k\sigma} \left(V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right) + \sum_{\sigma} \epsilon_{d\sigma} \left(\tau_{d\sigma} + \frac{1}{2} \right) \\
&\quad + U \left(\tau_{d\uparrow} + \frac{1}{2} \right) \left(\tau_{d\downarrow} + \frac{1}{2} \right) \\
&= \frac{1}{2} \sum_{k\sigma} \epsilon_k + \frac{1}{2} \sum_{\sigma} \epsilon_{d\sigma} + \frac{1}{4} U + \sum_{k\sigma} \epsilon_k \tau_{k\sigma} + \sum_{k\sigma} \left(V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right) + \sum_{\sigma} \epsilon_{d\sigma} \tau_{d\sigma} \quad (4.26) \\
&\quad + U \tau_{d\uparrow} \tau_{d\downarrow} + \frac{1}{2} U \sum_{\sigma} \tau_{d\sigma} \\
&= \xi_0 + \sum_{k\sigma} \epsilon_k \tau_{k\sigma} + \sum_{k\sigma} \left(V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right) + \sum_{\sigma} \left(\epsilon_{d\sigma} + \frac{U}{2} \right) \tau_{d\sigma} + U \tau_{d\uparrow} \tau_{d\downarrow} \\
&= \xi_0 + \sum_{k\sigma} \epsilon_k \tau_{k\sigma} + \sum_{k\sigma} \left(V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right) + \sum_{\sigma} \xi_{d\sigma} \tau_{d\sigma} + U \tau_{d\uparrow} \tau_{d\downarrow}
\end{aligned}$$

ξ_0 is the constant background energy $\frac{1}{2} \sum_{k\sigma} \epsilon_k + \frac{1}{2} \sum_{\sigma} \epsilon_{d\sigma} + \frac{1}{4} U$ which we will drop henceforth. $\xi_{d\sigma} = \epsilon_{d\sigma} + \frac{U}{2}$ is a modified impurity-site energy. U remains unchanged in the process. The renormalized Hamiltonian (up to first order in τ) after disentangling the electron at $q\beta$ is

$$\mathcal{H}_{q\beta} = \frac{1}{2} \text{Tr}_{q\beta} \mathcal{H}_N + \tau_{q\beta} \left\{ c_{q\beta}^\dagger \text{Tr}_{q\beta} (\mathcal{H}_N c_{q\beta}), \eta_{q\beta} \right\} \quad (4.27)$$

The calculations follow. As a first approximation, we will consider just one electron on the outermost shell Λ_N .

$$\mathcal{H}_N = \sum_{k\sigma}^< \left(\epsilon_k \tau_{k\sigma} + V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right) + \sum_{\sigma} \xi_{d\sigma} \tau_{d\sigma} + U \tau_{d\uparrow} \tau_{d\downarrow} + \epsilon_q \tau_{q\beta} + V_q c_{q\beta}^\dagger c_{d\beta} + h.c. \quad (4.28)$$

The sum $\sum^<$ runs over all shells below Λ_N . The first term gives

$$\begin{aligned}
\frac{1}{2} \text{Tr}_{q\beta} \mathcal{H}_N &= \frac{1}{2} \text{Tr}_{q\beta} \left[\sum_{k\sigma}^< \left(\epsilon_k \tau_{k\sigma} + V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right) + \sum_{\sigma} \xi_{d\sigma} \tau_{d\sigma} + U \tau_{d\uparrow} \tau_{d\downarrow} \right] \\
&\quad + \frac{1}{2} \text{Tr}_{q\beta} \left(\epsilon_q \tau_{q\beta} + V_q c_{q\beta}^\dagger c_{d\beta} + h.c. \right) \quad (4.29)
\end{aligned}$$

The first trace, involving terms not having $q\beta$, simply give a factor of 2 which is canceled by the half in front. Tracing over $\epsilon_q \tau_{q\beta}$ gives zero because the eigenvalues of $\tau_{q\beta}$ are $\pm \frac{1}{2}$.

Therefore,

$$\frac{1}{2}\text{Tr}_{q\beta}\mathcal{H}_N = \sum_{k\sigma}^< \left(\epsilon_k \tau_{k\sigma} + V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right) + \sum_{\sigma} \xi_{d\sigma} \tau_{d\sigma} + U \tau_{d\uparrow} \tau_{d\downarrow} \quad (4.30)$$

To calculate the second term, we note

$$c_{q\beta}^\dagger \text{Tr}_{q\beta} (\mathcal{H}_N c_{q\beta}) = V_q c_{q\beta}^\dagger c_{d\beta} \quad (4.31)$$

$$\text{Tr}_{q\beta} \left(c_{q\beta}^\dagger \mathcal{H}_N \right) c_{q\beta} = V_q^* c_{d\beta}^\dagger c_{q\beta} \quad (4.32)$$

$$\text{Tr}_{q\beta} (\mathcal{H}_N^D \hat{n}_{q\beta}) \hat{n}_{q\beta} = \left[\sum_{k\sigma}^< \left(\epsilon_k \tau_{k\sigma} + V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right) + \sum_{\sigma} \xi_{d\sigma} \tau_{d\sigma} + U \tau_{d\uparrow} \tau_{d\downarrow} + \frac{1}{2} \epsilon_q \right] \hat{n}_{q\beta} \quad (4.33)$$

$$\begin{aligned} \eta_{q\beta} &= \text{Tr}_{q\beta} \left(c_{q\beta}^\dagger \mathcal{H}_N \right) c_{q\beta} \frac{1}{\hat{\omega} - \text{Tr}_{q\beta} (\mathcal{H}_N^D \hat{n}_{q\beta}) \hat{n}_{q\beta}} \\ &= V_q^* c_{d\beta}^\dagger c_{q\beta} \frac{1}{\hat{\omega} - \left(\sum_{\sigma} \xi_{d\sigma} \tau_{d\sigma} + U \tau_{d\uparrow} \tau_{d\downarrow} + \frac{1}{2} \epsilon_q \right) \hat{n}_{q\beta}} \end{aligned} \quad (4.34)$$

where I absorbed the part below the shell into the $\hat{\omega}$. We can also absorb a $\frac{1}{2} \times \left(\sum_{\sigma} \xi_{d\sigma} \tau_{d\sigma} + U \tau_{d\uparrow} \tau_{d\downarrow} + \frac{1}{2} \epsilon_q \right) \hat{n}_{q\beta}$ into $\hat{\omega}$ to convert the $\hat{n}_{q\beta}$ into $\tau_{q\beta}$. Then we replace $\hat{\omega}$ with $\omega \tau_{q\beta}$:

$$\eta_{q\beta} = V_q^* c_{d\beta}^\dagger c_{q\beta} \frac{1}{\omega \tau_{q\beta} - \left(\sum_{\sigma} \xi_{d\sigma} \tau_{d\sigma} + U \tau_{d\uparrow} \tau_{d\downarrow} + \frac{1}{2} \epsilon_q \right) \tau_{q\beta}} \quad (4.35)$$

Since this term has a $c_{q\beta}$, it will survive only when acting on $|\tau_{q\beta} = \frac{1}{2}\rangle$, so we can replace the $\tau_{q\beta}$ in the denominator with $\frac{1}{2}$. Also, since there is a $c_{d\beta}^\dagger$, we can similarly replace $\tau_{d\beta} = -\frac{1}{2}$.

$$\begin{aligned} \eta_{q\beta} &= V_q^* c_{d\beta}^\dagger c_{q\beta} \frac{2}{\omega + \frac{1}{2} \xi_{d\beta} - \xi_{d\bar{\beta}} \tau_{d\bar{\beta}} + \frac{1}{2} U \tau_{d\bar{\beta}} - \frac{1}{2} \epsilon_q} \\ &= V_q^* c_{d\beta}^\dagger c_{q\beta} \left[\frac{\frac{1}{2} + \tau_{d\bar{\beta}}}{\omega + \frac{1}{2} \xi_{d\beta} - \frac{1}{2} \xi_{d\bar{\beta}} + \frac{1}{4} U - \frac{1}{2} \epsilon_q} + \frac{\frac{1}{2} - \tau_{d\bar{\beta}}}{\omega + \frac{1}{2} \xi_{d\beta} + \frac{1}{2} \xi_{d\bar{\beta}} - \frac{1}{4} U - \frac{1}{2} \epsilon_q} \right] \\ &= V_q^* c_{d\beta}^\dagger c_{q\beta} \frac{\omega + \frac{1}{2} \xi_{d\beta} - \frac{1}{2} \epsilon_q - \left(\frac{1}{2} U - \xi_{d\bar{\beta}} \right) \tau_{q\bar{\beta}}}{\left(\omega + \frac{1}{2} \xi_{d\beta} - \frac{1}{2} \epsilon_q \right)^2 - \left(\frac{1}{4} U - \frac{1}{2} \xi_{d\bar{\beta}} \right)^2} \end{aligned} \quad (4.36)$$

Then,

$$\begin{aligned}
\tau_{q\beta} \left\{ c_{q\beta}^\dagger \text{Tr}_{q\beta} (\mathcal{H}_N c_{q\beta}) , \eta_{q\beta} \right\} &= \tau_{q\beta} |V_q|^2 \frac{\omega + \frac{1}{2}\xi_{d\beta} - \frac{1}{2}\epsilon_q - \left(\frac{1}{2}U - \xi_{d\bar{\beta}}\right) \tau_{q\bar{\beta}}}{\left(\omega + \frac{1}{2}\xi_{d\beta} - \frac{1}{2}\epsilon_q\right)^2 - \left(\frac{1}{4}U - \frac{1}{2}\xi_{d\bar{\beta}}\right)^2} \left\{ c_{q\beta}^\dagger c_{d\beta}, c_{d\beta}^\dagger c_{q\beta} \right\} \\
&= \tau_{q\beta} |V_q|^2 \frac{\omega + \frac{1}{2}\xi_{d\beta} - \frac{1}{2}\epsilon_q - \left(\frac{1}{2}U - \xi_{d\bar{\beta}}\right) \tau_{q\bar{\beta}}}{\left(\omega + \frac{1}{2}\xi_{d\beta} - \frac{1}{2}\epsilon_q\right)^2 - \left(\frac{1}{4}U - \frac{1}{2}\xi_{d\bar{\beta}}\right)^2} (\hat{n}_{q\beta} - \hat{n}_{d\beta}) \\
&= \tau_{q\beta} |V_q|^2 \frac{\omega + \frac{1}{2}\xi_{d\beta} - \frac{1}{2}\epsilon_q - \left(\frac{1}{2}U - \xi_{d\bar{\beta}}\right) \tau_{q\bar{\beta}}}{\left(\omega + \frac{1}{2}\xi_{d\beta} - \frac{1}{2}\epsilon_q\right)^2 - \left(\frac{1}{4}U - \frac{1}{2}\xi_{d\bar{\beta}}\right)^2} (\tau_{q\beta} - \tau_{d\beta}) \\
&= |V_q|^2 \frac{\omega + \frac{1}{2}\xi_{d\beta} - \frac{1}{2}\epsilon_q - \left(\frac{1}{2}U - \xi_{d\bar{\beta}}\right) \tau_{q\bar{\beta}}}{\left(\omega + \frac{1}{2}\xi_{d\beta} - \frac{1}{2}\epsilon_q\right)^2 - \left(\frac{1}{4}U - \frac{1}{2}\xi_{d\bar{\beta}}\right)^2} \left(\frac{1}{4} - \tau_{q\beta} \tau_{d\beta} \right)
\end{aligned} \tag{4.37}$$

Putting $\tau_{q\beta} = \frac{1}{2}$,

$$\begin{aligned}
\tau_{q\beta} \left\{ c_{q\beta}^\dagger \text{Tr}_{q\beta} (\mathcal{H}_N c_{q\beta}) , \eta_{q\beta} \right\} &= \frac{1}{2} |V_q|^2 \frac{\omega + \frac{1}{2}\xi_{d\beta} - \frac{1}{2}\epsilon_q - \left(\frac{1}{2}U - \xi_{d\bar{\beta}}\right) \tau_{q\bar{\beta}}}{\left(\omega + \frac{1}{2}\xi_{d\beta} - \frac{1}{2}\epsilon_q\right)^2 - \left(\frac{1}{4}U - \frac{1}{2}\xi_{d\bar{\beta}}\right)^2} \left(\frac{1}{2} - \tau_{d\beta} \right) \\
&= \frac{1}{4} |V_q|^2 \frac{\omega + \frac{1}{2}\xi_{d\beta} - \frac{1}{2}\epsilon_q}{\left(\omega + \frac{1}{2}\xi_{d\beta} - \frac{1}{2}\epsilon_q\right)^2 - \left(\frac{1}{4}U - \frac{1}{2}\xi_{d\bar{\beta}}\right)^2} \\
&\quad - \frac{1}{4} |V_q|^2 \frac{\frac{1}{2}U - \xi_{d\bar{\beta}}}{\left(\omega + \frac{1}{2}\xi_{d\beta} - \frac{1}{2}\epsilon_q\right)^2 - \left(\frac{1}{4}U - \frac{1}{2}\xi_{d\bar{\beta}}\right)^2} \tau_{q\bar{\beta}} \\
&\quad - \frac{1}{2} |V_q|^2 \frac{\omega + \frac{1}{2}\xi_{d\beta} - \frac{1}{2}\epsilon_q}{\left(\omega + \frac{1}{2}\xi_{d\beta} - \frac{1}{2}\epsilon_q\right)^2 - \left(\frac{1}{4}U - \frac{1}{2}\xi_{d\bar{\beta}}\right)^2} \tau_{q\beta} \\
&\quad + \frac{1}{2} |V_q|^2 \frac{\frac{1}{2}U - \xi_{d\bar{\beta}}}{\left(\omega + \frac{1}{2}\xi_{d\beta} - \frac{1}{2}\epsilon_q\right)^2 - \left(\frac{1}{4}U - \frac{1}{2}\xi_{d\bar{\beta}}\right)^2} \tau_{q\beta} \tau_{q\bar{\beta}} \\
&= \Delta\xi_q + \Delta\xi_{d\bar{\beta}} \tau_{q\bar{\beta}} + \Delta\xi_{d\beta} \tau_{q\beta} + \Delta U \tau_{q\beta} \tau_{q\bar{\beta}}
\end{aligned} \tag{4.38}$$

The first term is a renormalization in the kinetic energy of the disentangled electrons. The rest of the terms are self-explanatory.

These are the changes after disentangling just one electron, $q\beta$:

$$\xi_{d\beta} \rightarrow \xi'_{d\beta} = \xi_{d\beta} + \Delta\xi_{d\beta} \tag{4.39}$$

$$\xi_{d\bar{\beta}} \rightarrow \xi'_{d\bar{\beta}} = \xi_{d\bar{\beta}} + \Delta\xi_{d\bar{\beta}} \tag{4.40}$$

If we now disentangle the electron $q\bar{\beta}$, the changes will get exchanged:

$$\begin{aligned}
\xi'_{d\beta} &\rightarrow \xi''_{d\beta} = \xi'_{d\beta} + \Delta\xi_{d\bar{\beta}} = \xi_{d\beta} + \Delta\xi_{d\beta} + \Delta\xi_{d\bar{\beta}} \equiv \Delta\xi_{dq} \\
\xi'_{d\bar{\beta}} &\rightarrow \xi''_{d\bar{\beta}} = \xi'_{d\bar{\beta}} + \Delta\xi_{d\beta} = \xi_{d\bar{\beta}} + \Delta\xi_{d\bar{\beta}} + \Delta\xi_{d\beta} \equiv \Delta\xi_{dq}
\end{aligned} \tag{4.41}$$

where

$$\begin{aligned}\Delta\xi_{dq} &= \frac{1}{2}|V_q|^2 \left[\frac{\frac{1}{2}U - \xi_{d\bar{\beta}}}{\left(\omega + \frac{1}{2}\xi_{d\beta} - \frac{1}{2}\epsilon_q\right)^2 - \left(\frac{1}{4}U - \frac{1}{2}\xi_{d\bar{\beta}}\right)^2} - \frac{\omega + \frac{1}{2}\xi_{d\beta} - \frac{1}{2}\epsilon_q}{\left(\omega + \frac{1}{2}\xi_{d\beta} - \frac{1}{2}\epsilon_q\right)^2 - \left(\frac{1}{4}U - \frac{1}{2}\xi_{d\bar{\beta}}\right)^2} \right] \\ &= \frac{1}{2}|V_q|^2 \frac{\frac{1}{2}U - \xi_{d\bar{\beta}} - \omega - \frac{1}{2}\xi_{d\beta} + \frac{1}{2}\epsilon_q}{\left(\omega + \frac{1}{2}\xi_{d\beta} - \frac{1}{2}\epsilon_q\right)^2 - \left(\frac{1}{4}U - \frac{1}{2}\xi_{d\bar{\beta}}\right)^2}\end{aligned}\tag{4.42}$$

Since, initially, $\xi_{d\beta} = \xi_{d\bar{\beta}} \equiv \xi_d$, this simplifies to

$$\Delta\xi_{dq} = \frac{1}{2}|V_q|^2 \frac{\frac{1}{2}U - \frac{3}{2}\xi_d - \omega + \frac{1}{2}\epsilon_q}{\left(\omega + \frac{1}{2}\xi_d - \frac{1}{2}\epsilon_q\right)^2 - \left(\frac{1}{4}U - \frac{1}{2}\xi_d\right)^2}\tag{4.43}$$

Similarly, after two disentanglings, U changes by

$$\Delta U = |V_q|^2 \frac{\frac{1}{2}U - \xi_d}{\left(\omega + \frac{1}{2}\xi_d - \frac{1}{2}\epsilon_q\right)^2 - \left(\frac{1}{4}U - \frac{1}{2}\xi_d\right)^2}\tag{4.44}$$

Disentangling the entire shell (all q) gives

$$\begin{aligned}\Delta\xi_d &= \frac{1}{2} \sum_q |V_q|^2 \frac{\frac{1}{2}U - \frac{3}{2}\xi_d - \omega + \frac{1}{2}\epsilon_q}{\left(\omega + \frac{1}{2}\xi_d - \frac{1}{2}\epsilon_q\right)^2 - \left(\frac{1}{4}U - \frac{1}{2}\xi_d\right)^2} \\ \Delta U &= \sum_q |V_q|^2 \frac{\frac{1}{2}U - \xi_d}{\left(\omega + \frac{1}{2}\xi_d - \frac{1}{2}\epsilon_q\right)^2 - \left(\frac{1}{4}U - \frac{1}{2}\xi_d\right)^2}\end{aligned}\tag{4.45}$$

Assuming spherically-symmetric scattering, we can take out $|V_q|^2 = |V|^2$. For a spherical shell, we can set $\epsilon_q = D$, and the summation will produce a factor $n(D)$, the number of states on the shell.

$$\begin{aligned}\Delta\xi_d &= \frac{1}{2}|V|^2 n(D) \frac{\frac{1}{2}U - \frac{3}{2}\xi_d - \omega + \frac{1}{2}D}{\left(\omega + \frac{1}{2}\xi_d - \frac{1}{2}D\right)^2 - \left(\frac{1}{4}U - \frac{1}{2}\xi_d\right)^2} \\ \Delta U &= |V|^2 n(D) \frac{\frac{1}{2}U - \xi_d}{\left(\omega + \frac{1}{2}\xi_d - \frac{1}{2}D\right)^2 - \left(\frac{1}{4}U - \frac{1}{2}\xi_d\right)^2}\end{aligned}\tag{4.46}$$