

We can rewrite the trace of Green's function as

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

such that

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

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

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

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

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

The change in the dos becomes

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

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

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

Hence,

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

From eq. 2.1.34, we get

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

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

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

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

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

2.1.3 An identity

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

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

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

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

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

2.2 Landau's theory of Fermi liquids

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

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

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

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

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

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

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

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

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

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

$$(2.2.6)$$

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

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

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

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

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

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

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

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

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

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

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

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

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

Then, up to first order,

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

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

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

Eq. 2.2.12 then becomes

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

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

Since the quasiparticles are in direct correspondence with the Fermionic particles, they

must also be fermions. This allows us to write down the probability of finding a quasiparticle at energy ξ ,

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

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

A temperature-dependent free energy can be concocted using

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

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

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

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

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

2.3 The single-impurity Anderson model (SIAM)

The SIAM consists of a single localized impurity site talking to a conduction bath. The impurity site has an energy ϵ_d which is typically below the Fermi surface and hence favours a bound state. We will assume the impurities are from a d or f-electron such that the orbitals are localized and there is a local repulsion U produced by the localized orbitals.

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

The SIAM involves the following energy scales:

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

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

- $U \gg \epsilon_d \gg \Delta$: Double occupation is not possible. Δ being small means very small hybridisation. So, d-site is either up or down, hence magnetic.

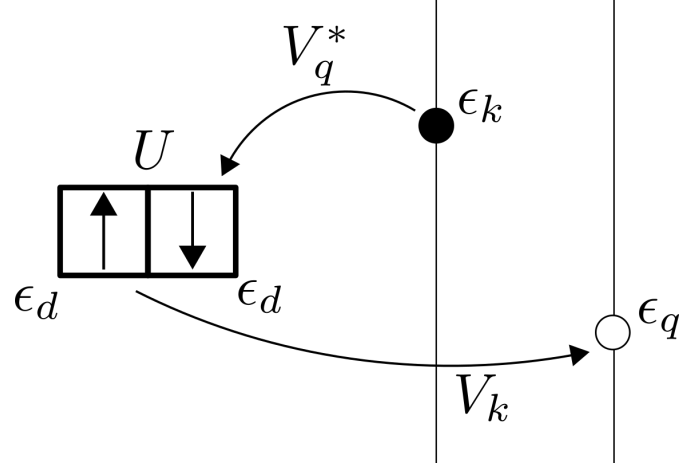


Figure 2.1: The single-impurity Anderson model Hamiltonian

- $U \gg \Delta \gg \epsilon_d$: Double occupation is still not possible, but now hybridisation will allows the up and down spins to fluctuate on the d-site, leading to zero average magnetization.
- $\Delta \gg U \gg \epsilon_d$: Hybridisation now fluctuates the up and down spins , leading to zero average magnetization.

To get a feel for the dynamic of the model, we can consider the very simple atomic limit ($V = 0$).

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

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

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

For a magnetic solution, we need

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

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

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

2.3.1 The non-interacting limit

The non-interacting limit consists of a non-interacting impurity site ($U = 0$). This is often referred to as the resonant-level model.

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

Green's function of impurity site:

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

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

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

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

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

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

Now,

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

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

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

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

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

Therefore,

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

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

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

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

The first density of states is delta function, because ϵ_d is an eigenstate in that case, and the poles of the corresponding Green's function are real poles. But the presence of the hybridisation means that is no longer the case in the second density of states, so the delta function fades into a Lorentzian in that case, and the poles of the Greens function move off the real axis.

The total number of d-electrons can be calculated as:

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

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

T -matrix is defined by

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

We also have

$$\begin{aligned} G &= G_0 + G_0VG = G_0 + G_0T \frac{1}{1 + GT} G \\ &= G_0 + G_0T(1 - GT + \dots)(G_0 + G_0VG_0 + \dots) \\ &= G_0 + G_0TG_0 \end{aligned} \quad (2.3.19)$$

The conduction electron Green's function can be calculated as

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

Noting that

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

we have

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

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

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

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

$$\text{Im}[T] = -\frac{t^2 \Delta}{(E - \epsilon_d)^2 + \Delta^2} = -\pi t^2 \rho_d \quad (2.3.24)$$

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

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

This relation will hold as long as the T -matrix is of the form $t^2 G_d$.

If the phase shift of the conduction electrons due to scattering off the impurity is δ , we have

$$T = e^{2i\delta} - 1 = e^{i\delta} (e^{i\delta} - e^{-i\delta}) \sim \frac{1}{\cot \delta - i} \quad (2.3.26)$$

Comparing with eq. 2.3.23, we can write

$$\delta(E) = \cot^{-1} \left(\frac{\epsilon_d - E}{\Delta} \right) \quad (2.3.27)$$

When $E = \epsilon_d$, the phase shift is π , and the scattering is head on (the conduction electron is reflected back). Comparing with eq. 2.3.17,

$$\frac{2}{\pi} \delta(0) = \langle n_d \rangle \quad (2.3.28)$$

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

Coulomb blockade

This section follows the discussion in reference [14]. A quantum dot is a set of electrons that are localized in a sufficiently small region so that their spectrum is quantized. The localization means that double occupation will come at a cost of U .

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

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

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

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

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

Tuning the voltage can make these two levels degenerate.

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

At this voltage, the two levels have the same energy and double occupancy becomes possible. Electrons can flow from the source to the sink via double occupation on the dot.

For a non-interacting resonance, the conductance can be calculated as follows. The conductance for perfect transmission is given by the quantum of conductance $G_0 = \frac{2e^2}{h}$. In this case, the transmission is not perfect, but is modulated by the density of states of the dot at the Fermi surface. Hence,

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

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

2.3.2 Total Hamiltonian: Mean field treatment

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

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

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

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

An alternative way of writing that is

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

Introducing $n_d = \langle n_{d\uparrow} \rangle + \langle n_{d\downarrow} \rangle$ and $m = \langle n_{d\uparrow} \rangle - \langle n_{d\downarrow} \rangle$, we can write

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

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

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

we get

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

At $m = 0$, $\langle n_{d\uparrow} \rangle = \langle n_{d\downarrow} \rangle$, therefore $\cot \frac{\pi n_d}{2} = \frac{U n_d}{2\Delta} + \frac{\epsilon_d}{\Delta}$. Substituting in eq. 2.3.40,

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

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

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

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

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

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

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

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

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

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

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

2.3.3 Some conclusions and observations

- The mean field solution predicts that local moments are sustained in the limit of large U and small $|\epsilon_d|$. However, this treatment becomes faulty at low temperatures.
- At low temperatures, the resistivity is found to reach a minimum and then vary as $\ln T$. This behavior stops at some very low temperature T_K . The temperature T_K is also that at which the magnetization vanishes, and the susceptibility becomes constant, suggesting that the impurity spin has condensed into a singlet.
- Since the disappearance of the $\ln T$ behavior is coincident with the condensation of the spin degree of freedom, it is natural to hope that the resistivity minimum is a result of the interaction between the impurity and the conduction spins.
- To describe such an interaction, the way to proceed is to strip the model of the charge excitations (via a *Schrieffer-Wolff transformation*). The resultant Hamiltonian consists of an anti-ferromagnetic interaction between the itinerant spins and the impurity spin, and is called the Kondo model.

- Calculating the scattering rate up to second order using the Kondo model produces a logarithmic term, which explains the log-dependence. Since this perturbative treatment will fail at small temperatures (where the log term diverges), we need some other technique to find out the fate of the model at low temperatures.
- Anderson's poor man's scaling wraps the effects of high energy scatterings into the low energy model, showing that the anti-ferromagnetic coupling diverges at low temperatures, producing a singlet.
- There are two routes that one can follow to note the changes in the system; one is by reducing the temperature which is equivalent to folding in the high energy fluctuations, aka scaling. The other is to reduce the onsite interaction U and note the changes in state.
- Reducing the temperature or performing the RG takes the model from the Anderson model ($T > 0$) to the Fermi liquid state ($T \sim T_K$). This Fermi liquid may have interactions, depending on the value of U we are working in.
- Coming down to $T < T_K$, we can now modify the U from ∞ to 0. Large U means the Fermi liquid has large interactions. Reducing U means coming down to a Fermi gas. For $T \neq 0$, reducing U means going from local moment regime to non-magnetic regime. For $T = 0$, local moments persist for all $U > 0$.
- It will be seen that in the large U regime, the singlet channel scattering phase shift (phase shift incurred when one singlet state scatters into another singlet state) at the Fermi energy is $\propto \tan^{-1} J_{\text{eff}}$. This effective coupling J_{eff} flows to ∞ under poor man's scaling as $T \rightarrow 0$. Thus, the singlet phase shift at ϵ_F approaches $\frac{\pi}{2}$ as $T \rightarrow 0$.

2.4 The Kondo model

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

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

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

2.4.1 Derivation of the Kondo Hamiltonian

Deriving the Kondo Hamiltonian involves separating the impurity spinon subspace ($\hat{n}_{d\uparrow} \neq \hat{n}_{d\downarrow}$) from the doublon and holon subspaces ($\hat{n}_{d\uparrow} = \hat{n}_{d\downarrow}$). The canonical (pun intended) way

of doing this is via a Schrieffer-Wolff transformation [15]. It involves applying a unitary transformation on the original Hamiltonian such that the terms that scatter between the two subspaces disappear, up to leading order. We are then left with a higher order intra-subspace scattering. It is often referred to as a one-shot renormalization group method, because it kills all the off-diagonal terms in one iteration. The approach here follows that in [14]. An alternate derivation via a projector operator method due to [12] is shown in 4.2.1.

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

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

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

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

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

$$\bar{H} = e^{-S} H e^S = H_0 + \left(V + [H_0, S] \right) + \frac{1}{2} \left([V, S] + [[H_0, S], S] \right) \quad (2.4.5)$$

Defining S such that the first order term vanishes,

$$V = [S, H_0] \quad (2.4.6)$$

$$\bar{H} = H_0 + \frac{1}{2} [V, S] \quad (2.4.7)$$

Take $S = \begin{pmatrix} 0 & -s^\dagger \\ s & 0 \end{pmatrix}$. From eq. 2.4.6,

$$\begin{aligned} V &= \begin{pmatrix} 0 & -s^\dagger \\ s & 0 \end{pmatrix} \begin{pmatrix} H^L & 0 \\ 0 & H^H \end{pmatrix} - \begin{pmatrix} H^L & 0 \\ 0 & H^H \end{pmatrix} \begin{pmatrix} 0 & -s^\dagger \\ s & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & -s^\dagger H^H + H^L s^\dagger \\ s H^L - H^H s & 0 \end{pmatrix} \end{aligned} \quad (2.4.8)$$

Comparing with the definition of V , we can write

$$v_{ij}^\dagger = s_{ij}^\dagger (E_i^L - E_j^H), v_{ij} = s_{ij} (E_j^L - E_i^H) \quad (2.4.9)$$

$$\implies s_{ij}^\dagger = \frac{v_{ij}^\dagger}{E_i^L - E_j^H}, s_{ij} = \frac{v_{ij}}{E_j^L - E_i^H} \quad (2.4.10)$$

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

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

Hence,

$$\bar{H} = H_0 + \frac{[V, S]}{2} = \begin{pmatrix} H^L + \frac{1}{2} (v^\dagger s + s^\dagger v) & 0 \\ 0 & H^H - v s^\dagger - s v^\dagger \end{pmatrix} \quad (2.4.12)$$

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

$$\mathcal{H} = \langle L | \bar{H} | L \rangle = H^L + \frac{1}{2} (v^\dagger s + s^\dagger v) \quad (2.4.13)$$

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

$$\begin{aligned} \Delta H &= \frac{1}{2} (v^\dagger s + s^\dagger v) = \frac{1}{2} \left(v^\dagger \sum_{HL} s_{HL} |H\rangle \langle L| + \text{h.c.} \right) \\ &= \frac{1}{2} \sum_{HL} \left[v^\dagger |H\rangle \langle L| \frac{v_{HL}}{E_L - E_H} + |L\rangle \langle H| \frac{v_{LH}^\dagger}{E_L - E_H} v \right] \end{aligned} \quad (2.4.14)$$

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

$$\Delta H_{ll'} = \langle l | \Delta H | l' \rangle = \frac{1}{2} \sum_H v_{lH}^\dagger v_{Hl'} \left(\frac{1}{E_{l'} - E_H} + \frac{1}{E_l - E_H} \right) \quad (2.4.15)$$

This can also be written as

$$\Delta H_{ll'} = \frac{1}{2} [T_{ll'}(E_l) + T_{ll'}(E_{l'})] \quad (2.4.16)$$

where

$$T_{ll'}(E) = \sum_H \frac{v_{lH}^\dagger v_{Hl'}}{E - E_H} = \sum_H \frac{V_{lH}^\dagger V_{Hl'}}{E - E_H} \quad (2.4.17)$$

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

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

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

where $\Delta_{LH} = E_L - E_H$ is the energy difference between the low energy subspace and the high energy state $|H\rangle$. For our Hamiltonian, $|H_1\rangle = |0\rangle, |H_2\rangle = |\uparrow\downarrow\rangle$. Therefore,

$$\Delta_{LH_1} = \epsilon_d - 0 = \epsilon_d, \Delta_{LH_2} = \epsilon_d - (2\epsilon_d + U) = -\epsilon_d - U \quad (2.4.19)$$

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

$$\begin{aligned} \Delta H &= V \frac{|0\rangle \langle 0|}{\epsilon_d} V - V \frac{|\uparrow\downarrow\rangle \langle \uparrow\downarrow|}{\epsilon_d + U} V \\ &= \sum_{k_1, k_2, \sigma_1, \sigma_2} V(k_1) V^*(k_2) \left[\frac{c_{d\sigma_2}^\dagger c_{k_2\sigma_2} |0\rangle \langle 0| c_{k_1\sigma_1}^\dagger c_{d\sigma_1}}{\epsilon_d} - \frac{c_{k_1\sigma_1}^\dagger c_{d\sigma_1} |\uparrow\downarrow\rangle \langle \uparrow\downarrow| c_{d\sigma_2}^\dagger c_{k_2\sigma_2}}{\epsilon_d + U} \right] \\ &= \sum_{k_1, k_2, \sigma_1, \sigma_2} V(k_1) V^*(k_2) \frac{c_{d\sigma_2}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_1} |d\sigma_1, h_{k_1\sigma_1}\rangle \langle d\sigma_1, h_{k_1\sigma_1}|}{\epsilon_d} \\ &\quad - \sum_{k_1, k_2, \sigma_1, \sigma_2} V(k_1) V^*(k_2) \frac{c_{k_1\sigma_1}^\dagger c_{d\sigma_1} c_{d\sigma_2}^\dagger c_{k_2\sigma_2} |d\bar{\sigma}_2, e_{k_2\sigma_2}\rangle \langle d\bar{\sigma}_2, e_{k_2\sigma_2}|}{\epsilon_d + U} \\ &= \sum_{k_1, k_2, \sigma_1, \sigma_2} V(k_1) V^*(k_2) \left[\frac{c_{d\sigma_2}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_1}}{\epsilon_d} - \frac{c_{k_1\sigma_1}^\dagger c_{d\sigma_1} c_{d\sigma_2}^\dagger c_{k_2\sigma_2}}{\epsilon_d + U} \right] P_{n_d=1} \end{aligned} \quad (2.4.20)$$

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

$$\begin{aligned} c_{d\sigma_2}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_1} &= \sum_{\sigma_3,\sigma_4} c_{d\sigma_3}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_4} \delta_{\sigma_1\sigma_3} \delta_{\sigma_4\sigma_2} \\ &= \frac{1}{2} \sum_{\sigma_3,\sigma_4} c_{d\sigma_3}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_4} \left(\delta_{\sigma_1\sigma_2} \delta_{\sigma_3\sigma_4} + \vec{\sigma}_{\sigma_1\sigma_2} \cdot \vec{\sigma}_{\sigma_3\sigma_4} \right) \\ &= \frac{1}{2} c_{k_2\sigma_1} c_{k_1\sigma_1}^\dagger n_d + c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} \cdot \sum_{\sigma_3,\sigma_4} c_{d\sigma_3}^\dagger \frac{\vec{\sigma}_{\sigma_3\sigma_4}}{2} c_{d\sigma_4} \end{aligned} \quad (2.4.21)$$

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

$$c_{d\sigma_2}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_1} = -\frac{1}{2} c_{k_1\sigma_1}^\dagger c_{k_2\sigma_1} - c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2} \cdot \sum_{\sigma_3,\sigma_4} c_{d\sigma_3}^\dagger \frac{\vec{\sigma}_{\sigma_3\sigma_4}}{2} c_{d\sigma_4} \quad (2.4.22)$$

Since the first term does not have any spin-spin interaction, we drop that term.

Defining $\vec{\sigma}_d = \sum_{\sigma_3,\sigma_4} c_{d\sigma_3}^\dagger \vec{\sigma}_{\sigma_3\sigma_4} c_{d\sigma_4}$, we have

$$c_{d\sigma_2}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_1} = -\frac{1}{2} c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2} \cdot \vec{\sigma}_d \quad (2.4.23)$$

Similarly,

$$c_{k_1\sigma_1}^\dagger c_{d\sigma_1} c_{d\sigma_2}^\dagger c_{k_2\sigma_2} = -\frac{1}{2} c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2} \cdot \vec{\sigma}_d \quad (2.4.24)$$

Finally, putting all this together,

$$\begin{aligned} \Delta H &= \frac{1}{2} \sum_{k_1,k_2,\sigma_1,\sigma_2} V(k_1) V^*(k_2) \left[\frac{1}{\epsilon_d + U} - \frac{1}{\epsilon_d} \right] c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2} \cdot \vec{\sigma}_d \\ &= \frac{1}{2} \sum_{k_1,k_2,\sigma_1,\sigma_2} J(k_1, k_2) c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2} \cdot \vec{\sigma}_d \end{aligned} \quad (2.4.25)$$

where

$$J(k_1, k_2) = V(k_1) V^*(k_2) \left[\frac{1}{\epsilon_d + U} - \frac{1}{\epsilon_d} \right] \quad (2.4.26)$$

Assuming $V(k) \equiv t$,

$$H_K = \sum_k \epsilon_k n_k + \frac{J}{2} \vec{\sigma}_e \cdot \vec{\sigma}_d \quad (2.4.27)$$

where

$$\vec{\sigma}_e = \sum_{k_1,k_2,\sigma_1,\sigma_2} c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2} = \sum_{\sigma_1,\sigma_2} c_{\sigma_1}^\dagger(\vec{r}=0) \vec{\sigma}_{\sigma_1\sigma_2} c_{\sigma_2}(\vec{r}=0) \quad (2.4.28)$$

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

2.4.2 Obtaining the resistivity minimum and log-dependence

The next few sections follow the approach in [16]. The model we are working with is

$$H_K = H_0 + V = \sum_k \epsilon_k n_k + \frac{J}{2} \sum_{k_1, k_2, \sigma_1, \sigma_2} c_{k_1 \sigma_1}^\dagger \vec{\sigma}_d \cdot \vec{\sigma}_{\sigma_1 \sigma_2} c_{k_2 \sigma_2} \quad (2.4.29)$$

$$\begin{aligned} \sum_{\sigma_1, \sigma_2} c_{k_1 \sigma_1}^\dagger \vec{\sigma}_d \cdot \vec{\sigma}_{\sigma_1 \sigma_2} c_{k_2 \sigma_2} &= \sigma_d^z \left(c_{k_1 \uparrow}^\dagger c_{k_2 \uparrow} - c_{k_1 \downarrow}^\dagger c_{k_2 \downarrow} \right) + \sigma_d^x \left(c_{k_1 \downarrow}^\dagger c_{k_2 \uparrow} + c_{k_1 \uparrow}^\dagger c_{k_2 \downarrow} \right) \\ &\quad - i \sigma_d^y \left(c_{k_1 \uparrow}^\dagger c_{k_2 \downarrow} - c_{k_1 \downarrow}^\dagger c_{k_2 \uparrow} \right) \end{aligned} \quad (2.4.30)$$

$$= \sigma_d^z \left(c_{k_1 \uparrow}^\dagger c_{k_2 \uparrow} - c_{k_1 \downarrow}^\dagger c_{k_2 \downarrow} \right) + c_{k_1 \downarrow}^\dagger c_{k_2 \uparrow} \sigma_d^+ + c_{k_1 \uparrow}^\dagger c_{k_2 \downarrow} \sigma_d^- \quad (2.4.31)$$

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

$$\begin{aligned} H_K &= \sum_k \epsilon_k n_k + \frac{J}{2} \sum_{k_1, k_2} \left[\sigma_d^z \left(c_{k_1 \uparrow}^\dagger c_{k_2 \uparrow} - c_{k_1 \downarrow}^\dagger c_{k_2 \downarrow} \right) + \sigma_d^+ c_{k_1 \downarrow}^\dagger c_{k_2 \uparrow} + \sigma_d^- c_{k_1 \uparrow}^\dagger c_{k_2 \downarrow} \right] \\ &= \sum_k \epsilon_k n_k + J \sum_{k_1, k_2} \left[S_d^z \left(c_{k_1 \uparrow}^\dagger c_{k_2 \uparrow} - c_{k_1 \downarrow}^\dagger c_{k_2 \downarrow} \right) + S_d^+ c_{k_1 \downarrow}^\dagger c_{k_2 \uparrow} + S_d^- c_{k_1 \uparrow}^\dagger c_{k_2 \downarrow} \right] \end{aligned} \quad (2.4.32)$$

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

$$T = V + V G_0 V \quad (2.4.33)$$

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

First order scattering

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

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

$$T_{\text{non-flip}}^{(1)} = T_{k_\uparrow, d_\sigma \rightarrow q_\uparrow, d_\sigma} = \langle q_\uparrow, d_\sigma | V | k_\uparrow, d_\sigma \rangle = m_d J \quad (2.4.34)$$

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

$$\mathcal{P}_{k_\sigma, d_{\sigma'} \rightarrow q_\sigma, d_{\sigma'}} = 2\pi \sum_\epsilon \rho(\epsilon) T_{k_\uparrow, d_\sigma \rightarrow q_\uparrow, d_\sigma}^2 = 2\pi \rho(0) J^2 m_d^2 \quad (2.4.35)$$

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

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

For spin-flip, the matrix element is

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

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

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

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

$$\begin{aligned} \mathcal{P}^{(1)} &= \frac{1}{2s_d + 1} \sum_{m_d = -s_d}^{s_d} (\mathcal{P}_1 + \mathcal{P}_2) = \frac{2\pi\rho(0)J^2}{(2s_d + 1)} \sum_{m_d = -s_d}^{s_d} (s_d(s_d + 1) - m_d) \\ &= 2\pi\rho(0)J^2 s_d(s_d + 1) \end{aligned} \quad (2.4.39)$$

Second order scattering

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

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

The second order transition matrix contribution is of the form

$$T_{i \rightarrow j}^{(2)} = \langle j | V G_0 V | i \rangle = \sum_l \frac{\langle j | V | l \rangle \langle l | V | i \rangle}{E_i - E_l} \quad (2.4.40)$$

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

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

where $m_d = \langle d_\sigma | S_d^z | d_\sigma \rangle$ and $1 - P(q)$ is the probability that the state $q \uparrow$ is empty. For the second process,

$$T_{12}^{(2)} = \sum_q \frac{\langle q_\uparrow k'_\uparrow d_\sigma | V | k'_\uparrow k_\uparrow d_\sigma \rangle \langle k'_\uparrow k_\uparrow d_\sigma | V | q_\uparrow k_\uparrow d_\sigma \rangle}{\epsilon_q - \epsilon_{k'}} P(q) \quad (2.4.42)$$

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

$$T_{12}^{(2)} = -J^2 m_d^2 \sum_q \frac{P(q)}{\epsilon_q - \epsilon_k} = J^2 m_d^2 \sum_q \frac{P(q)}{\epsilon_k - \epsilon_q} \quad (2.4.43)$$

For the third process,

$$T_{13}^{(2)} = \sum_q \frac{\langle k'_\uparrow d_\downarrow | V | q_\downarrow d_\uparrow \rangle \langle q_\downarrow d_\uparrow | V | k_\uparrow d_\downarrow \rangle}{\epsilon_k - \epsilon_q} \quad (2.4.44)$$

Using $\langle m_d \pm 1 | S_d^\pm | m_d \rangle = \sqrt{s_d(s_d + 1) - m_d(m_d \pm 1)} = \lambda_\pm$, we get

$$T_{13}^{(2)} = \lambda_+^2 J^2 \sum_q \frac{1 - P(q)}{\epsilon_k - \epsilon_q} \quad (2.4.45)$$

For the fourth process,

$$\begin{aligned} T_{14}^{(2)} &= \sum_q \frac{\langle q_\downarrow k'_\uparrow d_\uparrow | V | k'_\uparrow k_\uparrow d_\downarrow \rangle \langle k'_\uparrow k_\uparrow d_\downarrow | V | q_\downarrow k_\uparrow d_\uparrow \rangle}{\epsilon_q - \epsilon'_k} \\ &= -\lambda_-^2 J^2 \sum_q \frac{P(q)}{\epsilon_q - \epsilon_k} \\ &= \lambda_-^2 J^2 \sum_q \frac{P(q)}{\epsilon_k - \epsilon_q} \end{aligned} \quad (2.4.46)$$

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

$$\begin{aligned} T_{\text{nonflip}}^{(2)} &= \sum_{i=1}^4 T_{1i}^{(2)} = J^2 \sum_q \frac{m_d^2 + \lambda_+^2 - P(q) (\lambda_+^2 - \lambda_-^2)}{\epsilon_k - \epsilon_q} \\ &= J^2 \sum_q \frac{s(s+1) - m_d + 2m_d P(q)}{\epsilon_k - \epsilon_q} \\ &= J^2 [s(s+1) - m_d] (\alpha + \gamma) + 2J^2 m_d \gamma \end{aligned} \quad (2.4.47)$$

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

$$\begin{aligned} T_{\text{nonflip}}^{(2)} &= 2J^2 m_d \gamma \\ &= 2J^2 m_d \int d\epsilon N(\epsilon) \frac{P(\epsilon)}{\epsilon_k - \epsilon} = \frac{\sqrt{2}J^2 m_d m^{\frac{3}{2}}}{\pi^2 \hbar^3} \int d\epsilon \frac{\sqrt{\epsilon} P(\epsilon)}{\epsilon_k - \epsilon} \end{aligned} \quad (2.4.48)$$

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

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

For $T > 0$ but $\ll T_F$, the excitation energy of the electrons is very small and of the order of $k_B T$. Hence, we can replace $\epsilon_k - \epsilon_F = k_B T$ and everywhere else replace $\epsilon_k = \epsilon_F$.

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

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

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

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

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

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

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

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

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

$$\begin{aligned} T_{\text{flip}}^{(2)} &= 2J^2 \lambda_+ \sum_q \frac{P(q)}{\epsilon_k - \epsilon_q} \\ &= 2J^2 \lambda_+ N(\epsilon_F) \ln \left| \frac{T_F}{T} \right| \end{aligned} \quad (2.4.55)$$

Adding the first order contribution,

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

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

$$\mathcal{P} = \mathcal{P}^{(2)} \left[1 + 2JN(\epsilon_F) \ln \frac{T_F}{T} \right] \quad (2.4.57)$$

2.4.3 The Kondo resonance

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

$$T_{a \rightarrow b} = \sum_{s, m_s} |\langle s, m_s | a \rangle|^2 T_s \quad (2.4.58)$$

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

$$T_{|k \uparrow, d_\uparrow\rangle \rightarrow |k' \uparrow, d_\uparrow\rangle} = T_1 \quad (2.4.59)$$

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

$$T_{|k \uparrow, d_\downarrow\rangle \rightarrow |k' \uparrow, d_\downarrow\rangle} = \frac{T_1 + T_0}{2} \quad (2.4.60)$$

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

$$T_{|k \uparrow, d_\downarrow\rangle \rightarrow |k' \downarrow, d_\uparrow\rangle} = \frac{T_1 - T_0}{2} \quad (2.4.61)$$

Therefore,

$$\begin{aligned} T_1 &= T_{|k \uparrow, d_\downarrow\rangle \rightarrow |k' \uparrow, d_\downarrow\rangle} + T_{|k \uparrow, d_\downarrow\rangle \rightarrow |k' \downarrow, d_\uparrow\rangle} = T_{\text{nonflip}} + T_{\text{flip}} \\ T_0 &= T_{|k \uparrow, d_\downarrow\rangle \rightarrow |k' \uparrow, d_\downarrow\rangle} - T_{|k \uparrow, d_\downarrow\rangle \rightarrow |k' \downarrow, d_\uparrow\rangle} = T_{\text{nonflip}} - T_{\text{flip}} \end{aligned} \quad (2.4.62)$$

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

$$T_{\text{nonflip}} = J \left[m_d + \frac{J}{4} \{ 3(\alpha + \gamma) + 4m_d(\gamma - \alpha) \} \right] \quad (2.4.63)$$

$$T_{\text{flip}} = J \left[1 + J(\gamma - \alpha) \right] \quad (2.4.64)$$

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

$$\begin{aligned} T_1 &= \frac{J}{2} \left[1 + \frac{J}{2} (\alpha + 5\gamma) \right] \\ T_0 &= -\frac{3J}{2} \left[1 - \frac{3J}{2} \left(\alpha - \frac{\gamma}{3} \right) \right] \end{aligned} \quad (2.4.65)$$

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

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

Hence, the pre-factors are just the bare values of the interaction Hamiltonian, V . Hence, the equations 2.4.65 can be written as

$$T = V(1 + TG) \quad (2.4.67)$$

For the singlet and triplet T -matrices, it becomes

$$\begin{aligned} T_1 &= \frac{J}{2} \left[1 + T_1 (\alpha + 5\gamma) \right] \implies T_1 = \frac{J/2}{1 - \frac{J}{2}(\alpha + 5\gamma)} \\ T_0 &= -\frac{3J}{2} \left[1 + T_0 \left(\alpha - \frac{\gamma}{3} \right) \right] \implies T_0 = \frac{-3J/2}{1 + \frac{3J}{2}(\alpha - \gamma/3)} \end{aligned} \quad (2.4.68)$$

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

$$T_1 = \frac{1}{2/J - 5\gamma - \alpha} \quad (2.4.69)$$

$$T_0 = \frac{1}{-2/3J + \gamma/2 - \alpha} \quad (2.4.70)$$

For excitations (k) just above the Fermi surface, α will encounter a zero in its denominator, because the integral in α is outside the Fermi surface. On the other hand, the integral in γ is inside the Fermi surface, so the denominator in γ will never become zero for k just outside the Fermi surface. Hence, $\alpha = \text{real part} - i\pi N(0)$, $\gamma = \text{real part}$. Accordingly, the expressions for T_s can be written as

$$T_s = \frac{1}{\text{real part} + i\pi N(0)} \quad (2.4.71)$$

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

$$|T_s| \leq \frac{1}{\pi N_0} \quad (2.4.72)$$

From eq. 2.1.30, we can write

$$T_s = -\frac{e^{i\delta_s} \sin \delta_s}{\pi N(0)} \quad (2.4.73)$$

Eq. 2.3.24 allows us to write

$$\rho_{d\sigma}(0) = -\frac{\text{Im}[T]}{t^2\pi} = \frac{\sin^2 \delta_s}{t^2\pi^2 N(0)} = \frac{\sin^2 \delta_s}{\pi\Delta} = \frac{1}{\pi\Delta} \sin^2 \left(\frac{\pi n_c}{2} \right) \quad (2.4.74)$$

where $n_c = \langle n_{d\uparrow} + n_{d\downarrow} \rangle$. This is in contrast to the value obtained from the mean field analysis of the Anderson model, eq. 2.3.36,

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

For $n_c = 1$ (half-filling), the mean field value is less than the one obtained from the spin-spin scattering. This is because the mean-field analysis does not take these scatterings into account. The large density of states at the Fermi level means that the spectral function has three peaks in general, two of which are revealed in the mean field analysis, but a third one exists, which is of a width of the order of a very low temperature T_K , and hence is not noticed at higher temperatures.

Eq. 2.4.68 can be written as

$$T_1 = \frac{J/2}{1 - 2J\gamma - \frac{J}{2}(\alpha + \gamma)} \quad (2.4.76)$$

$$T_0 = \frac{-3J/2}{1 - 2J\gamma + \frac{3J}{2}(\alpha + \gamma)} \quad (2.4.77)$$

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

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

$\alpha + \gamma$ can be calculated as

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

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

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

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

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

Since

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

we can write

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

Similarly,

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

giving

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

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

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

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

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

This scattered wave is thus another radial wave but its phase is shifted by an amount $\Delta r = \frac{\delta_d}{k_F}$. For a positive Δr (and hence a positive δ_d), the wave will be drawn inward. Hence, the singlet channel having a positive δ will lead to formation of bound states. On the other hand, the triplet channel has a negative phase shift, meaning it is repulsive.

2.4.4 Adiabatic route to the Kondo resonance

Assuming $T = 0$, the interactions due to a single impurity are unlikely to break adiabaticity. Hence, we replace the effect of the U on the impurity by adding a self energy $\Sigma(\omega)$ to the bare energy ϵ_d . This self energy can be Taylor-expanded about $E = 0$:

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

Defining

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

we can write

$$\Sigma(E) = \Sigma(0) + \left(1 - Z^{-1}\right) E \quad (2.4.90)$$

The interacting Green's function for the impurity becomes

$$G_d(E) = \frac{1}{E - \epsilon_d - \Sigma - i\Delta} \quad (2.4.91)$$

where Δ is the result of the hybridisation. Substituting eq. 2.4.90 and gathering the terms gives

$$G_d(E) = \frac{Z}{E - Z(\epsilon_d + \Sigma(0)) - iZ\Delta} \quad (2.4.92)$$

Defining the renormalised parameters

$$\epsilon_d^* = Z(\epsilon_d + \Sigma(0)) \quad (2.4.93)$$

$$\Delta^* = Z\Delta \quad (2.4.94)$$

we have

$$G_d(E) = \frac{Z}{E - \epsilon_d^* - i\Delta^*} \quad (2.4.95)$$

What this means is that as we adiabatically vary the interaction U , the parameters ϵ_d^* and Δ^* also morph, keeping the form of the Greens's function constant. In the non-interacting limit ($U = 0$), we have

$$Z = 1, \Sigma = 0 \implies \epsilon_d^* = \epsilon_d, \Delta^* = \Delta \quad (2.4.96)$$

We then recover the atomic form of the Green's function. Z varies from 0 to 1. $Z = 1$ is the non-interacting limit, $Z = 0$ is the limit of $U = \infty$. The phase shift due to scattering can be calculated by looking at eq.2.3.27, and replacing the bare quantities with the renormalised versions:

$$\delta_d(0) = \cot^{-1} \frac{\epsilon_d^*}{\Delta^*} \quad (2.4.97)$$

Similarly, the renormalised version of eq. 2.3.16 is

$$\rho_d(0) = \frac{1}{\pi} \frac{\Delta^*}{\epsilon_d^{*2} + \Delta^{*2}} \quad (2.4.98)$$

Using eq. 2.4.97 gives

$$\rho_d(0) = \frac{1}{\pi} \frac{\Delta^*}{\Delta^{*2} \cot^2 \delta_d + \Delta^{*2}} = \frac{\sin^2 \delta_d}{\pi \Delta} \quad (2.4.99)$$

2.4.5 The Kondo temperature

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

$$H_K = \sum_{k > k_F} \epsilon_k n_k - \frac{3J}{2} \sum_{k, k' > k_F} c_{k'\sigma}^\dagger c_{k\sigma} \quad (2.4.100)$$

The operator to create the singlet state $|S_k\rangle = \frac{1}{\sqrt{2}} (|k \uparrow, d \downarrow\rangle - |k \downarrow, d \uparrow\rangle)$ off the Fermi sea ($|\Phi\rangle$) is

$$b_k^\dagger = \frac{1}{\sqrt{2}} (c_{k\uparrow}^\dagger c_{d\downarrow}^\dagger - c_{k\downarrow}^\dagger c_{d\uparrow}^\dagger) \quad (2.4.101)$$

Hence the total wavefunction of singlet+Fermi-sea is

$$|\Psi\rangle = \sum_{k>k_F} a_k b_k^\dagger |\Phi\rangle = |\Phi\rangle \otimes \sum_{k>k_F} a_k |S_k\rangle \quad (2.4.102)$$

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

$$a_q = \langle \Phi | \langle S_q | \sum_k a_k |S_k\rangle | \Phi \rangle = \langle \Phi | b_q | \Psi \rangle \quad (2.4.103)$$

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

$$\begin{aligned} E |\Psi\rangle &= H_K |\Psi\rangle = |\Phi\rangle \otimes H_K \sum_{k>k_F} a_k |S_k\rangle \\ &= |\Phi\rangle \otimes \sum_{k>k_F} a_k \left(\epsilon_k |S_k\rangle - \frac{3J}{2} \sum_{k'>k_F} |S_{k'}\rangle \right) \\ &= \sum_{k>k_F} a_k \left(\epsilon_k b_k^\dagger - \frac{3J}{2} \sum_{k'>k_F} b_{k'}^\dagger \right) |\Phi\rangle \end{aligned} \quad (2.4.104)$$

Multiplying b_q from left gives

$$E b_q |\Psi\rangle = \epsilon_q a_q |\Phi\rangle - \frac{3J}{2} \sum_{k>k_F} a_k |\Phi\rangle \quad (2.4.105)$$

Multiplying $\langle \Phi |$ from left and looking at eq. 2.4.103 gives

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

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

$$1 = \frac{3J}{2} \sum_{q>k_F} \frac{1}{\epsilon_q - E} \quad (2.4.107)$$

Converting to integral,

$$1 = \frac{3J}{2} \int_{\epsilon_F}^D d\epsilon \frac{N(\epsilon)}{\epsilon - E} \quad (2.4.108)$$