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0.1 T -matrix and S -matrix

It is defined as

$$V\psi = T\phi \quad (1)$$

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

$$H_0\phi = E\phi \quad (2)$$

$$(H_0 + V)\psi = E\psi \quad (3)$$

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

$$\psi = \phi + G_0V\psi \quad (4)$$

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

$$\begin{aligned} \psi &= \phi + G_0T\phi \\ \implies \psi &= (1 + G_0T)\phi \end{aligned} \quad (5)$$

Eq. 4 can also be written as

$$\psi = (1 - G_0 V)^{-1} \phi \quad (6)$$

Comparing the last two equations gives

$$\begin{aligned} 1 &= (1 - G_0 V)(1 + G_0 T) \\ \implies T &= V + V G_0 T \end{aligned} \quad (7)$$

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

$$T = V + V G_0 V + V G_0 V G_0 V + \dots \quad (8)$$

From scattering theory, we can write

$$\psi = (2\pi)^{-\frac{3}{2}} \left[e^{ikx} + f \frac{e^{ikr}}{r} \right] \quad (9)$$

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

$$f(k', k) \sim \langle k' | T | k \rangle \quad (10)$$

By definition, the S -matrix is

$$S(\omega) = e^{2i\pi\delta(\omega)} \quad (11)$$

Also,

$$S = 1 - 2i\pi\rho T \quad (12)$$

Therefore,

$$T = \frac{1}{2i\pi\rho} \left(1 - e^{2i\pi\delta(\omega)} \right) = -\frac{e^{i\delta} \sin \delta}{\pi\rho} \quad (13)$$

0.2 An identity

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

$$HA = A(\lambda + H) \quad (14)$$

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

$$(E - H)A = AE - A(\lambda + H) = A(E - \lambda - H) \quad (15)$$

$$\implies A(E - \lambda - H)^{-1} = (E - H)^{-1}A \quad (16)$$

0.3 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,

$$n_{k\sigma} = \begin{cases} 1 & k \leq k_F \\ 0 & k > k_F \end{cases} \quad (17)$$

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.

$$\Psi^* \xrightarrow{\text{turn interactions off}} \Phi \quad (18)$$

$$\Phi^* \xrightarrow{\text{turn interactions off}} \Psi \quad (19)$$

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,

$$|IGS\rangle \otimes |k_+\rangle \xrightarrow{\text{turn interactions on}} |RGS\rangle \otimes |k_+\rangle^* \quad (20)$$

$$|IGS\rangle \otimes |k_-\rangle \xrightarrow{\text{turn interactions on}} |RGS\rangle \otimes |k_-\rangle^* \quad (21)$$

$$(22)$$

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

$$c_{k_+}^\dagger |IGS\rangle \xrightarrow{\text{turn interactions on}} \eta_{k_+}^\dagger |RGS\rangle \quad (23)$$

$$c_{k_-} |IGS\rangle \xrightarrow{\text{turn interactions on}} \eta_{k_-} |RGS\rangle \quad (24)$$

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

$$\delta n_k = n_k - n_k^0 \quad (25)$$

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.

$$\mathcal{E}^0[n_k] = \sum_k n_k \epsilon_k \quad (26)$$

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

$$\mathcal{E}[n_k] = \mathcal{E}[n_k^0] + \sum_k \frac{\partial \mathcal{E}}{\partial n_k} \delta n_k \quad (27)$$

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

$$\delta \mathcal{E} \equiv \mathcal{E}[n_k] - \mathcal{E}[n_k^0] = \sum_k \xi_k \delta n_k \quad (28)$$

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

$$n_k^2 - n_k^1 = \begin{cases} 0 & k \neq q \\ 1 & k = q \end{cases} \quad (29)$$

Then, up to first order,

$$\mathcal{E}[n_k^2] - \mathcal{E}[n_k^1] = \sum_k \xi_k (n_k^2 - n_k^1) = \xi_q \quad (30)$$

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.

$$\xi_k = \xi_k^0 + \sum_q \frac{\partial \xi_k}{\partial n_q} \delta n_q \quad (31)$$

Eq. 28 then becomes

$$\delta \mathcal{E} = \sum_k \xi_k^0 \delta n_k + \sum_{k,q} f(k,q) \delta n_k \delta n_q \quad (32)$$

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 ,

$$f(\xi) = \left[e^{(\xi - \mu)\beta} + 1 \right]^{-1} \quad (33)$$

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

$$F[\delta n_k] = \delta \mathcal{E}[\delta n_k] - TS[\delta n_k] \quad (34)$$

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

$$\xi_k(T) = \xi_k^0 + \sum_q f(k,q) \langle \delta n_q \rangle \quad (35)$$

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

$$\left. \frac{dF}{d\delta n_q} \right|_{\delta n_q = \langle \delta n_q \rangle} = 0 \quad (36)$$

0.4 The model

$$H = \epsilon_d \hat{n}_d + \sum_k \epsilon_k \hat{n}_k + \sum_{k\sigma} t \left(c_{k\sigma}^\dagger c_{d\sigma} + c_{d\sigma}^\dagger c_{k\sigma} \right) + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \quad (37)$$

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.

0.5 Atomic limit ($t = 0$)

$$H_{\text{atomic}} = E_d + E_{CB} + U n_{d\uparrow} n_{d\downarrow} \quad (38)$$

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

$$H_{\text{atomic}} = \epsilon_d n_d + U n_{d\uparrow} n_{d\downarrow} \quad (39)$$

For a magnetic solution, we need

$$(\epsilon_\uparrow = \epsilon_\downarrow) \epsilon_d < (\epsilon_0, \epsilon_{\uparrow\downarrow}) 0, 2\epsilon_d + U \quad (40)$$

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

$$\epsilon_d > -U \quad (41)$$

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

$$H_{\text{non-int}} = \epsilon_d n_d + \sum_k \epsilon_k n_k + \sum_{k\sigma} t \left(c_{k\sigma}^\dagger c_{d\sigma} + c_{d\sigma}^\dagger c_{k\sigma} \right) \quad (42)$$

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

$$G_d^0(E) = \frac{1}{E - \epsilon_d} \quad (43)$$

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

$$G_d^0 \Sigma_c G_d^0, \text{ where } \Sigma_c = t \left(\sum_k G_k^0 \right) t = \sum_k \frac{t^2}{E - \epsilon_k} \quad (44)$$

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

$$\begin{aligned} G_d(E) &= G_d^0 + G_d^0 \Sigma_c G_d^0 + G_d^0 \Sigma_c G_d^0 \Sigma_c G_d^0 + G_d^0 \Sigma_c G_d^0 \Sigma_c G_d^0 \Sigma_c G_d^0 + \dots \\ &= G_d^0 \left[1 + (\Sigma_c G_d^0)^2 + \dots \right] = G_d^0 \frac{1}{1 - \Sigma_c G_d^0} = \frac{1}{E - \epsilon_d - \Sigma_c(E)} \end{aligned} \quad (45)$$

Now,

$$\frac{1}{t^2} \Sigma_c(E) = \sum_k \frac{1}{E - \epsilon_k} = \lim_{\eta \rightarrow 0} \int_{-W}^W d\epsilon \rho(\epsilon) \frac{1}{E - \epsilon + i\eta} \quad (46)$$

$$\Rightarrow \frac{1}{t^2} \text{Re} [\Sigma_c(E)] = \int_{-W}^W d\epsilon \rho(\epsilon) \frac{1}{E - \epsilon}, \text{ and} \quad (47)$$

$$\frac{1}{t^2} \text{Im} [\Sigma_c(E)] = \int_{-W}^W d\epsilon \rho(\epsilon) (-i\pi) \delta(E - \epsilon) \quad (48)$$

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

$$\Sigma_c(E) = \text{Im} [\Sigma_c(E)] = -i\pi t^2 \rho(E) = -i\Delta \quad (49)$$

Therefore,

$$G_d(E) = \frac{1}{E - \epsilon_d + i\Delta} \quad (50)$$

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

$$\rho_d^0(E) = -\frac{1}{\pi} \text{Im} [G_f^0] = -\frac{1}{\pi} \lim_{\eta \rightarrow 0} \frac{1}{E - \epsilon_d + i\eta} = \delta(E - \epsilon_d) \quad (51)$$

$$\rho_d(E) = -\frac{1}{\pi} \text{Im} [G_f] = -\frac{1}{\pi} \lim_{\eta \rightarrow 0} \frac{1}{E - \epsilon_d + i(\eta + \Delta)} = \frac{1}{\pi} \frac{\Delta}{(E - \epsilon_d)^2 + \Delta^2} \quad (52)$$

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:

$$\langle n_d \rangle = 2 \int d\epsilon \rho_d(\epsilon) = \frac{2\Delta}{\pi} \int \frac{d\epsilon}{(\epsilon - \epsilon_d)^2 + \Delta^2} = \frac{2}{\pi} \cot^{-1} \left(\frac{\epsilon_d}{\Delta} \right) \quad (53)$$

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

T -matrix is defined by

$$T = V + VGT \quad (54)$$

We also have

$$\begin{aligned} G &= G_0 + G_0VG = G_0 + G_0T \frac{1}{1 + GT} G \\ &= G_0 + G_0T(1 - GT + \dots)(G_0 + G_0VG_0 + \dots) \\ &= G_0 + G_0TG_0 \end{aligned} \quad (55)$$

The conduction electron Green's function can be calculated as

$$\begin{aligned} G_c(k, k', E) &= \delta_{k,k'} G_c^0(k, E) + G_c^0(k) t G_f^0 t G_c^0(k') + \\ &G_c^0(k) t G_f^0 t \sum_q G_c^0(q) t G_f^0 t G_c^0(k') + \dots \end{aligned} \quad (56)$$

Noting that

$$t \sum_q G_c^0(q) t = \Sigma_c, \quad (57)$$

we have

$$G_c(k, k', E) = \delta_{k,k'} G_c^0(k, E) + G_c^0(k) t^2 G_f(E) G_c^0(k) \quad (58)$$

Comparing with the final form of G in eq. 55, we can write

$$T(k, k', E) = t^2 G_d(E) = \frac{t^2}{E - \epsilon_d + i\Delta} = -\frac{t^2}{\Delta} \frac{1}{\frac{\epsilon_d - E}{\Delta} - i} \quad (59)$$

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

$$\text{Im}[T] = -\frac{t^2 \Delta}{(E - \epsilon_d)^2 + \Delta^2} = -\pi t^2 \rho_d \quad (60)$$

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

$$\rho_d = -\frac{1}{\pi} \text{Im}[G_d] = -\frac{1}{\pi t^2} \text{Im}[t^2 G_d] = -\frac{1}{\pi t^2} \text{Im}[T] \quad (61)$$

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

$$T = e^{2i\delta} - 1 = e^{i\delta} (e^{i\delta} - e^{-i\delta}) \sim \frac{1}{\cot \delta - i} \quad (62)$$

Comparing with eq. 59, we can write

$$\delta(E) = \cot^{-1} \left(\frac{\epsilon_d - E}{\Delta} \right) \quad (63)$$

When $E = \epsilon_d$, the phase shift is π , and the scattering is head on (the conduction electron is reflected back). Comparing with eq. 53,

$$\frac{2}{\pi} \delta(0) = \langle n_d \rangle \quad (64)$$

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

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 .

$$H_{\text{dot}} = \sum_{m\sigma} \epsilon_m n_{m\sigma} + U \frac{N(N+1)}{2} \quad (65)$$

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.

$$H_{\text{dot}} = \sum_{m\sigma} (\epsilon_m - eV) n_{m\sigma} + U \frac{N(N+1)}{2} \quad (66)$$

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

$$\Delta E = UN + \epsilon_N - eV \quad (67)$$

Tuning the voltage can make these two levels degenerate.

$$eV^* = UN + \epsilon_N \quad (68)$$

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,

$$G(V) = G_0 \rho(0) = \frac{2e^2}{h} \frac{\Delta^2}{(\epsilon_m - eV)^2 + \Delta^2} \quad (69)$$

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

0.7 Total Hamiltonian: Mean field treatment

$$n_{d\uparrow}n_{d\downarrow} \approx n_{d\uparrow}\langle n_{d\downarrow} \rangle + n_{d\downarrow}\langle n_{d\uparrow} \rangle + \text{constant} \quad (70)$$

$$H \approx \sum_k \epsilon_k n_k + \sum_\sigma [\epsilon_d + U\langle n_{d\bar{\sigma}} \rangle] n_{d\sigma} + t \sum_{k\sigma} \left(c_{k\sigma}^\dagger c_{d\sigma} + c_{d\sigma}^\dagger c_{k\sigma} \right) \quad (71)$$

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

$$\rho_{d\sigma} = \frac{1}{\pi} \frac{\Delta}{(E - \epsilon_{d\sigma})^2 + \Delta^2} \implies \langle n_{d\sigma} \rangle = \int \rho_{d\sigma} = \frac{1}{\pi} \cot^{-1} \left(\frac{\epsilon_{d\sigma}}{\Delta} \right) \quad (72)$$

An alternative way of writing that is

$$\frac{\epsilon_{d\sigma}}{\Delta} = \frac{\epsilon_d + U\langle n_{d\bar{\sigma}} \rangle}{\Delta} = \cot(\pi\langle n_{d\sigma} \rangle) \implies \langle n_{d\sigma} \rangle = \frac{\Delta}{U} \left[\cot(\pi\langle n_{d\bar{\sigma}} \rangle) - \frac{\epsilon_d}{\Delta} \right] \quad (73)$$

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

$$\begin{aligned} \langle n_{d\uparrow} - n_{d\downarrow} \rangle &\equiv m = \frac{\Delta}{U} [\cot(\pi\langle n_{d\downarrow} \rangle) - \cot(\pi\langle n_{d\uparrow} \rangle)] \\ &= \frac{\Delta}{U} \left[\cot \frac{\pi}{2} (n_d - m) - \cot \frac{\pi}{2} (n_d + m) \right] \end{aligned} \quad (74)$$

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

$$\cot(a+x) \approx \cot a - x (\sin a)^{-2} \implies \cot(a-x) - \cot(a+x) \approx 2x (\sin a)^{-2} \quad (75)$$

we get

$$m = \frac{\Delta}{U} \left[-\pi \frac{m}{\sin^2 \frac{\pi n_d}{2}} \right] \implies 1 = \lim_{m \rightarrow 0} \frac{U}{\pi \Delta} \frac{1}{1 + \cot^2 \frac{\pi n_d}{2}} \quad (76)$$

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. 76,

$$1 = \frac{U_c}{\pi} \frac{\Delta}{\Delta^2 + \left(\frac{U_c n_d}{2} + \epsilon_d \right)^2} \quad (77)$$

Magnetism will prevail for $U \geq U_c$. Comparing with eq. 73,

$$1 = U_c \rho_d(E=0) \quad (78)$$

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

$$U_c = \pi \Delta \quad (79)$$

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

$$\langle n_{d\uparrow} \rangle = \frac{1+m}{2} \quad (80)$$

$$\langle n_{d\downarrow} \rangle = \frac{1-m}{2} \quad (81)$$

$$\epsilon_{d\sigma} = \epsilon_d + U \langle n_{d\sigma} \rangle = \epsilon_d + \frac{U}{2} \pm \frac{U}{2} m = \pm \frac{U}{2} m \quad (82)$$

$$\rho_d = \rho_{d\uparrow} + \rho_{d\downarrow} = \frac{\Delta}{\pi} \left[\frac{1}{\Delta^2 + \left(E - \frac{U m}{2} \right)^2} + \frac{1}{\Delta^2 + \left(E + \frac{U m}{2} \right)^2} \right] \quad (83)$$

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

0.8 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 $T \rightarrow 0$.

0.9 Derivation of the Kondo Hamiltonian:

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

$$\begin{aligned} \text{low energy (L)} &\rightarrow \begin{cases} |\uparrow\rangle \\ |\downarrow\rangle \end{cases} \\ \text{high energy (H)} &\rightarrow \begin{cases} | \rangle \\ |\uparrow\downarrow\rangle \end{cases} \end{aligned} \quad (84)$$

$$H = H_0 + V = \begin{matrix} & \begin{matrix} \text{low} & \text{high} \end{matrix} \\ \begin{matrix} \text{low} \\ \text{high} \end{matrix} & \begin{pmatrix} H^L & v^\dagger \\ v & H^H \end{pmatrix} \end{matrix} \quad (85)$$

$$H_0 = \sum_k \epsilon_k n_k + \epsilon_d n_d + U n_{d\uparrow} n_{d\downarrow}, V = \sum_{k\sigma} \left(V_k c_{k\sigma}^\dagger c_{d\sigma} + V_k^* c_{d\sigma}^\dagger c_{k\sigma} \right) \quad (86)$$

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

$$\bar{H} = e^{-S} H e^S = H_0 + (V + [H_0, S]) + \frac{1}{2} ([V, S] + [[H_0, S], S]) \quad (87)$$

Defining S such that the first order term vanishes,

$$V = [S, H_0] \quad (88)$$

$$\bar{H} = H_0 + \frac{1}{2} [V, S] \quad (89)$$

Take $S = \begin{pmatrix} 0 & -s^\dagger \\ s & 0 \end{pmatrix}$. From eq. 88,

$$\begin{aligned} V &= \begin{pmatrix} 0 & -s^\dagger \\ s & 0 \end{pmatrix} \begin{pmatrix} H^L & 0 \\ 0 & H^H \end{pmatrix} - \begin{pmatrix} H^L & 0 \\ 0 & H^H \end{pmatrix} \begin{pmatrix} 0 & -s^\dagger \\ s & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & -s^\dagger H^H + H^L s^\dagger \\ s H^L - H^H s & 0 \end{pmatrix} \end{aligned} \quad (90)$$

Comparing with the definition of V , we can write

$$v_{ij}^\dagger = s_{ij}^\dagger (E_i^L - E_j^H), v_{ij} = s_{ij} (E_j^L - E_i^H) \quad (91)$$

$$\Rightarrow s_{ij}^\dagger = \frac{v_{ij}^\dagger}{E_i^L - E_j^H}, s_{ij} = \frac{v_{ij}}{E_j^L - E_i^H} \quad (92)$$

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

$$[V, S] = \begin{pmatrix} 0 & v^\dagger \\ v & 0 \end{pmatrix} \begin{pmatrix} 0 & -s^\dagger \\ s & 0 \end{pmatrix} - \begin{pmatrix} 0 & -s^\dagger \\ s & 0 \end{pmatrix} \begin{pmatrix} 0 & v^\dagger \\ v & 0 \end{pmatrix} = \begin{pmatrix} v^\dagger s + s^\dagger v & 0 \\ 0 & -v s^\dagger - s v^\dagger \end{pmatrix} \quad (93)$$

Hence,

$$\overline{H} = H_0 + \frac{[V, S]}{2} = \begin{pmatrix} H^L + \frac{1}{2} (v^\dagger s + s^\dagger v) & 0 \\ 0 & H^H - v s^\dagger - s v^\dagger \end{pmatrix} \quad (94)$$

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

$$\mathcal{H} = \langle L | \overline{H} | L \rangle = H^L + \frac{1}{2} (v^\dagger s + s^\dagger v) \quad (95)$$

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

$$\begin{aligned} \Delta H &= \frac{1}{2} (v^\dagger s + s^\dagger v) = \frac{1}{2} \left(v^\dagger \sum_{HL} s_{HL} |H\rangle \langle L| + \text{h.c.} \right) \\ &= \frac{1}{2} \sum_{HL} \left[v^\dagger |H\rangle \langle L| \frac{v_{HL}}{E_L - E_H} + |L\rangle \langle H| \frac{v_{LH}^\dagger}{E_L - E_H} v \right] \end{aligned} \quad (96)$$

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

$$\Delta H_{ll'} = \langle l | \Delta H | l' \rangle = \frac{1}{2} \sum_H v_{lH}^\dagger v_{Hl'} \left(\frac{1}{E_{l'} - E_H} + \frac{1}{E_l - E_H} \right) \quad (97)$$

This can also be written as

$$\Delta H_{ll'} = \frac{1}{2} [T_{ll'}(E_l) + T_{ll'}(E_{l'})] \quad (98)$$

where

$$T_{ll'}(E) = \sum_H \frac{v_{lH}^\dagger v_{Hl'}}{E - E_H} = \sum_H \frac{V_{lH}^\dagger V_{Hl'}}{E - E_H} \quad (99)$$

$T(E)$, 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

$$\begin{aligned} \Delta H_{ll'} &= \sum_H v_{lH}^\dagger v_{Hl'} \frac{1}{E_L - E_H} \\ \Rightarrow \Delta H &= V \left(\sum_H \frac{1}{\Delta_{LH}} |H\rangle \langle H| \right) V \end{aligned} \quad (100)$$

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,

$$\Delta_{LH_1} = \epsilon_d - 0 = \epsilon_d, \Delta_{LH_2} = \epsilon_d - (2\epsilon_d + U) = -\epsilon_d - U \quad (101)$$

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

$$\begin{aligned} \Delta H &= V \frac{|0\rangle \langle 0|}{\epsilon_d} V - V \frac{|\uparrow\downarrow\rangle \langle \uparrow\downarrow|}{\epsilon_d + U} V \\ &= \sum_{k_1, k_2, \sigma_1, \sigma_2} V(k_1) V^*(k_2) \left[\frac{c_{d\sigma_2}^\dagger c_{k_2\sigma_2} |0\rangle \langle 0| c_{k_1\sigma_1}^\dagger c_{d\sigma_1}}{\epsilon_d} - \frac{c_{k_1\sigma_1}^\dagger c_{d\sigma_1} |\uparrow\downarrow\rangle \langle \uparrow\downarrow| c_{d\sigma_2}^\dagger c_{k_2\sigma_2}}{\epsilon_d + U} \right] \\ &= \sum_{k_1, k_2, \sigma_1, \sigma_2} V(k_1) V^*(k_2) \frac{c_{d\sigma_2}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_1} |d\sigma_1, h_{k_1\sigma_1}\rangle \langle d\sigma_1, h_{k_1\sigma_1}|}{\epsilon_d} \\ &\quad - \sum_{k_1, k_2, \sigma_1, \sigma_2} V(k_1) V^*(k_2) \frac{c_{k_1\sigma_1}^\dagger c_{d\sigma_1} c_{d\sigma_2}^\dagger c_{k_2\sigma_2} |d\bar{\sigma}_2, e_{k_2\sigma_2}\rangle \langle d\bar{\sigma}_2, e_{k_2\sigma_2}|}{\epsilon_d + U} \\ &= \sum_{k_1, k_2, \sigma_1, \sigma_2} V(k_1) V^*(k_2) \left[\frac{c_{d\sigma_2}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_1}}{\epsilon_d} - \frac{c_{k_1\sigma_1}^\dagger c_{d\sigma_1} c_{d\sigma_2}^\dagger c_{k_2\sigma_2}}{\epsilon_d + U} \right] P_{n_d=1} \end{aligned} \quad (102)$$

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

$$\begin{aligned} c_{d\sigma_2}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_1} &= \sum_{\sigma_3, \sigma_4} c_{d\sigma_3}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_4} \delta_{\sigma_1\sigma_3} \delta_{\sigma_4\sigma_2} \\ &= \frac{1}{2} \sum_{\sigma_3, \sigma_4} c_{d\sigma_3}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_4} (\delta_{\sigma_1\sigma_2} \delta_{\sigma_3\sigma_4} + \vec{\sigma}_{\sigma_1\sigma_2} \cdot \vec{\sigma}_{\sigma_3\sigma_4}) \\ &= \frac{1}{2} c_{k_2\sigma_1} c_{k_1\sigma_1}^\dagger n_d + c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} \cdot \sum_{\sigma_3, \sigma_4} c_{d\sigma_3}^\dagger \frac{\vec{\sigma}_{\sigma_3\sigma_4}}{2} c_{d\sigma_4} \end{aligned} \quad (103)$$

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 $n_d = 1$.

$$c_{d\sigma_2}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_1} = -\frac{1}{2}c_{k_1\sigma_1}^\dagger c_{k_2\sigma_1} - c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2} \cdot \sum_{\sigma_3,\sigma_4} c_{d\sigma_3}^\dagger \frac{\vec{\sigma}_{\sigma_3\sigma_4}}{2} c_{d\sigma_4} \quad (104)$$

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

$$c_{d\sigma_2}^\dagger c_{k_2\sigma_2} c_{k_1\sigma_1}^\dagger c_{d\sigma_1} = -\frac{1}{2}c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2} \cdot \vec{\sigma}_d \quad (105)$$

Similarly,

$$c_{k_1\sigma_1}^\dagger c_{d\sigma_1} c_{d\sigma_2}^\dagger c_{k_2\sigma_2} = -\frac{1}{2}c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2} \cdot \vec{\sigma}_d \quad (106)$$

Finally, putting all this together,

$$\begin{aligned} \Delta H &= \frac{1}{2} \sum_{k_1,k_2,\sigma_1,\sigma_2} V(k_1)V^*(k_2) \left[\frac{1}{\epsilon_d + U} - \frac{1}{\epsilon_d} \right] c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2} \cdot \vec{\sigma}_d \\ &= \frac{1}{2} \sum_{k_1,k_2,\sigma_1,\sigma_2} J(k_1,k_2) c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2} \cdot \vec{\sigma}_d \end{aligned} \quad (107)$$

where

$$J(k_1,k_2) = V(k_1)V^*(k_2) \left[\frac{1}{\epsilon_d + U} - \frac{1}{\epsilon_d} \right] \quad (108)$$

Assuming $V(k) \equiv t$,

$$H_K = \sum_k \epsilon_k n_k + \frac{J}{2} \vec{\sigma}_e \cdot \vec{\sigma}_d \quad (109)$$

where

$$\vec{\sigma}_e = \sum_{k_1,k_2,\sigma_1,\sigma_2} c_{k_1\sigma_1}^\dagger \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2} = \sum_{\sigma_1,\sigma_2} c_{\sigma_1}^\dagger(\vec{r}=0) \vec{\sigma}_{\sigma_1\sigma_2} c_{\sigma_2}(\vec{r}=0) \quad (110)$$

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

0.10 Obtaining the resistivity minimum and log-dependence

The model we are working with is

$$H_K = H_0 + V = \sum_k \epsilon_k n_k + \frac{J}{2} \sum_{k_1,k_2,\sigma_1,\sigma_2} c_{k_1\sigma_1}^\dagger \vec{\sigma}_d \cdot \vec{\sigma}_{\sigma_1\sigma_2} c_{k_2\sigma_2} \quad (111)$$

$$\sum_{\sigma_1, \sigma_2} c_{k_1 \sigma_1}^\dagger \vec{\sigma}_d \cdot \vec{\sigma}_{\sigma_1 \sigma_2} c_{k_2 \sigma_2} = \sigma_d^z \left(c_{k_1 \uparrow}^\dagger c_{k_2 \uparrow} - c_{k_1 \downarrow}^\dagger c_{k_2 \downarrow} \right) + \sigma_d^x \left(c_{k_1 \downarrow}^\dagger c_{k_2 \uparrow} + c_{k_1 \uparrow}^\dagger c_{k_2 \downarrow} \right) - i \sigma_d^y \left(c_{k_1 \uparrow}^\dagger c_{k_2 \downarrow} - c_{k_1 \downarrow}^\dagger c_{k_2 \uparrow} \right) \quad (112)$$

$$= \sigma_d^z \left(c_{k_1 \uparrow}^\dagger c_{k_2 \uparrow} - c_{k_1 \downarrow}^\dagger c_{k_2 \downarrow} \right) + c_{k_1 \downarrow}^\dagger c_{k_2 \uparrow} \sigma_d^+ + c_{k_1 \uparrow}^\dagger c_{k_2 \downarrow} \sigma_d^- \quad (113)$$

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

$$\begin{aligned} H_K &= \sum_k \epsilon_k n_k + \frac{J}{2} \sum_{k_1, k_2} \left[\sigma_d^z \left(c_{k_1 \uparrow}^\dagger c_{k_2 \uparrow} - c_{k_1 \downarrow}^\dagger c_{k_2 \downarrow} \right) + \sigma_d^+ c_{k_1 \downarrow}^\dagger c_{k_2 \uparrow} + \sigma_d^- c_{k_1 \uparrow}^\dagger c_{k_2 \downarrow} \right] \\ &= \sum_k \epsilon_k n_k + J \sum_{k_1, k_2} \left[S_d^z \left(c_{k_1 \uparrow}^\dagger c_{k_2 \uparrow} - c_{k_1 \downarrow}^\dagger c_{k_2 \downarrow} \right) + S_d^+ c_{k_1 \downarrow}^\dagger c_{k_2 \uparrow} + S_d^- c_{k_1 \uparrow}^\dagger c_{k_2 \downarrow} \right] \end{aligned} \quad (114)$$

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

$$T = V + V G_0 V \quad (115)$$

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

First order scattering

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

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

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

$$T_{\text{nonflip}}^{(1)} = T_{k_\uparrow, d_\sigma \rightarrow q_\uparrow, d_\sigma} = \langle q_\uparrow, d_\sigma | V | k_\uparrow, d_\sigma \rangle = m_d J \quad (116)$$

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

$$\mathcal{P}_{k_\sigma, d_{\sigma'} \rightarrow q_\sigma, d_{\sigma'}} = 2\pi \sum_\epsilon \rho(\epsilon) T_{k_\uparrow, d_\sigma \rightarrow q_\uparrow, d_\sigma}^2 = 2\pi \rho(0) J^2 m_d^2 \quad (117)$$

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

$$\mathcal{P}_1 = 2\pi \rho(0) J^2 m_d^2 \quad (118)$$

For spin-flip, the matrix element is

$$T_{\text{flip}}^{(1)} = T_{k_\uparrow, d_\downarrow \rightarrow q_\downarrow, d_\uparrow} = \langle q_\downarrow, d_\uparrow | V | k_\uparrow, d_\downarrow \rangle = \lambda_+ J \quad (119)$$

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

$$\mathcal{P}_2 = \mathcal{P}_{k_\uparrow, d_\downarrow \rightarrow q_\downarrow, d_\uparrow} = 2\pi \rho(0) J [s_d(s_d + 1) - m_d(m_d + 1)] \quad (120)$$

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

$$\mathcal{P}^{(1)} = \frac{1}{2s_d + 1} \sum_{m_d = -s_d}^{s_d} (\mathcal{P}_1 + \mathcal{P}_2) = \frac{2\pi\rho(0)J^2}{(2s_d + 1)} \sum_{m_d = -s_d}^{s_d} (s_d(s_d + 1) - m_d) \quad (121)$$

$$= 2\pi\rho(0)J^2 s_d(s_d + 1)$$

Second order scattering

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

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

The second order transition matrix contribution is of the form

$$T_{i \rightarrow j}^{(2)} = \langle j | V G_0 V | i \rangle = \sum_l \frac{\langle j | V | l \rangle \langle l | V | i \rangle}{E_i - E_l} \quad (122)$$

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:

$$T_{11}^{(2)} = \sum_q \frac{\langle k'_\uparrow d_\sigma | V | q_\uparrow d_\sigma \rangle \langle q_\uparrow d_\sigma | V | k_\uparrow d_\sigma \rangle}{\epsilon_k - \epsilon_q} \quad (123)$$

$$= (Jm_d)^2 \sum_q \frac{1 - P(q)}{\epsilon_k - \epsilon_q} = J^2 m_d^2 \sum_q \frac{1 - P(q)}{\epsilon_k - \epsilon_q}$$

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,

$$T_{12}^{(2)} = \sum_q \frac{\langle q_\uparrow k'_\uparrow d_\sigma | V | k'_\uparrow k_\uparrow d_\sigma \rangle \langle k'_\uparrow k_\uparrow d_\sigma | V | q_\uparrow k_\uparrow d_\sigma \rangle}{\epsilon_q - \epsilon_{k'}} P(q) \quad (124)$$

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

$$T_{12}^{(2)} = -J^2 m_d^2 \sum_q \frac{P(q)}{\epsilon_q - \epsilon_k} = J^2 m_d^2 \sum_q \frac{P(q)}{\epsilon_k - \epsilon_q} \quad (125)$$

For the third process,

$$T_{13}^{(2)} = \sum_q \frac{\langle k'_\uparrow d_\downarrow | V | q_\downarrow d_\uparrow \rangle \langle q_\downarrow d_\uparrow | V | k_\uparrow d_\downarrow \rangle}{\epsilon_k - \epsilon_q} \quad (126)$$

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

$$T_{13}^{(2)} = \lambda_+^2 J^2 \sum_q \frac{1 - P(q)}{\epsilon_k - \epsilon_q} \quad (127)$$

For the fourth process,

$$\begin{aligned} T_{14}^{(2)} &= \sum_q \frac{\langle q_\downarrow k'_\uparrow d_\uparrow | V | k'_\uparrow k_\uparrow d_\downarrow \rangle \langle k'_\uparrow k_\uparrow d_\downarrow | V | q_\downarrow k_\uparrow d_\uparrow \rangle}{\epsilon_q - \epsilon'_k} \\ &= -\lambda_-^2 J^2 \sum_q \frac{P(q)}{\epsilon_q - \epsilon_k} \\ &= \lambda_-^2 J^2 \sum_q \frac{P(q)}{\epsilon_k - \epsilon_q} \end{aligned} \quad (128)$$

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

$$\begin{aligned} T_{\text{nonflip}}^{(2)} &= \sum_{i=1}^4 T_{1i}^{(2)} = J^2 \sum_q \frac{m_d^2 + \lambda_+^2 - P(q)(\lambda_+^2 - \lambda_-^2)}{\epsilon_k - \epsilon_q} \\ &= J^2 \sum_q \frac{s(s+1) - m_d + 2m_d P(q)}{\epsilon_k - \epsilon_q} \\ &= J^2 [s(s+1) - m_d] (\alpha + \gamma) + 2J^2 m_d \gamma \end{aligned} \quad (129)$$

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

$$\begin{aligned} T_{\text{nonflip}}^{(2)} &= 2J^2 m_d \gamma \\ &= 2J^2 m_d \int d\epsilon N(\epsilon) \frac{P(\epsilon)}{\epsilon_k - \epsilon} = \frac{\sqrt{2} J^2 m_d m^{\frac{3}{2}}}{\pi^2 \hbar^3} \int d\epsilon \frac{\sqrt{\epsilon} P(\epsilon)}{\epsilon_k - \epsilon} \end{aligned} \quad (130)$$

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

$$\begin{aligned} T_{\text{nonflip}}^{(2)} &= \frac{\sqrt{2}J^2m_d m^{\frac{3}{2}}}{\pi^2\hbar^3} \sqrt{\epsilon_k} \ln \left| \frac{\sqrt{\epsilon_k} + \sqrt{\epsilon_F}}{\sqrt{\epsilon_k} - \sqrt{\epsilon_F}} \right| \\ &= \frac{\sqrt{2}J^2m_d m^{\frac{3}{2}}}{\pi^2\hbar^3} \sqrt{\epsilon_k} \ln \left| \frac{\epsilon_k + \epsilon_F + 2\sqrt{\epsilon_k\epsilon_F}}{\epsilon_k - \epsilon_F} \right| \end{aligned} \quad (131)$$

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 $\epsilon_k = \epsilon_F$.

$$T_{\text{nonflip}}^{(2)} = \frac{\sqrt{2}J^2m_d m^{\frac{3}{2}}}{\pi^2\hbar^3} \sqrt{\epsilon_F} \ln \left| \frac{4T_F}{T} \right| \quad (132)$$

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

$$T_{\text{nonflip}}^{(2)} = 2J^2m_d N(\epsilon_F) \ln \left| \frac{T_F}{T} \right| \quad (133)$$

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

$$T_{\text{nonflip}} = Jm_d \left[1 + 2N(\epsilon_F)J \ln \frac{T_F}{T} \right] \quad (134)$$

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),

$$\begin{aligned} T_{21}^{(2)} &= -J^2(m_d + 1)\lambda_+ \sum_q \frac{1 - P_q}{\epsilon_k - \epsilon_q} \\ T_{23}^{(2)} &= J^2m_d\lambda_+ \sum_q \frac{1 - P_q}{\epsilon_k - \epsilon_q} \\ T_{22}^{(2)} &= J^2(m_d + 1)\lambda_+ \sum_q \frac{P(q)}{\epsilon_k - \epsilon_q} \\ T_{24}^{(2)} &= -\lambda_+m_dJ^2 \sum_q \frac{P(q)}{\epsilon_k - \epsilon_q} \end{aligned} \quad (135)$$

$$T_{\text{flip}}^{(2)} = -J^2\lambda_+ (\alpha - \gamma) \quad (136)$$

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

$$\begin{aligned} T_{\text{flip}}^{(2)} &= 2J^2\lambda_+ \sum_q \frac{P(q)}{\epsilon_k - \epsilon_q} \\ &= 2J^2\lambda_+ N(\epsilon_F) \ln \left| \frac{T_F}{T} \right| \end{aligned} \quad (137)$$

Adding the first order contribution,

$$T_{\text{flip}} = \lambda_+ J \left[1 + 2N(\epsilon_F) J \ln \frac{T}{T_F} \right] \quad (138)$$

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

$$\mathcal{P} = \mathcal{P}^{(2)} \left[1 + 2JN(\epsilon_F) \ln \frac{T_F}{T} \right] \quad (139)$$

0.11 The Kondo resonance

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

$$T_{a \rightarrow b} = \sum_{s, m_s} |\langle s, m_s | a \rangle|^2 T_s \quad (140)$$

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

$$T_{|k \uparrow, d_\uparrow\rangle \rightarrow |k' \uparrow d_\uparrow\rangle} = T_1 \quad (141)$$

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

$$T_{|k \uparrow, d_\downarrow\rangle \rightarrow |k' \uparrow d_\downarrow\rangle} = \frac{T_1 + T_0}{2} \quad (142)$$

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

$$T_{|k \uparrow, d_\downarrow\rangle \rightarrow |k' \downarrow d_\uparrow\rangle} = \frac{T_1 - T_0}{2} \quad (143)$$

Therefore,

$$\begin{aligned} T_1 &= T_{|k \uparrow, d_\downarrow\rangle \rightarrow |k' \uparrow d_\downarrow\rangle} + T_{|k \uparrow, d_\downarrow\rangle \rightarrow |k' \downarrow d_\uparrow\rangle} = T_{\text{nonflip}} + T_{\text{flip}} \\ T_0 &= T_{|k \uparrow, d_\downarrow\rangle \rightarrow |k' \uparrow d_\downarrow\rangle} - T_{|k \uparrow, d_\downarrow\rangle \rightarrow |k' \downarrow d_\uparrow\rangle} = T_{\text{nonflip}} - T_{\text{flip}} \end{aligned} \quad (144)$$

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

$$T_{\text{nonflip}} = J \left[m_d + \frac{J}{4} \{ 3(\alpha + \gamma) + 4m_d(\gamma - \alpha) \} \right] \quad (145)$$

$$T_{\text{flip}} = J [1 + J(\gamma - \alpha)] \quad (146)$$

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

$$\begin{aligned} T_1 &= \frac{J}{2} \left[1 + \frac{J}{2} (\alpha + 5\gamma) \right] \\ T_0 &= -\frac{3J}{2} \left[1 - \frac{3J}{2} \left(\alpha - \frac{\gamma}{3} \right) \right] \end{aligned} \quad (147)$$

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

$$J\vec{S}_d \cdot \vec{\sigma}_e = 2J\vec{S}_d \cdot \vec{S}_e = J(S^2 - S_d^2 - S_e^2) = J\left(s(s+1) - \frac{3}{2}\right) = \begin{cases} -\frac{3J}{2} & \text{(singlet)} \\ \frac{J}{2} & \text{(triplet)} \end{cases} \quad (148)$$

Hence, the pre-factors are just the bare values of the interaction Hamiltonian, V . Hence, the equations 147 can be written as

$$T = V(1 + TG) \quad (149)$$

For the singlet and triplet T -matrices, it becomes

$$\begin{aligned} T_1 &= \frac{J}{2} [1 + T_1(\alpha + 5\gamma)] \implies T_1 = \frac{J/2}{1 - \frac{J}{2}(\alpha + 5\gamma)} \\ T_0 &= -\frac{3J}{2} \left[1 + T_0\left(\alpha - \frac{\gamma}{3}\right)\right] \implies T_0 = \frac{-3J/2}{1 + \frac{3J}{2}(\alpha - \gamma/3)} \end{aligned} \quad (150)$$

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

$$T_1 = \frac{1}{2/J - 5\gamma - \alpha} \quad (151)$$

$$T_0 = \frac{1}{-2/3J + \gamma/2 - \alpha} \quad (152)$$

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

$$T_s = \frac{1}{\text{real part} + i\pi N(0)} \quad (153)$$

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

$$|T_s| \leq \frac{1}{\pi N_0} \quad (154)$$

From eq. 13, we can write

$$T_s = -\frac{e^{i\delta_s} \sin \delta_s}{\pi N(0)} \quad (155)$$

Eq. 60 allows us to write

$$\rho_{d\sigma}(0) = -\frac{\text{Im}[T]}{t^2\pi} = \frac{\sin^2 \delta_s}{t^2\pi^2 N(0)} = \frac{\sin^2 \delta_s}{\pi\Delta} = \frac{1}{\pi\Delta} \sin^2\left(\frac{\pi n_c}{2}\right) \quad (156)$$

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, 72,

$$\rho_{d\sigma}(0) = \frac{1}{\pi\Delta} \left[1 + \left(\frac{\epsilon_d + Un_c}{\Delta} \right)^2 \right]^{-1} \quad (157)$$

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. 150 can be written as

$$T_1 = \frac{J/2}{1 - 2J\gamma - \frac{J}{2}(\alpha + \gamma)} \quad (158)$$

$$T_0 = \frac{-3J/2}{1 - 2J\gamma + \frac{3J}{2}(\alpha + \gamma)} \quad (159)$$

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

$$\begin{aligned} T_1 &= \frac{1}{\frac{2}{J_{\text{eff}}} - (\alpha + \gamma)} \\ T_0 &= \frac{-1}{\frac{2}{3J_{\text{eff}}} + \alpha + \gamma} \end{aligned} \quad (160)$$

$\alpha + \gamma$ can be calculated as

$$\begin{aligned} \alpha + \gamma &= \lim_{\eta \rightarrow 0} \int_0^\infty d\epsilon \frac{N(\epsilon)}{\epsilon_k - \epsilon + i\eta} \\ &\sim \lim_{\epsilon_{\text{up}} \rightarrow \infty} \ln \left| \frac{\sqrt{\epsilon_k} - \sqrt{\epsilon_{\text{up}}}}{\sqrt{\epsilon_k} + \sqrt{\epsilon_{\text{up}}}} \right| - i\pi N(0) \end{aligned} \quad (161)$$

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

$$\left| \frac{\sqrt{\epsilon_k} - \sqrt{\epsilon_{\text{up}}}}{\sqrt{\epsilon_k} + \sqrt{\epsilon_{\text{up}}}} \right| \approx \left| \frac{-\sqrt{\epsilon_{\text{up}}}}{\sqrt{\epsilon_{\text{up}}}} \right| = 1 \quad (162)$$

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

$$T_1 = \frac{1}{2J_{\text{eff}}^{-1} + i\pi N(0)} \sim \frac{1}{\frac{2}{\pi N(0)J_{\text{eff}}} + i} \quad (163)$$

Since

$$T_s \sim e^{i\delta_s} \sin \delta_s = \frac{1}{\cot \delta_s - i} \quad (164)$$

we can write

$$\cot \delta_1 = -\frac{2}{\pi N(0) J_{\text{eff}}} \implies \tan \delta_1 = -\frac{\pi}{2} N(0) J_{\text{eff}} \quad (165)$$

Similarly,

$$T_0 = \frac{-1}{\frac{2}{3J_{\text{eff}}} - i\pi N(0)} \sim \frac{-1}{\frac{2}{3J_{\text{eff}}\pi N(0)} - i} \quad (166)$$

giving

$$\cot \delta_0 = \frac{2}{3J_{\text{eff}}\pi N(0)} \implies \tan \delta_0 = \frac{3\pi}{2} J_{\text{eff}} N(0) \quad (167)$$

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

$$\psi \sim \psi_{\text{in}} - e^{2i\delta_d} \psi_{\text{out}} \quad (168)$$

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,

$$\psi = \frac{e^{i\delta}}{r} \left(e^{-i(k_F r + \delta_d)} - e^{i(k_F r + \delta_d)} \right) \sim \frac{e^{i\delta}}{r} \sin [k_F (r + \Delta r)] \quad (169)$$

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.

0.12 Adiabatic route to the Kondo resonance

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

$$\Sigma(E) = \Sigma(0) + E \frac{d\Sigma}{dE} \Big|_{E=0} + O(E^2) \quad (170)$$

Defining

$$Z^{-1} \equiv 1 - \frac{d\Sigma}{dE} \Big|_{E=0} \quad (171)$$

we can write

$$\Sigma(E) = \Sigma(0) + (1 - Z^{-1}) E \quad (172)$$

The interacting Green's function for the impurity becomes

$$G_f(E) = \frac{1}{E - \epsilon_d - \Sigma - i\Delta} \quad (173)$$

where Δ is the result of the hybridisation. Substituting eq. 172 and gathering the terms gives

$$G_f(E) = \frac{Z}{E - Z(\epsilon_d + \Sigma(0)) - iZ\Delta} \quad (174)$$

Defining the renormalised parameters

$$\epsilon_d^* = Z(\epsilon_d + \Sigma(0)) \quad (175)$$

$$\Delta^* = Z\Delta \quad (176)$$

we have

$$G_f(E) = \frac{Z}{E - \epsilon_d^* - i\Delta^*} \quad (177)$$

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

$$Z = 1, \Sigma = 0 \implies \epsilon_d^* = \epsilon_d, \Delta^* = \Delta \quad (178)$$

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

$$\delta_d(0) = \cot^{-1} \frac{\epsilon_d^*}{\Delta^*} \quad (179)$$

Similarly, the renormalised version of eq. 52 is

$$\rho_d(0) = \frac{1}{\pi} \frac{\Delta^*}{\epsilon_d^{*2} + \Delta^{*2}} \quad (180)$$

Using eq. 179 gives

$$\rho_d(0) = \frac{1}{\pi} \frac{\Delta^*}{\Delta^{*2} \cot^2 \delta_d + \Delta^{*2}} = \frac{\sin^2 \delta_d}{\pi \Delta} \quad (181)$$

0.13 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,

$$H_K = \sum_{k > k_F} \epsilon_k n_k - \frac{3J}{2} \sum_{k, k' > k_F} c_{k'\sigma}^\dagger c_{k\sigma} \quad (182)$$

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

$$b_k^\dagger = \frac{1}{\sqrt{2}} (c_{k\uparrow}^\dagger c_{d\downarrow}^\dagger - c_{k\downarrow}^\dagger c_{d\uparrow}^\dagger) \quad (183)$$

Hence the total wavefunction of singlet+Fermi-sea is

$$|\Psi\rangle = \sum_{k > k_F} a_k b_k^\dagger |\Phi\rangle = |\Phi\rangle \otimes \sum_{k > k_F} a_k |S_k\rangle \quad (184)$$

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

$$a_q = \langle \Phi | \langle S_q | \sum_k a_k |S_k\rangle | \Phi \rangle = \langle \Phi | b_q | \Psi \rangle \quad (185)$$

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

$$\begin{aligned} E |\Psi\rangle &= H_K |\Psi\rangle = |\Phi\rangle \otimes H_k \sum_{k > k_F} a_k |S_k\rangle \\ &= |\Phi\rangle \otimes \sum_{k > k_F} a_k \left(\epsilon_k |S_k\rangle - \frac{3J}{2} \sum_{k' > k_F} |S_{k'}\rangle \right) \\ &= \sum_{k > k_F} a_k \left(\epsilon_k b_k^\dagger - \frac{3J}{2} \sum_{k' > k_F} b_{k'}^\dagger \right) |\Phi\rangle \end{aligned} \quad (186)$$

Multiplying b_q from left gives

$$E b_q |\Psi\rangle = \epsilon_q a_q |\Phi\rangle - \frac{3J}{2} \sum_{k > k_F} a_k |\Phi\rangle \quad (187)$$

Multiplying $\langle \Phi |$ from left and looking at eq. 185 gives

$$\begin{aligned} E \langle \Phi | b_q | \Psi \rangle &= E a_q = a_q \epsilon_q - \frac{3J}{2} \sum_k a_k \\ &\implies a_q = \frac{3J/2}{\epsilon_q - E} \sum_k a_k \\ &\implies \sum_q a_q = \sum_q \frac{3J/2}{\epsilon_q - E} \sum_k a_k \end{aligned} \quad (188)$$

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

$$1 = \frac{3J}{2} \sum_{q > k_F} \frac{1}{\epsilon_q - E} \quad (189)$$

Converting to integral,

$$1 = \frac{3J}{2} \int_{\epsilon_F}^D d\epsilon \frac{N(\epsilon)}{\epsilon - E} \quad (190)$$

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

$$\begin{aligned} \frac{2}{3JN(0)} &= \ln \left| \frac{D - E}{\epsilon_F - E} \right| \approx \ln \left| \frac{D}{\epsilon_F - E} \right| \\ \implies E &= \epsilon_F - D e^{-\frac{2}{3N(0)J}} \end{aligned} \quad (191)$$

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

$$E_b = D e^{-\frac{2}{3N(0)J}} \quad (192)$$

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

$$k_B T_K \sim E_b \implies T_K = \frac{D}{k_B} e^{-\frac{2}{3N(0)J}} \quad (193)$$

0.14 Poor man's scaling

The idea is to reduce the bandwidth from D to $D - \delta D$, by considering all possible excitations in that range, up to second order. The transition matrix second order contributions in that range

$$T^{(2)} = V G_0 V \quad (194)$$

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

$$H' = J_z \sum_{k_1, k_2} S_d^z \left(c_{k_1 \uparrow}^\dagger c_{k_2 \uparrow} - c_{k_1 \downarrow}^\dagger c_{k_2 \downarrow} \right) + J_T \sum_{k_1, k_2} \left(S_d^+ c_{k_1 \downarrow}^\dagger c_{k_2 \uparrow} + S_d^- c_{k_1 \uparrow}^\dagger c_{k_2 \downarrow} \right) \quad (195)$$

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 .

Renormalization of J_z

First consider the process

$$k \uparrow, d \downarrow \rightarrow q \downarrow d \uparrow \rightarrow k' \uparrow d \downarrow \quad (196)$$

The T -matrix term is

$$T_1 = J_T^2 \sum_q S_d^- c_{k'\uparrow}^\dagger c_{q\downarrow} \frac{1}{E - H_0} S_d^+ c_{q\downarrow}^\dagger c_{k\uparrow} \quad (197)$$

Using eq. 16, we can write

$$(E - H_0)^{-1} c_{q\downarrow}^\dagger c_{k\uparrow} = c_{q\downarrow}^\dagger c_{k\uparrow} (E - \lambda - H_0)^{-1} \quad (198)$$

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,

$$T_1 = J_T^2 S_d^- S_d^+ \sum_q c_{k'\uparrow}^\dagger c_{q\downarrow} c_{q\downarrow}^\dagger c_{k\uparrow} (E - \epsilon_q + \epsilon_k - H_0)^{-1} \quad (199)$$

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

$$T_1 = J_T^2 S_d^- S_d^+ c_{k'\uparrow}^\dagger c_{k\uparrow} \sum_q (E - \epsilon_q + \epsilon_k - H_0)^{-1} \quad (200)$$

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

$$\sum_q (E - \epsilon_q + \epsilon_k - H_0)^{-1} = N |\delta D| \frac{1}{E - D + \epsilon_k} \quad (201)$$

N is the density of states. Also,

$$S^- S^+ = (S^x - iS^y) (S^x + iS^y) = \frac{1}{2} + i[S^x, S^y] = \frac{1}{2} - S^z \quad (202)$$

Putting it all together,

$$T_1 = J_T^2 \left(\frac{1}{2} - S_d^z \right) N |\delta D| c_{k'\uparrow}^\dagger c_{k\uparrow} \frac{1}{E - D + \epsilon_k} \quad (203)$$

For the second possible scattering,

$$q \downarrow k \uparrow d \uparrow \rightarrow k' \uparrow k \uparrow d \downarrow \rightarrow k' \uparrow q \downarrow d \uparrow \quad (204)$$

we get

$$T_2 = J_T^2 \sum_q S_d^+ S_d^- c_{q\downarrow}^\dagger c_{k\uparrow} \frac{1}{E - H_0} c_{k'\uparrow}^\dagger c_{q\downarrow} \quad (205)$$

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

$$\begin{aligned} T_2 &= J_T^2 \left(\frac{1}{2} + S_d^z \right) N |\delta D| c_{k\uparrow}^\dagger c_{k'\uparrow} \frac{1}{E - D - \epsilon_{k'}} \\ &= -J_T^2 \left(\frac{1}{2} + S_d^z \right) N |\delta D| c_{k'\uparrow}^\dagger c_{k\uparrow} \frac{1}{E - D - \epsilon_{k'}} \end{aligned} \quad (206)$$

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 :

$$k \downarrow, d \uparrow \rightarrow q \uparrow d \downarrow \rightarrow k' \downarrow d \uparrow \quad (207)$$

$$q \uparrow k \downarrow d \downarrow \rightarrow k' \downarrow k \downarrow d \uparrow \rightarrow k' \downarrow q \uparrow d \downarrow \quad (208)$$

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

$$T_3 = J_T^2 \left(\frac{1}{2} + S_d^z \right) N |\delta D| c_{k'\downarrow}^\dagger c_{k\downarrow} \frac{1}{E - D + \epsilon_k} \quad (209)$$

$$T_4 = -J_T^2 \left(\frac{1}{2} - S_d^z \right) N |\delta D| c_{k'\downarrow}^\dagger c_{k\downarrow} \frac{1}{E - D - \epsilon_{k'}} \quad (210)$$

The total second order contribution is

$$T^{(2)} = -J_T^2 S_d^z N |\delta D| \left(\frac{1}{E - D + \epsilon_k} + \frac{1}{E - D - \epsilon_{k'}} \right) \left(c_{k'\uparrow}^\dagger c_{k\uparrow} - c_{k'\downarrow}^\dagger c_{k\downarrow} \right) \quad (211)$$

Comparing this with the S_d^z term in the Hamiltonian

$$J_z S_d^z \left(c_{k'\uparrow}^\dagger c_{k\uparrow} - c_{k'\downarrow}^\dagger c_{k\downarrow} \right) \quad (212)$$

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

$$\delta J_d^z = -J_T^2 N |\delta D| \left(\frac{1}{E - D + \epsilon_k} + \frac{1}{E - D - \epsilon_{k'}} \right) \quad (213)$$

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

$$\frac{dJ_d^z}{dD} = -J_T^2 N \frac{2}{D} \quad (214)$$

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

Renormalization of J_T

Consider the scattering

$$k \uparrow d \downarrow \rightarrow q \downarrow d \uparrow \rightarrow k' \downarrow d \uparrow \quad (215)$$

$$T_1 = -J_T J_z S_d^z S_d^+ N |\delta D| c_{k'\downarrow}^\dagger c_{k\uparrow} \frac{1}{E - D + \epsilon_k} \quad (216)$$

The minus sign at the front comes from the term

$$-S_d^z c_{k'\downarrow}^\dagger c_{q\downarrow} \quad (217)$$

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

$$T_1 = -J_T J_z \frac{S_d^+}{2} N |\delta D| c_{k'\downarrow}^\dagger c_{k\uparrow} \frac{1}{E - D + \epsilon_k} \quad (218)$$

The second process is

$$q \uparrow k \uparrow d \downarrow \rightarrow k' \downarrow k \uparrow d \uparrow \rightarrow q \uparrow k' \downarrow d \uparrow \quad (219)$$

$$T_2 = -J_T J_z \frac{S_d^+}{2} N |\delta D| c_{k'\downarrow}^\dagger c_{k\uparrow} \frac{1}{E - D - \epsilon_{k'}} \quad (220)$$

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

$$+S_d^z c_{k'\uparrow}^\dagger c_{q\uparrow} \quad (221)$$

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

$$-S_d^z c_{k'\downarrow}^\dagger c_{q\downarrow} \quad (222)$$

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.

$$T_3 = T_1 \quad (223)$$

$$T_4 = T_2 \quad (224)$$

The total contribution is

$$T^{(2)} = -J_T J_z S_d^+ N |\delta D| c_{k'\downarrow}^\dagger c_{k\uparrow} \left(\frac{1}{E - D - \epsilon_{k'}} + \frac{1}{E - D + \epsilon_k} \right) \quad (225)$$

Comparing with the S_d^+ term in the Hamiltonian

$$J_T S_d^+ c_{k'\downarrow}^\dagger c_{k\uparrow} \quad (226)$$

we can write

$$\delta J_T = -J_T J_z N |\delta D| \left(\frac{1}{E - D - \epsilon_{k'}} + \frac{1}{E - D + \epsilon_k} \right) \quad (227)$$

Again neglecting the terms in the denominator, we get

$$\frac{dJ_T}{dD} = -J_T J_z N \frac{2}{D} \quad (228)$$

This is the scaling equation for J_T .

Flow of the couplings

Switching to the dimensionless couplings

$$g_1 = N J_z, g_2 = N J_T \quad (229)$$

the equations become

$$\frac{dg_1}{dD} = -\frac{2g_2^2}{D} \quad (230)$$

$$\frac{dg_2}{dD} = -\frac{2g_1 g_2}{D} \quad (231)$$

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

$$\frac{dg_1}{dg_2} = \frac{g_2}{g_1} \implies g_1^2 - g_2^2 = \text{constant} \quad (232)$$

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

$$\begin{aligned} g(D') &= \frac{g_0}{1 - 2g_0 \ln \frac{D}{D'}} \\ \implies 2g(D') &= \frac{1}{\ln \frac{D'}{T_K}} \end{aligned} \quad (233)$$

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. 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.

$$g(D') = \frac{g_0}{1 - 2g_0 \ln \frac{D}{D'}} = -\frac{|g_0|}{1 + 2|g_0| \ln \frac{D}{D'}} \quad (234)$$

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

Alternate way of obtaining the scaling equations

From eq. 98, the interaction part can be written as

$$\Delta H_{ll'} = \frac{1}{2} [T_{ll'}(E_l) + T_{ll'}(E_{l'})] \quad (235)$$

where the transition matrix T is

$$T_{ll'}(E) = \sum_H \frac{V_{lH} V_{Hl'}}{E - E_H} \quad (236)$$

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

$$V = J \vec{S}_d \cdot \sum_{k,k',\alpha,\alpha'} c_{k\alpha}^\dagger \vec{\sigma}_{\alpha\alpha'} c_{k'\alpha'} \quad (237)$$

The first process is

$$k\alpha \xrightarrow{\sigma^b} q\lambda \xrightarrow{\sigma^a} k'\beta \quad (238)$$

$$d\sigma \xrightarrow{S_d^b} d\sigma'' \xrightarrow{S_d^a} d\sigma' \quad (239)$$

The transition matrix element is

$$\begin{aligned} T_1 &= \sum_{q \in \{D-\delta D\}, \lambda, \sigma''} \langle k'\beta, \sigma' | V | q\lambda, \sigma'' \rangle \langle q\lambda, \sigma'' | V | k\alpha, \sigma \rangle \frac{1}{E - E_q} \\ &= J^2 \sum_{\sigma''} (S_d^a)_{\sigma'\sigma''} (S_d^b)_{\sigma''\sigma} \sum_{\lambda} (\sigma^a)_{\beta\lambda} (\sigma^b)_{\lambda\alpha} \sum_{q \in \{D-\delta D\}} \frac{1}{E - E_q} \\ &\approx J^2 (S_d^a S_d^b)_{\sigma'\sigma} (\sigma^a \sigma^b)_{\beta\alpha} \frac{N|\delta D|}{E - D} \end{aligned} \quad (240)$$

The second process is

$$k\alpha \longrightarrow k\alpha \xrightarrow{\sigma^a} q\lambda \quad (241)$$

$$q\lambda \xrightarrow{\sigma^b} k'\beta \longrightarrow k'\beta \quad (242)$$

$$d\sigma \xrightarrow{S_d^b} d\sigma'' \xrightarrow{S_d^a} d\sigma' \quad (243)$$

Here the intermediate state consists of two electrons with energy $E_k, E_{k'}$ and a hole with energy $-E_q$. The transition matrix element is

$$\begin{aligned} T_2 &= \sum_{q \in \{D-|\delta D|\}, \lambda, \sigma''} \langle q\lambda, k'\beta, \sigma' | V | k'\beta, k\alpha, \sigma'' \rangle \langle k'\beta, k\alpha, \sigma'' | V | q\lambda, k\alpha, \sigma \rangle \frac{1}{E - (E_k + E_{k'} - E_q)} \\ &\approx -J^2 (S_d^a S_d^b)_{\sigma'\sigma} (\sigma^b \sigma^a)_{\beta\alpha} \frac{N|\delta D|}{E - D} \end{aligned} \quad (244)$$

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

$$\begin{aligned} T &= \frac{J^2 N |\delta D|}{D} (S_d^a S_d^b)_{\sigma'\sigma} [\sigma^b, \sigma^a]_{\beta\alpha} \\ &= \frac{J^2 N |\delta D|}{2D} [S_d^a, S_d^b]_{\sigma'\sigma} [\sigma^b, \sigma^a]_{\beta\alpha} \end{aligned} \quad (245)$$

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

$$\begin{aligned} [S_d^a, S_d^b]_{\sigma'\sigma} [\sigma^b, \sigma^a]_{\beta\alpha} &= -[S_d^a, S_d^b]_{\sigma'\sigma} [\sigma^a, \sigma^b]_{\beta\alpha} \\ &= -i\epsilon_{abc} S_{\sigma\sigma'}^c 2i\epsilon_{abd} \sigma_{\beta\alpha}^d \\ &= 4\delta_{cd} S_{\sigma\sigma'}^c \sigma_{\beta\alpha}^d \\ &= 4\vec{S}_{\sigma\sigma'} \cdot \vec{\sigma}_{\beta\alpha} \end{aligned} \quad (246)$$

Therefore,

$$T = \frac{2J^2 N |\delta D|}{D} \vec{S}_{\sigma\sigma'} \cdot \vec{\sigma}_{\beta\alpha} \quad (247)$$

The correction to the coupling J can be read off:

$$J(D - \delta D) = J(D) - \frac{2J^2 N \delta D}{D} \quad (248)$$

This gives the same scaling equations we found earlier.

0.15 Universality

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

$$\frac{\partial g}{\partial \ln D} = -2g^2 + 2g^3 \quad (249)$$

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

$$\ln \frac{D'}{D} = - \int_{g_0}^g \frac{dg}{2g^2 - 2g^3} = - \int_{g_0}^g \frac{dg}{2g^2} (1 + g) \quad (250)$$

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

$$\begin{aligned} \ln \frac{k_B T_K}{D} &= - \int_{g_0}^1 \frac{dg}{2g^2} (1 + g) = -\frac{1}{2g_0} + \frac{1}{2} \ln g_0 + O(1) \\ &= -\frac{1}{2g_0} + \frac{1}{2} \ln 2g_0 + O(1) \end{aligned} \quad (251)$$

This gives a better estimate of the Kondo temperature

$$T_K = \frac{D}{k_B} \sqrt{2g_0} \exp\left(-\frac{1}{2g_0}\right) \quad (252)$$

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

$$k_B T_K = D y(g) \quad (253)$$

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

$$\frac{dT_K}{dD} = 0 \quad (254)$$

Substituting the form of T_K , eq. 253, in this equation gives

$$\begin{aligned} y(g) + D \frac{dy(g)}{dD} &= 0 \\ \implies y + D \frac{dy}{dg} \frac{dg}{dD} &= 0 \\ \implies y - 2g^2 \frac{dy}{dg} &= 0 \\ \implies y &= e^{-\frac{1}{2g}} \end{aligned} \quad (255)$$

This gives almost the same solution as eq. 252:

$$T_K = \frac{D}{k_B} e^{-\frac{1}{2g}} \quad (256)$$

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. 233, up to second order, we can write

$$g(D') = g_0 \left(1 + 2g_0^2 \ln \frac{D}{D'}\right) \quad (257)$$

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

$$g_0 \rightarrow g = g_0 \left(1 + 2g_0 \ln \frac{T_F}{T}\right) \quad (258)$$

Since $g \equiv NJ$, we have recovered eq. 139. Since eq. 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.

0.16 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,

$$S^z = \frac{\sigma^z}{2} = \sum_{ij} c_i^\dagger \frac{\sigma_{ij}^z}{2} c_j = \frac{1}{2} (c_\uparrow^\dagger c_\uparrow - c_\downarrow^\dagger c_\downarrow) \quad (259)$$

Similarly,

$$\begin{aligned} S^x &= \frac{1}{2} (c_\uparrow^\dagger c_\downarrow + c_\downarrow^\dagger c_\uparrow) \\ S^y &= \frac{-i}{2} (c_\uparrow^\dagger c_\downarrow - c_\downarrow^\dagger c_\uparrow) \end{aligned} \quad (260)$$

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

$$|\uparrow\rangle = c_\uparrow^\dagger |0\rangle \quad (261)$$

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

$$\mu = -i\frac{\pi}{2}k_B T \quad (262)$$

The new Hamiltonian is

$$\tilde{H} = H - \mu(n_d - 1) \quad (263)$$

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

$$Z = \text{Tr} [\exp(-\beta H)] = \sum_{\sigma_d=\uparrow,\downarrow} \sum_k [\exp(-\beta H)] \quad (264)$$

The modified partition function is

$$\begin{aligned} \tilde{Z} &= \text{Tr} [\exp(-\beta (H - \mu(n_d - 1)))] \\ &= \text{Tr} \left[\exp \left(-\beta H - i\frac{\pi}{2}(n_d - 1) \right) \right] \\ &= \sum_{\sigma_d=\uparrow,\downarrow} \sum_k [\exp(-\beta H)] + \sum_k \exp \left(-\beta H + i\frac{\pi}{2} \right) + \sum_k \exp \left(-\beta H - i\frac{\pi}{2} \right) \\ &= Z \Big|_{n_d=1} + iZ \Big|_{n_d=0} - iZ \Big|_{n_d=0} \end{aligned} \quad (265)$$

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

$$Z \Big|_{n_d=0} = Z \Big|_{n_d=0} \quad (266)$$

Hence,

$$\tilde{Z} = Z \quad (267)$$

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

0.17 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

$$C_V = \gamma T \quad (268)$$

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

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

$$E_g = J \left[2\vec{S}_e \cdot \vec{S}_d \right] = J \left[S^2 - S_d^2 - S_e^2 \right] = J \left[s(s+1) - \frac{3}{2} \right] = -\frac{3J}{2} \quad (269)$$

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,

$$\frac{|0_\uparrow, d \downarrow\rangle - |0_\downarrow, d \uparrow\rangle}{\sqrt{2}} \quad (270)$$

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

$$E_1 = -\frac{3}{2}J + \frac{3}{2}J = 0 \quad (271)$$

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

$$\psi \sim \frac{\sin[kr + \delta(E_k)]}{r} \quad (272)$$

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.

$$n = \sum_{\sigma} \frac{\delta}{\pi} \implies 1 = \frac{2\delta}{\pi} \implies \delta = \frac{\pi}{2} \quad (273)$$

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

$$k_F a = \delta(0) \implies \delta(0) = \frac{\pi}{2a} 2 = \frac{\pi}{2} \quad (274)$$

where the formula for k_F was used.

In a Fermi gas, the energy levels are separated by

$$\Delta\epsilon = \frac{\partial\epsilon}{\partial k} \Delta k \quad (275)$$

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

$$\Delta\epsilon = \frac{\partial\epsilon}{\partial k} \frac{\pi}{L} \quad (276)$$

However, this changes in the presence of the impurity. Because of eq. 272, the boundary condition becomes

$$k_n L + \delta(\epsilon_k) = n\pi \implies k_n = \frac{n\pi}{L} - \frac{\delta}{L} = k_n^0 - \frac{\delta(\epsilon_k)}{L} \quad (277)$$

The energy becomes

$$\begin{aligned}\epsilon(k) &= \epsilon(k^0) + \frac{\partial \epsilon}{\partial k} (k - k_0) \\ &= \epsilon_k - \frac{\partial \epsilon}{\partial k} \frac{\delta(\epsilon_k)}{L}\end{aligned}\quad (278)$$

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

$$\tilde{\epsilon}_\sigma(k) = \epsilon_k - \frac{\partial \epsilon}{\partial k} \frac{\delta_\sigma(\epsilon_k, \{n_{q,\sigma}\})}{L} \quad (279)$$

In bulk Fermi liquid, we expand the quasiparticle energy in the deviation of the quasiparticle distribution n_k from the ideal Fermi-Dirac distribution n_k^0 ,

$$\begin{aligned}\tilde{\epsilon}_p &= \underbrace{\epsilon_F}_{\text{Fermi gas}} + \overbrace{\frac{p_F^*}{m} (p - p_F)}^{\text{linear contribution for } p \text{ close to } p_F} \\ &\quad + \underbrace{\sum_{q\sigma} f(p, q) (n_q - n_q^0)}_{\text{interacting between two quasiparticles at momenta } p \text{ and } q}\end{aligned}\quad (280)$$

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,

$$\delta_\sigma(\tilde{\epsilon}, \{n_{q,\sigma}\}) = \delta_\sigma(\tilde{\epsilon} = \epsilon_F, n_k = n_k^0) + \alpha (\tilde{\epsilon} - \epsilon_F) + \Phi \sum_{q\sigma'} (n_{q\sigma'} - n_{q\sigma'}^0) \quad (281)$$

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

$$\alpha = \frac{d\delta_\sigma}{dE} \quad (282)$$

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

$$\delta_\sigma(\tilde{\epsilon}, \{n_{q,\sigma}\}) = \delta_\sigma(\tilde{\epsilon} = \epsilon_F, n_k = n_k^0) + \alpha (\tilde{\epsilon} - \epsilon_F) + \Phi \sum_q \delta n_{q,-\sigma} \quad (283)$$

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,

$$\delta_{\uparrow}^0 = \frac{\pi}{2} + \Phi \sum_q \delta n_{q\downarrow}^0 \quad (284)$$

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

$$\delta_{\uparrow}^0 = \frac{\pi}{2} \quad (285)$$

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

$$N(\mu = 0) = N^0 \quad (286)$$

$$N(E' = E + \mu) = N(E' = E) + \frac{dN}{dE'} (E' - E) = N^0 + \rho \Delta\mu \quad (287)$$

$$\implies \sum_q \delta n_q = N - N^0 = \rho \Delta\mu \quad (288)$$

Hence, from eq. 283,

$$\begin{aligned} \delta_{\uparrow} &= \frac{\pi}{2} + \alpha (\epsilon'_F - \epsilon_F) + \Phi \sum_q \delta n_{q\downarrow} \\ &= \delta_{\uparrow}^0 + \alpha \Delta\mu + \Phi \rho \Delta\mu \end{aligned} \quad (289)$$

Hence the change in the phase is

$$0 = \Delta\delta_{\uparrow} = \Delta\mu (\alpha + \Phi\rho) \implies \alpha = -\Phi\rho \quad (290)$$

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

$$n_{\sigma} = \frac{kL}{\pi} + \frac{\delta_{\sigma}(E)}{\pi} = n^0 + \frac{\delta_{\sigma}(E)}{\pi} \quad (291)$$

Hence,

$$\begin{aligned} \rho &= \frac{dn_{\sigma}}{dE} = \rho^0 + \frac{1}{\pi} \frac{d\delta_{\sigma}}{dE} \\ \implies \rho &= \rho^0 + \frac{1}{\pi} \alpha \end{aligned} \quad (292)$$

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

$$C_v^0 = \gamma T = \frac{\pi^2 k_B^2}{3} \mathcal{N}(0) T \quad (293)$$

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

$$\begin{aligned} C_v &= \frac{\pi^2 k_B^2}{3} (\rho_\uparrow + \rho_\downarrow) T \\ &= \frac{2\alpha}{\pi} \frac{\pi^2 k_B^2}{3} T \end{aligned} \quad (294)$$

In presence of a magnetic field B , the magnetization is

$$m = \delta n \times \mu \quad (295)$$

where μ is the magnetic moment

$$\mu = -\frac{g}{2} \mu_B \quad (296)$$

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

$$\delta n = \langle n_\uparrow \rangle - \langle n_\downarrow \rangle = \frac{1}{\pi} (\delta_\uparrow - \delta_\downarrow) \quad (297)$$

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

$$E_\sigma^B = E - \sigma \frac{g\mu_B}{2} B \quad (298)$$

Hence,

$$\sum_k \delta n_{k\sigma} = N_\sigma(E_\sigma^B) - N(E) = \frac{dN}{dE^B} (E^B - E) = -\rho \frac{g\mu_B}{2} \sigma B \quad (299)$$

This modifies the phase shift at the Fermi surface,

$$\begin{aligned} \delta_\sigma(\epsilon_F) &= \frac{\pi}{2} + \alpha \left(\epsilon_F - \frac{g\mu_B}{2} \sigma B - \epsilon_F \right) + \Phi \sum_q \delta n_{q,-\sigma} \\ &= \frac{\pi}{2} - \sigma \frac{g\mu_B}{2} \alpha B + \Phi \rho \frac{g\mu_B}{2} \sigma B \\ &= \frac{\pi}{2} - 2\alpha \frac{g\mu_B}{2} \sigma B \end{aligned} \quad (300)$$

Hence,

$$\delta n = \frac{1}{\pi} (\delta_\uparrow - \delta_\downarrow) = -\frac{4\alpha B}{\pi} \frac{g\mu_B}{2} \quad (301)$$

The susceptibility is

$$\chi = \frac{\partial m}{\partial B} = \frac{\partial}{\partial B} \mu \delta n = \frac{4\alpha}{\pi} \left(\frac{g\mu_B}{2} \right)^2 \quad (302)$$

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

$$\mu = -\frac{g}{2} \mu_B \quad (303)$$

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

$$\delta n = n_{\uparrow}(0) - n_{\downarrow}(0) = n_{\uparrow}(\epsilon_F - \frac{g}{2} \mu_B B) - n_{\downarrow}(\epsilon_F + \frac{g}{2} \mu_B B) = -\frac{1}{2} \mathcal{N}(0) g B \mu_B \quad (304)$$

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

$$m = \delta n \times \mu = \mathcal{N}(0) \left(\frac{g}{2} \mu_B \right)^2 B \quad (305)$$

The magnetic susceptibility comes out to be

$$\chi^0 = \left. \frac{\partial m}{\partial B} \right|_{B \rightarrow 0} = \mathcal{N}(0) \left(\frac{g}{2} \mu_B \right)^2 \quad (306)$$

The Wilson ratio R can now be computed,

$$R = \frac{\chi/\chi_0}{C_v/C_v^0} = \frac{4\alpha/\pi \mathcal{N}(0)}{2\alpha/\pi \mathcal{N}(0)} = 2 \quad (307)$$

0.18 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

$$H = \sum_k \epsilon_k n_k + J \vec{S}_d \cdot \vec{\sigma}_e \quad (308)$$

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 $H_c|0\rangle$,

$$|1\rangle = (\lambda_1 H_c|0\rangle + \lambda_2 |0\rangle) \quad (309)$$

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:

$$|1\rangle = \frac{1}{\gamma_0} (H_c|0\rangle + \lambda |0\rangle) \quad (310)$$

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

$$\lambda = -\langle 0|H_c|0\rangle \quad (311)$$

Therefore,

$$|1\rangle = \frac{1}{\gamma_0} (H_c|0\rangle - \langle 0|H_c|0\rangle |0\rangle) \quad (312)$$

The general state can be shown to be

$$|n+1\rangle = \frac{1}{\gamma_n} (H_c|n\rangle - |n\rangle \langle n|H_c|n-1\rangle - |n-1\rangle \langle n-1|H_c|n\rangle) \quad (313)$$

From eq. 313, by multiplying $\langle n'|$ from left, we get

$$\delta_{n',n+1} = \frac{1}{\gamma_n} \left[(H_c)_{n',n} + (H_c)_{n,n-1} \delta_{n',n} + (H_c)_{n-1,n} \delta_{n',n-1} \right] \quad (314)$$

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

$$(H_c)_{n',n} = 0 \quad (315)$$

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

$$(H_c)_{n+1,n} = \gamma_n \quad (316)$$

Taking the complex conjugate of this gives

$$\gamma_n^* = (H_c^\dagger)_{n,n+1} = (H_c)_{n,n+1} \quad (317)$$

Defining

$$(H_c)_{n,n} = \epsilon_n \quad (318)$$

we can write

$$\begin{aligned}
H_c &= \sum_{n_1, n_2} |n_1\rangle \langle n_1| H_c |n_2\rangle \langle n_2| \\
&= \sum_n \epsilon_n |n\rangle \langle n| + \sum_n (\gamma_n |n\rangle \langle n+1| + \gamma_n^* |n+1\rangle \langle n|) \\
&= \sum_n \epsilon_n \hat{n}_n + \sum_n \left(\gamma_n c_n^\dagger c_{n+1} + \gamma_n^* c_{n+1}^\dagger c_n \right)
\end{aligned} \tag{319}$$

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 Hilbert space (and hence the matrices) manageable. Another problem is that as one goes on adding sites to the chain, the couplings need to die off, otherwise this process will never converge.

Logarithmic discretization

First, note that up to first order

$$\epsilon_k = \epsilon_F + (k - k_F) \frac{\partial \epsilon_k}{\partial k} \tag{320}$$

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

$$d_n = \Lambda^{-n} (1 - \Lambda^{-1}) \tag{321}$$

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

$$\psi_{m,n}(k) = \frac{1}{\sqrt{d_n}} \exp\left(\frac{2\pi i m}{d_n} k\right) \tag{322}$$

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

$$a_{m,n}^\dagger = \sum_k \psi_m(k) c_k^\dagger \tag{323}$$

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

$$\phi_{m,n}(k) = \frac{1}{\sqrt{d_n}} \exp\left(-\frac{2\pi i m}{d_n} k\right) \tag{324}$$

$$b_{m,n}^\dagger = \sum_k \phi_m(k) c_k^\dagger \tag{325}$$

Then,

$$a_{m,n}^\dagger + b_{m,n}^\dagger = \frac{2}{\sqrt{d_n}} \sum_{\pm k \in \mathbb{Z}} \cos\left(\frac{2\pi mk}{d_n}\right) c_k^\dagger \quad (326)$$

Summing over n involves summing over all momenta.

$$\begin{aligned} \sum_n (a_{m,n}^\dagger + b_{m,n}^\dagger) &= \frac{2}{\sqrt{d_n}} \sum_k \cos\left(\frac{2\pi mk}{d_n}\right) c_k^\dagger \\ \Rightarrow \sum_n (a_{0,n}^\dagger + b_{0,n}^\dagger) &= \frac{2}{\sqrt{d_n}} \sum_k c_k^\dagger \end{aligned} \quad (327)$$

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

$$\sum_{k,q} c_k^\dagger c_q = \sum_k c_k^\dagger \sum_q c_q \quad (328)$$

Looking at eq. 327, 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

$$\epsilon_n = 0, \gamma = D' \Lambda^{-\frac{n}{2}} \quad (329)$$

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

$$H_N = D' \sum_{n=0}^{N-1} \Lambda^{-\frac{n}{2}} \left(c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n \right) + 2J \vec{S}_d \cdot \vec{S}_e \quad (330)$$

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

$$H_{N+1} = H_N + D' \Lambda^{-\frac{N}{2}} \left(c_N^\dagger c_{N+1} + c_{N+1}^\dagger c_N \right) \quad (331)$$

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

$$\overline{H}_N = \frac{H_N}{\Gamma_N} = \frac{\Lambda^{\frac{N-1}{2}}}{D'} H_N \quad (332)$$

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

$$\begin{aligned} \overline{H}_{N+1} &= \frac{\Lambda^{\frac{N}{2}}}{D'} \left[H_N + \Lambda^{-\frac{N}{2}} D' \left(c_N^\dagger c_{N+1} + c_{N+1}^\dagger c_N \right) \right] \\ \Rightarrow \overline{H}_{N+1} &= \Lambda^{\frac{1}{2}} \overline{H}_N + \left(c_N^\dagger c_{N+1} + c_{N+1}^\dagger c_N \right) \end{aligned} \quad (333)$$

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

$$H = \lim_{N \rightarrow \infty} H_N = \lim_{N \rightarrow \infty} D' \Lambda^{\frac{1-N}{2}} \bar{H}_N \quad (334)$$

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

$$\bar{H}_N = \sum_m E_m |m\rangle \langle m| \quad (335)$$

The next Hamiltonian is then

$$\bar{H}_{N+1} = \Lambda^{\frac{1}{2}} \sum_m E_m |m\rangle \langle m| + \sum_{m,m'} (C(m, m') |m\rangle \langle m'| + \text{h.c.}) \quad (336)$$

This is the same equation as eq. 333, with \bar{H}_N expressed in its eigenbasis and the creation and annihilation operators also expressed in that basis; the $C(m, m')$ are just the matrix elements of c and c^\dagger in that basis.

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

0.19 Correspondence between the Anderson model fixed-point Hamiltonian and a 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,

$$H_{\text{eff}} = \sum_k \epsilon_k n_k + \sum_k V_k c_d^\dagger c_k + \text{h.c.} + U n_{d\uparrow} n_{d\downarrow} \quad (337)$$

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 \tilde{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,

$$n_{d\uparrow}n_{d\downarrow} \approx n_{d\uparrow}\langle n_{d\downarrow} \rangle + n_{d\downarrow}\langle n_{d\uparrow} \rangle = \sum_{k,q,\sigma} |\alpha_q|^2 |\alpha_k|^2 n_{k\sigma} \langle n_{q,-\sigma} \rangle \quad (338)$$

Since the α are pure phases, their mod-square are unity. The effective one-particle energy becomes

$$\tilde{\epsilon}_{k\sigma} = \epsilon_k + U \sum_q \langle \delta n_{q,-\sigma} \rangle = \epsilon_k + U \eta_\sigma \quad (339)$$

This is analogous to the Landau quasiparticle energy functional, eq. 35, U acting as the interaction between the quasiparticles. δn acts as the excitations from the ground state.

$$\langle \delta n_{k,\sigma} \rangle = \begin{cases} \langle n_{k\sigma} \rangle, & \tilde{\epsilon}_k > \epsilon_F \\ -\langle n_{k\sigma} \rangle, & \tilde{\epsilon}_k < \epsilon_F \end{cases} \quad (340)$$

This quantity $\gamma = \frac{C_v}{T}$ is

$$\gamma_{\text{imp}} = \frac{2\pi^2 k_B^2}{3} \rho_d(0) \quad (341)$$

Under a magnetic field B , $\tilde{\epsilon}_{k\sigma} = \epsilon_k + U \eta_\sigma + \sigma h$, where $h = \frac{1}{2} g B \mu_B$. The magnetic susceptibility is

$$\begin{aligned} \chi_m &= \frac{g\mu_B}{2} \frac{\partial}{\partial B} \langle \delta n_\uparrow(\tilde{\epsilon}_F) - \delta n_\downarrow(\tilde{\epsilon}_F) \rangle \\ &= \frac{g\mu_B}{2} \frac{\partial}{\partial B} \sum_\sigma \sigma \langle \delta n(\tilde{\epsilon}_F, \sigma) \rangle \\ &= \frac{g\mu_B}{2} \sum_{k,\sigma} \sigma \frac{\partial}{\partial \tilde{\epsilon}_{k\sigma}} \langle \delta n(\tilde{\epsilon}_F, \sigma) \rangle \frac{\partial \tilde{\epsilon}_{k\sigma}}{\partial B} \end{aligned} \quad (342)$$

The term $\frac{\partial}{\partial \tilde{\epsilon}_{k\sigma}} \langle \delta n(\tilde{\epsilon}_F, \sigma) \rangle$ is the density of states of the whole system.

$$\frac{\partial}{\partial \tilde{\epsilon}_k} \langle \delta n(\tilde{\epsilon}_F, \sigma) \rangle = \delta(\tilde{\epsilon}_{k\sigma} - \epsilon_F) \quad (343)$$

In the limit of $T \rightarrow 0$ and $h \rightarrow 0$, the quasiparticle energy becomes that of a non-interacting system.

$$\lim_{T \rightarrow 0, h \rightarrow 0} \frac{\partial}{\partial \tilde{\epsilon}_{k\sigma}} \langle \delta n(\tilde{\epsilon}_F, \sigma) \rangle = \delta(\tilde{\epsilon}_k - \epsilon_F) \quad (344)$$

Therefore,

$$\chi_m = -\frac{g\mu_B}{2} \sum_k \delta(\tilde{\epsilon}_k - \epsilon_F) \sum_\sigma \sigma \frac{\partial \tilde{\epsilon}_{k\sigma}}{\partial B} \quad (345)$$

Now, the remaining derivative can be evaluated as

$$\frac{\partial \tilde{\epsilon}_{k\sigma}}{\partial B} = \frac{\partial}{\partial B} (\epsilon_k + \sigma h + U\eta_\sigma) = \frac{g\mu_B}{2} \frac{\partial}{\partial h} (+\sigma h + U\eta_\sigma) = \frac{g\mu_B}{2} \sigma [1 + U\rho_d] \quad (346)$$

The impurity contribution is

$$\chi_{m,\text{imp}} = \left(\frac{g\mu_B}{2}\right)^2 \rho_d(0) \sum_\sigma [1 + U\rho_d(0)] = \frac{(g\mu_B)^2}{2} \rho_d(0) [1 + U\rho_d(0)] \quad (347)$$

Similarly, the charge susceptibility is

$$\chi_{c,\text{imp}} = 2\rho_d(0) (1 - U\rho_d(0)) \quad (348)$$

where $\rho_d(E)$ is the density of states in the non-interacting limit. χ_m and χ_c are the magnetic and charge susceptibilities. Eliminating $\rho_d(0)$ between eqs. 341, 347 and 348 gives

$$\frac{4}{g^2\mu_B^2} \chi_{m,\text{imp}} + \chi_{c,\text{imp}} = \frac{6}{\pi^2 k_B^2} \gamma_{\text{imp}} \quad (349)$$

The Wilson ratio is

$$R = 1 + U\rho_d(0) \quad (350)$$

From the expressions of χ_m and χ_c , its easy to prove

$$U\rho_d(0) = \frac{4\chi_m - g^2\mu_B^2\chi_c^2}{4\chi_m + g^2\mu_B^2\chi_c^2} \quad (351)$$

Substituting that in the Wilson ratio gives

$$R = \frac{2}{1 + \frac{g^2\mu_B^2}{4} \frac{\chi_c}{\chi_m}} \quad (352)$$

At the strong-coupling limit, the impurity is localised at the 0th site, so the charge susceptibility must go to zero. This gives

$$\chi_c = 0 \quad (353)$$

Substituting this in the Wilson ratio gives

$$R = 2 \quad (354)$$

We thus see that a mean-field treatment of the Anderson model gives results similar to Landau's phenomenological treatment of the Fermi liquid.

0.20 Microscopic approach

The average occupation for the non-interacting quasiparticles can be similarly written from eq. 365.

$$\langle \tilde{n}_d \rangle = \frac{1}{2} - \frac{1}{\pi} \tan^{-1} \frac{\tilde{\epsilon}_d}{\tilde{\Delta}} = \frac{1}{2} - \frac{1}{\pi} \tan^{-1} \frac{\epsilon_d - \Sigma(0)}{\Delta} = \langle n_d \rangle \quad (355)$$

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

$$\gamma_{\text{imp}} = \frac{2\pi k_B^2}{3} \frac{\tilde{\Delta}}{\tilde{\epsilon}_d^2 + \tilde{\Delta}^2} \quad (356)$$

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

$$\chi_{\text{m,imp}} = \frac{g^2 \mu_B^2}{2} \alpha' \rho_d(0) \quad (357)$$

$$\chi_{\text{c,imp}} = 2\alpha'' \rho_d(0) \quad (358)$$

where

$$\alpha' = \frac{1 - \partial_h \Sigma_\sigma(\epsilon_F, 0)}{1 - \partial_E \Sigma_\sigma(\epsilon_F, 0)} \quad (359)$$

$$\alpha'' = \frac{1 + \partial_\mu \Sigma_\sigma(\epsilon_F, 0)}{1 - \partial_E \Sigma_\sigma(\epsilon_F, 0)} \quad (360)$$

Renormalized perturbation

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 $T, h \rightarrow 0..$ This approach is obviously more general as all terms in the original Hamiltonian are retained.

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

$$G_d^0 = \frac{1}{E - \epsilon_d + i\Delta} \quad (361)$$

Including the self energy gives

$$G_d = \frac{1}{E - \epsilon_d + i\Delta - \Sigma(E)} \quad (362)$$

As shown previously in section 0.12, the impurity Green's function can be shown to take the form

$$G_d = \frac{Z}{E - \tilde{\epsilon}_d + i\tilde{\Delta} - \tilde{\Sigma}(E)} \quad (363)$$

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

$$\begin{aligned} \tilde{\epsilon}_d &= Z(\epsilon_d + \Sigma(0)) \\ \tilde{\Delta} &= Z\Delta \\ \tilde{\Sigma} &= Z\Sigma^{\text{rem}}(E) \\ Z^{-1} &= 1 - \Sigma(0)' \\ \tilde{\Gamma}_{\sigma\sigma'}(E, E') &= z^2\Gamma_{\sigma\sigma'}(E, E') \\ \tilde{U} &= z^2\Gamma_{\uparrow\downarrow}(0, 0) \end{aligned} \quad (364)$$

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

$$\tilde{G}_d = \frac{1}{E - \tilde{\epsilon}_d + i\tilde{\Delta}} \quad (365)$$

The Anderson hamiltonian

$$H = \epsilon_d n_d + U n_{d\uparrow} n_{d\downarrow} + \sum_k \epsilon_k n_k + \sum_k \left(V_k c_{d\sigma}^\dagger c_{k\sigma} + V_k^* c_{k\sigma}^\dagger c_{d\sigma} \right) \quad (366)$$

can be written in the form

$$H = \tilde{H}_{qp} - \tilde{H}_c \quad (367)$$

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

$$\tilde{H}_{qp}^0 = \tilde{\epsilon}_d \tilde{n}_d + \sum_k \epsilon_k n_k + \sum_k \left(\tilde{V}_k \tilde{c}_{d\sigma}^\dagger c_{k\sigma} + \tilde{V}_k^* c_{k\sigma}^\dagger \tilde{c}_{d\sigma} \right) \quad (368)$$

$$\tilde{H}_{qp}^I = \tilde{U} \tilde{n}_{d\uparrow} \tilde{n}_{d\downarrow} \quad (369)$$

The renormalised parameters are defined in eq. 364. The renormalised operators are

$$\tilde{c}_d^\dagger = \sqrt{z} c_d^\dagger \quad (370)$$

$$\tilde{c}_d = \sqrt{z} c_d \quad (371)$$

The \tilde{H}_c that satisfies eq. 367 is

$$\tilde{H}_c = \lambda_1 \tilde{n}_d + \lambda_2 n_{d\uparrow} n_{d\downarrow} \quad (372)$$

where

$$\lambda_1 = z\Sigma(0, 0) \quad (373)$$

$$\lambda_2 = z^2 [\Gamma_{\uparrow\downarrow}(0, 0) - U] \quad (374)$$

\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

$$\begin{aligned} \tilde{\Sigma}(0) &= 0 \\ \tilde{\Sigma}'(0) &= 0 \end{aligned} \quad (375)$$

Close to the Fermi surface, we also have

$$\tilde{\Gamma}_{\uparrow\downarrow}(0) = \tilde{U} \quad (376)$$

$$\tilde{\Gamma}_{\sigma\sigma}(0) = 0 \quad (377)$$

$$\implies \Gamma_{\sigma\sigma'}(0) = \tilde{U}(1 - \delta_{\sigma\sigma'}) \quad (378)$$

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} .

$$\lambda_i = \sum_n \lambda_i^{(n)} \tilde{U}^n \quad (379)$$

$$z = \sum_n z^{(n)} \tilde{U}^n \quad (380)$$

$$(381)$$

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

$$G^0 = \frac{1}{E - \tilde{\epsilon}_d + i\tilde{\Delta}} \quad (382)$$

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

$$\langle n_{d\sigma} \rangle = \frac{1}{\pi} \tan^{-1} \frac{\Delta}{\epsilon_d + \Sigma(0, h)} \quad (383)$$

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

$$\langle n_{d\sigma} \rangle = \frac{1}{\pi} \tan^{-1} \frac{\tilde{\Delta}}{\tilde{\epsilon}_d + \tilde{\Sigma}(0, h)} \quad (384)$$

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. 375. 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.

By considering diagrams for the self energy, we get

$$\left(\frac{\partial}{\partial E} + \frac{\partial}{\partial \mu} \right) \Sigma(E) \Big|_{E=0} = -\rho_{d\sigma}(0) \Gamma_{\uparrow\downarrow}(0, 0) \quad (385)$$

$$\left(\frac{\partial}{\partial h} - \frac{\partial}{\partial E} \right) \Sigma(E) \Big|_{E=0} = -\rho_{d\sigma}(0) \Gamma_{\uparrow\downarrow}(0, 0) \quad (386)$$

Multiplying both equations throughout by Z , we get

$$\left(\frac{\partial}{\partial E} + \frac{\partial}{\partial \mu} \right) \tilde{\Sigma}(E) \Big|_{E=0} = -Z \rho_{d\sigma}(0) \Gamma_{\uparrow\downarrow}(0, 0) = -\frac{1}{Z} \rho_{d\sigma}(0) \tilde{U} \quad (387)$$

$$\left(\frac{\partial}{\partial h} - \frac{\partial}{\partial E} \right) \tilde{\Sigma}(E) \Big|_{E=0} = -Z \rho_{d\sigma}(0) \Gamma_{\uparrow\downarrow}(0, 0) = -\frac{1}{Z} \rho_{d\sigma}(0) \tilde{U} \quad (388)$$

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

$$\tilde{\rho}(0) \sim \frac{\tilde{\Delta}}{\tilde{\epsilon}_d^2 + \tilde{\Delta}^2} = \frac{1}{Z} \frac{\Delta}{\epsilon_d^2 + \Delta^2} = \frac{1}{Z} \rho_d(0) \quad (389)$$

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

$$\frac{\partial \tilde{\Sigma}(E)}{\partial \mu} \Big|_{E=0} = \frac{\partial \tilde{\Sigma}(E)}{\partial h} \Big|_{E=0} = -\tilde{\rho}_{d\sigma}(0) \tilde{U} \quad (390)$$

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.

$$\tilde{\gamma} \sim \tilde{\rho}_d(0) \quad (391)$$

The susceptibilities are given by

$$\chi_m = - \left(\frac{g\mu_B}{2} \right)^2 \tilde{\rho}_d \sum_{\sigma} \frac{\partial (\epsilon_k - h\sigma + \tilde{\Sigma})}{\partial h} = \frac{g^2 \mu_B^2}{2} \tilde{\rho}_d \left(1 - \frac{\partial \tilde{\Sigma}}{\partial h} \right) \quad (392)$$

Substituting from eq. 390,

$$\chi_m = \frac{g^2 \mu_B^2}{2} \tilde{\rho}_d \left(1 + \tilde{U} \tilde{\rho}_d(0) \right) \quad (393)$$

Similarly,

$$\chi_c = \frac{dn}{d\mu} = \tilde{\rho}_d(0) \sum_{\sigma} \frac{d(\epsilon_F + \tilde{\Sigma})}{d\mu} = 2\tilde{\rho}_d(0) \left(1 + \frac{\partial \tilde{\Sigma}}{\partial \mu} \right) = 2\tilde{\rho}_d(0) \left(1 - \tilde{U} \tilde{\rho}_d(0) \right) \quad (394)$$

Friedel sum rule

Looking at eq. 362, we can write down the density of states and hence the average occupancy of the impurity site

$$\rho_{d\sigma} = \frac{-1}{\pi} \text{Im} [G_d] \quad (395)$$

$$\langle n_{d\sigma} \rangle = \int_{-\infty}^0 dE \rho_{d\sigma} = -\frac{1}{\pi} \text{Im} \int_{-\infty}^0 dE G_d(E) \quad (396)$$

Luttinger proved that

$$\int_{-\infty}^0 \Sigma' G dE = 0 \quad (397)$$

In order to use this, note that

$$\begin{aligned} \ln G_d^{-1} &= \ln (E - \epsilon_d + i\Delta - \Sigma) \\ \implies \frac{d \ln G_d^{-1}}{dE} &= \frac{1}{E - \epsilon_d + i\Delta - \Sigma} (1 - \Sigma') = G_d - \Sigma' G_d \\ \implies G_d &= \Sigma' G_d - \frac{d \ln G_d}{dE} \end{aligned} \quad (398)$$

Substituting this expression for G_d in eq. 396,

$$\langle n_{d\sigma} \rangle = -\frac{1}{\pi} \text{Im} \int_{-\infty}^0 \Sigma' G dE + \frac{1}{\pi} \text{Im} \int_{-\infty}^0 \frac{d \ln G_d}{dE} dE \quad (399)$$

The first integral is zero, courtesy Luttinger. We get

$$\begin{aligned}
\langle n_{d\sigma} \rangle &= \frac{1}{\pi} \text{Im} \left[\ln \frac{1}{E - \epsilon_d + i\Delta - \Sigma} \right]_{-\infty}^0 \\
&= -\frac{1}{\pi} \text{Im} [\ln (E - \epsilon_d + i\Delta - \Sigma)]_{-\infty}^0 \\
&= -\frac{1}{\pi} \text{Im} [\ln e^{i\theta}]_{-\infty}^0 \quad \left[\tan \theta = \frac{\Delta}{E - \epsilon_d - \Sigma} \right] \\
&= -\frac{1}{\pi} [\theta(0) - \theta(-\infty)] \\
&= \frac{1}{\pi} \tan^{-1} \frac{\Delta}{\epsilon_d + \Sigma(0, h)} \\
&= \frac{1}{2} - \frac{1}{\pi} \tan^{-1} \frac{\epsilon_d + \Sigma(0, h)}{\Delta}
\end{aligned} \tag{400}$$

We can now relate the average occupancy with the density of states. From eq. 395,

$$\begin{aligned}
\rho_{d\sigma} &= \frac{1}{\pi} \frac{\Delta}{(\epsilon_d + \Sigma(0))^2 + \Delta^2} \\
&= \frac{1}{\pi\Delta} \left[1 + \left(\frac{\epsilon_d + \Sigma(0)}{\Delta} \right)^2 \right]^{-1} \\
&= \frac{1}{\pi\Delta} [1 + \cot^2 \pi \langle n_{d\sigma} \rangle]^{-1} \\
&= \frac{\sin^2 \pi \langle n_{d\sigma} \rangle}{\pi\Delta}
\end{aligned} \tag{401}$$