

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

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

Hence the total wavefunction of singlet+Fermi-sea is

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

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

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

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

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

Multiplying b_q from left gives

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

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

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

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

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

Converting to integral,

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

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

$$\begin{aligned} \frac{2}{3JN(0)} &= \ln \left| \frac{D-E}{\epsilon_F-E} \right| \approx \ln \left| \frac{D}{\epsilon_F-E} \right| \\ \implies E &= \epsilon_F - De^{-\frac{2}{3N(0)J}} \end{aligned} \quad (2.4.109)$$

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

$$E_b = De^{-\frac{2}{3N(0)J}} \quad (2.4.110)$$

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

$$k_B T_K \sim E_b \implies T_K = \frac{D}{k_B} e^{-\frac{2}{3N(0)J}} \quad (2.4.111)$$

2.4.6 Poor man's scaling

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

$$T^{(2)} = VG_0V \quad (2.4.112)$$

can be clubbed into a term ΔV . This term is a representative of the scatterings from that range. After reducing the bandwidth to $D - \delta D$, the effect of the excluded region can be incorporated by changing the interaction term $V \rightarrow V' = V + \Delta V$. The interaction part is

$$H' = J_z \sum_{k_1, k_2} S_d^z \left(c_{k_1\uparrow}^\dagger c_{k_2\uparrow} - c_{k_1\downarrow}^\dagger c_{k_2\downarrow} \right) + J_T \sum_{k_1, k_2} \left(S_d^+ c_{k_1\downarrow}^\dagger c_{k_2\uparrow} + S_d^- c_{k_1\uparrow}^\dagger c_{k_2\downarrow} \right) \quad (2.4.113)$$

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

$$k \uparrow, d \downarrow \rightarrow q \downarrow d \uparrow \rightarrow k' \uparrow d \downarrow \quad (2.4.114)$$

The T -matrix term is

$$T_1 = J_T^2 \sum_q S_d^- c_{k'\uparrow}^\dagger c_{q\downarrow} \frac{1}{E - H_0} S_d^+ c_{q\downarrow}^\dagger c_{k\uparrow} \quad (2.4.115)$$

Using eq. 2.1.53, we can write

$$(E - H_0)^{-1} c_{q\downarrow}^\dagger c_{k\uparrow} = c_{q\downarrow}^\dagger c_{k\uparrow} (E - \lambda - H_0)^{-1} \quad (2.4.116)$$

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

$$T_1 = J_T^2 S_d^- S_d^+ \sum_q c_{k'\uparrow}^\dagger c_{q\downarrow} c_{q\downarrow}^\dagger c_{k\uparrow} (E - \epsilon_q + \epsilon_k - H_0)^{-1} \quad (2.4.117)$$

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

$$T_1 = J_T^2 S_d^- S_d^+ c_{k'\uparrow}^\dagger c_{k\uparrow} \sum_q (E - \epsilon_q + \epsilon_k - H_0)^{-1} \quad (2.4.118)$$

If we set the Fermi level to 0, $H_0 = 0$. Since the summation is over the narrow band $\{D - \delta D, D\}$, we can approximate the result of the summation as

$$\sum_q (E - \epsilon_q + \epsilon_k - H_0)^{-1} = N |\delta D| \frac{1}{E - D + \epsilon_k} \quad (2.4.119)$$

N is the density of states. Also,

$$S^- S^+ = (S^x - iS^y) (S^x + iS^y) = \frac{1}{2} + i [S^x, S^y] = \frac{1}{2} - S^z \quad (2.4.120)$$

Putting it all together,

$$T_1 = J_T^2 \left(\frac{1}{2} - S_d^z \right) N |\delta D| c_{k'\uparrow}^\dagger c_{k\uparrow} \frac{1}{E - D + \epsilon_k} \quad (2.4.121)$$

For the second possible scattering,

$$q \downarrow k \uparrow d \uparrow \rightarrow k' \uparrow k \uparrow d \downarrow \rightarrow k' \uparrow q \downarrow d \uparrow \quad (2.4.122)$$

we get

$$T_2 = J_T^2 \sum_q S_d^+ S_d^- c_{q\downarrow}^\dagger c_{k\uparrow} \frac{1}{E - H_0} c_{k'\uparrow}^\dagger c_{q\downarrow} \quad (2.4.123)$$

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

$$\begin{aligned} T_2 &= J_T^2 \left(\frac{1}{2} + S_d^z \right) N |\delta D| c_{k\uparrow} c_{k'\uparrow}^\dagger \frac{1}{E - D - \epsilon_{k'}} \\ &= -J_T^2 \left(\frac{1}{2} + S_d^z \right) N |\delta D| c_{k'\uparrow}^\dagger c_{k\uparrow} \frac{1}{E - D - \epsilon_{k'}} \end{aligned} \quad (2.4.124)$$

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

$$k \downarrow, d \uparrow \rightarrow q \uparrow d \downarrow \rightarrow k' \downarrow d \uparrow \quad (2.4.125)$$

$$q \uparrow k \downarrow d \downarrow \rightarrow k' \downarrow k \downarrow d \uparrow \rightarrow k' \downarrow q \uparrow d \downarrow \quad (2.4.126)$$

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

$$T_3 = J_T^2 \left(\frac{1}{2} + S_d^z \right) N |\delta D| c_{k'\downarrow}^\dagger c_{k\downarrow} \frac{1}{E - D + \epsilon_k} \quad (2.4.127)$$

$$T_4 = -J_T^2 \left(\frac{1}{2} - S_d^z \right) N |\delta D| c_{k'\downarrow}^\dagger c_{k\downarrow} \frac{1}{E - D - \epsilon_{k'}} \quad (2.4.128)$$

The total second order contribution is

$$T^{(2)} = -J_T^2 S_d^z N |\delta D| \left(\frac{1}{E - D + \epsilon_k} + \frac{1}{E - D - \epsilon_{k'}} \right) (c_{k'\uparrow}^\dagger c_{k\uparrow} - c_{k'\downarrow}^\dagger c_{k\downarrow}) \quad (2.4.129)$$

Comparing this with the S_d^z term in the Hamiltonian

$$J_z S_d^z (c_{k'\uparrow}^\dagger c_{k\uparrow} - c_{k'\downarrow}^\dagger c_{k\downarrow}) \quad (2.4.130)$$

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

$$\delta J_d^z = -J_T^2 N |\delta D| \left(\frac{1}{E - D + \epsilon_k} + \frac{1}{E - D - \epsilon_{k'}} \right) \quad (2.4.131)$$

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

$$\frac{dJ_d^z}{dD} = -J_T^2 N \frac{2}{D} \quad (2.4.132)$$

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

Renormalization of J_T

Consider the scattering

$$k \uparrow d \downarrow \rightarrow q \downarrow d \uparrow \rightarrow k' \downarrow d \uparrow \quad (2.4.133)$$

$$T_1 = -J_T J_z S_d^z S_d^+ N |\delta D| c_{k'\downarrow}^\dagger c_{k\uparrow} \frac{1}{E - D + \epsilon_k} \quad (2.4.134)$$

The minus sign at the front comes from the term

$$-S_d^z c_{k'\downarrow}^\dagger c_{q\downarrow} \quad (2.4.135)$$

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

$$T_1 = -J_T J_z \frac{S_d^+}{2} N |\delta D| c_{k'\downarrow}^\dagger c_{k\uparrow} \frac{1}{E - D + \epsilon_k} \quad (2.4.136)$$

The second process is

$$q \uparrow k \uparrow d \downarrow \rightarrow k' \downarrow k \uparrow d \uparrow \rightarrow q \uparrow k' \downarrow d \uparrow \quad (2.4.137)$$

$$T_2 = -J_T J_z \frac{S_d^+}{2} N |\delta D| c_{k'\downarrow}^\dagger c_{k\uparrow} \frac{1}{E - D - \epsilon_{k'}} \quad (2.4.138)$$

Two more processes can be constructed from the above two processes, by switching the S_d^+ and S_d^z operations. The change in the first process is that the S_d^z term will now become

$$+S_d^z c_{k'\uparrow}^\dagger c_{q\uparrow} \quad (2.4.139)$$

so that will invert the sign. The change in the second process is that now the q -electron has to start off as \downarrow , which means that the S_d^z term for this process becomes

$$-S_d^z c_{k'\downarrow}^\dagger c_{q\downarrow} \quad (2.4.140)$$

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

$$T_3 = T_1 \quad (2.4.141)$$

$$T_4 = T_2 \quad (2.4.142)$$

The total contribution is

$$T^{(2)} = -J_T J_z S_d^+ N |\delta D| c_{k'\downarrow}^\dagger c_{k\uparrow} \left(\frac{1}{E - D - \epsilon_{k'}} + \frac{1}{E - D + \epsilon_k} \right) \quad (2.4.143)$$

Comparing with the S_d^+ term in the Hamiltonian

$$J_T S_d^+ c_{k'\downarrow}^\dagger c_{k\uparrow} \quad (2.4.144)$$

we can write

$$\delta J_T = -J_T J_z N |\delta D| \left(\frac{1}{E - D - \epsilon_{k'}} + \frac{1}{E - D + \epsilon_k} \right) \quad (2.4.145)$$

Again neglecting the terms in the denominator, we get

$$\frac{dJ_T}{dD} = -J_T J_z N \frac{2}{D} \quad (2.4.146)$$

This is the scaling equation for J_T .

Flow of the couplings

Switching to the dimensionless couplings

$$g_1 = NJ_z, g_2 = NJ_T \quad (2.4.147)$$

the equations become

$$\frac{dg_1}{dD} = -\frac{2g_2^2}{D} \quad (2.4.148)$$

$$\frac{dg_2}{dD} = -\frac{2g_1 g_2}{D} \quad (2.4.149)$$

The first equation says that as the cutoff decreases, g_1 will always increase. For $g < 0$ (ferromagnetic coupling), the coupling will go to zero. That is, at sufficiently low temperatures, the impurity electron becomes effectively decoupled from the conduction band. The phenomenon is called asymptotic freedom. For the antiferromagnetic case, the coupling should go to infinity. This means that at sufficiently low temperatures, the coupling will necessarily become appreciable large so as to render perturbation theory inapplicable. Dividing the two coupling equations gives

$$\frac{dg_1}{dg_2} = \frac{g_2}{g_1} \implies g_1^2 - g_2^2 = \text{constant} \quad (2.4.150)$$

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

$$\begin{aligned} g(D') &= \frac{g_0}{1 - 2g_0 \ln \frac{D}{D'}} \\ \Rightarrow 2g(D') &= \frac{1}{\ln \frac{D'}{T_K}} \end{aligned} \quad (2.4.151)$$

where $T_K = \frac{D}{k_B} \exp\left(-\frac{1}{2g_0}\right)$. D' is the running bandwidth and D is the original bandwidth. This is almost the same as the one obtained in eq. 2.4.111, because $g = NJ$. The expression for $g_{D'}$ shows that perturbation theory will work only for $T \gg T_K$, because close to T_K , the expression becomes non-analytic.

The ferromagnetic case ($g < 0$), on the other hand, remains perturbative.

$$g(D') = \frac{g_0}{1 - 2g_0 \ln \frac{D}{D'}} = -\frac{|g_0|}{1 + 2|g_0| \ln \frac{D}{D'}} \quad (2.4.152)$$

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

Alternate way of obtaining the scaling equations

From eq. 2.4.16, the interaction part can be written as

$$\Delta H_{ll'} = \frac{1}{2} [T_{ll'}(E_l) + T_{ll'}(E_{l'})] \quad (2.4.153)$$

where the transition matrix T is

$$T_{ll'}(E) = \sum_H \frac{V_{lH} V_{Hl'}}{E - E_H} \quad (2.4.154)$$

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

$$V = J \vec{S}_d \cdot \sum_{k,k',\alpha,\alpha'} c_{k\alpha}^\dagger \vec{\sigma}_{\alpha\alpha'} c_{k'\alpha'} \quad (2.4.155)$$

The first process is

$$k\alpha \xrightarrow{\sigma^b} q\lambda \xrightarrow{\sigma^a} k'\beta \quad (2.4.156)$$

$$d\sigma \xrightarrow{S_d^b} d\sigma'' \xrightarrow{S_d^a} d\sigma' \quad (2.4.157)$$

The transition matrix element is

$$\begin{aligned} T_1 &= \sum_{q \in \{D-\delta D\}, \lambda, \sigma''} \langle k'\beta, \sigma' | V | q\lambda, \sigma'' \rangle \langle q\lambda, \sigma'' | V | k\alpha, \sigma \rangle \frac{1}{E - E_q} \\ &= J^2 \sum_{\sigma''} \left(S_d^a \right)_{\sigma'\sigma''} \left(S_d^b \right)_{\sigma''\sigma} \sum_{\lambda} \left(\sigma^a \right)_{\beta\lambda} \left(\sigma^b \right)_{\lambda\alpha} \sum_{q \in \{D-\delta D\}} \frac{1}{E - E_q} \\ &\approx J^2 \left(S_d^a S_d^b \right)_{\sigma'\sigma} \left(\sigma^a \sigma^b \right)_{\beta\alpha} \frac{N|\delta D|}{E - D} \end{aligned} \quad (2.4.158)$$

The second process is

$$k\alpha \longrightarrow k\alpha \xrightarrow{\sigma^a} q\lambda \quad (2.4.159)$$

$$q\lambda \xrightarrow{\sigma^b} k'\beta \longrightarrow k'\beta \quad (2.4.160)$$

$$d\sigma \xrightarrow{S_d^b} d\sigma'' \xrightarrow{S_d^a} d\sigma' \quad (2.4.161)$$

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

$$\begin{aligned} T_2 &= \sum_{q \in \{D - |\delta D|\}, \lambda, \sigma''} \langle q\lambda, k'\beta, \sigma' | V | k'\beta, k\alpha, \sigma'' \rangle \langle k'\beta, k\alpha, \sigma'' | V | q\lambda, k\alpha, \sigma \rangle \frac{1}{E - (E_k + E_{k'} - E_q)} \\ &\approx -J^2 \left(S_d^a S_d^b \right)_{\sigma'\sigma} \left(\sigma^b \sigma^a \right)_{\beta\alpha} \frac{N|\delta D|}{E - D} \end{aligned} \quad (2.4.162)$$

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

$$\begin{aligned} T &= \frac{J^2 N |\delta D|}{D} \left(S_d^a S_d^b \right)_{\sigma'\sigma} \left[\sigma^b, \sigma^a \right]_{\beta\alpha} \\ &= \frac{J^2 N |\delta D|}{2D} \left[S_d^a, S_d^b \right]_{\sigma'\sigma} \left[\sigma^b, \sigma^a \right]_{\beta\alpha} \end{aligned} \quad (2.4.163)$$

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

$$\begin{aligned} \left[S_d^a, S_d^b \right]_{\sigma'\sigma} \left[\sigma^b, \sigma^a \right]_{\beta\alpha} &= - \left[S_d^a, S_d^b \right]_{\sigma'\sigma} \left[\sigma^a, \sigma^b \right]_{\beta\alpha} \\ &= -i\epsilon_{abc} S_{\sigma\sigma'}^c 2i\epsilon_{abd} \sigma_{\beta\alpha}^d \\ &= 4\delta_{cd} S_{\sigma\sigma'}^c \sigma_{\beta\alpha}^d \\ &= 4\vec{S}_{\sigma\sigma'} \cdot \vec{\sigma}_{\beta\alpha} \end{aligned} \quad (2.4.164)$$

Therefore,

$$T = \frac{2J^2 N |\delta D|}{D} \vec{S}_{\sigma\sigma'} \cdot \vec{\sigma}_{\beta\alpha} \quad (2.4.165)$$

The correction to the coupling J can be read off:

$$J(D - \delta D) = J(D) - \frac{2J^2 N \delta D}{D} \quad (2.4.166)$$

This gives the same scaling equations we found earlier.

2.4.7 Universality

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

$$\frac{\partial g}{\partial \ln D} = -2g^2 + 2g^3 \quad (2.4.167)$$

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

$$\ln \frac{D'}{D} = - \int_{g_0}^g \frac{dg}{2g^2 - 2g^3} = - \int_{g_0}^g \frac{dg}{2g^2} (1 + g) \quad (2.4.168)$$

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

$$\begin{aligned} \ln \frac{k_B T_K}{D} &= - \int_{g_0}^1 \frac{dg}{2g^2} (1 + g) = - \frac{1}{2g_0} + \frac{1}{2} \ln g_0 + O(1) \\ &= - \frac{1}{2g_0} + \frac{1}{2} \ln 2g_0 + O(1) \end{aligned} \quad (2.4.169)$$

This gives a better estimate of the Kondo temperature

$$T_K = \frac{D}{k_B} \sqrt{2g_0} \exp \left(- \frac{1}{2g_0} \right) \quad (2.4.170)$$

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

$$k_B T_K = D y(g) \quad (2.4.171)$$

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

$$\frac{dT_K}{dD} = 0 \quad (2.4.172)$$

Substituting the form of T_K , eq. 2.4.171, in this equation gives

$$\begin{aligned} y(g) + D \frac{dy(g)}{dD} &= 0 \\ \implies y + D \frac{dy}{dg} \frac{dg}{dD} &= 0 \\ \implies y - 2g^2 \frac{dy}{dg} &= 0 \\ \implies y &= e^{-\frac{1}{2g}} \end{aligned} \quad (2.4.173)$$

This gives almost the same solution as eq. 2.4.170:

$$T_K = \frac{D}{k_B} e^{-\frac{1}{2g}} \quad (2.4.174)$$

The difference in the pre-factor arises from the extra contribution incorporated in that solution.

The fact that the scaling equations are universal can be seen by noting that from eq. 2.4.151, up to second order, we can write

$$g(D') = g_0 \left(1 + 2g_0^2 \ln \frac{D}{D'} \right) \quad (2.4.175)$$

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

$$g_0 \rightarrow g = g_0 \left(1 + 2g_0 \ln \frac{T_F}{T} \right) \quad (2.4.176)$$

Since $g \equiv NJ$, we have recovered eq. 2.4.57. Since eq. 2.4.57 was obtained as a perturbation calculation, it should have been valid only at $T \gg T_K$, but the scaling relation holds at all temperatures.

2.4.8 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 [17]. For example,

$$S^z = \frac{\sigma^z}{2} = \sum_{ij} c_i^\dagger \frac{\sigma_{ij}^z}{2} c_j = \frac{1}{2} (c_\uparrow^\dagger c_\uparrow - c_\downarrow^\dagger c_\downarrow) \quad (2.4.177)$$

Similarly,

$$\begin{aligned} S^x &= \frac{1}{2} (c_\uparrow^\dagger c_\downarrow + c_\downarrow^\dagger c_\uparrow) \\ S^y &= \frac{-i}{2} (c_\uparrow^\dagger c_\downarrow - c_\downarrow^\dagger c_\uparrow) \end{aligned} \quad (2.4.178)$$

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

$$|\uparrow\rangle = c_\uparrow^\dagger |0\rangle \quad (2.4.179)$$

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 [18]

$$\mu = -i \frac{\pi}{2} k_B T \quad (2.4.180)$$

The new Hamiltonian is

$$\tilde{H} = H - \mu(n_d - 1) \quad (2.4.181)$$

The new partition function is then allowed to run over the entire Hilbert space, including the unphysical states. The actual partition function for the original Hamiltonian H is

$$Z = \text{Tr} [\exp(-\beta H)] = \sum_{\sigma_d=\uparrow,\downarrow} \sum_k [\exp(-\beta H)] \quad (2.4.182)$$

The modified partition function is

$$\begin{aligned}
 \tilde{Z} &= \text{Tr} \left[\exp \left(-\beta (H - \mu(n_d - 1)) \right) \right] \\
 &= \text{Tr} \left[\exp \left(-\beta H - i\frac{\pi}{2}(n_d - 1) \right) \right] \\
 &= \sum_{\sigma_d=\uparrow,\downarrow} \sum_k \left[\exp(-\beta H) \right] + \sum_k \exp \left(-\beta H + i\frac{\pi}{2} \right) + \sum_k \exp \left(-\beta H - i\frac{\pi}{2} \right) \\
 &= Z \Big|_{n_d=1} + iZ \Big|_{n_d=0} - iZ \Big|_{n_d=0}
 \end{aligned} \tag{2.4.183}$$

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

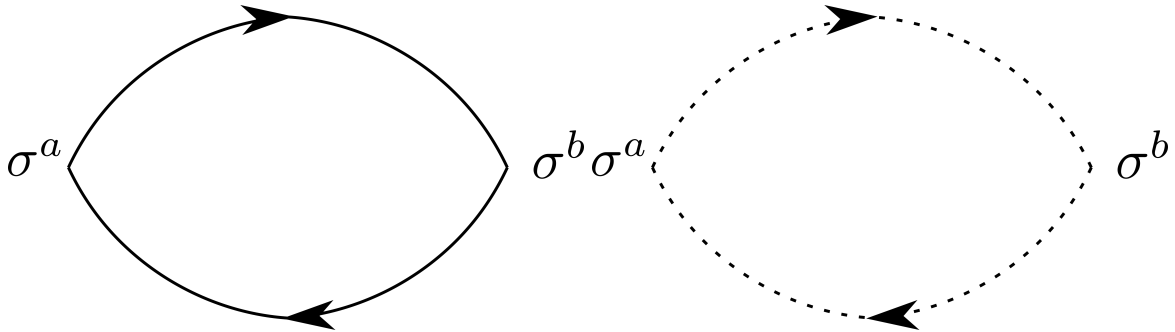
$$Z \Big|_{n_d=0} = Z \Big|_{n_d=0} \tag{2.4.184}$$

Hence,

$$\tilde{Z} = Z \tag{2.4.185}$$

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

This method can also be used to determine the higher order corrections to the susceptibility. The zeroth order diagrams are



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

$$\chi_c = -k_B T \sum_{k, \omega_n, \phi_0} \langle \phi_0 | \sigma^a G(k, i\omega_n) \sigma^b G_k(i\omega_n) | \phi_0 \rangle \tag{2.4.186}$$

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

$$\begin{aligned}
 \chi_c &= -k_B T \sum_{k, \omega_n} \text{Tr} \left[\sigma^a G(k, i\omega_n) \sigma^b G(k, i\omega_n) \right] \\
 &= -2k_B T \sum_{k, \omega_n} G^2(k, i\omega_n) \\
 &= -2k_B T \sum_{k, \omega_n} (i\omega_n - \epsilon_k)^{-2} \\
 &= 2 \sum_k \frac{d}{d\epsilon_k} k_B T \sum_{\omega_n} (i\omega_n - \epsilon_k)^{-1}
 \end{aligned} \tag{2.4.187}$$

Now, it can be shown that

$$k_B T \sum_{\omega_n} (i\omega_n - \epsilon_k)^{-1} = f(\epsilon_k) - \frac{1}{2} \tag{2.4.188}$$

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

$$\chi_c = 2 \sum_k \frac{df(\epsilon_k)}{d\epsilon_k} = 2 \sum_k \rho(\epsilon_k) = 2N(0) \tag{2.4.189}$$

The second diagram gives

$$\chi_d^{(0)} = -k_B T \sum_{\omega_n} \text{Tr} \left[\sigma^a G_d(i\omega_n) \sigma^b G_d(i\omega_n) \right] \tag{2.4.190}$$

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

$$G_d = \frac{1}{i\omega_n - \lambda_d} \tag{2.4.191}$$

where $\lambda_d = i\pi \frac{1}{2\beta}$ is the imaginary chemical potential introduced. Since this is, for mathematical purposes, the same as the conduction Greens function with λ_d replacing ϵ_k , we again get

$$\chi_d^{(0)} = 2 \frac{df(\lambda_d)}{d\lambda_d} = -2\beta \frac{e^{\beta\lambda_d}}{(1 + e^{\beta\lambda_d})^2} = \beta \tag{2.4.192}$$

The first order diagrams are The first diagram gives

$$\chi^{(1)} = \chi_c \left(-\frac{J}{2} \right) \chi_d = -\beta J N(0) \tag{2.4.193}$$

The second one gives

$$\chi_d^{(1)} = \chi_d \left(-\frac{J}{2} \right) \chi_c = -\beta J N(0) \tag{2.4.194}$$

The total susceptibility is

$$\chi_d = \chi_d^{(0)} + \chi_d^{(1)} = \beta (1 - 2JN(0)) \tag{2.4.195}$$

2.4.9 Nozières' local Fermi liquid theory

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

$$C_V = \gamma T \quad (2.4.196)$$

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

$$E_g = J \left[2\vec{S}_e \cdot \vec{S}_d \right] = J \left[S^2 - S_d^2 - S_e^2 \right] = J \left[s(s+1) - \frac{3}{2} \right] = -\frac{3J}{2} \quad (2.4.197)$$

Since the interaction term is spherically symmetric, it suffices to consider a one dimensional chain of conduction electrons with the impurity site coupling to the conduction electron at the origin. This electron forms a singlet with the impurity electron,

$$\frac{|0_\uparrow, d \downarrow\rangle - |0_\downarrow, d \uparrow\rangle}{\sqrt{2}} \quad (2.4.198)$$

Considering a tight-binding model, the only electron that can hop to the zeroth site is the one on the first site. The hopping of this electron on to the zeroth site would lead to an energy of

$$E_1 = -\frac{3}{2}J + \frac{3}{2}J = 0 \quad (2.4.199)$$

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

$$\psi \sim \frac{\sin [kr + \delta(E_k)]}{r} \quad (2.4.200)$$

That is, the phase shift is only a function of the energy. At the Fermi surface, this value $\delta(0)$ is $\frac{\pi}{2}$, as known from the Friedel sum rule.

$$n = \sum_{\sigma} \frac{\delta}{\pi} \implies 1 = \frac{2\delta}{\pi} \implies \delta = \frac{\pi}{2} \quad (2.4.201)$$

n is the number of conduction electrons bound in the resonance and the sum is over the possible quantum numbers (spin in this case). $\delta(0)$ can also be obtained directly from eq. 2.4.200, by substituting $k = k_F$ and noting that the isolation of the 0th site means all wavefunctions should shift by $\Delta r = a$:

$$k_F a = \delta(0) \implies \delta(0) = \frac{\pi}{2a} 2 = \frac{\pi}{2} \quad (2.4.202)$$

where the formula for k_F was used.

In a Fermi gas, the energy levels are separated by

$$\Delta \epsilon = \frac{\partial \epsilon}{\partial k} \Delta k \quad (2.4.203)$$

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

$$\Delta \epsilon = \frac{\partial \epsilon}{\partial k} \frac{\pi}{L} \quad (2.4.204)$$

However, this changes in the presence of the impurity. Because of eq. 2.4.200, the boundary condition becomes

$$k_n L + \delta(\epsilon_k) = n\pi \implies k_n = \frac{n\pi}{L} - \frac{\delta}{L} = k_n^0 - \frac{\delta(\epsilon_k)}{L} \quad (2.4.205)$$

The energy becomes

$$\begin{aligned} \epsilon(k) &= \epsilon(k^0) + \frac{\partial \epsilon}{\partial k} (k - k_0) \\ &= \epsilon_k - \frac{\partial \epsilon}{\partial k} \frac{\delta(\epsilon_k)}{L} \end{aligned} \quad (2.4.206)$$

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

$$\tilde{\epsilon}_{\sigma}(k) = \epsilon_k - \frac{\partial \epsilon}{\partial k} \frac{\delta_{\sigma}(\epsilon_k, \{n_{q,\sigma}\})}{L} \quad (2.4.207)$$

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 ,

$$\begin{aligned} \tilde{\epsilon}_p &= \underbrace{\epsilon_F}_{\text{Fermi gas}} + \overbrace{\frac{p_F^*}{m} (p - p_F)}^{\text{linear contribution for } p \text{ close to } p_F} \\ &\quad + \underbrace{\sum_{q\sigma} f(p, q) (n_q - n_q^0)}_{\text{interacting between two quasiparticles at momenta } p \text{ and } q} \end{aligned} \quad (2.4.208)$$

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

$$\delta_\sigma(\tilde{\epsilon}, \{n_{q,\sigma}\}) = \delta_\sigma(\tilde{\epsilon} = \epsilon_F, n_k = n_k^0) + \alpha(\tilde{\epsilon} - \epsilon_F) + \Phi \sum_{q\sigma'} (n_{q\sigma'} - n_{q\sigma'}^0) \quad (2.4.209)$$

This is just a Taylor expansion of δ_σ around $\tilde{\epsilon} = \epsilon_F$ and $n_q = n_q^0$. Φ and α play the same role as f and $\frac{p_F^*}{m}$ in eq. 2.4.208. Specifically, Φ represents the onsite interaction between quasiparticles of opposite spin and

$$\alpha = \frac{d\delta_\sigma}{dE} \quad (2.4.210)$$

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

$$\delta_\sigma(\tilde{\epsilon}, \{n_{q,\sigma}\}) = \delta_\sigma(\tilde{\epsilon} = \epsilon_F, n_k = n_k^0) + \alpha(\tilde{\epsilon} - \epsilon_F) + \Phi \sum_q \delta n_{q,-\sigma} \quad (2.4.211)$$

Since the singlet is isolated from the Fermi liquid, any change in the chemical potential will not affect the average occupation of the impurity site $\langle n_d \rangle$, and since we know that $\langle n_d \rangle = \frac{2\delta(0)}{\pi}$, this means that $\delta(0)$, the phase shift at the Fermi surface, is invariant under a change of the chemical potential. This in turn means that the resonance scattering ($\delta = \frac{\pi}{2}$) will always be pinned to the Fermi surface. With this knowledge, let us explicitly try to calculate the change in the phase shift at Fermi surface when we change the chemical potential by $\Delta\mu$. Before the change in chemical potential,

$$\delta_\uparrow^0 = \frac{\pi}{2} + \Phi \sum_q \delta n_{q\downarrow}^0 \quad (2.4.212)$$

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

$$\delta_\uparrow^0 = \frac{\pi}{2} \quad (2.4.213)$$

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

$$N(\mu = 0) = N^0 \quad (2.4.214)$$

$$N(E' = E + \mu) = N(E' = E) + \frac{dN}{dE'} (E' - E) = N^0 + \rho\Delta\mu \quad (2.4.215)$$

$$\implies \sum_q \delta n_q = N - N^0 = \rho\Delta\mu \quad (2.4.216)$$

Hence, from eq. 2.4.211,

$$\begin{aligned} \delta_\uparrow &= \frac{\pi}{2} + \alpha(\epsilon'_F - \epsilon_F) + \Phi \sum_q \delta n_{q\downarrow} \\ &= \delta_\uparrow^0 + \alpha\Delta\mu + \Phi\rho\Delta\mu \end{aligned} \quad (2.4.217)$$

Hence the change in the phase is

$$0 = \Delta\delta_\uparrow = \Delta\mu (\alpha + \Phi\rho) \implies \alpha = -\Phi\rho \quad (2.4.218)$$

This shows that the interaction term Φ is responsible for pinning the resonance at the Fermi level; without that term in the formalism, the occupancy of the impurity site will change. This is similar to the fact that the interaction term $f(k, k')$ in the bulk Fermi liquid is responsible for making the Landau theory invariant under Galilean transformations.

Now we can calculate the density of states. From the boundary condition, we have

$$n_\sigma = \frac{kL}{\pi} + \frac{\delta_\sigma(E)}{\pi} = n^0 + \frac{\delta_\sigma(E)}{\pi} \quad (2.4.219)$$

Hence,

$$\begin{aligned} \rho &= \frac{dn_\sigma}{dE} = \rho^0 + \frac{1}{\pi} \frac{d\delta_\sigma}{dE} \\ \Rightarrow \rho &= \rho^0 + \frac{1}{\pi} \alpha \end{aligned} \quad (2.4.220)$$

ρ^0 is the density of states in absence of the impurity. The low temperature specific heat of an ideal Fermi liquid can be shown to be

$$C_v^0 = \gamma T = \frac{\pi^2 k_B^2}{3} \mathcal{N}(0) T \quad (2.4.221)$$

The interacting Fermi liquid is just a renormalised version of the Fermi gas, with a modified density of states $\frac{1}{\pi} \alpha$. Hence, the impurity contribution to the specific heat is

$$\begin{aligned} C_v &= \frac{\pi^2 k_B^2}{3} (\rho_\uparrow + \rho_\downarrow) T \\ &= \frac{2\alpha}{\pi} \frac{\pi^2 k_B^2}{3} T \end{aligned} \quad (2.4.222)$$

In presence of a magnetic field B , the magnetization is

$$m = \delta n \times \mu \quad (2.4.223)$$

where μ is the magnetic moment

$$\mu = -\frac{g}{2} \mu_B \quad (2.4.224)$$

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

$$\delta n = \langle n_\uparrow \rangle - \langle n_\downarrow \rangle = \frac{1}{\pi} (\delta_\uparrow - \delta_\downarrow) \quad (2.4.225)$$

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

$$E_\sigma^B = E - \sigma \frac{g\mu_B}{2} B \quad (2.4.226)$$

Hence,

$$\sum_k \delta n_{k\sigma} = N_\sigma(E_\sigma^B) - N(E) = \frac{dN}{dE^B} (E^B - E) = -\rho \frac{g\mu_B}{2} \sigma B \quad (2.4.227)$$

This modifies the phase shift at the Fermi surface,

$$\begin{aligned} \delta_\sigma(\epsilon_F) &= \frac{\pi}{2} + \alpha \left(\epsilon_F - \frac{g\mu_B}{2} \sigma B - \epsilon_F \right) + \Phi \sum_q \delta n_{q,-\sigma} \\ &= \frac{\pi}{2} - \sigma \frac{g\mu_B}{2} \alpha B + \Phi \rho \frac{g\mu_B}{2} \sigma B \\ &= \frac{\pi}{2} - 2\alpha \frac{g\mu_B}{2} \sigma B \end{aligned} \quad (2.4.228)$$

Hence,

$$\delta n = \frac{1}{\pi} (\delta_\uparrow - \delta_\downarrow) = -\frac{4\alpha B}{\pi} \frac{g\mu_B}{2} \quad (2.4.229)$$

The susceptibility is

$$\chi = \frac{\partial m}{\partial B} = \frac{\partial}{\partial B} \mu \delta n = \frac{4\alpha}{\pi} \left(\frac{g\mu_B}{2} \right)^2 \quad (2.4.230)$$

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

$$\mu = -\frac{g}{2} \mu_B \quad (2.4.231)$$

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

$$\delta n = n_\uparrow(0) - n_\downarrow(0) = n_\uparrow(\epsilon_F - \frac{g}{2} \mu_B B) - n_\downarrow(\epsilon_F + \frac{g}{2} \mu_B B) = -\frac{1}{2} \mathcal{N}(0) g B \mu_B \quad (2.4.232)$$

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

$$m = \delta n \times \mu = \mathcal{N}(0) \left(\frac{g}{2} \mu_B \right)^2 B \quad (2.4.233)$$

The magnetic susceptibility comes out to be

$$\chi^0 = \left. \frac{\partial m}{\partial B} \right|_{B \rightarrow 0} = \mathcal{N}(0) \left(\frac{g}{2} \mu_B \right)^2 \quad (2.4.234)$$

The Wilson ratio R can now be computed,

$$R = \frac{\chi/\chi_0}{C_v/C_v^0} = \frac{4\alpha/\pi \mathcal{N}(0)}{2\alpha/\pi \mathcal{N}(0)} = 2 \quad (2.4.235)$$

2.5 Numerical renormalization group calculation

Wilson's idea [19] was to remove the limitations of the perturbative nature of Anderson's scaling method. To that end, we transformed the Hamiltonian into a one-dimensional chain, and then iteratively diagonalised chains of increasing length. The Hamiltonian we are working with is

$$H = \sum_k \epsilon_k n_k + J \vec{S}_d \cdot \vec{\sigma}_e \quad (2.5.1)$$

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

$$|1\rangle = (\lambda_1 H_c |0\rangle + \lambda_2 |0\rangle) \quad (2.5.2)$$

This is a general form for any ket in the subspace spanned by $|0\rangle$ and $H_c |0\rangle$. Since we want the state to be normalised, we can shift one of the parameters to the denominator:

$$|1\rangle = \frac{1}{\gamma_0} (H_c |0\rangle + \lambda |0\rangle) \quad (2.5.3)$$

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

$$\lambda = -\langle 0|H_c|0\rangle \quad (2.5.4)$$

Therefore,

$$|1\rangle = \frac{1}{\gamma_0} (H_c |0\rangle - \langle 0|H_c|0\rangle |0\rangle) \quad (2.5.5)$$

The general state can be shown to be

$$|n+1\rangle = \frac{1}{\gamma_n} (H_c |n\rangle - |n\rangle \langle n|H_c|n-1\rangle - |n-1\rangle \langle n-1|H_c|n\rangle) \quad (2.5.6)$$

From eq. 2.5.6, by multiplying $\langle n'|$ from left, we get

$$\delta_{n',n+1} = \frac{1}{\gamma_n} \left[(H_c)_{n',n} + (H_c)_{n,n-1} \delta_{n',n} + (H_c)_{n-1,n} \delta_{n',n-1} \right] \quad (2.5.7)$$

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

$$(H_c)_{n',n} = 0 \quad (2.5.8)$$

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

$$(H_c)_{n+1,n} = \gamma_n \quad (2.5.9)$$

Taking the complex conjugate of this gives

$$\gamma_n^* = \left(H_c^\dagger\right)_{n,n+1} = (H_c)_{n,n+1} \quad (2.5.10)$$

Defining

$$(H_c)_{n,n} = \epsilon_n \quad (2.5.11)$$

we can write

$$\begin{aligned} H_c &= \sum_{n_1, n_2} |n_1\rangle \langle n_1| H_c |n_2\rangle \langle n_2| \\ &= \sum_n \epsilon_n |n\rangle \langle n| + \sum_n \left(\gamma_n |n\rangle \langle n+1| + \gamma_n^* |n+1\rangle \langle n| \right) \\ &= \sum_n \epsilon_n \hat{n}_n + \sum_n \left(\gamma_n c_n^\dagger c_{n+1} + \gamma_n^* c_{n+1}^\dagger c_n \right) \end{aligned} \quad (2.5.12)$$

The diagonalization of these chains become impossible for $n > 8$. To remedy this problem, Wilson, after diagonalization a chain of a particular length, retained only the lowest parts of the spectrum, and the Hamiltonian for the next stage was formed out of these low-lying states. This keeps the size of the Hilber space (and hence the matrices) manageable. Another problem is that as one goes on adding sites to the chain, the couplings need to die off, otherwise this process will never converge.

Logarithmic discretization

First, note that up to first order

$$\epsilon_k = \epsilon_F + (k - k_F) \frac{\partial \epsilon_k}{\partial k} \quad (2.5.13)$$

By choosing $k_F = \epsilon_F = 0$, we get $\epsilon_k = k$.

Wilson divided the conduction band into patches, $[\Lambda^{-(n+1)}, \Lambda^{-n}]$, for $n = 1, 2, 3...$ The width of each interval is

$$d_n = \Lambda^{-n} (1 - \Lambda^{-1}) \quad (2.5.14)$$

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

$$\psi_{m,n}(k) = \frac{1}{\sqrt{d_n}} \exp\left(\frac{2\pi i m}{d_n} k\right) \quad (2.5.15)$$

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

$$a_{m,n}^\dagger = \sum_k \psi_m(k) c_k^\dagger \quad (2.5.16)$$

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

$$\phi_{m,n}(k) = \frac{1}{\sqrt{d_n}} \exp\left(-\frac{2\pi i m}{d_n} k\right) \quad (2.5.17)$$

$$b_{m,n}^\dagger = \sum_k \phi_m(k) c_k^\dagger \quad (2.5.18)$$

Then,

$$a_{m,n}^\dagger + b_{m,n}^\dagger = \frac{2}{\sqrt{d_n}} \sum_{\pm k \in []} \cos\left(\frac{2\pi m k}{d_n}\right) c_k^\dagger \quad (2.5.19)$$

Summing over n involves summing over all momenta.

$$\begin{aligned} \sum_n (a_{m,n}^\dagger + b_{m,n}^\dagger) &= \frac{2}{\sqrt{d_n}} \sum_k \cos\left(\frac{2\pi m k}{d_n}\right) c_k^\dagger \\ \Rightarrow \sum_n (a_{0,n}^\dagger + b_{0,n}^\dagger) &= \frac{2}{\sqrt{d_n}} \sum_k c_k^\dagger \end{aligned} \quad (2.5.20)$$

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

$$\sum_{k,q} c_k^\dagger c_q = \sum_k c_k^\dagger \sum_q c_q \quad (2.5.21)$$

Looking at eq. 2.5.20, we see that the impurity spin is coupled only to the $m = 0$ operators. This is where the approximation comes in, in Wilson's scheme. All the m values other than $m = 0$ are ignored.

Wilson chose

$$\epsilon_n = 0, \gamma = D' \Lambda^{-\frac{n}{2}} \quad (2.5.22)$$

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

$$H_N = D' \sum_{n=0}^{N-1} \Lambda^{-\frac{n}{2}} \left(c_n^\dagger c_{n+1} + c_{n+1}^\dagger c_n \right) + 2J \vec{S}_d \cdot \vec{S}_e \quad (2.5.23)$$

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

$$H_{N+1} = H_N + D' \Lambda^{-\frac{N}{2}} \left(c_N^\dagger c_{N+1} + c_{N+1}^\dagger c_N \right) \quad (2.5.24)$$

To compare the couplings, and hence the Hamiltonians, at each value of N , we need to rescale the Hamiltonians H_N so that the lowest energy scale is independent of the running index N . Looking at eq. 2.5.23, the lowest energy scale is $\Gamma_N = D' \Lambda^{-\frac{N-1}{2}}$. Hence, the rescaled Hamiltonian is

$$\bar{H}_N = \frac{H_N}{\Gamma_N} = \frac{\Lambda^{\frac{N-1}{2}}}{D'} H_N \quad (2.5.25)$$

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

$$\begin{aligned} \bar{H}_{N+1} &= \frac{\Lambda^{\frac{N}{2}}}{D'} \left[H_N + \Lambda^{-\frac{N}{2}} D' \left(c_N^\dagger c_{N+1} + c_{N+1}^\dagger c_N \right) \right] \\ \Rightarrow \bar{H}_{N+1} &= \Lambda^{\frac{1}{2}} \bar{H}_N + \left(c_N^\dagger c_{N+1} + c_{N+1}^\dagger c_N \right) \end{aligned} \quad (2.5.26)$$

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

$$H = \lim_{N \rightarrow \infty} H_N = \lim_{N \rightarrow \infty} D' \Lambda^{\frac{1-N}{2}} \bar{H}_N \quad (2.5.27)$$

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

$$\bar{H}_N = \sum_m E_m |m\rangle \langle m| \quad (2.5.28)$$

The next Hamiltonian is then

$$\bar{H}_{N+1} = \Lambda^{\frac{1}{2}} \sum_m E_m |m\rangle \langle m| + \sum_{m,m'} \left(C(m, m') |m\rangle \langle m'| + \text{h.c.} \right) \quad (2.5.29)$$

This is the same equation as eq. 2.5.26, with \bar{H}_N expressed in its eigenbasis and the creation and annihilation operators also expressed in that basis; the $C(m, m')$ are just the matrix elements of c and c^\dagger in that basis.

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

2.6 Correspondence between the Kondo model fixed-point and a local Fermi liquid

Local Fermi liquid

The fixed-point Hamiltonians [20] are found to represent interacting Fermi liquids. The effective Hamiltonian can be shown to resemble the Anderson model, but with modified parameters,

$$H_{\text{eff}} = \sum_k \epsilon_k n_k + \sum_k V_k c_d^\dagger c_k + \text{h.c.} + U n_{d\uparrow} n_{d\downarrow} \quad (2.6.1)$$

The parameters ϵ_k, V_k, U are not the same as the Anderson model we start with, but I am using the same symbols for convenience. The interaction term U is the leading irrelevant operator near the low-energy fixed point. For $T \rightarrow 0$, assuming only single excitations, the interacting term will not get invoked.

Under mean-field,

$$\begin{aligned} n_{d\uparrow} n_{d\downarrow} &\approx n_{d\uparrow} \langle n_{d\downarrow} \rangle + \langle n_{d\uparrow} \rangle n_{d\downarrow} - \langle n_{d\uparrow} \rangle \langle n_{d\downarrow} \rangle \\ \implies \langle n_{d\uparrow} n_{d\downarrow} \rangle &= \langle n_{d\uparrow} \rangle \langle n_{d\downarrow} \rangle \\ &= \sum_{k,q} \langle n_{k\sigma} \rangle \langle n_{q,-\sigma} \rangle \end{aligned} \quad (2.6.2)$$

where N is the number of sites. Note that the number of excitations, $\langle n_q \rangle$ has to be defined differently for the states above and below the Fermi surface. For excited states above ϵ_F , the number of excitations is given usually:

$$\langle n_q^> \rangle = \langle \psi^> | c_k^\dagger c_k | \psi^> \rangle = n_k^p \quad (2.6.3)$$

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

$$\langle n_q^< \rangle = \langle \psi^< | c_k^\dagger c_k | \psi^< \rangle = -\langle \psi^< | c_k c_k^\dagger | \psi^< \rangle = -n_k^h \quad (2.6.4)$$

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

$$\langle \delta n_{k,\sigma} \rangle = \begin{cases} n_k^p, & \epsilon_k > \epsilon_F \\ -n_k^h, & \epsilon_k < \epsilon_F \end{cases} \quad (2.6.5)$$

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

$$\epsilon_{k\sigma} = \epsilon_k + U \sum_q \langle \delta n_{q,-\sigma} \rangle \equiv \epsilon_k + U \langle \delta n_{-\sigma} \rangle \quad (2.6.6)$$

This is analogous to the Landau quasiparticle energy functional, eq. 2.2.19, U acting as the interaction between the quasiparticles. $\delta n > 0$ acts as the excitations from the ground state.

The interacting density of states is

$$\rho_{d\sigma}(\omega) = \frac{\Delta}{\pi} \frac{1}{\left(\omega - \epsilon_d^*\right)^2 + \Delta^2} \quad (2.6.7)$$

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

Calculation of C_v

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

$$\frac{d\langle E \rangle}{dT} = \sum_{k,\sigma} \epsilon_{k\sigma} \frac{d\langle \delta n_{k\sigma} \rangle}{dT} \quad (2.6.8)$$

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

$$\begin{aligned} \langle \delta n_{k\sigma} \rangle(T) &= \frac{1}{e^{\beta \epsilon_{k\sigma}} + 1} \\ \Rightarrow \frac{d\langle \delta n_{k\sigma} \rangle}{dT} &= \frac{e^{\beta \epsilon_{k\sigma}}}{(e^{\beta \epsilon_{k\sigma}} + 1)^2} \left[\frac{1}{k_B T^2} \epsilon_{k\sigma} - \frac{1}{k_B T} (2\epsilon_{k\sigma} - \epsilon_k) \frac{d\langle \delta n_{k\sigma} \rangle}{dT} \right] \end{aligned} \quad (2.6.9)$$

At sufficiently low temperatures, the first term will dominate over the others ($T^{-2} \gg T^{-1}$). Hence the low temperature specific heat can be written as

$$\begin{aligned} \frac{d\langle E \rangle}{dT} &= \sum_{k,\sigma} \epsilon_{k\sigma} \frac{e^{\beta \epsilon_{k\sigma}}}{(e^{\beta \epsilon_{k\sigma}} + 1)^2} \frac{1}{k_B T^2} \epsilon_{k\sigma} \\ &= \frac{1}{k_B T^2} \sum_{k,\sigma} \epsilon_{k\sigma}^2 \frac{e^{\beta \epsilon_{k\sigma}}}{(e^{\beta \epsilon_{k\sigma}} + 1)^2} \\ &= \frac{1}{k_B T^2} \sum_{\sigma} \int d\epsilon_{\sigma} \rho(\epsilon_{\sigma}) \epsilon_{\sigma}^2 \frac{e^{\beta \epsilon_{\sigma}}}{(e^{\beta \epsilon_{\sigma}} + 1)^2} \end{aligned} \quad (2.6.10)$$

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

$$\begin{aligned} \frac{d\langle E \rangle}{dT} &= \frac{1}{k_B T^2} \sum_{\sigma} \rho_{\sigma}(0) \int_{-\infty}^{\infty} d\epsilon_{\sigma} \epsilon_{\sigma}^2 \frac{e^{\beta \epsilon_{\sigma}}}{(e^{\beta \epsilon_{\sigma}} + 1)^2} \\ &= -\frac{1}{T} \sum_{\sigma} \rho_{\sigma}(0) \int_{-\infty}^{\infty} d\epsilon_{\sigma} \epsilon_{\sigma}^2 f'(\epsilon_{\sigma}) \\ &= -\frac{1}{T} \sum_{\sigma} \rho_{\sigma}(0) \int_1^0 df \epsilon_{\sigma}^2 \end{aligned} \quad (2.6.11)$$

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

$$\epsilon = k_B T \ln(f^{-1} - 1) \Rightarrow \epsilon^2 = k_B^2 T^2 \left[\ln(f^{-1} - 1) \right]^2 \quad (2.6.12)$$

Therefore,

$$\frac{d\langle E \rangle}{dT} = -k_B^2 T \sum_{\sigma} \rho_{\sigma}(0) \int_1^0 df \left[\ln(f^{-1} - 1) \right]^2 \quad (2.6.13)$$

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

$$\begin{aligned}\frac{d\langle E \rangle}{dT} &= k_B^2 T \sum_{\sigma} \rho_d(0) \frac{\pi^2}{3} \\ &= 2k_B^2 T \rho_d(0) \frac{\pi^2}{3} \\ &= \gamma_{\text{imp}} T\end{aligned}\tag{2.6.14}$$

where

$$\gamma_{\text{imp}} \equiv \frac{C_v}{T} = \frac{2\pi^2}{3} k_B^2 \rho_d(0)\tag{2.6.15}$$

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

$$\frac{\gamma_{\text{imp}}}{\gamma^{(0)}} = \frac{\rho_d(0)}{\rho_d^{(0)}(0)}\tag{2.6.16}$$

Calculation of χ

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

$$\begin{aligned}m &= \frac{g\mu_B}{2} (\delta n_{\uparrow} - \delta n_{\downarrow}) \\ &= \frac{g\mu_B}{2} \sum_{\sigma} \sigma \delta n_{\sigma} \\ &= \frac{g\mu_B}{2} \sum_{k\sigma} \sigma \frac{\partial n_{\sigma}}{\partial \epsilon_{k\sigma}} \delta \epsilon_{k\sigma} \\ &= \frac{g\mu_B}{2} \sum_{k\sigma} \sigma \rho_{k\sigma} (\sigma h + U \delta n_{-\sigma}) \\ &= \frac{g\mu_B}{2} \sum_{\sigma} \sigma \rho_{\sigma} (\sigma h + U \delta n_{-\sigma})\end{aligned}\tag{2.6.17}$$

On applying the magnetic field, the Fermi energy of spin $-\sigma$ decreases as $\epsilon_F - \sigma h$. Hence, more number of spin $-\sigma$ electrons will get excited, the number of such excitations being

$$\delta n_{-\sigma} = \sum_q \delta n_{q,-\sigma} = \sum_q \Delta \epsilon_F \rho_{q,-\sigma} = \sigma h \rho_{-\sigma}(0)\tag{2.6.18}$$

In the last step, I used the fact that the density of states is non-zero only very close to the Fermi surface. Substituting this in the magnetization gives

$$\begin{aligned}m &= \frac{g\mu_B}{2} h \sum_{\sigma} \sigma^2 \rho_{\sigma}(0) (1 + U \rho_{-\sigma}(0)) \\ &= \left(\frac{g\mu_B}{2} \right)^2 B \sum_{\sigma} \rho_{\sigma}(0) [1 + U \rho_{-\sigma}(0)]\end{aligned}\tag{2.6.19}$$

The susceptibility is

$$\begin{aligned}
 \chi_{\text{imp}} &= \lim_{h \rightarrow 0} \frac{\partial m}{\partial B} \\
 &= \left(\frac{g\mu_B}{2} \right)^2 \rho_d(0) [1 + U\rho_d(0)] \sum_{\sigma} \\
 &= \frac{(g\mu_B)^2}{2} \rho_d(0) [1 + U\rho_d(0)] \\
 &= \chi^{(0)} \frac{\rho_d(0)}{\rho_d^{(0)}(0)} [1 + U\rho_d(0)]
 \end{aligned} \tag{2.6.20}$$

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

The Wilson ratio is

$$R \equiv \frac{\chi_{\text{imp}}}{\chi^{(0)}} \frac{\gamma^{(0)}}{\gamma_{\text{imp}}} = 1 + U\rho_d(0) \tag{2.6.21}$$

Relation between the density of states and scattering phase shift

The Green's function is of the general form

$$G_d(\omega) = \frac{1}{\omega - \epsilon_d - i\Delta - \Sigma(\omega)} \tag{2.6.22}$$

Close to the Fermi surface, the imaginary part of the self energy goes as ω^2 . Therefore, up to first order in ω , the self energy is completely real close to the Fermi surface:

$$\begin{aligned}
 \Sigma(\omega) &= \Sigma(0, 0) + \omega\Sigma'(0) + O(i\omega^2) \\
 &\equiv \Sigma(0) + \left(1 - Z^{-1}\right) \omega
 \end{aligned} \tag{2.6.23}$$

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

$$\begin{aligned}
 G_d(\omega) &= \frac{1}{\omega - \epsilon_d - i\Delta - \Sigma(0) - \left(1 - Z^{-1}\right) \omega} \\
 &= \frac{Z}{Z\omega - Z\epsilon_d - iZ\Delta - Z\Sigma(0) - Z\omega + \omega} \\
 &= \frac{Z}{\omega - Z(\epsilon_d + \Sigma(0)) - iZ\Delta} \\
 &\equiv \frac{Z}{\omega - \epsilon_d^* - i\Delta^*}
 \end{aligned} \tag{2.6.24}$$

The density of states at the Fermi surface is given by

$$\begin{aligned}
 \rho_d(0) &= \frac{1}{\pi} \text{Im } G_d(\omega) \Big|_{\omega=0} \\
 &= \frac{1}{\pi} \frac{Z\Delta^*}{\left(\omega - \epsilon_d^*\right)^2 + \Delta^{*2}} \Big|_{\omega=0} \\
 &= \frac{1}{\pi} \frac{Z\Delta^*}{\epsilon_d^{*2} + \Delta^{*2}}
 \end{aligned} \tag{2.6.25}$$

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

$$\begin{aligned}
 G &= G^{(0)} + G^{(0)}VG_d^{(0)}VG^{(0)} + G^{(0)}VG_d^{(0)}VG^{(0)}VG_d^{(0)}VG^{(0)} + \dots \\
 &= G^{(0)} + G^{(0)}V \left[G_d^{(0)} + G_d^{(0)}VG^{(0)}VG_d^{(0)} \right] VG^{(0)} \\
 &= G^{(0)} + G^{(0)}V^2G_dG^{(0)}
 \end{aligned} \tag{2.6.26}$$

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

$$G = G_0 + G_0TG_0 \tag{2.6.27}$$

we can write

$$T = V^2G_d \tag{2.6.28}$$

where T is the T -matrix for scattering of conduction electrons off the impurity. From the optical theorem, we know that the S -matrix ($S(\omega) \equiv e^{2i\delta(\omega)}$) is related to the T -matrix as

$$\begin{aligned}
 e^{2i\delta(\omega)} &= 1 - 2\pi i \rho T(\omega) \\
 \implies T &= V^2G_d = \frac{1}{2\pi i \rho} \left(1 - e^{2i\delta(\omega)} \right) = \frac{e^{i\delta(\omega)}}{2\pi i \rho} (-2i \sin \delta) \\
 \implies G_d &= -\frac{e^{i\delta(\omega)}}{V^2 \pi \rho} \sin \delta
 \end{aligned} \tag{2.6.29}$$

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

$$G_d = |G_d| e^{i\delta(\omega)} \tag{2.6.30}$$

From the expression for G_d in eq. 2.6.24, we can find the phase of G_d :

$$\begin{aligned}
 \delta(\omega) &= \tan^{-1} \frac{\Delta^*}{\omega - \epsilon_d^*} \\
 \implies \epsilon_d^* &= -\Delta^* \cot \delta(0)
 \end{aligned} \tag{2.6.31}$$

Substituting this in the density of states expression gives

$$\rho_d(0) = \frac{Z \sin^2 \delta(0)}{\pi \Delta^*} \tag{2.6.32}$$