MANY BODY PHYSICS: 621. Spring 2024

Exercise 1 solutions. Kondo Effect.

1. (a) In a non-interacting impurity problem, the asymptotic wavefunction's experience a scattering phase shift, with a radial wavefunction that takes the form

$$\psi(r) \sim \frac{\sin(kr + \delta(E_k))}{r}. \tag{1}$$

If we put the system inside a sphere of radius R, and the boundary condition $\psi(R) = 0$, then $kR + \delta(E_k) = n\pi$ determines the allowed momenta of the quasiparticles, given by $k_n = n\frac{\pi}{R} - \frac{\delta(E_k)}{R}$, separated in momentum by $\Delta k = \frac{\pi}{R}$. The level spacing in the absence of scattering is $\Delta\epsilon = \frac{\partial\epsilon}{\partial k}\Delta k = \frac{\partial\epsilon}{\partial k}\frac{\pi}{R}$. Now in the presence of the scattering phase shift, momenta are reduced by an amount $\Delta k = -\frac{\delta[E_k]}{R}$, so the corresponding energy levels are shifted downwards by an amount

$$E_k \to \epsilon_k - \frac{\partial\epsilon}{\partial k}\frac{\delta(E_k)}{R} = \epsilon_k - \frac{\delta(E_k)}{\pi}\Delta\epsilon. \tag{2}$$

(b) Since there is a one-to-one correspondence between the original states with energy ϵ and the scattered eigenstates with energy E, we can write

$$N(\epsilon)d\epsilon = N^*(E)dE \tag{3}$$

where $N(\epsilon)$ and $N^*(E)$ are the unscattered and scattered density of states, respectively. It thus follows that

$$N^*(E) = N(\epsilon)\frac{d\epsilon}{dE} \tag{4}$$

Now from (2) we have

$$E = \epsilon - \frac{\delta(E)}{\pi}\Delta\epsilon \tag{5}$$

so that

$$\frac{d\epsilon}{dE} = 1 + \frac{\Delta\epsilon}{\pi}\frac{\partial\delta(E)}{\partial E} \tag{6}$$

Combining this with (4) we thus obtain

$$N^*(E) = N(E)\left(1 + \frac{\Delta\epsilon}{\pi}\frac{d\delta(E)}{dE}\right) \tag{7}$$

where we have replaced $N(\epsilon) \to N(E)$, because E and ϵ differ by the infinitesimal $\Delta\epsilon$. But $N(E) = \frac{1}{\Delta\epsilon}$, so that

$$N^*(E) = N(E) + \frac{1}{\pi}\frac{d\delta(E)}{dE} \tag{8}$$

2. (a) Let us write the basis of singlet states as

$$\{|1\rangle, |2\rangle, |3\rangle\} = \left\{\psi^\dagger_\uparrow\psi^\dagger_\downarrow|0\rangle, \frac{1}{\sqrt{2}}\left(\psi^\dagger_\uparrow f^\dagger_\downarrow + f^\dagger_\uparrow\psi^\dagger_\downarrow\right)|0\rangle, f^\dagger_\uparrow f^\dagger_\downarrow|0\rangle\right\}, \tag{9}$$

then the action of the Hamiltonian

$$H = \sum_{\sigma=\uparrow,\downarrow}\left[\epsilon\psi^\dagger_\sigma\psi_\sigma + V[\psi^\dagger_\sigma f_\sigma + \text{H.c}] + E_f n_{f\sigma}\right] + U n_{f\uparrow}n_{f\downarrow}, \tag{10}$$

on these states is

$$H|1\rangle = \left(2\epsilon\psi^\dagger_\uparrow\psi^\dagger_\downarrow + V\sum(f^\dagger_\uparrow\psi^\dagger_\downarrow + \psi^\dagger_\uparrow f^\dagger_\downarrow)\right)|0\rangle = 2\epsilon|1\rangle + \sqrt{2}V|2\rangle \tag{11}$$

similarly ,

$$H|2\rangle = (\epsilon + E_f)|2\rangle + \sqrt{2}V(|1\rangle + |3\rangle), \tag{12}$$

and

$$H|3\rangle = (2E_f + U)|3\rangle + \sqrt{2}V|2\rangle. \tag{13}$$

Note the appearance of U in the last equaation From this we see that $H|i\rangle = |j\rangle H_{ij} = |j\rangle\langle j|H|i\rangle$, where

$$H_{ij} = \begin{pmatrix} 2\epsilon & \sqrt{2}V & 0 \\ \sqrt{2}V & \epsilon + E_f & \sqrt{2}V \\ 0 & \sqrt{2}V & 2E_f + U \end{pmatrix} = \mathcal{H} \tag{14}$$

(b) The determinantal equation for the eigenvalues E of $\mathcal{H}$ is

$$\begin{aligned} \det[E\underline{1} - \mathcal{H}] &= (E - 2\epsilon)\left[(E - (\epsilon + E_f))(E - 2E_f - U) - 2V^2\right] - 2V^2\left[E - 2E_f - U\right] \\ &= (E - 2\epsilon)(E - 2E_f - U)\left[E - \epsilon - E_f - \Sigma(E)\right], \end{aligned} \tag{15}$$

where the "self energy"

$$\Sigma(E) = \frac{2V^2}{E - 2E_f - U} + \frac{2V^2}{E - 2\epsilon}. \tag{16}$$

It follows that the three energy eigenvalues are roots of the equation

$$E = (\epsilon + E_f) + \Sigma(E) \tag{17}$$

(c) The triplet states

$$\begin{cases} \psi^\dagger_\uparrow f^\dagger_\uparrow|0\rangle, \\ \psi^\dagger_\downarrow f^\dagger_\downarrow|0\rangle, \\ (\psi^\dagger_\uparrow f^\dagger_\downarrow + \psi^\dagger_\downarrow f^\dagger_\uparrow)|0\rangle, \end{cases} \tag{18}$$

do not hybridize with each other, and have energies $E_f + \epsilon$.

(d) To obtain the energy eigenstates to leading order in V^2, we can use second-order perturbation theory, to obtain

$$
\begin{aligned}
E_1^* &= 2\epsilon - \frac{2V^2}{E_f - \epsilon} \\
E_2^* &= \epsilon + E_f - \frac{2V^2}{\epsilon - E_f} - \frac{2V^2}{E_f + U - \epsilon} \\
E_3^* &= 2E_f + U - \frac{2V^2}{\epsilon - E_f - U}
\end{aligned}
\tag{19}
$$

(e) When $\epsilon - E_f > 0$ and $E_f + U - \epsilon > 0$, then the lowest energy eigenvalue of the singlet states is $E_2^* \approx \epsilon + E_f$, corresponding to a state with one f-electron: a stable local moment, bound-into a singlet with a conduction electron. The energy of this singlet state is, to leading order in perturbation theory

$$
E_2^* = \epsilon + E_f - \frac{2V^2}{\epsilon - E_f} - \frac{2V^2}{E_f + U - \epsilon} = \epsilon + E_f - 2J \tag{20}
$$

where

$$
J = \frac{V^2}{\epsilon - E_f} + \frac{V^2}{E_f + U - \epsilon} \tag{21}
$$

If we project into the sub-space with 1 f-electron, then the energy of the triplet state is $\epsilon n_c + E_f - 2J$ for the singlet state and $\epsilon n_c + E_f$ otherwise, so that in this case, the effective Hamiltonian is

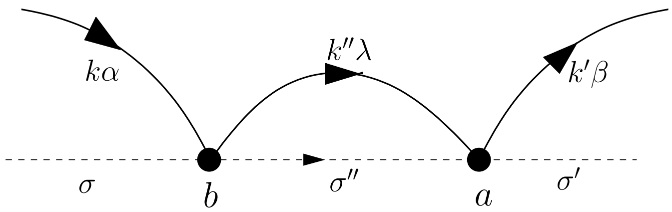
$$
H = \sum_\sigma \epsilon \psi_\sigma^\dagger \psi_\sigma - 2J P_{S=0,n_c=1} \tag{22}
$$

where

$$
P_{S=0,n_c=1} = \frac{1}{4} P_{n_c=1} - \frac{1}{2} (\psi_\alpha^\dagger \vec{\sigma}_{\alpha\beta} \psi_\beta) \cdot \vec{S}_f \tag{23}
$$

where $P_{n_c=1} = n_c - 2n_{c\uparrow} n_{c\downarrow}$ projects into the state with $n_c = 1$, Where $n_{c\sigma} = \psi_\sigma^\dagger \psi_\sigma$, $n_c = n_{c\uparrow} + n_{c\downarrow}$. Notice how this Hamiltonian contains a potential and a Kondo scattering term.

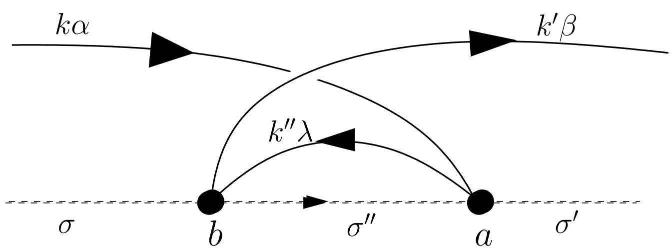
3. (a) The one loop Feynman diagrams for the anisotropic Kondo model are basically the same as for the isotropic case. There are two contributions to the t-matrix. Process I is



for which the T-matrix for scattering into a high energy electron state is

$$\begin{aligned} T^{(I)}(E)_{k'\beta\sigma';k\alpha\sigma} &= \sum_{\epsilon_{k''}\in[D-\delta D,D]} \left[\frac{1}{E-\epsilon_{k''}}\right] J_a J_b (\sigma^a\sigma^b)_{\beta\alpha}(S^a S^b)_{\sigma'\sigma} \\ &\approx J_a J_b \rho \delta D \left[\frac{1}{E-D}\right](\sigma^a\sigma^b)_{\beta\alpha}(S^a S^b)_{\sigma'\sigma} \end{aligned} \tag{24}$$

In process (II),



the formation of a particle-hole pair involves a conduction electron line that crosses itself, leading to a negative sign. Notice how the spin operators of the conduction sea and antiferromagnet reverse their relative order in process II, so that the T-matrix for scattering into a high-energy hole-state is given by

$$\begin{aligned} T^{(II)}(E)_{k'\beta\sigma';k\alpha\sigma} &= -\sum_{\epsilon_{k''}\in[-D,-D+\delta D]} \left[\frac{1}{E-(\epsilon_k+\epsilon_{k'}-\epsilon_{k''})}\right] J_a J_b (\sigma^b\sigma^a)_{\beta\alpha}(S^a S^b)_{\sigma'\sigma} \\ &= -J_a J_b \rho \delta D \left[\frac{1}{E-D}\right](\sigma^b\sigma^a)_{\beta\alpha}(S^a S^b)_{\sigma'\sigma} \end{aligned} \tag{25}$$

where we have assumed that the energies ϵ_k and $\epsilon_{k'}$ are negligible compared with D. Adding (Eq. 24) and (Eq. 25) gives

$$\begin{aligned} \delta H^{int}_{k'\beta\sigma';k\alpha\sigma} &= \hat{T}^I + \hat{T}^{II} = -\frac{J_a J_b \rho |\delta D|}{D}[\sigma^a,\sigma^b]_{\beta\alpha} S^a S^b \\ &= -\frac{1}{2}\frac{J_a J_b \rho |\delta D|}{D} \overbrace{[\sigma^a,\sigma^b]_{\beta\alpha}}^{2i\epsilon^{abc}\sigma^c} \overbrace{[S^a,S^b]}^{i\epsilon^{abd}S^d} \\ &= \frac{\rho|\delta D|}{D} J_a J_b \overbrace{\epsilon^{abc}\epsilon^{abd}}^{|\epsilon_{abc}|\delta_{cd}} \sigma^c_{\beta\alpha} S^d \\ &= \frac{\rho|\delta D|}{D} J_a J_b |\epsilon_{abc}| \sigma^c{}_{\beta\alpha} S^c{}_{\sigma'\sigma}, \end{aligned} \tag{26}$$

where we are using a summation convention throughout. In this way we see that the virtual emission of a high energy electron and hole generates an antiferromagnetic correction to the original Kondo coupling constant

$$J_a(D-|\delta D|) = J_a(D) + 2J_bJ_c\rho\frac{|\delta D|}{D} = J_a(D) - J_bJ_c\rho\frac{\delta D}{D}, \qquad (b \neq c \neq a), \quad (27)$$

since we have reduced the band-width, $\delta D = -|\delta D|$. Note that in removing the summation convention, and the $|\epsilon_{abc}|$, we pick up a factor of two and must now impose the condition $a \neq b \neq c$ In other words,

$$\frac{\partial J_a\rho}{\partial \ln D} = -2J_bJ_c, \qquad (a \neq b \neq c). \quad (28)$$

(b) In the easy-plane/easy axis case where $J_x = J_y = J_\perp$, the three scaling equations in (28) become

$$\begin{aligned} \frac{\partial J_\perp}{\partial \ln D} &= -2J_zJ_\perp\rho + O(J^3), \\ \frac{\partial J_z}{\partial \ln D} &= -2(J_z)^2\rho + O(J^3), \end{aligned} \quad (29)$$

Multiplying the first equation by $J_\perp$ and the second equation by J_z, and subtracting the two we then get

$$\frac{\partial}{\partial D}(J_z^2 - J_\perp^2) = 0, \qquad \Rightarrow J_z^2 - J_\perp^2 = \text{constant}. \quad (30)$$

(c) The scaling flows contain three domains of attraction corresponding to three stable fixed points: (Fig. 1):

- Fully Screened Kondo singlet, with domain of attraction $J_\perp > 0,\ J_z > -|J_\perp|$.
- Unscreened local moment, with domain of attraction $J_z < -|J_\perp|$.
- Entangled Kondo triplet, with domain of attraction $J_\perp < 0,\ J_z > -|J_\perp|$.

(d) In the easy-plane ferromagnetic Kondo model, $J_\perp < 0$. Provided $J_z > -|J_\perp|$, i.e providing the Ising part of the Kondo coupling is not too ferromagnetic, a "triplet Kondo" effect will take place, scaling to strong coupling to produce a S=1, triplet entangled Kondo state.

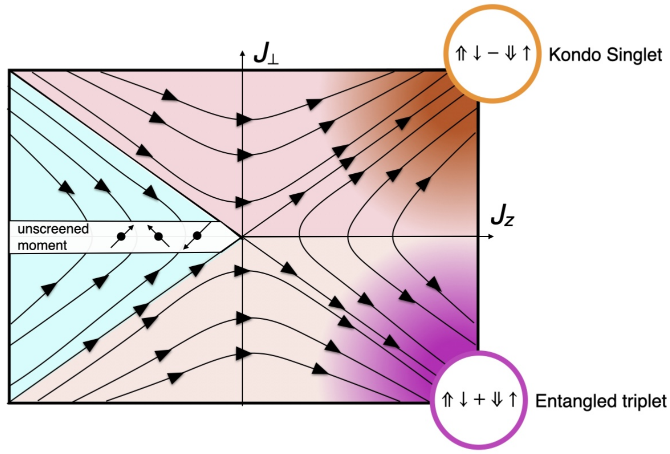


FIG. 1: Scaling flows for the anisotropic Kondo model, showing three stable fixed points: the Kondo singlet, the entangled triplet and unscreened moment fixed points.