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

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

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

\[ k_n = \frac{n\pi - \delta(E_k)}{R}, \]

separated in momentum by \( \Delta k = \frac{\pi}{R} \). The level spacing in the absence of scattering is \( \Delta\epsilon = \frac{\partial\epsilon}{\partial k} \Delta k = \frac{\partial\epsilon \pi}{\partial k R} \). 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

\[ E_k \rightarrow \epsilon_k - \frac{\partial\epsilon \delta(E_k)}{\partial k} = \epsilon_k - \frac{\delta(E_k)}{\pi R} \Delta\epsilon. \]

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

\[ N(\epsilon)d\epsilon = N'(E)dE \]  

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

\[ N'(E) = N(\epsilon) \frac{d\epsilon}{dE} \]

Now from (2) we have

\[ E = \epsilon - \frac{\delta(E) \Delta\epsilon}{\pi} \]

so that

\[ \frac{d\epsilon}{dE} = 1 + \frac{\Delta\epsilon \partial\delta(E)}{\pi \partial E} \]  

Combining this with (4) we thus obtain

\[ N'(E) = N(E) \left(1 + \frac{\Delta\epsilon d\delta(E)}{\pi dE}\right) \]

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

\[ N'(E) = N(E) + \frac{1}{\pi} \frac{d\delta(E)}{dE} \]
2. (a) Let us write the basis of singlet states as
\[ |1\rangle, |2\rangle, |3\rangle = \left\{ |\psi\uparrow\uparrow\rangle, \frac{1}{\sqrt{2}} (|\psi\uparrow\downarrow\rangle + |\psi\downarrow\uparrow\rangle), |\psi\downarrow\downarrow\rangle \right\}, \]
then the action of the Hamiltonian
\[ H = \sum_{\sigma = \uparrow, \downarrow} \left[ \epsilon \psi\uparrow\sigma \psi\downarrow\sigma + V[\psi\uparrow\sigma f\uparrow\sigma + \text{H.c.}] + E_\sigma n_{\sigma f} \right] + U n_{\uparrow f} n_{\downarrow f}, \]
on these states is
\[ H|1\rangle = \left( 2\epsilon |\psi\uparrow\psi\uparrow\rangle + V \sum (f\uparrow\psi\downarrow + \psi\uparrow f\downarrow)|0\rangle \right) = 2\epsilon|1\rangle + \sqrt{2}V|2\rangle \]
similarly,
\[ H|2\rangle = (\epsilon + E_f)|2\rangle + \sqrt{2}V(|1\rangle + |3\rangle), \]
and
\[ H|3\rangle = (2E_f + U)|3\rangle + \sqrt{2}V|2\rangle. \]
Note the appearance of $U$ in the last equation. From this we see that $H|i\rangle = |j\rangle H_{ij} = |j\rangle \langle j|H|i\rangle$, where
\[ H_{ij} = \begin{pmatrix} 2\epsilon & \sqrt{2}V & 0 \\ \sqrt{2}V & \epsilon + E_f & \sqrt{2}V \\ 0 & \sqrt{2}V & 2E_f + U \end{pmatrix} = \mathcal{H} \]
(b) The determinantal equation for the eigenvalues $E$ of $\mathcal{H}$ is
\[ \det[E - \mathcal{H}] = (E - 2\epsilon) \left[ (E - (\epsilon + E_f))(E - 2E_f - U) - 2V^2 \right] - 2V^2 \left[ E - 2E_f - U \right] \]
\[ = (E - 2\epsilon)(E - 2E_f - U) \left[ E - \epsilon - E_f - \Sigma(E) \right], \]
where the “self energy”
\[ \Sigma(E) = \frac{2V^2}{E - 2E_f - U} + \frac{2V^2}{E - 2\epsilon}. \]
It follows that the three energy eigenvalues are roots of the equation
\[ E = (\epsilon + E_f) + \Sigma(E) \]
(c) The triplet states
\[ \left\{ \begin{array}{l} |\psi\uparrow\uparrow\rangle, \\ |\psi\uparrow\downarrow\rangle, \\ (|\psi\uparrow\downarrow\rangle + |\psi\downarrow\uparrow\rangle) \end{array} \right\}, \]
do not hybridize with each other, and have energies $E_f + \epsilon$. 

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

$$
E_1^* = 2\epsilon - \frac{2V^2}{E_f - \epsilon}
$$

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

$$
E_3^* = 2E_f + U - \frac{2V^2}{\epsilon - E_f - U}
$$

(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

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

(20)

where

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

(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

$$
H = \sum_{\sigma} \epsilon \psi_{\sigma}^\dagger \psi_{\sigma} - 2JP_{S=0,n_c=1}
$$

(22)

where

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

(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

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

$$\approx J_a J_b \delta D \left[ \frac{1}{E - D} \right] (\sigma^a \sigma^b)_{\beta\alpha} (S^a S^b)_{\sigma'\sigma}$$  \hspace{1cm} (24)

In process (II),

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

$$= -J_a J_b \delta D \left[ \frac{1}{E - D} \right] (\sigma^b \sigma^a)_{\beta\alpha} (S^a S^b)_{\sigma'\sigma}$$  \hspace{1cm} (25)

where we have assumed that the energies \(\epsilon_k\) and \(\epsilon_{k'}\) are negligible compared with \(D\).

Adding (Eq. 24) and (Eq. 25) gives

$$\delta H_{k'\beta\sigma';k\alpha\sigma}^{(I)} = \hat{T}^{I} + \hat{T}^{II} = -\frac{J_a J_b \delta D}{D} \left[ \frac{1}{2\epsilon_{ab} \epsilon_{cd}} \left[ \sigma^a \sigma^b \right]_{\beta\alpha} (S^a S^b)_{\sigma'\sigma} \right]$$

$$= -\frac{1}{2} \frac{J_a J_b \delta D}{D} \left[ \frac{1}{\epsilon_{ab} \epsilon_{cd}} \right] \left[ \sigma^a \sigma^b \right]_{\beta\alpha} (S^a S^b)_{\sigma'\sigma}$$

$$= \rho \frac{\delta D}{D} J_a J_b \epsilon_{abc} \epsilon_{dab} \sigma^c_{\beta\alpha} S^d$$

$$= \rho \frac{\delta D}{D} J_a J_b \epsilon_{abc} \sigma^c_{\beta\alpha} S^d$$  \hspace{1cm} (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

\[ J_a(D - |\delta D|) = J_a(D) + 2J_bJ_c\rho \frac{\delta D}{D} = J_a(D) - J_bJ_c\rho \frac{\delta D}{D}, \quad (b \neq c \neq a), \quad (27) \]
since we have reduced the band-width, \( \delta D = -|\delta D| \). Note that in removing the sum-
mation 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,

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

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

\[ \frac{\partial J_\perp}{\partial \ln D} = -2J_zJ_\parallel \rho + O(J^3), \]

\[ \frac{\partial J_z}{\partial \ln D} = -2(J_z)^2 \rho + O(J^3), \quad (29) \]

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

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

(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 
etangled 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.