Kondo singlet - variational solution

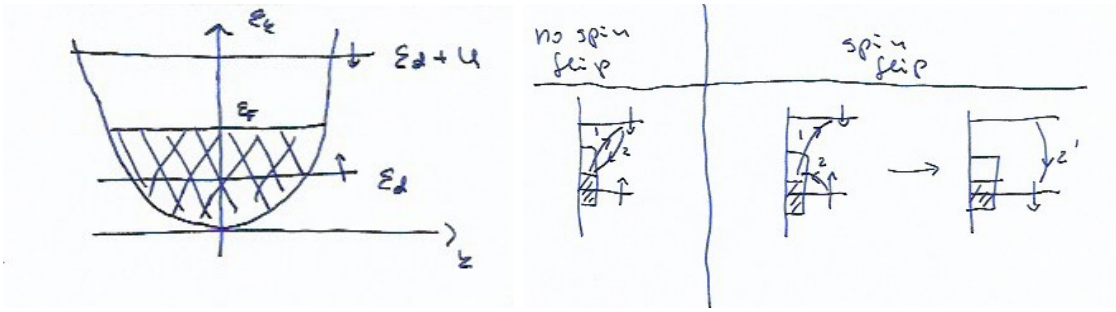
Krzysztof Byczuk, University of Warsaw

11 January 2021

Problem 1. Kondo singlet binding energy - To a system of N non-interacting electrons with a dispersion relation ϵ_k we add one electron on a localized site with an energy ϵ_d. This localized (impurity) state is coupled to the conducting electrons via a hybridization function V_k. The symbol k represents a wave vector in d-dimensional space. When the impurity site is occupied by two electrons with opposite spins the energy of the system increases by $U > 0$. This system is described by the following single impurity Anderson Hamiltonian

$$H = \epsilon_d \sum_\sigma d^\dagger_\sigma d_\sigma + \sum_{k\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_{k\sigma} (V_k c^\dagger_{k\sigma} d_\sigma + V^*_k d^\dagger_\sigma c_{k\sigma}) + U n^d_\uparrow n^d_\downarrow,$$

where $\sigma = \uparrow$ or $\downarrow$ represents a spin projection and $n^d_\sigma = d^\dagger_\sigma d_\sigma$. All operators obey canonical anticommutation relations. When U ($\gg \epsilon_d$, V_k, and ϵ_F - the Fermi energy) is the highest energy in the system a double occupancy of the impurity site is desfavorable. Instead, a second order processes in V_k can lead to a hopping of a conducting electron on ϵ_d site and back, yielding an impurity spin's flips. As a result a singlet bound state between an impurity electron and conducting electrons is formed and, therefore, a local magnetic moment on the impurity site is screened. This is known as the Kondo effect.



In this problem find a binding energy E_b of the Kondo singlet using the variational principle and the following trial state

$$|\Psi\rangle = [\alpha + \sum_{k<k_F,\sigma} \beta_k d^\dagger_\sigma c_{k\sigma}]|FS(N+1)\rangle,$$

where $|FS(N+1)\rangle$ is the non-interacting Fermi sea with $N+1$ electrons with the Fermi wave vector k_F and α and β_k are complex variational parameters. Explicitly:
1. find a normalization condition on α and β_k,
2. determine the energy functional $E[\alpha, \beta_k] = \langle\Psi|H|\Psi\rangle$,
3. minimize the energy functional $F[\alpha, \beta_k\lambda] = E[\alpha, \beta] + \lambda(\langle\Psi|\Psi\rangle - 1)$ with Lagrange method to incorporate the normalization constrain and find an equation on the energy λ,
4. taking a constant density of states at the Fermi level $\rho(\epsilon_F)$, the k-independent and real hybridization function $V_k = V$, and using that the binding energy must be small $|E_b| \ll \epsilon_d$, ϵ_F, U, find an explicit expression for E_b and show that it is negative, thereby the system energy is lowered due to the formation of the Kondo singlet,
5. show that $\sum_{k<k_F,\sigma} \beta_k d^\dagger_\sigma c_{k\sigma}|FS(N+1)\rangle = \sum_{k>k_F} \beta_k (d^\dagger_\uparrow c^\dagger_{k\downarrow} - d^\dagger_\downarrow c^\dagger_{k\uparrow})FS(N-1)\rangle$, therefore the trial state indeed describes a singlet state in a superposition with the $N+1$ particle Fermi sea.

Solution

1. Normalization

Let $|FS(N+1)\rangle$ is a Fermi sea with $N+1$ electrons. If $N+1$ is even then all states with $k \leq k_F$ are occupied by two electrons with opposite spins. If $N+1$ is odd the the last energy state is single occupied with spin up or down in equal probable superposition. Therefore,

$$\langle\Psi|\Psi\rangle = \langle FS(N+1)|[\alpha^* + \sum_{k<k_F,\sigma} \beta_k^* c_{k\sigma}^\dagger d_\sigma][\alpha + \sum_{k<k_F,\sigma} \beta_k d_\sigma^\dagger c_{k\sigma}]|FS(N+1)\rangle =$$

$$= |\alpha|^2 + \sum_{k<k_F,\sigma} \sum_{k'<k_F,\sigma'} \beta_k^* \beta_k' \langle FS(N+1)|c_{k\sigma}^\dagger \underbrace{d_\sigma d_{\sigma'}^\dagger}_{\delta_{\sigma\sigma'} - d_{\sigma'}^\dagger d_\sigma} c_{k'\sigma}|FS(N+1)\rangle =$$

$$= |\alpha|^2 + 2\sum_{k<k_F} |\beta_k|^2 = 1,$$

where $\langle FS(N+1)|c_{k\sigma}^\dagger c_{k'\sigma}|FS(N+1)\rangle = \delta_{kk'}\Theta(k_F - k)$ and $d_{\sigma'}^\dagger d_\sigma|FS(N+1)\rangle = 0$.

2. Energy functional

$$E[\alpha, \beta_k] = \langle\Psi|H|\Psi\rangle = 2\epsilon_d \sum_{k<k_F} |\beta_k|^2 + 2\sum_{k<k_F} \epsilon_k |\alpha|^2 - 2\sum_{k<k_F} \epsilon_k |\beta_k|^2 + 4\sum_{k<k_F} \sum_{k'<k_F} \epsilon_k |\beta_{k'}|^2 +$$

$$+2\sum_{k<k_F} V_k \beta_k \alpha^* + 2\sum_{k<k_F} V_k^* \beta_k^* \alpha.$$

3. Minimization

$$F[\alpha, \beta_k\lambda] = E[\alpha, \beta] + \lambda(|\alpha|^2 + 2\sum_{k<k_F} |\beta_k|^2 - 1).$$

$$\frac{\partial F}{\partial \alpha^*} = 2\sum_{k<k_F} \epsilon_k \alpha + 2\sum_{k<k_F} V_k \beta_k - \lambda\alpha = 0,$$

$$\frac{\partial F}{\partial \beta_k^*} = 2\epsilon_d \beta_k - 2\epsilon_k \beta_k + 4\sum_{k'<k_F} \epsilon_{k'} \beta_k + V_k^* \alpha - 2\lambda\beta_k = 0.$$

Let $\tilde{\lambda} = \lambda - \sum_{k<k_F} \epsilon_k$ is the energy measured with respect to the energy of the free electron gas we get

$$\begin{cases} \tilde{\lambda}\alpha = 2\sum_{k<k_F} V_k \beta_k \\ 2(\tilde{\lambda} - \epsilon_d + \epsilon_k)\beta_k = V_k^* \alpha. \end{cases}$$

From the first equation we find

$$\alpha = \frac{2}{\tilde{\lambda}} \sum_{k<k_F} V_k \beta_k.$$

And eliminating α from the second equation we get

$$\beta_k = \frac{V_k^*}{2(\tilde{\lambda} - \epsilon_d + \epsilon_k)} \frac{2}{\tilde{\lambda}} \sum_{k<k_F} V_k \beta_k.$$

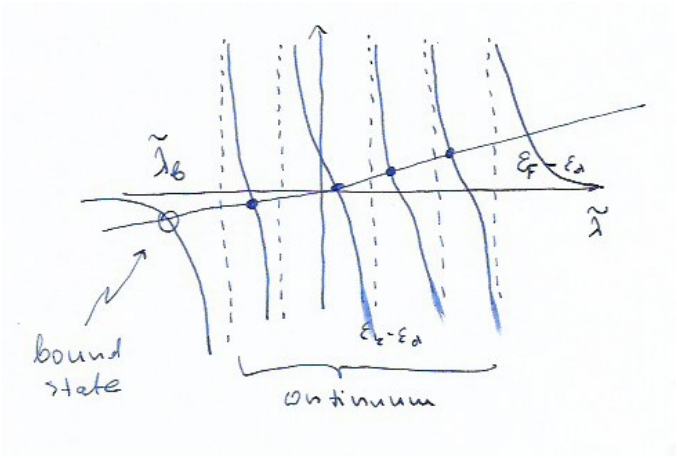
Multiplying both sides by V_k and taking the sum $\sum_{k<k_F}$ we obtain

$$\sum_{k<k_F} V_k \beta_k = \sum_{k'<k_F} \frac{|V_{k'}|^2}{\tilde{\lambda} - \epsilon_d + \epsilon_{k'}} \frac{1}{\tilde{\lambda}} \sum_{k<k_F} V_k \beta_k.$$

Canceling the same terms on both sides we finally find the equation on $\tilde{\lambda}$

$$\tilde{\lambda} = \sum_{k<k_F} \frac{|V_k|^2}{\tilde{\lambda} - \epsilon_d + \epsilon_k}.$$

The graphical solution is presented in the figure



4. Solution for binding energy

Let $V_k = V \in R$ and we get

$$\tilde{\lambda} = \int_0^{\epsilon_F} d\epsilon \rho(\epsilon) \frac{V^2}{\tilde{\lambda} - \epsilon_d + \epsilon} \approx \rho(\epsilon_F) V^2 \int_0^{\epsilon_F} d\epsilon \frac{1}{\tilde{\lambda} - \epsilon_d + \epsilon} = \rho(\epsilon_F) V^2 \ln \left| \frac{\epsilon_F - \epsilon_d + \tilde{\lambda}}{-\epsilon_d + \tilde{\lambda}} \right|.$$

Defining the binding energy E_b vi $E_b = \tilde{\lambda} - \epsilon_d$ we write the last equation in the form

$$E_b + \epsilon_d = \rho(\epsilon_F) V^2 \ln \left| \frac{\epsilon_F - E_b}{E_b} \right|.$$

Next we observe that $E_b < 0$ and $|E_b| \ll \epsilon_d$ together with $|E_b| \ll \epsilon_F$. Therefore we approximate the last equation as

$$\epsilon_d \approx \rho(\epsilon_F) V^2 \ln \left| \frac{\epsilon_F}{E_b} \right|,$$

and find the binding energy in the explicit form

$$E_b = -\epsilon_F e^{-\frac{\epsilon_d}{\rho(\epsilon_F) V^2}} = -\epsilon_F e^{-\frac{1}{\rho(\epsilon_F) J}},$$

where $J = V^2/\epsilon_d$ is the effective exchange coupling.

5. Singlet state

Observe that for $k > k_F^{(N-1)}$

$$c_{k\downarrow}^\dagger |FS(N-1)\rangle = c_{k\downarrow}^\dagger \underbrace{(1 - n_{k\uparrow})}_{=1 - c_{k\uparrow}^\dagger c_{k\uparrow} = c_{k\uparrow} c_{k\uparrow}^\dagger} |FS(N-1)\rangle = c_{k\downarrow}^\dagger c_{k\uparrow} c_{k\uparrow}^\dagger |FS(N-1)\rangle = c_{k\uparrow} |FS(N+1)\rangle$$

with $k < k_F^{(N+1)}$, and similarly for $k > k_F^{(N-1)}$

$$c_{k\uparrow}^\dagger |FS(N-1)\rangle = c_{k\uparrow}^\dagger \underbrace{(1-n_{k\downarrow})}_{=1-c_{k\downarrow}^\dagger c_{k\downarrow}=c_{k\downarrow}c_{k\downarrow}^\dagger} |FS(N-1)\rangle = c_{k\uparrow}^\dagger c_{k\downarrow} c_{k\downarrow}^\dagger |FS(N-1)\rangle = -c_{k\downarrow}|FS(N+1)\rangle$$

with $k < k_F^{(N+1)}$. Therefore,

$$\sum_{k<k_F} \beta_k (d_\uparrow^\dagger c_{k\uparrow} + d_\downarrow^\dagger c_{k\downarrow})|FS(N+1)\rangle = \sum_{k>k_F} \beta_k (d_\uparrow^\dagger c_{k\downarrow}^\dagger - d_\downarrow^\dagger c_{k\uparrow}^\dagger)|FS(N-1)\rangle,$$

and it is indeed a singlet state.