Hubbard - Anderson - Kondo model with two elctrones

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In the Anderson model, an electron can occupy energy levels above the Fermi level or an impurity level below the Fermi level. If two Electrons occupying the impurity level, there is a large energetic coast u_0. Also if the impurity level is empty there is a large energetic coast u_f.
Let us focus on the Hubbard model of two sites (0,ε) with two electrons. In this model the transition amplitude from one site to another is W.If two electrons occupy the same site the system will gain energy u_0.

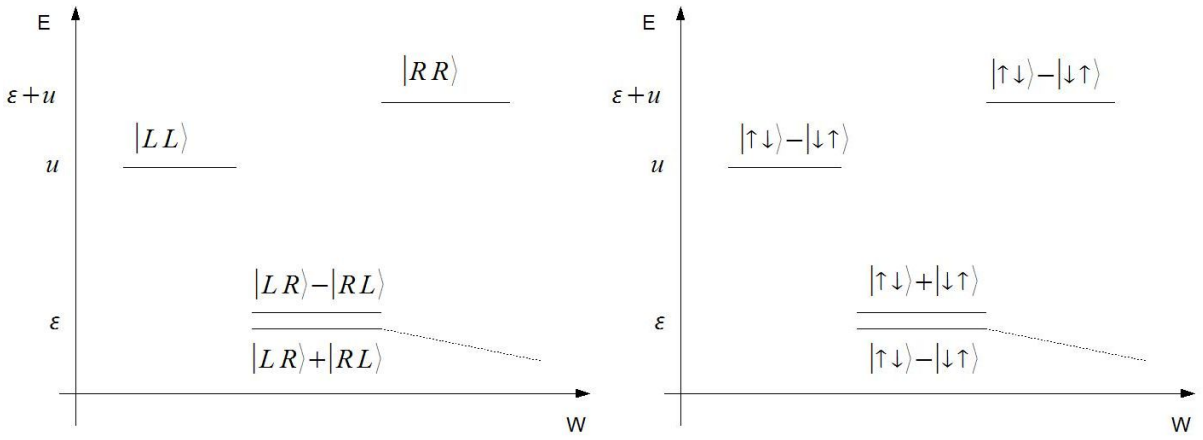
1. Write down the permitted states of the system in first and second quantization language.
2. Write down the Hamiltonian of the system.
3. Use perturbation theory to define the ground state and define by the spinorical part of the wave function for all the states whether they belongs to the triplet or to the singlet.
4. Returning to the Anderson model, Assuming there is a band of energy levels. Find a condition on u_0 and u_f so that the lower energy states will be separated into tow groups. Generally, we can't assume that this condition is valid but the ground state is still singlet. Explain the phenomenon.
5. Find the effective scattering potential (second order) of electron in the band with "P+Q" formalism .
6. Define by the previous part the value of J in Kondo's effective Hamiltonian:
$$\mathcal{H} = \mathcal{H}_0 + JS_{impurity} \cdot S(x=0)$$
7. Write down Kondo's Hamiltonian in second quantization language.

Solution:

1. Let us first define the permitted states in the location presentation and then multiply it with the appropriate spinoric state.
While the location states are $|LL\rangle, |RL\rangle, |LR\rangle, |RR\rangle$ we will transform to the base of symmetric and anti-simetric states getting:
$$triplet \rightarrow \begin{cases} |LL\rangle \\ |LR\rangle + |RL\rangle \\ |RR\rangle \end{cases}$$
$singlet \rightarrow |LR\rangle - |RL\rangle$
Because we are dealing with fermions the wave functions that represent them should be anti-simetric. Using this assumption, the triplet states representing the location of the electron should be multiplied in an anti symmetric spinoric state, $|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$ .On the other hand the singlet state should be multiplied in a symmetric spinoric state, $|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$. Although there are three symmetric states that are satisfying the symmetry term, tow of them are not full filing the demand that two fermions cannot obtain the same location and have the same spin.
$|LL\rangle \otimes (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$
$(|LR\rangle + |RL\rangle) \otimes (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$
$|RR\rangle \otimes (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$
$(|LR\rangle - |RL\rangle) \otimes (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$
By defining the states in second quantization as $|n_{L\uparrow}n_{L\downarrow}n_{R\uparrow}n_{R\downarrow}\rangle$. We get that the states in second quantization are:
$|LL\rangle \otimes (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) = \left(a^\dagger_{L\downarrow}a^\dagger_{L\uparrow} - a^\dagger_{L\uparrow}a^\dagger_{L\downarrow}\right)|\phi\rangle = |1100\rangle$
$(|LR\rangle + |RL\rangle) \otimes (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) = \left(a^\dagger_{R\downarrow}a^\dagger_{L\uparrow} + a^\dagger_{L\downarrow}a^\dagger_{R\uparrow} - a^\dagger_{R\uparrow}a^\dagger_{L\downarrow} - a^\dagger_{L\uparrow}a^\dagger_{R\downarrow}\right)|\phi\rangle = |1001\rangle - |0110\rangle$
$|RR\rangle \otimes (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) = \left(a^\dagger_{R\downarrow}a^\dagger_{R\uparrow} - a^\dagger_{R\uparrow}a^\dagger_{R\downarrow}\right)|\phi\rangle = |0011\rangle$
$(|LR\rangle - |RL\rangle) \otimes (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) = \left(a^\dagger_{R\downarrow}a^\dagger_{L\uparrow} - a^\dagger_{L\downarrow}a^\dagger_{R\uparrow} + a^\dagger_{R\uparrow}a^\dagger_{L\downarrow} - a^\dagger_{L\uparrow}a^\dagger_{R\downarrow}\right)|\phi\rangle = |1001\rangle + |0110\rangle$

2. The Hamiltonian in first quantization, assuming the electrons do not change their spin is :
$$\begin{pmatrix} u_0 & W & W & 0 \\ W & \varepsilon & 0 & W \\ W & 0 & \varepsilon & W \\ 0 & W & W & 2\varepsilon + u_0 \end{pmatrix}$$
After changing base the Hamiltonian is:
$$\begin{pmatrix} u_0 & \sqrt{2}W & 0 & 0 \\ \sqrt{2}W & \varepsilon & 0 & \sqrt{2}W \\ 0 & 0 & \varepsilon & 0 \\ 0 & \sqrt{2}W & 0 & 2\varepsilon + u_0 \end{pmatrix}$$

3. Because the states of the system obtained by multiplying representations of the location and the spin, we can regroup the states of the system by one of the representations used in the product. Regrouping the Eugen states by the spinoric representation leads us to the conclusion that there are **3** states belonging to the *singlet* states and **1** to the triplet.



Diagrams of the energy levels by the multiplied representations

From the Hamiltonian we can see that the triplet state is not coupled. Therefore the energy splitting achieved from the perturbation theory will lead us to one ground state, the singlet.
$E_0 \approx E^{[1]} + \sum_{n=1}^{3} \frac{|W_{0,n}|^2}{E_0 - E_n} = \varepsilon - 2W^2 \left(\frac{1}{u_0 - \varepsilon} + \frac{1}{u_0 + \varepsilon} \right)$

4. Using the energy shift that we got in the previous part, and changing the Hamiltonian so it will describe the Anderson model we get:
$$\mathcal{H} = \begin{pmatrix} u_0 & \sqrt{2}W & 0 & 0 \\ \sqrt{2}W & \varepsilon & 0 & \sqrt{2}W \\ 0 & 0 & \varepsilon & 0 \\ 0 & \sqrt{2}W & 0 & 2\varepsilon + u_f \end{pmatrix}$$
and the ground state energy is:
$E_0 \approx E^{[1]} + \sum_{n=1}^{3} \frac{|W_{0,n}|^2}{E_0 - E_n} = \varepsilon - 2W^2 \left(\frac{1}{u_0 - \varepsilon} + \frac{1}{u_f + \varepsilon} \right)$
from the energy of the ground state we can see that if the energy shift is 0 we can't distinguish between the two states (the triplet and the singlet).Hence our term is:
$\frac{1}{u_0 - \varepsilon} + \frac{1}{u_f + \varepsilon} \neq 0 \Rightarrow u_f \neq -u_0$
Besides that we can see that the triplet state is not coupled,so if the electron is prepared in this state it is stuck there. so it cannot be the ground state because it's not actually part of the system.

5. $\mathcal{H} = \begin{pmatrix} \varepsilon & W & 0 & \cdots & W & W \\ W & \varepsilon & W & \cdots & W & W \\ 0 & W & \varepsilon & \cdots & W & W \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ W & W & W & \cdots & u_0 & 0 \\ W & W & W & \cdots & 0 & 2\varepsilon_f + u_f \end{pmatrix} = \begin{pmatrix} \mathcal{H}^{\mathcal{P}} & 0 \\ 0 & \mathcal{H}^{\mathcal{Q}} \end{pmatrix} + \begin{pmatrix} 0 & V^{\mathcal{PQ}} \\ V^{\mathcal{QP}} & 0 \end{pmatrix}$
   The effective Hamiltonian is:
   $\mathcal{H} = \mathcal{H}_0^{\mathcal{P}} + \Sigma^{\mathcal{P}}$
   So as we can see, if we know the prefactor of $\Sigma^{\mathcal{P}}$ we can find J in Kondo's Hamiltonian.
   Where $\Sigma^{\mathcal{P}} = V^{\mathcal{PQ}} G_0^{\mathcal{Q}} V^{\mathcal{QP}}$ we get:
   $\Sigma^{\mathcal{P}} = \sum_k \langle k'| V^{\mathcal{PQ}} |k\rangle \langle k| G_0 |k\rangle \langle k| V^{\mathcal{QP}} |k'\rangle = \sum_k \frac{\langle k'|W^2|k'\rangle}{E - E_k + i0} = \sum_k \frac{|W|^2}{E - E_k} - i\pi \sum_k |W|^2 \delta(E - E_k)$
   $\Sigma^{\mathcal{P}} = \left(\sum_k \frac{|W|^2}{E - E_k} - i\pi W^2 \nu \right) \begin{pmatrix} 1 & \cdots & 1 \\ \vdots & \ddots & \vdots \\ 1 & \cdots & 1 \end{pmatrix}$
   Let us change the result to the momentum base in order to fit the potential into a scattering problem:
   $\langle k| \Sigma^{\mathcal{P}} |k'\rangle = \langle k| \left(\left(\sum_k \frac{|W|^2}{E - E_k} - i\pi W^2 \nu \right) \sum_x \sum_{x'} |x\rangle \langle x'| \right) |k'\rangle =$
   $\left(\sum_k \frac{|W|^2}{E - E_k} - i\pi W^2 \nu \right) \sum_x \frac{e^{ikx}}{\sqrt{N}} \sum_{x'} \frac{e^{ik'x'}}{\sqrt{N}}$
   $\Rightarrow JS_{impurity} \cdot S(x = 0) = \left(\sum_k \frac{|W|^2}{E - E_k} - i\pi W^2 \nu \right) N \delta_{k,0} \delta_{0,k'}$

6. and therefore:
   $J = \sum_k \frac{|W|^2}{E - E_k} - i\pi W^2 \nu N$

7. $\mathcal{H} = \mathcal{H}_0 + JS_{impurity} \cdot S(x = 0)$
   $\mathcal{H}_0$ represent all the states in the band($E = \varepsilon$) and therefore we can express it as:
   $\mathcal{H}_0 = \sum_{k,l,k',l'} \hat{n}_{kl} \cdot \varepsilon + \hat{a}_{kl}^{\dagger} W \hat{a}_{k'l}$
   Using EX.1002:
   $S_z = \frac{1}{2} \left(\hat{a}_{0,\uparrow}^{\dagger} \hat{a}_{0,\uparrow} - \hat{a}_{0,\downarrow}^{\dagger} \hat{a}_{0,\downarrow} \right)$
   $S_+ = \hat{a}_{0,\uparrow}^{\dagger} \hat{a}_{0,\downarrow}$
   $S_- = \hat{a}_{0,\downarrow}^{\dagger} \hat{a}_{0,\uparrow}$