EX1017: Kondo Scattering

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The problem:

In problem 904, we studied the scattering of a single particle, moving in an energy band gap, on a delta function potential. The result was, that as long as we are far enough from the band gap "edges", we get a clean normal result, but as we approach the edges (in this problem we will concentrate on the lower bound) we discover a singularity.
(1) Assume now that below E_F all states are full. Using the many-particle formalism show how this gets rid of the singularity.
(2) Explain why the singularity reapeares if the scattering potential, also flips the spin of the electron.

The solution:

The first page by D.C. is aimed in clarifying the main point of the calculation.

The scattering is described by

$$V = \sum_{k',k} a_k^\dagger V_{k',k} a_k$$

hence

$$T^{[2]} = \left\langle k_2 \left| V \frac{1}{E-\mathcal{H}} V \right| k_1 \right\rangle \quad = \quad \sum_{k'_b,k_b} \sum_{k'_a,k_a} \left\langle k_2 \left| a_{k'_b}^\dagger V_{k'_b,k_b} a_{k_b} \frac{1}{E-\mathcal{H}} a_{k'_a}^\dagger V_{k'_a,k_a} a_{k_a} \right| k_1 \right\rangle$$

where both the initial and the final states are zero temperature Fermi sea with one additional electron above the Fermi energy. The initial and final states have the same energy:

$$E \quad = \quad E_0 + \epsilon_{k_1} \quad = \quad E_0 + \epsilon_{k_2}$$

where E_0 is the total energy of the zero temperature Fermi sea. The key observation is that all the intermediate states are with definite occupation. therefore we can pull out the resolvent:

$$T^{[2]} = \sum_{k'_b,k_b,k'_a,k_a} \frac{V_{k'_b,k_b} V_{k'_a,k_a}}{E - E_{k_a,k'_a}} \left\langle k_2 \left| a_{k'_b}^\dagger a_{k_b} a_{k'_a}^\dagger a_{k_a} \right| k_1 \right\rangle$$

where

$$E_{k_a,k'_a} \quad = \quad E_0 + \epsilon_{k_1} - \epsilon_{k_a} + \epsilon_{k'_a}$$

As in the calculation of "exchange" we have two non-zero contribution to the sum. Either (k'_b, k_b, k'_a, k_a) equals (k_2, k', k', k_1) with k' above the Fermi energy, or (k', k_1, k_2, k') with k' below the Fermi energy. Accordingly $E - E_{k_a,k'_a}$ equals either $(\epsilon_{k'} - \epsilon_{k_1})$ or $-(\epsilon_{k'} - \epsilon_{k_1})$. Hence we get

$$T^{[2]} = \sum_{k'} \left[\frac{V_{k_2,k'} V_{k',k_1}}{+(\epsilon_{k'} - \epsilon_{k_1})} \left\langle k_2 \left| a_{k_2}^\dagger a_{k'} a_{k'}^\dagger a_{k_1} \right| k_1 \right\rangle + \frac{V_{k',k_1} V_{k_2,k'}}{-(\epsilon_{k'} - \epsilon_{k_1})} \left\langle k_2 \left| a_{k'}^\dagger a_{k_1} a_{k_2}^\dagger a_{k'} \right| k_1 \right\rangle \right] = \sum_{k'} \frac{V_{k_2,k'} V_{k',k_1}}{\epsilon_{k'} - \epsilon_{k_1}}$$

leading to a result which is not divergent at the Fermi energy, as if the Fermi energy does not exist at all:

$$T^{[2]} = \sum_{k'} \frac{V_{k_2,k'} V_{k',k_1}}{\epsilon_{k'} - \epsilon_{k_1}}$$

we have used

$$\left\langle k_2 \left| a^\dagger_{k_2} a_{k'} a^\dagger_{k'} a_{k_1} \right| k_1 \right\rangle = \left\langle k_2 \left| a^\dagger_{k_2} (1 - n_{k'}) a_{k_1} \right| k_1 \right\rangle = +1 \times \left\langle k_2 \left| a^\dagger_{k_2} a_{k_1} \right| k_1 \right\rangle$$

which holds if k' is above the Fermi energy (otherwise it is zero). And

$$\left\langle k_2 \left| a^\dagger_{k'} a_{k_1} a^\dagger_{k_2} a_{k'} \right| k_1 \right\rangle = \left\langle k_2 \left| a_{k_1} (n_{k'}) a^\dagger_{k_2} \right| k_1 \right\rangle = -1 \times \left\langle k_2 \left| a^\dagger_{k_2} a_{k_1} \right| k_1 \right\rangle$$

which holds if k' is below the Fermi energy (otherwise it is zero). Note that irrespective of gauge

$$\left\langle k_2 \left| a^\dagger_{k_2} a_{k_1} \right| k_1 \right\rangle^2 = 1$$

From here on starts the original version:

(1) The first thing that I want to do is to derive the integral of 904 through the second quantization formalism. This is quite trivial, but before I start, I would like to state that since the full solution and formulation was done in 904, in this problem I will concentrate only on the second order of scattering and only on the problematic $1/(E - E')$ of the resolvent. Now to formulate the problem in second quantization formalism, we simply follow the states of the system. First, we annihilate the initial state k_1 in other words we have the annihilation operator a_{k_1}, then through the potential $V_{k'k_1}$ we create a new intermediate state k' or in the language of second quantization, insert the creation operator $a^+_{k'}$ and so on... For the amplitude we also have to include the information of the initial and final states and we get:

$$T^{[1]} = \left\langle k_2 \left| V \frac{1}{E - H} V \right| k_1 \right\rangle$$

Now since we have the identity

$$V = \sum_{k,k'} a^+_k V_{k,k'} a_{k'}$$

We get:

$$T^{[1]} = \sum_{k,k',k'',k'''} \left\langle k_2 \left| a^+_k V_{k,k'} a_{k'} \frac{1}{E - H} a^+_{k''} V_{k'',k'''} a_{k'''} \right| k_1 \right\rangle$$

Now we must simplify this expression by choosing the sets of k, k', k'', k''' that contribute a non-trivial part to the amplitude.
Since:

$$a_k \left| k' \right\rangle = \delta_{k,k'} \left| 0 \right\rangle$$

$$\left\langle k' \right| a^+_k = \left\langle 0 \right| \delta_{k,k'}$$

keeping in mind also the fact that the resolvent is diagonal, we get:

$$T^{[1]} = \sum_{k,k',k'',k'''} \left\langle k_2 \left| a^+_k V_{k,k'} a_{k'} \frac{1}{E - H} a^+_{k''} V_{k'',k'''} a_{k'''} \right| k_1 \right\rangle = \sum_{k,k',k'',k'''} \left\langle 0 \left| \delta_{k,k_2} V_{k,k'} a_{k'} \frac{1}{E - H} a^+_{k''} V_{k'',k'''} \delta_{k''',k_1} \right| 0 \right\rangle =$$

$$= \sum_{k,k',k'',k'''} \delta_{k,k_2} V_{k,k'} \left\langle k' \left| \frac{1}{E-H} \right| k'' \right\rangle V_{k'',k'''} \delta_{k''',k_1} = \sum_{k,k',k'',k'''} V_{k,k'} \frac{1}{E-E'_{k'}} V_{k'',k'''} \delta_{k,k_2} \delta_{k''',k_1} \delta_{k',k''} =$$

$$= \sum_{k'} V_{k_2,k'} \frac{1}{E-E'_{k'}} V_{k',k_1}$$

And this brings us to the same integral that was evaluated in 904.
So the only contribution comes from $k = k_2, k''' = k_1, k' = k''$.
Now the question is what is missing? Simple! the initial state is not "k_1 is full and the rest are empty" but "k_1 is full and all states below the Fermi energy are also full" and the same for the final state. For this reason we will now add the fermi states to all states. This does not change the calculation of the term above, instead adds another term.
Now we have another second order process. I'll remind that the first was: the electron interacts with the potential and shifts to another state and then interacts again and shifts to the final state. The second possible process is: Another electron from the Fermi cluster interacts with the potential and shifts to the band gap and then the original electron interacts with the potential and shifts to fill the Fermi state that the other electron left empty.
Now I will show that the second process is mathematically equivalent to the first, thus simply completing the limit of the integration so that there is effectively no lower boundary and therefore no singularity.
Returning to the equation for the amplitude but the full fermi states we have:

$$T = \sum_{k,k',k'',k'''} \left\langle k_2, \text{Fermi} \left| a^+_k V_{k,k'} a_{k'} \frac{1}{E-H} a^+_{k''} V_{k'',k'''} a_{k'''} \right| k_1, \text{Fermi} \right\rangle$$

Now there are two terms contributing to the amplitude. The first one is the one we have analyzed before. However before we were limited to $k = k_2, k''' = k_1$ because the only states were k_2, k_1, however now we also have the fermi states. So now there are four possibilities: 1. $k = k_2, k''' = k_1$ 2. $k = k_{\text{Fermi}}, k''' = k_1$ 3. $k = k_2, k''' = k_{\text{Fermi}}$ 4. $k = k_{\text{Fermi}}, k''' = k_{\text{Fermi}}$. The first one is the regular amplitude that we calculated before. The second and third processes have zero amplitudes becuase of the diagonality (the right and left state simply cannot be the same) of the resolvent and the last one is our second term and is equal to:

$$T^{[2]} = \sum_{k'} \left\langle k_2, \text{Fermi} \left| a^+_{k'} V_{k',k_1} a_{k_1} \frac{1}{E-H} a^+_{k_2} V_{k_2,k'} a_{k'} \right| k_1, \text{Fermi} \right\rangle$$

Now let us compare the two terms. First the potential matrix elements are the same (in different order, but it doesn't matter) and therefore as far as the comparison goes, they can be left out. Now we turn to the energy term $\frac{1}{E-E''}$. Note that the intermediate energy E'' is not the same as E'. Since the state k' (which has the energy E') is annihilated and instead creates a state with the energy E and therefore $E'' = E + E - E'$ and $E - E'' = -(E - E')$, therefore the second term now has a sign difference. So we are left with the task of comparing the two following expressions:
(1)

$$\left\langle k_2, \text{Fermi} \left| a^+_{k_2} a_{k'} a^+_{k'} a_{k_1} \right| k_1, \text{Fermi} \right\rangle$$

(2)

$$- \left\langle k_2, \text{Fermi} \left| a^+_{k'} a_{k_1} a^+_{k_2} a_{k'} \right| k_2, \text{Fermi} \right\rangle$$

I will remind the anticommutation relations for the creation and annihilation operators:

$$(a_i, a_j) = (a^+_i, a^+_j) = 0$$

$$(a^+_i, a_j) = \delta_{ij}$$

Using the above, we can bring the second expression closer to the first, by placing the creation of k_2 to the end and the annihilation of k_1 to the beginning. This requires 3 permutations of order and therefore creates an additional minus sign. So now the second term looks like:

$$\left\langle k_2, \text{Fermi} \left| a^+_{k_2} a^+_{k'} a_{k'} a_{k_1} \right| k_1, \text{Fermi} \right\rangle$$

To the untrained eye, the only difference now between (1) and (2) is the order of the creation and annihilation of k' (and that is bad because we don't want any difference) but there is another important difference that hides in the initial and final states. Notice that in the first process, the state k' is unoccupied, both in the beginning and the end. Whereas in the second process it is the opposite and k' is occupied both in beginning and end. Keeping in mind also the fact that a^+a is the number operator, we have:
(1)

$$\left\langle k_2, \text{Fermi} \left| a^+_{k_2} (1 - N_{k'}) a_{k_1} \right| k_1, \text{Fermi} \right\rangle = \left\langle \text{Fermi} \left| (1 - N_{k'}) \right| \text{Fermi} \right\rangle = 1 - 0 = 1$$

(2)

$$\left\langle k_2, \text{Fermi} \left| a^+_{k_2} N_{k'} a_{k_1} \right| k_1, \text{Fermi} \right\rangle = \left\langle \text{Fermi} \left| N_{k'} \right| \text{Fermi} \right\rangle = 1$$

This concludes the proof, the two expressions are the same and therefore the singularity is removed.
(2) In the second case of spin flip, we need to include the spin explicitly rather than just through the anticommutation relations of the creation and annihilation operators. Therefore we must specify in the initial and final states the spin of the electron and the impurity (the scattering potential). Therefore when studying the scattering amplitude, we must study a specific amplitude. For example:

$$\langle k_2, \text{Fermi} \uparrow\Downarrow |T| \, k_1, \text{Fermi} \uparrow\Downarrow \rangle$$

Where the arrow represents the spin of the electron and the double arrow represents the spin of the impurity. Obviously the impurity can only flip the spin of the electron if their spin is opposite.
Now, the first process does contribute to the amplitude above, because in the first interaction the spin of the electron is flipped to down and the second interaction flips it up. However, what about the second process? Now, the second process has two options, since every state in the Fermi cluster is occupied by both up and down spin electrons, the impurity can excite any one of them to the band gap. If the excited electron has a spin up, then the impurity flips it to down and then the original electron gets affected, but the second electron is still down and therefore does not contribute to the above amplitude. If the excited electron has a spin down, then the impurity (which also has a spin down) does not flip the spin so that the electron remains with the spin down and again, does not contribute to the above amplitude. So the second process does not contribute to the amplitude and the singularity remains.