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Advanced Theoretical Condensed Matter Physics — SS11

Exercise 6

(Please return your solutions by Tues. 21.06.2011)

We have heard about the phenomenological basis of Anderson's Poor Man's Scaling approach to the Kondo problem in the lecture. In essence, the purpose of this approach is to integrate out degrees of freedom far away from the Fermi level, thereby reducing the bandwidth D, and hence reducing the logarithmic divergence proportional to kT/D which appears when one treats the Kondo model perturbatively. As the bandwidth is reduced, one would expect also a change in the values of the coupling constants $J_\pm$ and J_z of the Kondo Hamiltonian.

In the first part on this sheet we will recreate Anderson's arguments that led to his scaling equations for the different coupling constants $J_\pm$ and J_z in an anisotropic Kondo model. In the second part of the sheet we will solve the scaling equations and obtain the flow diagram for the model we are using. All these concepts (scaling equations, flow diagrams, renormalized coupling constants) are important in the theory of the renormalization group, which is in itself one of the most important concepts in condensed matter physics.

6.1. Anderson's Scaling Argument: Poor Man's Scaling Approach to the Kondo Model

We start from the *Kondo Hamiltonian*, written explicitly as

$$\mathcal{H} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}\sigma} \hat{c}^\dagger_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\mathbf{k}'} \Big[J_+ \hat{S}^+ \hat{c}^\dagger_{\mathbf{k}\downarrow} \hat{c}_{\mathbf{k}'\uparrow} + J_- \hat{S}^- \hat{c}^\dagger_{\mathbf{k}\uparrow} \hat{c}_{\mathbf{k}'\downarrow} + J_z \hat{S}^z (\hat{c}^\dagger_{\mathbf{k}\uparrow} \hat{c}_{\mathbf{k}'\uparrow} - \hat{c}^\dagger_{\mathbf{k}\downarrow} \hat{c}_{\mathbf{k}'\downarrow}) \Big] \tag{1}$$

where $J_\pm$ and J_z are simply coupling constants, while $\hat{S}^{\pm,z}$ are the transversal spin rising / lowering and longitudinal operators, respectively.

We start with the *T-matrix*:

$$\begin{aligned} \mathcal{T}(\varepsilon) &= \mathcal{V} + \mathcal{V} \frac{1}{\varepsilon - \mathcal{H}_0} \mathcal{V} + \ldots \\ &= \mathcal{V} + \mathcal{V} \frac{1}{\varepsilon - \mathcal{H}_0} \mathcal{T}(\varepsilon) \end{aligned}$$

where $\mathcal{V}$ is the "perturbation", and $\frac{1}{\epsilon - \mathcal{H}_0}$ is essentially the free propagator. These quantities will become clearer once a diagram has been drawn, see below. But first we state the question we want to ask, namely: can we invent a different perturbation $\tilde{\mathcal{V}}$ and a different "unperturbed" Hamiltonian $\tilde{\mathcal{H}}_0$ such that we have again the same T-matrix

$$\mathcal{T}(\epsilon) = \tilde{\mathcal{V}} + \tilde{\mathcal{V}} \frac{1}{\varepsilon - \tilde{\mathcal{H}}_0} \tilde{\mathcal{T}}(\varepsilon)$$

but with a reduced bandwidth, $-\tilde{D} < \varepsilon < \tilde{D}$, see the schematic in Fig. 1 of this procedure.

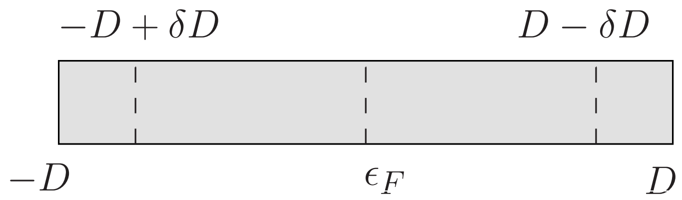

Figure 1: Integration of the higher-energy states

a) Define a projector P onto states with one or more excitations with energies $D > |\varepsilon| > \tilde{D} \equiv D - \delta D$. We would like to calculate the projected T-matrix

$$\tilde{\mathcal{T}}(\varepsilon) = (1-P)\mathcal{T}(\varepsilon)(1-P)$$

Using the fact that $(1-P)+P=1$, $(1-P)^2=(1-P)$, $[\mathcal{H}_0, P]=0$ and discarding a term which is small if $\mathcal{V}$ is small, show that

$$\mathcal{V} = (1-P)\mathcal{V}(1-P) + (1-P)\mathcal{V}P\frac{1}{\varepsilon - \mathcal{H}_0}\mathcal{V}(1-P) \tag{2}$$

$$\mathcal{H}_0 = (1-P)\mathcal{H}_0(1-P) \tag{3}$$

The second term in (2) is the change of the "perturbation" due to the reduction in the bandwidth. It is possible to look at the behaviour of this term under the action of the projector P and deduce the rescaling of the various parameters. We start by writing $P = P_1 + P_2$, where P_1 projects onto states which have at least one hole with energy $-D < \varepsilon < -D + \delta D$, and P_2 projects onto states which have at least one electron with energy $D - \delta D < \varepsilon < D$. Thus we will look at terms which look like, for example

$$\delta V_{1,2} = (1-P)\mathcal{V}P_{1,2}\frac{1}{\varepsilon - \mathcal{H}_0}P_{1,2}\mathcal{V}(1-P) \tag{4}$$

where the index i on δV_i would signify whether the process involves the projection only onto electron states, or involve hole states. Diagrams for the former process is shown in Fig. 2 while the latter in Fig. 3. In both diagrams the curved lines denote the incoming and outgoing electron (or hole) lines, respectively, while the horizontal line denote the spin state of the localized spin. Arrows denote spin states.

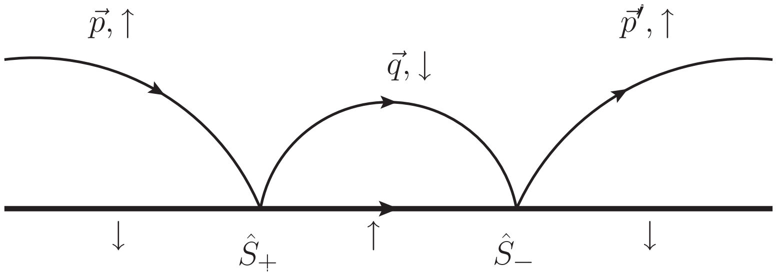

Figure 2: Diagram without spin flip with an electronic intermediate state

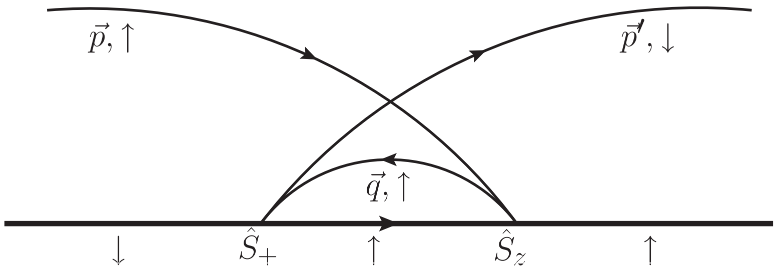

Figure 3: Diagram with spin flip with a hole intermediate state

b) You might have noticed that in Fig. 2 there is no spin flipping between the incoming and outgoing electrons, while in Fig. 3 there is flipping involved. Taking conservation of spin flips into account, draw all possible *distinct* diagrams that involve both electron and hole states, and also spin flipping / no flipping.
Hint: It is generally a good idea to categorize the diagrams in the following manner:

Spin Flip	Particle	Hole
No Spin Flip	Particle	Hole

From the diagrams sketched in (b), we can now see what happens when a particular term is evaluated. First note that a term such as

$$P_2\mathcal{V}(1-P) = \frac{1}{N}\sum_{\mathbf{qp}}\left(J_+\hat{S}^+\hat{c}^\dagger_{\mathbf{q}\downarrow}\hat{c}_{\mathbf{p}\uparrow} + J_-\hat{S}^-\hat{c}^\dagger_{\mathbf{q}\uparrow}\hat{c}_{\mathbf{p}\downarrow} + J_z\hat{S}^z(\hat{c}^\dagger_{\mathbf{q}\uparrow}\hat{c}_{\mathbf{p}\uparrow} - \hat{c}_{\mathbf{q}\downarrow}\hat{c}_{\mathbf{p}\downarrow})\right) \tag{5}$$

signifies a summation over wavevectors $\mathbf{p}$ such that $|\varepsilon_{\mathbf{p}}| < D - \delta D$ and the sum over $\mathbf{q}$ is such that $D - \delta D < \varepsilon_{\mathbf{q}} < D$. This means that the expression in (4) would be the multiplication of the propagator by (5) from the right, and the complex conjugate of (5) from the left. Usually this would entail the multiplication of all possible terms, but since we have drawn the relevant diagrams in (b), we need to only work with the diagrams and not look at the actual terms in (4). For example, the diagram in Fig. 2 would correspond to the expression

$$\frac{1}{N^2}\sum_{\mathbf{q'p'}}\sum_{\mathbf{qp}}\left(J_-J_+\hat{S}^-\hat{c}^\dagger_{\mathbf{p'}\uparrow}\hat{c}_{\mathbf{q'}\downarrow}\frac{1}{\varepsilon-\mathcal{H}_0}\hat{c}^\dagger_{\mathbf{q}\downarrow}\hat{c}_{\mathbf{p}\uparrow}\hat{S}^+\right) \tag{6}$$

c) **Intermezzo:** Show that the following holds: given the noninteracting part of our Kondo Hamiltonian $\mathcal{H}_0$, for any operator $\hat{A}$ such that $[\mathcal{H}_0, \hat{A}] = b\hat{A}$, where b is a c-number, then

$$\frac{1}{\varepsilon-\mathcal{H}_0}\hat{A} = \hat{A}\frac{1}{\varepsilon - b - \mathcal{H}_0} \tag{7}$$

d) Using (7), we can now work with expressions of the type (6). In (6), commute $\hat{c}^\dagger_{\mathbf{q}\downarrow}\hat{c}_{\mathbf{p}\uparrow}\hat{S}^+$ across the propagator (note that the spin rising / lowering operators do not commute with one another!). We now go to extensive approximations (these approximations were also performed in the original Anderson paper !).

 – First of all, since we have restricted the summation over $\mathbf{q}$ in (6) to the energy interval $D - \delta D < \varepsilon_{\mathbf{q}} < D$, we can approximate $\varepsilon_{\mathbf{q}} \approx D$.

- Also due to this reason, we can write $\hat{c}_{\mathbf{q}'\downarrow}\hat{c}^{\dagger}_{\mathbf{q}\downarrow} \approx \delta_{\mathbf{q}\mathbf{q}'}$. The summation over $\mathbf{q}'$ can now be done, and we are only left with a summation over $\mathbf{q}$.
- Since at this point, the summand is $\mathbf{q}$-independent, the summation over $\mathbf{q}$ simply gives us $N\nu(0)\delta D$.
- Finally, we can set $\mathcal{H}_0$ to zero in the denominator.

You should obtain finally, for the term (6)

$$\frac{\nu(0)\delta D}{N} J_- J_+ \hat{S}^- \hat{S}^+ \sum_{\mathbf{p}\mathbf{p}'} \hat{c}^{\dagger}_{\mathbf{p}'\uparrow}\hat{c}_{\mathbf{p}\uparrow} \frac{1}{\varepsilon - D + \varepsilon_{\mathbf{p}}} \tag{8}$$

Explain the reasoning behind the approximations done above, using Fig. 1 and the fact that we set our ground state energy to 0; otherwise let your tutor explain it in the exercise class and only use these approximations for the calculations here :-)

d) Do the same for all the diagrams in (b) using the same reasoning as in (c). The idea is now to sum up all the diagrams and simplify them. This can be done using the identities

$$\begin{aligned}
\hat{S}^+\hat{S}^- &= \frac{1}{2} + \hat{S}^z \\
\hat{S}^-\hat{S}^+ &= \frac{1}{2} - \hat{S}^z \\
\hat{S}^z\hat{S}^+ &= \frac{1}{2}\hat{S}^+ \\
\hat{S}^+\hat{S}^z &= -\frac{1}{2}\hat{S}^+
\end{aligned}$$

which are valid for $S = \frac{1}{2}$. Show that, at the end you get several terms, which are: *Hint: We note that we would like to ultimately compare the renormalized Hamiltonian to the original, which has the form* (1). *This means that it would be a good idea to get the arrangements of the creation / annihilation operators as close to the form in the Hamiltonian as possible.*

- a change in the ground state energy

$$\delta E_G = -\frac{\nu(0)\delta D}{N}\left(\frac{1}{2}J_z^2 + J_+ J_-\right)\sum_{\mathbf{p}} \frac{1}{D - \varepsilon + \varepsilon_{\mathbf{p}}}$$

  which can be absorbed in a redefinition of ε and is therefore unimportant.
- A term of order $\mathcal{O}(\delta D/D^2)$ which is small and can be discarded.
- Finally, the renormalized coupling constants J_z and $J_\pm$ have the form

$$J_z \to J_z + \nu(0)\delta D J_+ J_- \left(\frac{1}{D - \varepsilon - \varepsilon_{\mathbf{p}}} + \frac{1}{D - \varepsilon + \varepsilon_{\mathbf{p}'}}\right) \tag{9}$$

$$J_\pm \to J_\pm + \nu(0)\delta D J_z J_\pm \left(\frac{1}{D - \varepsilon - \varepsilon_{\mathbf{p}}} + \frac{1}{D - \varepsilon + \varepsilon_{\mathbf{p}'}}\right) \tag{10}$$

e) Discarding the energy dependence in the denominators in (9) and (10) to derive the scaling equations

$$\frac{\partial J_z}{\partial D} = -2\nu(0)\frac{J_\pm J_\mp}{D} \tag{11}$$

$$\frac{\partial J_\pm}{\partial D} = -2\nu(0)\frac{J_\pm J_z}{D} \tag{12}$$

Why are there extra minus signs?

Hint : For reference the following expressions, after inserting the spin operator identities, are what one expects.

$$\begin{aligned}\delta V_{\uparrow\uparrow} =& \frac{\nu(0)\delta D}{N} J_+ J_- \hat{S}^z \sum_{\mathbf{p}\mathbf{p}'} \hat{c}^\dagger_{\mathbf{p}'\uparrow}\hat{c}_{\mathbf{p}\uparrow}\left(\sum_{\mathbf{p}} \frac{1}{D-\varepsilon-\varepsilon_{\mathbf{p}}} + \frac{1}{D-\varepsilon+\varepsilon_{\mathbf{p}'}}\right) - \\ &- \frac{\nu(0)\delta D}{N}\left(\frac{1}{4}J_z^2 + \frac{1}{2}J_+J_-\right)\sum_{\mathbf{p}\mathbf{p}'} \hat{c}^\dagger_{\mathbf{p}'\uparrow}\hat{c}_{\mathbf{p}\uparrow}\frac{\varepsilon_{\mathbf{p}}+\varepsilon_{\mathbf{p}'}}{(D-\varepsilon-\varepsilon_{\mathbf{p}})((D-\varepsilon+\varepsilon_{\mathbf{p}'})} - \\ &- \frac{\nu(0)\delta D}{N}\left(\frac{1}{4}J_z^2 + \frac{1}{2}J_+J_- + J_-J_+\hat{S}^z\right)\sum_{\mathbf{p}'}\frac{1}{D-\varepsilon+\varepsilon_{\mathbf{p}'}}\end{aligned}$$

$$\delta V_{\uparrow\downarrow} = \frac{\nu(0)\delta D}{N} J_z J_- \hat{S}^- \sum_{\mathbf{p}\mathbf{p}'} \hat{c}^\dagger_{\mathbf{p}'\uparrow}\hat{c}_{\mathbf{p}\downarrow}\left(\frac{1}{D-\varepsilon-\varepsilon_{\mathbf{p}}} + \frac{1}{D-\varepsilon+\varepsilon_{\mathbf{p}'}}\right)$$

where $\delta V_{\uparrow\uparrow}$ is the total expression for no spin flipping, and $\delta V_{\uparrow\downarrow}$ is the total contribution from diagrams which flips the spin from up to down.

6.2. Solution of the Scaling Equations and the Flow Diagram

In this exercise we will solve the scaling equations in (9) and (10) and sketch the flow diagram associated with them.

a) Set the magnitudes of J_+ and J_- the same such that you can write $J_\pm J_\mp = J_\pm^2$. Solve (9) and (10) to obtain the additional condition

$$J_z^2 - J_\pm^2 = C \tag{13}$$

where C is a constant value which can take on values $C \lesseqgtr 0$.

b) To simplify the solution of the differential equation, rewrite (9) and (10) as differentials over the logarithms instead, i.e., $\frac{\partial J_z}{\partial \ln D}$ and $\frac{\partial J_\pm}{\partial \ln D}$. Decouple the rewritten scaling equations using (13) to obtain a differential equation for J_z (or $J_\pm$, depending on how you decoupled your equations). Refer to the lecture for an example of this procedure, in which the same procedure was done for the isotropic Kondo Hamiltonian.

c) Solve the differential equation in b), and sketch the scaling equation.