

# Scaling the Kondo problem: clever approach to a strongly correlated system

Igor Milat, University of Zagreb, Bijenicka c. 32

**Abstract.** This lecture presents a short introduction to Kondo effect, a strange low temperature behavior of some alloys containing rare-earth or transition element impurities. Starting from the Anderson model Hamiltonian it is first shown how the rare-earth type impurities can act as spin-flip scattering centers for the conduction electrons. Then, using the technique known as “poor man’s scaling” it is demonstrated how spin-flip scattering leads to divergent scaled coupling of conduction electrons to scattering centers. This divergence in coupling hints at the reasons for the anomalous behavior of rare-earth compounds at low-temperatures.

## 1. Introduction

It was observed in the early 1930’s that there exists a whole class of dilute alloys which show a resistance minimum at low temperatures of about 10K. This was considered strange since in most alloys resistance decreases rapidly with decreasing temperature and eventually saturates to a finite value as  $T \rightarrow 0$ . It was found that the position of the minimum depends linearly on the impurity concentration and that its occurrence is always accompanied by the existence of Curie type term in the magnetic susceptibility.

The first plausible theoretical explanation for the resistance minimum phenomenon was put forth by *Kondo* in 1964. He showed that the scattering of conduction electrons by magnetic impurities leads to logarithmic divergence of resistivity as  $T \rightarrow 0$  in higher orders of perturbational calculation. This logarithmic divergence is referred to as Kondo effect and it stirred up a lot of theoretical interest.

After this short introduction, in the second part I present a short derivation of Kondo model Hamiltonian starting from the well known Anderson model and show how a localized magnetic moment can survive in a metallic environment. In the third part I demonstrate a technique called “poor man’s scaling” to treat the Kondo model Hamiltonian. In the last part I summarize the results obtained and give a qualitative description of what is believed to be the correct picture of Kondo effect.

## 2. Theoretical models

### 2.1. Anderson model

The standard way to describe impurities in a metallic host is the Anderson model [1]. Electrons of the host metal form a conduction band. Let  $c_{\mathbf{k}\sigma}^\dagger$  be the creation operator

‡ The rapid decrease  $\propto T^5$  is due to decreasing number of thermal phonons and the finite value at zero temperature is due to impurity scattering

for a conduction electron with wave vector  $\mathbf{k}$  and spin  $\sigma$ . Additionally localized electron states are induced by the impurity atom. They usually have  $d$  or  $f$  like character. Let  $f_\sigma^\dagger$  be the creation operator for the electron in the localized impurity state with spin  $\sigma$ . The Anderson model Hamiltonian (AMH) is then

$$H_{AM} = \sum_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma} + \sum_{\sigma} \epsilon_f n_{f,\sigma} + \sum_{k\sigma} \left( V f_\sigma^\dagger c_{k\sigma} + V^* c_{k\sigma}^\dagger f_\sigma \right) + U n_{f,\uparrow} n_{f,\downarrow}. \quad (1)$$

Where  $n_{f,\sigma} = f_\sigma^\dagger f_\sigma$  is the localized electron number operator.

The first two terms in Hamiltonian (1) describe the electron band and localized electrons, respectively. The third term is the so called hybridization term. It accounts for the fact that there exists a residual interaction that mixes conduction and localized states §. The electrons can thus jump from the conduction band onto the impurity and from the impurity into the conduction band. The last term, the so called correlation term, represents the strong interaction between the electrons when they are localized on the impurity atom. The correlation term makes AMH very difficult to solve exactly. Formally, Anderson model depicts a single impurity system, but the results obtained can be also applied to dilute impurity systems where the interaction between the impurities or the coherent electron scattering by two or more impurities can be neglected.

## 2.2. Kondo model

Consider now a situation such that  $|\epsilon_f|, |\epsilon_f + U| \gg k_B T$ , so that the states in which there are two or no electrons at the impurity site are high in energy compared to the thermal excitations at temperature  $T$ . One can now try to write the effective Hamiltonian acting only on the thermally relevant states by calculating the effect of the virtual higher energy excitations by a simple perturbation treatment.

Let us divide the state space into subspaces  $\varepsilon_0, \varepsilon_1, \varepsilon_2$  be the subspaces in which there are 0, 1 or 2 electrons localized on the impurity and let  $\psi_0, \psi_1$  and  $\psi_2$  be the projections of the wave function on the respective subspaces. The Hamiltonian (1) can now be written in matrix form as

$$\begin{bmatrix} H_{00} & H_{01} & H_{02} \\ H_{10} & H_{11} & H_{12} \\ H_{20} & H_{21} & H_{22} \end{bmatrix} \begin{bmatrix} \psi_0 \\ \psi_1 \\ \psi_2 \end{bmatrix} = E \begin{bmatrix} \psi_0 \\ \psi_1 \\ \psi_2 \end{bmatrix}. \quad (2)$$

Where  $H_{ij}$  denotes the part of the Hamiltonian acting between subspaces  $\varepsilon_i$  and  $\varepsilon_j$ . Thus, for example

$$H_{10} = \sum_{k\sigma} V_{k\sigma} f_\sigma^\dagger c_{k\sigma} \quad H_{22} = \sum_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma} + 2\epsilon_d + U. \quad (3)$$

Formally one can now solve the matrix equation (2) to obtain the effective Hamiltonian in the  $\varepsilon_1$  subspace,

$$H_{eff} = H_{11} + H_{12} \frac{1}{E - H_{22}} H_{21} + H_{10} \frac{1}{E - H_{00}} H_{01}. \quad (4)$$

In the limit where both  $\epsilon_f$  and  $2\epsilon_f + U$  are much larger then  $E$  one can, consistently to the second order in  $V$ , replace the resolvent operators in equation (4) by

$$\frac{1}{E - H_{22}} \simeq \frac{1}{-\epsilon_d - U} \quad \frac{1}{E - H_{00}} \simeq \frac{1}{\epsilon_d}. \quad (5)$$

§ Although the hybridization matrix element  $V$  in general depends both on  $\mathbf{k}$  and  $\sigma$  it is customary to neglect this dependence and use the isotropic hybridization with absolute value equal to its average over the Fermi surface

Physically, this means that we have included effects of virtual fluctuations of impurity valence only in lowest order. Two such processes are possible. In the first an electron jumps from conduction band to the impurity and then and then one of the two electrons on the impurity jumps back and in the second, an electron first jumps of the impurity and then the impurity state is filled by an electron from a conduction band. Resolvents in equations (5) describe the propagation of the doubly occupied and unoccupied impurity.

Effective Hamiltonian which acts only in the  $\varepsilon_1$  subspace now becomes

$$H_K = \sum_{\mathbf{k}\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + J \sum_{\mathbf{k}\mathbf{k}'} \left[ S_+ c_{\mathbf{k}\downarrow}^\dagger c_{\mathbf{k}'\uparrow} + S_- c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}'\downarrow} + S_z (c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}'\uparrow} - c_{\mathbf{k}\downarrow}^\dagger c_{\mathbf{k}'\downarrow}) \right], \quad (6)$$

where we have used the restriction  $\sum_\sigma n_{f,\sigma} = 1$  and the following operator identities

$$f_\uparrow^\dagger f_\downarrow = S_+, \quad f_\downarrow^\dagger f_\uparrow = S_-, \quad \frac{1}{2} (n_{f,\uparrow} - n_{f,\downarrow}) = S_z \quad (7)$$

where  $S_+$ ,  $S_-$  and  $S_z$  are standard spin operators.

Equation (6) is the famous Kondo model Hamiltonian (KMH). Jumping of electrons to and from the impurity, which occurs in AMH, has been replaced by the spin flip interaction. The system behaves as if it consisted of conduction electrons and a *localized spin* which interact through a form of exchange. Exchange interaction constants are linked to the parameters of the Anderson model by

$$J = |V|^2 \left[ \frac{1}{U + \epsilon_f} - \frac{1}{\epsilon_f} \right] \quad (8)$$

If the interaction is weak, one can neglect it at high temperatures. Thus at high temperatures impurity behaves as a free spin and contributes the experimentally observed Curie type term to susceptibility.

### 3. Poor man's scaling

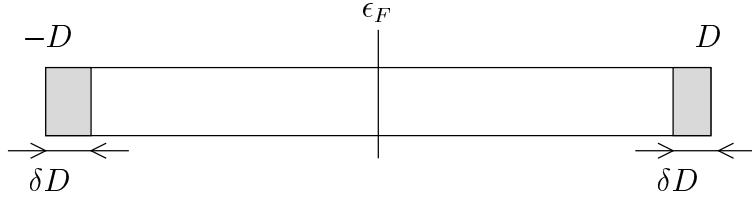
It was shown by Kondo [2] that the Hamiltonian 6 leads to a logarithmically divergent scattering cross-section for the conduction electrons in the  $T \rightarrow 0$  limit. He considered the problem of the impurity of spin  $S$  in the rectangular conduction band|| with density of states  $\rho$  and of half-width  $D$ . Using the third order Born expansion he obtained the following impurity contribution to the resistance

$$R_{imp} \propto J^2 S(S+1) \left( 1 - 4\rho J \ln \left( \frac{T}{D} \right) \right), \quad (9)$$

where half width  $D$  is conveniently measured in  $K$ . The problem with this result is that not only diverges in the low temperature limit but also in the infinite band limit ( $D \rightarrow \infty$ ). I will now use the scaling approach known as ‘‘Poor man’s scaling’’, originally due to Anderson [3] to hint at the origins of this ‘‘unphysical’’ behavior of the perturbational result.

The  $\ln D$  dependence of the scattering cross-section points to the fact that there exists no single energy scale in the problem and that all the excitations are important and have to be taken into account. The essence of the scaling approach is to exploit the idea of preceding section and in a way sum up the influence of the high energy excitations on the low energy ones in a form of an effective interaction.

|| In the rectangular conduction band electrons can have energy in the range  $-D < \epsilon < D$ . The energy of the conduction electron is independent of its momentum.



**Figure 1.** Division of the conduction band. Shaded states are “band edges”.

Let us to this end try to remove from the consideration the states which have at least one electron or hole in the “edges” of the band of very small width  $|\delta D|$  as shown on figure 1. The state space is divided in three subspaces. The subspace  $\varepsilon_1$  contains states with no excitations into band edges, and  $\varepsilon_0$  and  $\varepsilon_2$  states with at least one hole in the lower or one electron in the upper edge, respectively.

Hamiltonian can be again written in the matrix form formally the same as the equation 2.  $H_{ij}$  now denote parts of the KMH (6) acting between subspaces defined in the previous paragraph. Thus, for example,  $H_{21}$  scatters a conduction electron into a state with wave-vector  $\mathbf{q}$  in the unoccupied upper band edge

$$H_{21} = J \sum_{\mathbf{q}, \mathbf{k}} \left[ S^+ c_{\mathbf{q}, \downarrow}^\dagger c_{\mathbf{k}, \uparrow} + S^- c_{\mathbf{q}, \uparrow}^\dagger c_{\mathbf{k}, \downarrow} + S_z (c_{\mathbf{q}, \uparrow}^\dagger c_{\mathbf{k}, \uparrow} - c_{\mathbf{q}, \downarrow}^\dagger c_{\mathbf{k}, \downarrow}) \right]. \quad (10)$$

The Hamiltonian  $H_{01}$  is similar with  $\mathbf{k}$  and  $\mathbf{q}$  reversed and  $\mathbf{q}$  is then a state in the lower band edge.

Again, effective Hamiltonian in the  $\varepsilon_1$  subspace can be written in the form of equation (4). To second order in  $J$ , operator  $H_{12}(E - H_{22})^{-1}H_{21}$  describes a process in which an electron is first scattered into the upper band edge, then the state with an electron in band edge propagates and finally the electron is scattered from the band edge. Operator  $H_{10}(E - H_{00})^{-1}H_{01}$  represents, to same order in  $J$ , a process in which an electron is first scattered from the bottom band edge, then a state with a single hole in the lower band edge propagates until the hole finally filled by an electron from an occupied state not in the band edge. In either scattering electron can flip its spin, at the same time flipping the spin of the impurity in such a way that the total spin of the system remains conserved.

If we are interested only in the energies for which  $E \sim T \ll D$  we can safely neglect the  $E$  dependence of propagators and approximate

$$\frac{1}{E - H_{22}} \simeq \frac{1}{E - H_{00}} \simeq \frac{1}{D}. \quad (11)$$

When this is taken into account the contribution from the described virtual processes can be summarized in the effective interaction of the form

$$\delta H_I = -2\rho\delta D \frac{J^2}{D} \sum_{\mathbf{k}, \mathbf{k}'} \left[ S^+ c_{\mathbf{k}, \downarrow}^\dagger c_{\mathbf{k}', \uparrow} + S^- c_{\mathbf{k}, \uparrow}^\dagger c_{\mathbf{k}', \downarrow} + S_z (c_{\mathbf{k}, \uparrow}^\dagger c_{\mathbf{k}', \uparrow} - c_{\mathbf{k}, \downarrow}^\dagger c_{\mathbf{k}', \downarrow}) \right]. \quad (12)$$

The effective interaction has the same form as the initial interaction and it can be absorbed in the renormalization of coupling constant. Thus if we reduce the band width from  $D$  to  $D - |\delta D|$  and at the same time change the coupling constant to  $J + \delta J$  where

$$\delta J = -2\rho\delta D \frac{J^2}{D}, \quad (13)$$

the excitation energies of this new problem will be the same (to order  $J^2$ ) as the energies of the original system.

Since the new problem is formally the same as the initial one, one can apply the same procedure over and over and scale the band down to width  $\tilde{D} \ll D$ . The value of the coupling constant  $\tilde{J}$  is given by the differential equation

$$\frac{d(\rho J)}{d \ln D} = -2(\rho J)^2, \quad (14)$$

which is known as the *scaling equation*. Upon integrating it from  $D$  to  $\tilde{D}$  we obtain

$$D e^{-1/(2\rho J)} = \tilde{D} e^{-1/(2\rho\tilde{J})} \simeq T_K, \quad (15)$$

where  $T_K$  is the scaling invariant of the system and is known as the *Kondo temperature*

In the physically relevant case, that the initial coupling is antiferromagnetic ( $J > 0$ ),  $\tilde{J}$  increases in absolute value as  $\tilde{D}$  is reduced and would diverge¶ in the limit  $\tilde{D} \rightarrow T_K$ .

At temperatures  $T > T_K$  it is possible to reduce the band width all the way down to  $\tilde{D} \sim T$  and do the perturbational calculation for physical observables on this, renormalized, model. Equation (9) can be written in the form

$$R_{imp} \propto S(S+1)\tilde{J}^2 = S(S+1)\frac{1}{\ln^2 T/T_K} \quad (16)$$

where we have used equation (15) to obtain the expression for the scaled coupling  $\tilde{J}$  at  $\tilde{D} = T$ . All the terms proportional to  $\ln T/\tilde{D}$  drop out and the infinite band width divergence is removed. Low temperature divergence still remains, but is now the consequence of the divergent effective coupling  $\tilde{J}$ .

The growth of the effective coupling strength seems to point to the fact that at low temperatures conduction electrons bind with localized spin. Subsequent exact solutions to the single impurity Kondo problem [4] showed that this is the case.

## References

- [1] Hewson A *The Kondo Problem to Heavy Fermions*, Cambridge university press (1993)
- [2] Kondo J 1964 *Progr. Theor. Phys.* **32** 37-49
- [3] Anderson P W 1970 *J. Phys. C* **3** 2437-41
- [4] Wilson K G 1975 *Rev. Mod. Phys.* **47** 773

¶ This divergence is of course unphysical, since the derivation of the scaling equations ceases to be valid as soon as  $|J| \simeq 1$