

# The Kondo Problem

An overview of the history and two approaches to solutions

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## Abstract

This digest is intended to provide an overview of the developments in physics surrounding the Kondo problem. We briefly discuss the history of the Kondo problem. Then we describe some early models of magnetic impurities, after which we briefly discuss Kondo's solution to the resistance minimum and the Kondo problem which arises from this solution. After this, we follow in the footsteps of those who attempted to solve the Kondo problem by various means. First, we review Kenneth Wilson's 1975 approach through the method of the renormalization group. Then the exact solutions are found through the method of the Bethe Ansatz as described by Andrei and Wiegmann in 1980. Finally, we discuss the influence of the Kondo problem on further advances in physics.

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# 1 Introduction

The development of the Kondo problem provides an interesting insight into the interplay between theoretical and experimental condensed matter physics over the course of about fifty years. The seemingly simple theoretical problem has puzzled many theoreticians over the years and has had many attempts from different technical angles fired at it. Finally being solved from a side of physics quite unexpected, it proved to lay the foundation of a new era of theoretical condensed matter physics. The Kondo problem is also a striking example of how different approaches to the same problem can be equally valuable, shedding light on different parts of it, but that there is not one approach that describes all the aspects of the problem.

Anomalous behaviour was first observed by experimentalists at the beginning of the thirties, who were measuring the resistance of metals at low temperatures. Instead of monotonically decreasing with temperature, as one would expect due to the phonon contribution to the resistance decreasing with temperature, a finite resistance minimum was found as  $T \rightarrow 0$ . It was later found that this behaviour was due to magnetic impurities in the non-magnetic bulk metal, which affect the conduction electrons, resulting in a change in resistivity. At first, the way in which magnetic impurities influence resistance minima was entirely obscure [1]. Since this was found to be the cause of the resistance minimum, many models of magnetic impurities have been set up to attempt to describe the experimentally observed quantities theoretically. This proved to be a task more daunting than it first appeared. It was Jun Kondo who, in his 1964 paper on resistance minima in the s-d exchange model (to be described in section 2.3), was able to model the impurities successfully, retrieving the behaviour as observed in experiments [2].

Kondo's findings, however, caused new theoretical problems for our understanding of magnetic impurities. In his perturbational calculations, he retrieved a  $\ln T$  contribution to the resistivity, which solves the initial problem of the observed resistance minimum, but poses new questions as to how to describe the theory as  $T \rightarrow 0$ , since the  $\ln T$  diverges in this region. Thus spawned the search for a theory to describe the low temperature behaviour of systems with resistance minima. This search is called the Kondo problem and attracted the attention of many theoreticians over the course of ten years, finally being concluded by the groundbreaking work by Kenneth Wilson [3].

Wilson's landmark 1975 research article approaches the problem from a completely new angle, not previously attempted in this field of condensed matter physics. He constructed a non-perturbative method, involving renormalization group transformations from field theory and scaling ideas from condensed matter physics. This not only described the Kondo problem correctly in the low energy regime and obtained results for the ground state, but also provided a new powerful tool to be applied to other problems. Though this numerical renormalization method described the behaviour of the model very effectively, it proved difficult to obtain exact results for states other than the ground state, as this required great computing resources, especially at the time.

The exact solutions to the s-d exchange model were discovered by Andrei and Wiegmann in 1981, using the Bethe ansatz [4]. They retrieved analytical results which described the system over the full temperature range. Their work confirmed Wilson's ideas, which positively determined his method as a new tool to be applied to other physical problems.

The course of this digest will follow the chronological outline described above. First we will do a quick and dirty description of various models of magnetic impurities created over the years before Kondo. We will briefly show their shortcomings by calculating the resistance minima, thereby observing predictions which don't match experiment. After this we will have a run through of Kondo's perturbative approach, resulting in the  $\ln T$  problem named after him. The bulk of this digest will be the following in the footsteps of Wilson's renormalization group calculation and Andrei and Wiegmann's Bethe ansatz solution, respectively. Finally, we will comment on the impact the developments in the Kondo problem had on modern theoretical physics.

## 2 Models of magnetic impurities

When we make a first attempt at the problem of magnetic impurities, we formulate a general Hamiltonian from first principles and try to account for the low temperature behaviour. This Hamiltonian has the form,

$$\mathcal{H} = \sum_{i=0}^{N_0} \left( \frac{\mathbf{p}_i^2}{2m} + U(\mathbf{r}_i) + V_{imp}(\mathbf{r}_i) \right) + \frac{1}{2} \sum_{i \neq j}^{N_0} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} + \sum_{i=1}^{N_0} \lambda(\mathbf{r}_i) \mathbf{l}_i \cdot \boldsymbol{\sigma}_i, \quad (1)$$

for  $N_0$  electrons. The Hamiltonian in (1) possesses all kinetic and potential terms that you would expect. Including an electron-electron interaction term but the Coulomb term makes it impossible to do perturbative calculations. To deal with this Coulomb term we need the framework of model Hamiltonians, where you start off with an approximated Hamiltonian, where for example the lattice is used as input for the model. In the case of impurities we assume we're dealing with simple metals with broad conduction bands and, for now, we assume a non-interacting system of electrons. By doing so the Hamiltonian reduces to the form

$$\mathcal{H} = \sum_{\mathbf{k}, \sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}, \sigma}^\dagger c_{\mathbf{k}, \sigma}, \quad (2)$$

where the creation and annihilation operators,  $c^\dagger$  and  $c$  obey standard commutation relations for fermions. Before we can start thermodynamical calculations we need a density of states so that we can construct a partition function. To keep things simple we assume a basic density of states with the form,

$$\rho_0(\epsilon) = \sum_k \delta(\epsilon - \epsilon_k). \quad (3)$$

With these two basic ingredients it is straightforward to calculate the partition function  $Z_0$ ,

$$Z_0 = \text{Tr} e^{-\beta(H - \mu N)} = \prod_k \left( 1 + e^{\beta(\epsilon_k - \mu)} \right)^2. \quad (4)$$

Were the power of 2 is due to spin degeneracy. With this partition function we can perform thermodynamical calculations. To start off, we investigate the specific heat  $C(T)$  by using the Fermi-Dirac distribution function and performing a Sommerfeld expansion. This gives,

$$C(T) = \gamma T \left( 1 - \frac{\pi^2}{30} (k_B T)^2 \left( \left( \frac{\rho'_0}{\rho_0} \right)^2 - \left( \frac{\rho''_0}{\rho_0} \right) \right) \right)_{\epsilon = \epsilon_k} + O(T^5) \quad \text{where} \quad \gamma = \frac{2\pi^2 k_B^2}{3} \rho_0(\epsilon_F). \quad (5)$$

Secondly, for magnetic properties we couple the system to a magnetic field and by doing so the energy becomes spin dependent. This makes it possible to calculate the zero field paramagnetic susceptibility  $\chi(T)$ ,

$$\chi(T) = \chi(0) \left( 1 - \frac{\pi^2}{6} (k_B T)^2 \left( \left( \frac{\rho'_0}{\rho_0} \right)^2 - \left( \frac{\rho''_0}{\rho_0} \right) \right) \right)_{\epsilon = \epsilon} + O(T^4) \quad \text{where} \quad \chi(0) = 2\mu_B^2 \rho_0(\epsilon_F). \quad (6)$$

### 2.1 Potential scattering and Friedel sum rule

In the previous section we introduced a basic Hamiltonian, but that did not describe the physics of impurities in host metals. To improve on this we can introduce a potential term caused by the impurity. Because the impurity has a different electron configuration than the atoms of the host metal the potential term will be a Coulomb term. However the conduction electrons from the host metal will screen the charge of the impurity, so that it will not generate a macroscopic electrical field. By adding this effective potential term  $V_{eff}(\mathbf{r})$  to the Hamiltonian in (1) it changes to the form,

$$\mathcal{H} = \sum_{\mathbf{k}, \sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k}, \sigma}^\dagger c_{\mathbf{k}, \sigma} + \sum_{\mathbf{k}, \mathbf{k}', \sigma} V_{\mathbf{k}, \mathbf{k}'} c_{\mathbf{k}, \sigma}^\dagger c_{\mathbf{k}', \sigma}. \quad (7)$$

The thermodynamical properties of the new system are found by introducing a new basis  $\alpha$ . This basis changes the Hamiltonian to the form,

$$\mathcal{H} = \sum_{\alpha,\sigma} \epsilon_{\alpha} c_{\alpha,\sigma}^{\dagger} c_{\alpha,\sigma}, \quad (8)$$

and is again diagonalizable. The only thing that the introduced potential does is shift the energy levels of the Hamiltonian in (1). The shift in energy levels does not change the calculations performed in the previous section so it only changes  $\rho_0(\epsilon) \rightarrow \rho(\epsilon)$  in equations (5) and (6). The potential term did not account for interesting physical behaviour so far mainly because the impurity has a insignificant impact on the density of states. To see when it does, we need a different representation of the density of states, that is, one that allow perturbative calculations. This is possible with the machinery of Green's functions in the following form,

$$\rho(\epsilon) = \mp \frac{1}{\pi} \text{ImTr} G^{\pm}(\epsilon), \quad (9)$$

where  $G^+$  is the retarded Green's function and  $G^-$  is the Advanced Green's function. Before we can start perturbative calculations on the density equation in (9) we need to introduce a resolvent Green's function that satisfies

$$(\epsilon \pm is - \mathcal{H}) G^{\pm}(\epsilon) = I. \quad (10)$$

. The resolvent Green's function together with the Hamiltonian in the form  $\mathcal{H} = \mathcal{H}_0 + V$  allows us to find an expression for the full Green's function  $G^{\pm}$ ,

$$G^{\pm} = G_0^{\pm} + G_0^{\pm} V G^{\pm}. \quad (11)$$

By iterating this process we find a power series in  $V$  of the form,

$$G^+ = G_0^+ + G_0^+ T(\epsilon^+) G_0^+, \quad (12)$$

where the  $T$  matrix is given by

$$T(\epsilon^+) = V + V G_0^+ V + V G_0^+ V G_0^+ + \dots = V (I - G_0^+ V)^{-1}, \quad (13)$$

and we only regarded the retarded Green's function. The equation for the advanced Green's functions is found by changing  $is \rightarrow -is$  in 10. This machinery can be used to find an expression for the difference in the density of states  $\Delta\rho(\epsilon) = \rho(\epsilon) - \rho_0(\epsilon)$  by using (9)

$$\Delta\rho(\epsilon) = -\frac{1}{\pi} \text{ImTr} (G^+(\epsilon) - G_0^+(\epsilon)). \quad (14)$$

This expression can be rewritten, by using some identities from linear algebra, to a form

$$\Delta\rho(\epsilon) = \frac{1}{\pi} \text{Im} \frac{\partial}{\partial \epsilon} \ln (\det T(\epsilon^+)). \quad (15)$$

So the impurity creates an effective local potential where electrons from the host metal can scatter. The scattering process causes a phase shift in the electron wave functions as a result of a change in energy. If we integrate the difference in the density of states up to the Fermi level we find the expression

$$n_{imp} = \frac{\eta(\epsilon_F)}{\pi} \quad (16)$$

This relationship is called the *Friedel Sum Rule* and relates the valence differences and the phase shift. By introducing an impurity that has more valence electrons than the host material, every states that moves under the Fermi level picks up a phase difference of  $\pi$ .

When the effective potential is sufficiently large it can induce a bound state below the conduction band. Think of it as an attractive potential that localises the electrons of the host material for a period of time in the vicinity of the impurity. This generates a narrow peak in the conduction band and is called *virtual bound state resonance*. It is virtual because far from the impurity the wave function becomes a Bloch state. For a long time they thought virtual bound states explained the effects of impurities in metals.

## 2.2 From the Anderson model to the s-d exchange model

In the previous section we talked about virtual bound state resonance and this is the starting point for this section. Philip Warren Anderson looked at materials where the  $d$ - or  $f$ -levels lie in the conduction band. For these states there is an effective potential term due to angular momentum and localises the higher angular momentum states in such a way that an impurity ion resembles atomic  $d$ - or  $f$ -states. It is possible for electrons to tunnel through this barrier and create a virtual bound state. These states overlap with the Bloch states of the material and generate the following Hamiltonian,

$$\mathcal{H} = \sum_{\sigma} \epsilon_d c_{d,\sigma}^{\dagger} c_{d,\sigma} + \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k},\sigma}^{\dagger} c_{\mathbf{k},\sigma} + U n_{d,\uparrow} n_{d,\downarrow} + \sum_{\mathbf{k},\sigma} \left( V_{\mathbf{k}} c_{d,\sigma}^{\dagger} c_{\mathbf{k},\sigma} + V_{\mathbf{k}}^* c_{\mathbf{k},\sigma}^{\dagger} c_{d,\sigma} \right). \quad (17)$$

For  $U = 0$  the system is solvable, produces virtual bound state resonance and can account for the Friedel sum rule, but does not explain the resistance minimum. So far we considered models with a single impurity. But to have an impurity contribution we need a finite concentration  $c_{imp} = \frac{N_{imp}}{N_s}$  which is small enough so that we can neglect the interactions between the impurities. When this is the case, the leading term in the specific heat and paramagnetic susceptibility are

$$C_{imp} = \frac{2\pi^2}{3} k_b^2 T c_{imp} \Delta \rho(\epsilon_F) \quad \text{and} \quad \chi_{imp} = 2\mu_B^2 c_{imp} \Delta \rho(\epsilon). \quad (18)$$

When we look at the susceptibility we see that the leading term is independent of the temperature and the following term is of the order  $T^2$ . Estimations of the parameters of the one-body formalism are so high that it is unlikely that they produce the explanation for the problem.

## 2.3 The s-d Exchange model

In the limiting case of the Anderson problem where  $U \rightarrow \infty$  we obtain the *s-d exchange model* with the form

$$\mathcal{H}_{sd} = \sum_{\mathbf{k},\mathbf{k}'} J_{\mathbf{k},\mathbf{k}'} \left( S^+ c_{\mathbf{k},\downarrow}^{\dagger} c_{\mathbf{k}',\uparrow} + S^- c_{\mathbf{k},\uparrow}^{\dagger} c_{\mathbf{k}',\downarrow} + S_z \left( c_{\mathbf{k},\uparrow}^{\dagger} c_{\mathbf{k}',\uparrow} - c_{\mathbf{k},\downarrow}^{\dagger} c_{\mathbf{k}',\downarrow} \right) \right). \quad (19)$$

In this model it is assumed that the resistance effect can be explained by an interaction term  $J_{\mathbf{k},\mathbf{k}'}$  that represents an interaction between the local magnetic moment from the impurity and the conduction electrons. By performing perturbative calculation in  $J_{\mathbf{k},\mathbf{k}'}$  up to second order, and assuming that 19 is a perturbation on the full Hamiltonian 19 + 7, will result in the same behaviour as found for potential scattering.

## 3 The resistance minimum

Thus far we only used models that contain a single impurity and also pointed out that it is not likely that these can explain the resistance minimum. To generalize the Hamiltonian in (7) we take

$$\mathcal{H} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c_{\mathbf{k},\sigma}^{\dagger} c_{\mathbf{k},\sigma} + \sum_{\mathbf{K},\mathbf{q},\sigma} \sum_{\mathbf{R}_i} e^{i\mathbf{q}\cdot\mathbf{R}_i} V_{\mathbf{q}} c_{\mathbf{k}+\mathbf{q},\sigma}^{\dagger} c_{\mathbf{k},\sigma}. \quad (20)$$

In theory this model can work but in reality we do not know the impurity distribution. To deal with this problem, we average over random configurations by using *dynamical mean field theory*. This is a local theory and describes time dependent interactions but also generates a 'self-energy' term  $\Sigma(\mathbf{k}, \epsilon^+) = c_{imp} \langle \mathbf{k} | T(\epsilon^+) | \mathbf{k} \rangle$ . The self-energy term can be related to the cross-section by using the optical theorem of scattering theory, and after doing dimensional analysis we get an expression for the mean free path

$$Im\Sigma(\mathbf{k}, \epsilon_{\mathbf{k}}^+) = -\frac{\hbar}{2\tau(\mathbf{k})}. \quad (21)$$

From this expression we could use the Drude theory of electron conduction to find a form for the conductivity,

$$\sigma = \frac{ne^2\tau_{tr}}{m}, \quad (22)$$

where  $n$  is the number of conduction electrons per unit volume. But this form does not generate the correct results. To show this we use the Boltzmann theory to find a distribution function in the presence of a static field  $\mathbf{E}$ . When going through the calculation and restricting ourselves to potential scattering we end up with an expression for the resistivity  $R_{imp}$  due to the impurities of the form

$$R_{imp} = \frac{3\pi c_{imp} m V^2}{2e^2 \hbar \epsilon_F}. \quad (23)$$

But this term is temperature independent. Even if we look at corrections and combine it with phonon scattering it does not explain the resistance minimum.

The calculations in the s-d exchange model are different because you have to consider the degree of freedom in spin explicitly. When doing so, up to second order one ends up essentially with the same results as for potential scattering.

### 3.1 Kondo's solution and problem

In the year 1964 the field of magnetic impurities got an impulse thanks to Japanese physicist Jun Kondo [2]. At the ninth conference on magnetism and magnetic materials he saw the experimental data of [5] on resistivity minimum measurements on dilute alloys of  $Fe$  with different concentrations. He used two findings within this date to deduce a term that accounts for the resistance minimum. Firstly, the minimal temperature is proportional to  $c^{\frac{1}{3}}$ , where  $c$  is the concentration of the impurity atoms. Even at low concentrations the minimal temperature is remarkably high. This would suggest that the local spins are not correlated in the neighbourhood of  $T_{min}$ . Secondly the difference between the absolute resistivity and the resistivity at  $T_{min}$  is proportional to the concentration but  $\rho_{T_{min}}$  is also proportional to the concentration which means that the relative depth of the minimum is independent of the concentration. These two observations suggest that we need a model where the contribution is generated by addition of spin (a paramagnetic effect). Taking all this in consideration, Kondo concluded that the result must be deduced from the s-d exchange model where localised spins are not correlated. Thus far, calculations on the s-d exchange model did not give any interesting results for the problem at hand. But this was because only expansions up to second order in  $J_{\mathbf{k},\mathbf{k}'}$  were done. Kondo performed perturbative calculations up to third term, by not only taking the commutation relations between creation and annihilation operators into account, but also those for spin raising and lowering operators. To do so we need the  $T$  matrix up to second order,

$$\langle \mathbf{k}', \sigma' | T(\epsilon^+) | \mathbf{k}, \sigma \rangle_{(2)} = \langle \mathbf{k}', \sigma' | H_{sd} G_0^+(\epsilon) H_{sd} | \mathbf{k}, \sigma \rangle, \quad (24)$$

which generates a lot of terms, but the most important ones are the ones with spin exchange. One contribution is

$$\frac{J^2}{N_s^2} \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}'_1, \mathbf{k}'_2} \langle \mathbf{k}', \uparrow | S^- c_{\mathbf{k}_1, \uparrow}^\dagger c_{\mathbf{k}'_1, \downarrow} (\epsilon + is - H_0)^{-1} S^+ c_{\mathbf{k}_2, \uparrow}^\dagger c_{\mathbf{k}'_2} | \mathbf{k}, \uparrow \rangle. \quad (25)$$

This term contributes for  $\mathbf{k}_1 = \mathbf{k}'_1$ ,  $\mathbf{k}'_1 = \mathbf{k}_2$ ,  $\mathbf{k}'_2 = \mathbf{k}$ , and gives

$$\frac{J^2}{N_e^2} \sum_{\mathbf{k}_2} S^- S^+ \frac{(1 - f(\epsilon_{\mathbf{k}_2}))}{(\epsilon + is - \epsilon(\mathbf{k}_2))}, \quad (26)$$

where  $f(\epsilon_{\mathbf{k}})$  is the Fermi factor. When we switch the spins in the creation and annihilation operators, perform the same calculation and add the two terms together we get

$$S_z^2 \frac{J^2}{N_e^2} \sum_{\mathbf{k}_2} \frac{1}{(\epsilon + is - \epsilon(\mathbf{k}_2))}. \quad (27)$$

After collecting the first and second order terms together we find

$$\langle \mathbf{k}', \uparrow | T(\epsilon_+) | \mathbf{k}, \uparrow \rangle = s_z \frac{J}{N_s} (1 - 2Jg(\epsilon)) \quad \text{where} \quad g(\epsilon) = \frac{1}{N_s} \sum_{\mathbf{k}} \frac{f(\epsilon_{\mathbf{k}})}{\epsilon_{\mathbf{k}} - \epsilon - is}. \quad (28)$$

In a similar way, terms arise from  $\langle \mathbf{k}', \downarrow | T(\epsilon_+) | \mathbf{k}, \downarrow \rangle$ ,  $\langle \mathbf{k}', \uparrow | T(\epsilon_+) | \mathbf{k}, \downarrow \rangle$  and  $\langle \mathbf{k}', \downarrow | T(\epsilon_+) | \mathbf{k}, \uparrow \rangle$ . After collecting all the terms and using the Boltzmann theory we find the expression

$$\frac{1}{\tau(k)} = \frac{3nc_{imp}J^2S(S+1)}{2e^2\hbar\epsilon_F} (1 - 2J(g(\epsilon_{\mathbf{k}}) + g^*(\epsilon_{\mathbf{k}}))). \quad (29)$$

The only thing that remains is performing the complex integral over  $g(\epsilon)$ . The final result is

$$R_{imp}^{spin} = \frac{3\pi mJ^2S(S+1)}{2e^2\hbar\epsilon_F} \left( 1 - 4J\rho_0(\epsilon_F) \ln\left(\frac{k_B T}{D}\right) \right), \quad (30)$$

and the total resistivity term has the form,

$$R(T) = aT^5 + c_{imp}R_0 - c_{imp}R_1 \ln\left(k_B \frac{T}{D}\right), \quad (31)$$

where the phonon contribution is also considered. By looking at the expression  $T_{min}$  we find the same behaviour that Kondo saw in the data, namely,

$$T_{min} = \left(\frac{R_1}{5a}\right)^{\frac{1}{5}} c_{imp}^{\frac{1}{5}} \quad (32)$$

So far Kondo explained the resistance minimum but a new problem arose. When we look at the last term in the resistivity in (31) there is  $\ln(T)$  contribution. This term is problematic in the limit  $T \rightarrow 0$  because it diverges. Describing the behaviour in low temperature regime is called the *Kondo problem*

## 4 From Kondo to Wilson

As we have seen in the previous section, Kondo's third order perturbation solution to the s-d exchange model in the coupling parameter  $J$  gives rise to a  $\ln T$  term, which successfully describes the resistance minimum. However, we can also evidently see where this solution breaks down, as this term diverges as  $T \rightarrow 0$ . The search for a theory which correctly describes the low temperature regime of the system is known as the Kondo problem. Different approaches involving perturbation methods have been attempted, but all had their respective failures. It became clear that the aim was to find non-perturbative techniques for calculating quantities such as the magnetic susceptibility and the specific heat as  $T \rightarrow 0$  for the s-d exchange model.

The most important of these for our discussion was the development of ideas by Anderson, Yuval and Hamann [6]. They modeled the spin-flips due to the local moment as charged particles, effectively turning the problem into a classical one. This made it possible to incorporate scaling and renormalization ideas involving the conduction electron band width  $D$ . By doing so, Anderson showed that the energy of the conduction band width can be reduced from the order of electron volts down to thermal energy scales. In the ferromagnetic case, the perturbative scaling for  $T = 0$  can be continued down to  $D \rightarrow 0$ , resulting in a renormalised coupling  $J \rightarrow 0$ , and as such the impurity spin is uncoupled. Therefore, the ferromagnetic case is essentially solved. For the physically more interesting antiferromagnetic model, however, the conduction band width can only be reduced to the order of  $k_B T$ , after which the perturbative approach breaks down. Thus the antiferromagnetic case still remains unsolved and there still remains the challenge of continuing the scaling beyond the perturbative regime to create a model that could describe the lowest lying excitations, and hence the thermodynamic behaviour as  $T \rightarrow 0$ .

We realise that the above discussion is very hand-wavy and far from explanatory, but it should only serve as a conceptual bridge from the methods considered in Kondo's time to those proposed by Wilson, to be discussed in the next section. Anderson's incorporation of scaling and renormalization ideas paved the way for Wilson's successful, inventive approach to the Kondo problem.

## 5 The renormalization group approach

Wilson's successful line of attack to the Kondo problem was through the renormalization group approach. It required a conceptual leap which resulted in a powerful tool that could be applied to



other open problems in physics. Indeed, he did win the 1982 Nobel prize in physics for his work to be discussed below. The renormalization group approach was known to work for field theoretical problems and those systems which exhibit critical phenomena for phase transitions. After Wilson, though, it could also be applied to problems of the likes of the Kondo problem.

In this section, first of all, the conceptual foundation underlying the renormalization group approach will be discussed. After this, renormalization group transformations and renormalization group flows will be considered in a general nature. Then we will reformulate the Kondo Hamiltonian in a way fit for these renormalization group transformations, after which we will perform them. The last part of this section shows how Wilson went about calculating thermodynamical quantities for the system of magnetic impurities in the low temperature regime from the results obtained by performing the iterative renormalization group calculations. This section follows in the footsteps of Wilson's 1975 paper [3] and in parts uses the pedagogical approaches of [7] and [8].

## 5.1 The conceptual framework of 'the renormalization group'

As many names for phenomena in modern theoretical physics, the renormalization group, too, is an unfortunate one. As John Cardy explains eloquently in his book [8], all three the words have their respective failures. As is often the case, they are remnants of historical and by now certainly outdated terminology. The doctrine of the 60's had been that our world could be understood in terms of symmetries and their implementations on groups, rather than dynamics. The transformations actually have the mathematical structure of a semi-group, as the transformation cannot be inverted. Perhaps the most interesting misnomer is the definite article 'the'. It suggests the existence of a certain machine into which one can put some problem and the answers come rolling out. This is not the case with these methods, as they rely more on a framework of ideas that is to be adapted to any specific problem at hand. In this subsection, we will try to briefly lay a foundation for the concepts underlying the renormalization group, before we show how transformations are applied and understood in the next.

The area of physics to which renormalization group methods provide paths to solutions is that of problems which don't have a characteristic parameter scale. For instance, in field theory, one considers all available virtual momenta when describing interactions. Or in critical phenomena, all the fluctuations from the scale of atomic spacing up to the correlation length are equally important. When using techniques which don't involve renormalization group methods, it is in such situations that, when one wants to calculate certain physical quantities, one inevitably encounters divergences. The problem is that, though each order of magnitude range of parameters contributes a finite amount, the sum of these is infinite, because we consider an infinite amount of orders.

Basically, what the renormalization group approach aims to do is to divide the full range of parameter scales into smaller ones, which are each manageable in their size, to subsequently consider each subrange in sequence. Each subrange is then influenced by the previous and influences the next. Each one of such steps comes from a renormalization group transformation and at the end of each of the steps, one is left with a new effective Hamiltonian, which describes all the following subranges not yet solved. These steps keep reparameterising the Hamiltonian, though all the while, they still have the same form as the original Hamiltonian and the physics of the full system remains unchanged. Because the current discussion inevitably ends up too qualitative and abstract, we shall now consider these general renormalization group transformations and their behaviour in a general context.

## 5.2 General renormalization group transformations and renormalization group flows

Consider a general, unspecified Hamiltonian  $H$  with a set of interaction parameters  $\mathbf{K} = \{K_1, K_2, \dots\}$ . The renormalization group transformation is a mapping  $T$  from the original Hamiltonian  $H(\mathbf{K})$  to a new, effective, renormalised Hamiltonian  $H'(\mathbf{K}')$  of the same form, specified by a new set of interaction parameters  $\mathbf{K}' = \{K'_1, K'_2, \dots\}$ ,

$$T[H(\mathbf{K})] = H'(\mathbf{K}'). \quad (33)$$

These transformations are generally non-linear. This new Hamiltonian is valid over a reduced scale of the original interaction parameters, having essentially removed some of the old parameter scales. In order to have the resulting Hamiltonian look like the original one, we must rescale the parameters by a coefficient, let's call it  $\zeta$ , which specifies the ratio of the new parameter scale to the old one. In particular, after each transformation, the partition function of the system must remain the same. One can perform the above transformation in sequence, resulting in a new effective Hamiltonian at each step.

Now consider the parameter space of the original set  $\mathbf{K}$ . The Hamiltonian is at some point  $H(\mathbf{K})$ . As we perform subsequent renormalization group transformations, the new effective Hamiltonian will start to move in this parameter space. And once we let  $\zeta$  be a continuous variable, this movement will describe a trajectory. In fact, the purpose of changing the variables by rescaling, was to allow the existence of *fixed points* in the parameter space. A fixed point is a point  $\mathbf{K}^*$  in the parameter space which is invariant under the transformation,

$$T[H(\mathbf{K}^*)] = H(\mathbf{K}^*), \quad (34)$$

which we will henceforth abbreviate by

$$T[\mathbf{K}^*] = \mathbf{K}^*. \quad (35)$$

The trajectories obtained by subsequent renormalization group transformations either move towards or away from these fixed points. The behaviour of the trajectories near the fixed points can be analysed by linearising the renormalization group transformation near the fixed point. We will now consider such a linearisation process.

We assume differentiability of the renormalization group transformation near the fixed point. In the neighbourhood of a fixed point, we can write  $\mathbf{K} = \mathbf{K}^* + \delta\mathbf{K}$ . After performing the renormalization group transformation and expanding in powers of  $\delta\mathbf{K}$ , we have

$$T[\mathbf{K}^* + \delta\mathbf{K}] = \mathbf{K}^* + \mathbf{L}_\zeta^* \delta\mathbf{K} + \mathcal{O}(\delta\mathbf{K}^2), \quad (36)$$

where  $\mathbf{L}_\zeta^*$  is a linear transformation. Now we assume the linear transformation to have a complete basis of eigenvalues and eigenvectors,  $\lambda_n^*(\zeta)$  and  $\mathbf{O}_n^*(\zeta)$ , respectively. We can then use them as a basis for  $\delta\mathbf{K}$ ,

$$\delta\mathbf{K} = \sum_n \delta K_n \mathbf{O}_n^*(\zeta). \quad (37)$$

Now that we have linearised the renormalization group transformation, we can get a feeling for how successive applications of the transformation affect a point near a fixed point in parameter space. Say we act  $l$  times with  $T$ , we then get

$$T^l[\mathbf{K}^* + \delta\mathbf{K}] = \mathbf{K}^* + \sum_n \delta K_n \lambda_n^{*l} \mathbf{O}_n^*(\zeta). \quad (38)$$

As we can see, the direction of the trajectory near a fixed point depends on the value of  $\lambda_n^*$ . If the eigenvalues of the linearised equations are  $\lambda_n^* > 1$ , the terms are called relevant and if there are one or more such terms around a fixed point, we call it an unstable fixed point, as points in parameter space are pushed away from it. For eigenvalues  $\lambda_n^* < 1$ , we see that the components of  $\delta\mathbf{K}$  decrease with  $l$ . These terms are called irrelevant and if a fixed point has only irrelevant eigenvalues, we call it a stable fixed point, as all nearby points in parameter space are drawn toward it. Eigenvalues  $\lambda_n^* = 1$  are called marginal. Fixed points are only called marginal if there are no relevant eigenvalues and at least one marginal one. In this case, we cannot tell from the linearised equations whether the nearby point will move toward the fixed point or away from it, and the behaviour can often be deduced by performing perturbative methods on the problem at hand.

The picture of all these possible trajectories and all the various fixed points together in the parameter space is what is called the renormalization group flow. In particular, regions between unstable and stable fixed points are interesting, as they describe how points in between flow from the one to the other. This is called the cross-over region.

### 5.3 Redefining the Kondo problem

Before we can apply the methods of the renormalization group approach to the Kondo problem, we need to cast the Kondo Hamiltonian in a new form. The Kondo problem describes a spin- $\frac{1}{2}$  impurity coupled to the conduction band of a non-magnetic metal. Contrary to primary intuition, the Kondo problem's difficulties lie more in subtleties involving the conduction band, rather than the magnetic impurity. The effect of the impurity on the conduction band is quite simple. Instead of being able to treat the conduction band electrons as independent entities, they must be considered as a many-electron system. This is due to the fact that the magnetic impurity causes spin-flips, and these spin-flips cause the electrons to no longer be independent from one another. Imagine two spin-up electrons flying towards the spin-down impurity. The first electron to hit the impurity will exchange spin with it, but the second can no longer spin-flip scatter with the impurity since they are now both spin-up. Thus, the impurity is coupled to the entire bath of electrons, and we must modify the Hamiltonian in such a way that this coupled nature can be represented in a manner fit for the iterative renormalization group approach.

The Kondo Hamiltonian, as given by the man himself in 1969 [9], reads, in dimensionless form

$$H_K = \int_{-1}^1 dk a_k^\dagger a_k - JA^+ \boldsymbol{\sigma} A \cdot \boldsymbol{\tau}, \quad (39)$$

where

$$A = \int_{-1}^1 dk a_k, \quad \{a_k, a_{k'}^\dagger\} = \delta(k - k'). \quad (40)$$

The  $a_k$  is the annihilation operator for a conduction band electron with momentum  $k$  relative to the Fermi momentum  $k_F$ , where the spin index is omitted. Integration runs from  $-1$  to  $1$ , because  $k$  is measured in units of the band edge momentum, and the energy is rescaled such that there is no constant factor.  $A$  is an operator that annihilates electrons in the vicinity of the impurity. It has a spin index, and  $\boldsymbol{\sigma}$  is the corresponding Pauli matrix.  $\boldsymbol{\tau}$  are the Pauli matrices for the impurity spin.

It takes three steps to cast the Hamiltonian into an approximate form, such that Wilson's iterative renormalization group approach can be used. The first step is to discretise the operators  $a_k$ , by turning the continuum  $-1 < k < 1$  into a discrete set. The discrete values are  $\pm 1, \pm \Lambda^{-1}, \pm \Lambda^{-2}, \dots$ , where  $\Lambda$  is an arbitrary parameter  $> 1$ . Wilson's calculations were done for  $\Lambda = 2, 2.5$  and  $3$ , and the calculations for these values matched within 3% of experiment. The discretisation is done logarithmically, and the motivation for this is that each order of magnitude range of momentum  $k$  contributes equally to the logarithmic divergence found in Kondo's perturbative solution. This is exactly what is needed for a renormalization group approach to work, since we have equal contribution of all energy scales. This step contains Wilson's fundamental approximation. He generates a complete set of orthogonal electron creation and annihilation operators in each sub-interval by setting up a Fourier transform and subsequently neglects all but the first of these operators. The rejected states are not directly coupled to the impurity and the indirect coupling to the first states becomes small in the continuum limit. For a more thorough explanation of this approximation, the reader is referred to [3].

The Hamiltonian is now

$$H_a = \sum_{n=0}^{\infty} \Lambda^{-n} (a_n^\dagger a_n - b_n^\dagger b_n) - JA^+ \boldsymbol{\sigma} A \cdot \boldsymbol{\tau}, \quad (41)$$

where

$$A = \sum_{n=0}^{\infty} \Lambda^{-\frac{n}{2}} (a_n + b_n). \quad (42)$$

The  $a_n$  and  $b_n$  correspond to momenta  $k = \Lambda^{-n}$  and  $k = -\Lambda^{-n}$ , respectively.

The second step converts this Hamiltonian into a new orthogonal basis,

$$H_a = \sum_{n=0}^{\infty} \Lambda^{-\frac{n}{2}} \epsilon_n (f_n^\dagger f_{n+1} + f_{n+1}^\dagger f_n) - \tilde{J} f_0^\dagger \boldsymbol{\sigma} f_0 \cdot \boldsymbol{\tau}, \quad (43)$$

where the zero mode of  $f_n$  is chosen so as to correspond to  $A$  and is normalised to  $\{f_0, f_0^+\} = 1$ . The third step is to redefine  $\epsilon_n = [(1 + \Lambda^{-1})/2]^{-\frac{n}{2}}$  for all  $n$  and divide the Hamiltonian by  $(1 + \Lambda^{-1})/2\Lambda^{-\frac{n}{2}}$ . The  $\tilde{J}$  is then related to  $J$  by  $\tilde{J} = 4J(1 + \lambda^{-1})^{-1}$  and the resulting hopping Hamiltonian is

$$H = \sum_{n=0}^{\infty} \Lambda^{-\frac{n}{2}} (f_n^+ f_{n+1} + f_{n+1}^+ f_n) - \tilde{J} f_0^+ \boldsymbol{\sigma} f_0 \cdot \boldsymbol{\tau}. \quad (44)$$

This Hamiltonian now represents a semi-infinite linear chain of electrons, able to hop from site to site. The magnetic impurity is at the zeroth position open end of the chain. Each step along the chain represents an exponentially decreasing energy scale for the conduction band electrons. The justification for the redefinition of  $\epsilon_n$  is as follows. The problem to be analysed is that of the low-temperature regime of the magnetic impurity system. As we go along the chain, the conduction band energy decreases, corresponding to states nearer to the Fermi surface, which are the only ones that matter in the low temperature regime. In doing so, we increase  $n$  and as such, the original  $\epsilon_n = \frac{(1+\Lambda^{-1})}{2} \Lambda^{-\frac{n}{2}}$  limits to 1 anyway.

What is the physical picture that emerges from these transformations? We see that the impurity is coupled directly to a local orbital, which itself is coupled to the next, slightly more removed one, and so forth. There is a picture of shells of coupled electron orbitals on top of each other, much like the layers of an onion. As we go to the more distant shells, or equivalently, as we move to lower energy scales, they are built up of states near the Fermi level. These states are important in calculations of thermodynamical quantities near zero temperature, as this limit can only excite low energy conduction states.

We now have the set up to perform the iterative renormalization group calculation, which is described in the next section.

## 5.4 Renormalization group transformation of Kondo Hamiltonian

To perform the iterative procedure, it will be convenient to write the Hamiltonian in the following form

$$H_N = \Lambda^{(N-1)/2} \left[ \sum_{n=0}^{N-1} \Lambda^{-n/2} (f_n^+ f_{n+1} + f_{n+1}^+ f_n) - \tilde{J} f_0^+ \boldsymbol{\sigma} f_0 \cdot \boldsymbol{\tau} \right], \quad (45)$$

so that the original Hamiltonian can be recovered by

$$H = \lim_{N \rightarrow \infty} \Lambda^{-(N-1)/2} H_N. \quad (46)$$

The scaling factor of  $\Lambda^{(N-1)/2}$  will be useful for the discussion of fixed points, which follows later. Now we have a recursion relation for the Hamiltonians  $H_N$ ,

$$H_{N+1} = \Lambda^{1/2} H_N + f_{N+1}^+ f_N + f_N^+ f_N, \quad (47)$$

which is nearly the definition of the renormalization group transformation for this system. The strategy is as follows. Diagonalise each  $H_N$ , calculate the matrix elements of  $H_{N+1}$  in the representation in which  $H_N$  is diagonal, and finally diagonalise  $H_{N+1}$ . In very general terms, the diagonalised Hamiltonian  $H_N$  can be expressed as

$$H_N = \sum_{\mathbf{m}} E(\mathbf{m}) |\mathbf{m}\rangle \langle \mathbf{m}|, \quad (48)$$

with eigenstates  $|\mathbf{m}\rangle$ . The next Hamiltonian to be diagonalised is then

$$H_{N+1} = \sum_{\mathbf{m}}^{N_{max}} \tilde{E}(\mathbf{m}) |\mathbf{m}\rangle \langle \mathbf{m}| + \sum_{\mathbf{m}, \mathbf{m}'}^{N_{max}} [g(\mathbf{m}, \mathbf{m}') \langle \mathbf{m} | \mathbf{m}' \rangle + \text{h.c.}], \quad (49)$$

where  $g(\mathbf{m}, \mathbf{m}') = \langle \mathbf{m} | f_n^+ | \mathbf{m}' \rangle$  and  $\tilde{E}(\mathbf{m}) = \Lambda^{1/2} E(\mathbf{m})$ . The truncation of the sum to  $N_{max}$  is a practical matter for the numerical iteration, as the matrices become very large very soon. The

question is then, which states are to be retained in the calculation? The ultimate aim of the calculation is to determine the thermodynamic quantities at very low temperature. Therefore, only the  $N_{max}$  eigenstates with the lowest many-particle energies are kept, as the higher excited states are too high energetically to be important for the thermodynamics. What this number amounts to is dependent on the problem at hand. In Wilson's case, it proved accurate to keep  $N_{max} = 1000$  at each step. Also, in retaining a fixed number at each iteration, the old Hamiltonian is mapped onto a new one of the same form at each stage, with renormalized parameter set  $\{\tilde{E}(\mathbf{m}), g(\mathbf{m}, \mathbf{m}')\}$ .

The actual renormalization group transformation subtracts the ground state energy and thus reads

$$H_{N+1} = T[H_N] = \Lambda^{1/2}H_N + f_{N+1}^+ f_N + f_N^+ f_{N+1} - E_{G,N+1}, \quad (50)$$

where  $E_{G,N+1}$  is chosen such that the  $H_{N+1}$  has ground state energy 0. The transformation takes as input the eigenvalues  $H_N$  and the matrix elements  $f_N$  and puts out the eigenvalues of  $H_{N+1}$  and the matrix elements of  $f_{N+1}$ .

It can be seen that the renormalization group transformation has two fixed points, by looking at the form of  $H_N$  as  $N \rightarrow \infty$ . The two fixed points are  $\tilde{J} = 0$  and  $\tilde{J} = -\infty$ . The excitations in both cases correspond to a single particle Hamiltonian with the spin impurity decoupled.

For  $\tilde{J} = 0$ , the Hamiltonian describes a free electron and it can be solved by finding the single electron eigenstates. This procedure is done numerically, using the iterative renormalization group transformations on a computer. The result is what is called a limit cycle, where the renormalization group transformation goes back onto itself after two transformations instead of one. The fixed point is then for transformations  $T^2$ . One thus gets two sets of single particle energy levels, one for even  $N$  and one for odd  $N$ . This was the reason for introducing the factor  $\Lambda^{(N-1)/2}$  in the definition of  $H_N$ , because it is needed to have a fixed point in the large  $N$  limit for the low instead of the high eigenvalues of the Hamiltonian, as we truncate the higher ones during the process.

For the case of  $\tilde{J} = -\infty$ , which is the strongly coupled anti-ferromagnetic case, the  $\tilde{J}$  term in the Hamiltonian is much larger than the rest. This term is  $-\tilde{J}f_0^+ \boldsymbol{\sigma} f_0 \cdot \boldsymbol{\tau}$  and the impurity is coupled to the first site on the chain in a singlet ground state. The excited states of this term have infinite energy, and as such, the impurity and the first site are effectively decoupled from the rest of the chain. The states of the rest of the Hamiltonian are then free from this coupling and described by

$$H_N(\tilde{J} \rightarrow -\infty) = \text{constant} + \Lambda^{(N-1)/2} \sum_{n=1}^{N-1} \Lambda^{-n/2} (f_n^+ f_{n+1} + f_{n+1}^+ f_n). \quad (51)$$

We see that the low energy excitations of  $H_N(\tilde{J} = -\infty)$  and  $H_{N-1}(\tilde{J} = 0)$  are the same, though now with the even and odd single particle energy levels exchanged.

The big question now is, how do the Hamiltonians behave in the vicinity of the fixed points? Parts of this discussion are very technical in Wilson's account, so, for the sake of brevity, we will sometimes oversimplify and skip over some steps. The unsatisfied reader is referred to the original article [3].

We begin by searching for an effective Hamiltonian near the fixed points. Then we proceed by linearising these Hamiltonians around the fixed points to find out whether we are dealing with stable, unstable or marginal fixed points. This will provide us with the renormalization group flow of the system and thus the behaviour as we go to smaller energy regimes.

We look for a Hamiltonian of the form  $H' = H^* + \delta H$ , where  $H^*$  corresponds to a fixed point.  $\delta H$  depends only on  $\boldsymbol{\tau}$  and the first few  $f_n$ , as they are likely to be the most important interactions. We also assume  $\delta H$  to be small in the vicinity of the fixed point. We then have

$$H'_N = H_N^* + \Lambda^{(N-1)/2} \delta H, \quad (52)$$

where the factor  $\Lambda^{(N-1)/2}$  appears again to correspond with the definition of  $H$  earlier. Both  $H_N^*$  and  $H'_N$  satisfy the recursion relations (47). The difference  $H'_N - H_N^*$  then satisfies a linearised

renormalization group equation with a linear operator as discussed in section 5.2. We would like to expand  $\delta H$  in terms of the local interaction terms  $\delta H_m$ ,  $\delta H = \sum_m \delta H_m(N)$ . Since we are working in a limit cycle, the expansion of  $\delta H$  in terms of eigenvalues and eigenoperators should look like

$$\delta H = \sum_m c_m \lambda_m^{N/2} \mathbf{O}_m^*, \quad (53)$$

where  $\mathbf{O}_m^*$  are the eigenoperators,  $\lambda_m^{N/2}$  the eigenvalues and  $c_m$  constants, depending on the choice of  $\delta H_m$ .

To find the eigenvalues of the linear operator, we need a form for  $\delta H_m$ . There are a few physical considerations to take into account in choosing a suitable form for  $\delta H_m$ . First of all, we need the minimum possible number of operators  $f_0$  and  $f_1$ , since each contributes a factor of  $\Lambda^{-N/2}$  and  $\Lambda^{-3N/2}$  to the  $N$  dependence of the eigenvalues, respectively. Secondly, we want the  $\delta H_m$  to have the same symmetries as  $H$  itself. It must conserve charge, total spin and particle-hole symmetry. After these considerations, we are left with three possible forms for  $\delta H_m$ , namely

$$\begin{aligned} \delta H_1 &= f_0^+ \boldsymbol{\sigma} f_0 \cdot \boldsymbol{\tau}, \\ \delta H_2 &= f_0^+ f_1 + f_1^+ f_0, \\ \delta H_3 &= (f_0^+ f_0 - 1)^2. \end{aligned}$$

It may seem as though  $\delta H_3$  violates particle-hole conservation, but after multiplying out and converting to normal ordering, the  $f_0^+ f_0$  term is cancelled and one is only left with quartic terms. To simplify the technicalities performed by Wilson, consider the following. The operator  $f_0^+$  can be expressed in terms of operators for particles and holes,  $p_n^+$  and  $h_n$ , respectively. One can write

$$f_0^+ = \Lambda^{-(N-1)/4} \sum_n \alpha_{0,n} (p_n^+ + h_n), \quad (54)$$

where  $\alpha_{0,n}$  is a constant. The equation for  $f_1^+$  is similar, though has a prefactor  $\Lambda^{-3(N-1)/4}$ . To find the eigenvalues of the linearisation, we now plug equation (54) and the hermitian conjugates into the  $\delta H_m$  and compare these to (53). For  $\tilde{J} = 0$ , we find that  $\delta H_1$  has eigenvalue  $\Lambda^0$  and thus is a marginal operator.  $\delta H_{2,3}$  both return irrelevant eigenvalues. We conclude that  $\tilde{J} = 0$  is a marginal fixed point. Note that the operator  $\delta H_1$  only exists for the  $\tilde{J} = 0$  fixed point. The  $\tilde{J} = -\infty$  fixed point has no  $\boldsymbol{\tau}$  operator, because the coupling between the impurity and the first site removes these from the rest of the chain, as we have seen. Therefore,  $\tilde{J} = -\infty$  has only irrelevant eigenvalues, and as such,  $\tilde{J} = -\infty$  is a stable fixed point.

One can determine the behaviour of the cross-over region by performing numerical calculations with the effective Hamiltonian (51) for values near the  $\tilde{J} = 0$  fixed point. It is found that there is a crossover from  $\tilde{J} = 0$  fixed point for small  $N$  to  $\tilde{J} = -\infty$  fixed for large  $N$ . This numerical result confirms our analysis of the eigenvalues near the fixed point.

For calculations in the low temperature range for the magnetic susceptibility, it turns out to be necessary to know how the energy levels of  $H_N$  approach their limiting values for  $N \rightarrow \infty$ . From analytic analysis, one finds that these can be calculated from another effective Hamiltonian, involving a 'pseudo-potential'. This turns out to be our original Hamiltonian with exactly those terms added which we determined from our discussion of  $\delta H$ . Since we are interested in the low temperature regime, we need the effective Hamiltonian for the corresponding fixed point. Thus, for the  $\tilde{J} = -\infty$  fixed point, we have

$$H_N = \Lambda^{(N-1)/2} \left( \sum_{n=1}^{N-1} \Lambda^{n/2} (f_n^+ f_{n+1} + f_{n+1}^+ f_n) + w_1(\tilde{J}) (f_1^+ f_2 + f_2^+ f_1) + w_2(\tilde{J}) (f_1^+ f_1 - 1)^2 \right), \quad (55)$$

where  $w_1$  and  $w_2$  are parameters to be determined numerically.

## 5.5 Calculation of thermodynamical quantities

In this review, the consideration of the thermodynamical quantities of the Kondo problem will be restricted to the zero temperature limit of the magnetic susceptibility. This has a few reasons.

First of all, the primary aim of this review is to show how the renormalization group approach was able to reach these answers conceptually. Secondly, Wilson's steps in this part of the calculation are plenty, pretty technical and hardly summarisable. They also involve a lot of numerical calculations, which aren't interesting to sum up. Rather, a short general idea will be given of how Wilson came to the zero temperature magnetic susceptibility from where we left of in the last section. Once again, the eager eyes are referred to [3].

The impurity susceptibility is given by

$$\chi_{imp}(T) = \frac{(g\mu_B)^2}{k_B T} \left( \lim_{N \rightarrow \infty} \frac{\text{Tr} S_{N_z}^2 e^{-H_N(\tilde{J})/k_B T}}{\text{Tr} e^{-H_N(\tilde{J})/k_B T}} - \frac{\text{Tr} S_{N_z}^2 e^{-H_N(0)/k_B T}}{\text{Tr} e^{-H_N(0)/k_B T}} + \frac{1}{4} \right) \quad (56)$$

To calculate the low temperature range of the magnetic susceptibility, we need the effective Hamiltonian near the  $\tilde{J} = -\infty$  fixed point, that is, equation (55).  $w_1$  and  $w_2$  are parameters which are determined by fitting them to the lowest excitations of the numerical iterations of (55).  $w_2$  is compared with the single particle excitation  $E_{1,N}$  and for  $w_2$  this is done for the lowest two particle excitation  $E_{2,N}$ . Once this iteration approaches the large  $N$  limit, and as such, the strong coupling regime,  $w_1$  and  $w_2$  become smaller and smaller, because they represent the irrelevant operators in that region. The energy range of the full Hamiltonian become smaller as well, as we are moving to the outer shells of electron states. Once the temperature is low enough, the correction terms of (55) can be treated in lowest order perturbation theory. This is the strategy which Wilson followed to calculate the magnetic susceptibility in the very low temperature regime. The result is

$$\chi_{imp}(T) = \frac{(g\mu_B)^2 (0.4128 \pm .002)}{4k_B T_K}, \quad (57)$$

where  $T_K$  is the Kondo temperature. This is finite as  $T \rightarrow \infty$ , which was the ultimate aim of solving the Kondo problem. A satisfactory theory has been developed for describing the system of a magnetic impurity in a non-magnetic metal down to zero temperature range.

Wilson remarked at the end of his article that further studies on the subject would likely include the effects of potential scattering, studies of dynamical properties like the resistivity, attempts to include  $d$ -wave coupling to the impurity and the study of impurity-impurity effects. In the years following, it was thought that these were mere cases of rounding up calculations, but that they were inhibited by limited computing power. Researchers lost their attention and pursued other studies. At the start of the eighties, however, there was a new theoretical development. This will be discussed in the next section.

## 6 The Bethe Ansatz approach

In the previous section a qualitative understanding of the Kondo problem was obtained by Wilson in the seventies, which used the machinery of the renormalization group. The obtained results were confirmed by exact solutions to the Kondo problem found by two other physicists. Andrei and Wiegmann solved the s-d exchange model independently using an ansatz introduced by Bethe in 1931. By doing so they immensely increased the popularity of the branch of integrable systems and supported the method of the renormalization group by confirming its validity. In the next section we formulate a step by step methodology for applying the tool, which is followed by an implementation of the approach in the Kondo problem. The main resources used are [7], the lecture notes on the Bethe Ansatz from J.S. Caux and the original papers by Andrei [10] and Wiegmann [4].

### 6.1 The General Methodology

The Bethe ansatz can be used for extracting eigenvectors and eigenvalues of model Hamiltonians which describe short-range interactions. It does this by rewriting the many-body wave functions as products of separate two-body scattering events. In this section a general methodology is introduced based on the lecture notes on the Bethe ansatz from J. S. Caux and [11].

1. In the case of  $N$  particles, they are put on a ring with circumference  $L$ . This way we impose periodic boundary conditions and translational symmetry. For free particles the wave function is described by

$$\psi(x_1 \dots x_N) = \sum_{\mathcal{P} \in S_N} \prod_{i=1}^{N-1} \theta(x_{\mathcal{P}_{i+1}} - x_{\mathcal{P}_i}) A_{\mathcal{P}} e^{ix_1 k_1 + \dots + ix_N k_N}, \quad (58)$$

where, depending on whether it is a boson or a fermion, the equation should be symmetrised or anti-symmetrised. In case of spin dependence:  $\psi(x_1 \dots x_N) = \psi(x_1 \dots x_N)_{\alpha_1 \dots \alpha_N}$

2. Look for configurations that solve the Schrödinger equation at the point of local interactions. This way it is possible to find the scattering matrix  $S^{ij}$ .
3. We now have an expression for the scattering matrix but we need to check for consistency. Because we are dealing with identical particles we have to watch that permutations of the system that result in the same configuration of particles must have the same wave function. This constrains the two-body scattering and is known as the *Yang-Baxter equation*. Basically it dictates how a three-body problem is described in two-body matrices. The Yang-Baxter equation has the form:

$$S^{3,2} S^{1,3} S^{1,2} = S^{1,2} S^{1,3} S^{2,3}. \quad (59)$$

4. By imposing boundary conditions on the wave function proposed in (58) we find

$$e^{-\frac{ik_j L}{2}} A_{x_j, \mathcal{P}_{N-1}} = e^{\frac{ik_j L}{2}} A_{\mathcal{P}_{N-1}, x_j} \quad (60)$$

and swaps the most left particle  $x_j = -\frac{L}{2}$  with the most right particle  $x_j = \frac{L}{2}$ .

5. A different way to find an expression for  $A_{x_j, \mathcal{P}_{N-1}}$  is by starting in a configuration  $x_j, \mathcal{P}_{N-1}$  and scattering across all other particles using the scattering matrices  $S^{j,i}$  where, of course,  $j \neq i$ . The Yang-Baxter equation helps you with the identity  $\mathcal{P}_{N-1} = 1_{N-1}$  and you end up with

$$A_{1_{N-1}, x_j} = Z_j A_{x_j, 1_{N-1}} \quad \text{where} \quad Z_j = S^{j,N} \dots S^{j,j+1} S^{j,j-1} \dots S^{j,1}. \quad (61)$$

Combining the two expressions in (3) and (61) we get

$$Z_j A_{x_j, 1_{N-1}} = e^{-k_j L} A_{x_j, 1_{N-1}}, \quad (62)$$

which has reduced it to a set of eigenvalue problems.

6. The hardest part is solving this set of problems specified in (62) and by doing so you'll end up with the Bethe momenta and the total energy of the system.

When we spell it out like this, it looks very straightforward but especially finding solutions to the Yang-Baxter equation and of course the last step is certainly not trivial. In the next section we're going to implement these steps for the Kondo problem, resulting in an expression for the magnetic susceptibility.

## 6.2 Using the Bethe Ansatz to solve the Kondo problem

In class we used the Bethe Ansatz to solve the Lieb-Liniger model. The repulsion term in the Hamiltonian dictates how two particles scatter and in that case it was characterized by a simple phase shift. In the Kondo Hamiltonian this is not the case because the interaction is due to spin exchange and we somehow have to deal with this internal degree of freedom. The derivation in this section follows roughly the steps taken by Andrei in [10] and Wiegmann in [4]. To keep the derivation clear we sometimes used a different notation for certain formulas or expressions plus we had to make decisions on how thorough we could be on certain aspects of the derivation. For the sake of brevity, some steps are omitted.

The representation of the Kondo Hamiltonian used in this part has the following form

$$\mathcal{H} = -i\hbar v_F \sum_{\sigma=\uparrow\downarrow} \int_{-\frac{L}{2}}^{\frac{L}{2}} \psi_{\sigma}^{\dagger}(x) \partial_x \psi(x) dx + \frac{Ja}{2} \sum_{\sigma, \sigma'} \psi_{\sigma}^{\dagger}(0) \psi_{\sigma'}(0) \vec{\sigma}_{\sigma\sigma'} \cdot \vec{S} \quad (63)$$



where  $a$  is the lattice spacing,  $J$  the spin-exchange interaction and  $\vec{S}$  the impurity spin. Now we can start to implement the machinery from the previous section. First of all, we put the impurity on  $x = 0$  and order the  $N$  particles on a line segment of size  $L$ . The wave function has the shape of a plane wave with the form

$$\psi(x_1 \dots x_N)_{\alpha_1 \dots \alpha_N} = e^{i \sum_{j=1}^N k_j x_j} \sum_{\mathcal{P}} A_{\alpha_1 \dots \alpha_N, \alpha_0}^{\mathcal{P}}, \quad (64)$$

where the  $k_i$  are the momenta and  $a_i$  labels the spin at each site ( $a_0$  states the spin of the impurity). With this wave function we can start solving the schrödinger equation for particle  $j$  interacting with the impurity. Think of a certain ordering  $\mathcal{P}$  and a permutation  $\mathcal{Q}$  both containing  $N$  particles and the impurity site. In this case the scattering matrix connects the two in the following way

$$S^{0j} A_{\alpha_1 \dots, \alpha_j, \dots, \alpha_N, \alpha_0}^{\mathcal{P}} = A_{\alpha_1 \dots, \alpha'_j, \dots, \alpha_N, \alpha'_0}^{\mathcal{Q}}, \quad (65)$$

where the matrix  $S$  is the mapping between the amplitude  $A^{\mathcal{P}}$  of the configuration  $P$  on the left of the impurity and  $A^{\mathcal{Q}}$  is the amplitude of the configuration  $Q$ . The calculations for finding the scattering matrix for the problem at hand were based on the calculation of Yang published in 1966 ([12]) on spin interactions in a one dimensional Heisenberg chain and can be written in the following form

$$S^{0j} = \frac{I^{j0} - icP^{j0}}{1 - ic}, \quad (66)$$

where  $P^{j0} = \frac{1}{2} (I^{j0} + \vec{\sigma}_j \cdot \vec{\sigma}_0)$  exchanges the spin of the impurity and the conductivity electron  $j$ , and  $c$  is a function of  $J$ . With this scattering matrix we can check if the theory is still consistent. Because we are dealing with indistinguishable particles, a different order of interaction should not result in a different result. To check this, the following relation has to hold

$$S^{ij} S^{i0} S^{j0} = S^{j0} S^{i0} S^{ij}. \quad (67)$$

We can account for this with the choice  $S_{ij} = P^{ij}$ , which physically means that when one electrons crosses another, they interchange their spin labels. With the consistency check in place, we can enforce periodic boundary conditions to find an expression for the operator  $Z_j$ .  $Z_j$  represents a scattering process where a particle  $j$  interacts with all the particles on the circle, which stretches length  $L$ .

$$Z_j = P^{jj-1} \dots e^{-i\phi} \frac{I^{j0} - icP^{j0}}{1 - ic} \dots P^{jj+1}. \quad (68)$$

This operator can be related to an eigenvector  $e^{-k_j L}$  and it is the Bethe momentum  $k_j$  that we are after, because we can use these to calculate the energy of the system. Solving this eigenvalue problem is not trivial and can be done by using the quantum inverse scattering method together with the transfer matrix approach of Baxter. It goes under the name of the *algebraic Bethe Ansatz*. Doing so results in an expression for the Bethe momentum,

$$k_j = \frac{2\pi}{L} n_j + \frac{1}{L} \sum_{\gamma=1}^M [\Theta(2\Lambda_\gamma - 2) - \pi], \quad (69)$$

where  $\Theta(\Lambda) = -2\arctan(\frac{\Lambda}{c})$  and  $n_j$  are quantum numbers. This expression is characterized by the conservation of the total spin and projection of the spin on the  $z$ -axis and generates physical quantities  $\Theta_\gamma$  called spin momenta that are associated to down spins by  $M = \frac{N+1}{2} - S_z$ . The possible values for the spin moment  $\Theta_\gamma$  are determined by  $M$  equations and the set of quantum numbers  $I_\gamma$  via the formula

$$N\Theta(2\Lambda_\gamma - 2) + 2\Theta(2\Lambda) = -2\pi I_\gamma + \sum_{\delta}^M \Theta(\Lambda_\gamma - \Lambda_\delta) \quad (70)$$

The combination of the quantum numbers  $\{n_j\}$  and  $\{I_\gamma\}$  determine the shape of the ground state. The ground state is found by choosing  $I_\gamma$  to be consecutive as  $I_{\gamma+1} = I_\gamma + 1$ , take the minimal levels for  $n_j$  and look at the thermodynamical limit where  $N \rightarrow \infty$ . In that situation the spin momenta will become dense and consecutive levels should satisfy

$$\sigma(\Lambda) = f(\Lambda) - \int \frac{d\Lambda'}{\pi} \frac{c}{c^2 + (\Lambda - \Lambda')^2} \sigma(\Lambda'), \quad (71)$$

where  $f(\Lambda) = \frac{2c}{\pi} \left[ \frac{N}{c^2+4(\Lambda-1)^2} + \frac{1}{c^2+4\Lambda^2} \right]$ . This expression is solvable and results in an expression for the ground state. Excited states can be generated by changing the quantum numbers with respect to their ground state values. Now that we can find an expression for the ground state, we can discuss the magnetic susceptibility. The susceptibility is found with the formula  $\chi^{-1} = \mu^{-2} \left[ \frac{\partial^2 E(S)}{\partial S^2} \right]_{s=0}$  where  $E(S)$  is the minimum energy in the presence of magnetization  $\mu S$  and  $S = N - 2M$ . We can finally get to the expression for the magnetic susceptibility

$$\chi = \frac{1}{\pi} \mu^2 \frac{N^e + N^i \exp\left(\frac{\pi}{C}\right)}{\frac{N^e}{L} \exp^{-\frac{\pi}{C}}} \quad (72)$$

where the leading term is induced by the impurities.

We conclude that the Bethe ansatz approach leads to an exact solution for the magnetic susceptibility for the system of magnetic impurities in a non-magnetic metal.

## 7 Conclusion

The history of the Kondo problem has been discussed in broad terms. A seemingly simple problem has caused many physicists to come up with inventive approaches over the years. As such, the experimental anomaly of resistance minima in metals has contributed greatly to modern theoretical physics. Ideas from the renormalization group from field theory and critical phenomena have been generalised to be applicable to a broader set of physical problems. The Bethe ansatz has confirmed presumptions from the renormalization group approach. In doing so, it has contributed considerably to exact calculations on models that are experimentally testable. The further developments in theories surrounding magnetic impurities in non-magnetic metals have been used to try and describe high temperature superconductors too, among other phenomena. It is believed that the strongly correlated nature induced by the short range Coulomb interaction at the impurity sites is the key to understanding the anomalous behaviour of high temperature superconductors. Thus, the history of the Kondo problem as described in this review is only the beginning of an on-going story of strongly correlated systems.

## References

- [1] Alan Herries Wilson. The theory of metals. *American Journal of Physics*, 22(4):243–244, 1954.
- [2] Jun Kondo. Resistance minimum in dilute magnetic alloys. *Progress of theoretical physics*, 32(1):37–49, 1964.
- [3] Kenneth G Wilson. The renormalization group: Critical phenomena and the Kondo problem. *Reviews of modern physics*, 47(4):773, 1975.
- [4] P B Wiegmann. Exact solution of the sd exchange model (Kondo problem). *Journal of Physics C: Solid State Physics*, 14(10):1463, 1981.
- [5] M P Sarachik, E Corenzwit, and L D Longinotti. Resistivity of mo-nb and mo-re alloys containing 1% fe. *Physical Review*, 135(4A):A1041, 1964.
- [6] Philip W Anderson, G Yuval, and D R Hamann. Exact results in the Kondo problem. II. Scaling theory, qualitatively correct solution, and some new results on one-dimensional classical statistical models. *Physical Review B*, 1(11):4464, 1970.
- [7] Alexander Cyril Hewson. *The Kondo problem to heavy fermions*, volume 2. Cambridge university press, 1997.
- [8] John Cardy. *Scaling and renormalization in statistical physics*, volume 5. Cambridge university press, 1996.
- [9] J Kondo. Solid State Physics vol 23 ed F Seitz. *D Turnbull and H Ehrenreich (New York: Academic) p*, 183, 1969.
- [10] N Andrei. Diagonalization of the kondo hamiltonian. *Physical Review Letters*, 45(5):379, 1980.
- [11] Yuval Vinkler. Toward a Bethe Ansatz Treatment of Quantum Impurity Models with Momentum-Generating Scattering. 2009.
- [12] Chen-Ning Yang and Chen-Ping Yang. One-dimensional chain of anisotropic spin-spin interactions. I. Proof of Bethe’s hypothesis for ground state in a finite system. *Physical Review*, 150(1):321, 1966.