

Renormalization Group Approaches to the Kondo Effect

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Abstract

Kondo effect was first introduced by Kondo in 1964 for explaining the extraordinary resistivity of metals with magnetic impurities: The resistivity $\rho(T)$ increases as temperature T goes to zero. This problem can be well understood by the method of the renormalization group. In this essay, the renormalization group is used to analyze the effective coupling of the impurity with the conduction electrons. One finds that the effective coupling diverges towards a fixed point for antiferromagnetic case, and tends to zero for ferromagnetic case. We will discuss the low temperature behavior of the antiferromagnetic Kondo model, which is well characterized by the Landau Fermi liquid approach. Some physical quantities such as specific heat capacity, impurity entropy and susceptibility are obtained perturbatively in low temperature limit. The qualitative behaviors of those physical quantities for the whole temperature regime are also discussed in this essay.

1 Introduction

One of the old and fundamental questions in condensed matter physics is how the resistivity of metals depends on temperature. In usual solid state physics textbook, one finds the resistivity $\rho(T)$ decreases to zero as $T \rightarrow 0$ if phonons interaction is included. However, experimentally, one observes $\rho(T)$ increases as $T \rightarrow 0$

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if metals contain magnetic impurities. This anomalous behavior of the metals' resistivity was explained by Kondo in 1964. The Hamiltonian Kondo wrote was

$$H = \sum_{\vec{k}\alpha} \psi_{\vec{k}}^{\dagger\alpha} \psi_{\vec{k}\alpha} \varepsilon(k) + \lambda \vec{S} \cdot \sum_{\vec{k}\vec{k}'} \psi_{\vec{k}}^{\dagger} \frac{\vec{\sigma}}{2} \psi_{\vec{k}'} \quad (1)$$

where $\psi_{\vec{k}\alpha}$'s are conduction electron annihilation operators with momentum \vec{k} and spin α and \vec{S} is the spin of the magnetic impurity. This Hamiltonian represents the interaction between one impurity spin and electrons at $\vec{x} = 0$.

The perturbation theory up to second leading order terms gives divergent behavior of $\rho(T)$ at $T = 0$:

$$\rho(T) \sim \left[\lambda + v\lambda^2 \ln \frac{D}{T} + \dots \right]^2 \quad (2)$$

where D is the band width and v is the density of states. We can immediately ask one question: what happens at the temperature $T \sim T_K = D e^{-\frac{1}{v\lambda}}$? At this temperature, the second order $O(\lambda^2)$ term will be comparable to the first order term $O(\lambda)$. It is clear that the perturbation theory is no longer trustful in this case and we can expect that higher order terms in perturbation theory will also contribute to the expansion at sufficiently low temperature.

Wilson developed the idea of renormalization group approach, which provides a powerful tool to understand and solve such questions. Nozieres following the idea of Anderson and Wilson developed a simple picture of the low temperature behavior of Kondo problem in 1974. Kondo model was also solved by the method of Bethe ansatz in 1980, which gives the specific heat and magnetization.

2 Renormalization Group Approach to Kondo Effect

Like usual renormalization group method, we could integrate out $\psi(k)$ for k far from fermi wave-vector k_F , and successively reduce the band width D . We could obtain a new effective interaction after one renormalization transformation. We suppose the coupling is weak and hence we can do above procedure perturbatively in λ . We could expand the interaction term

$$T \exp \left[-i\lambda \int \vec{S}(t) \cdot \psi^{\dagger} \frac{\vec{\sigma}}{2} \psi(\vec{0}, t) \right] \quad (3)$$

in the interaction picture. Through expansion of this interaction term, we could arrange the terms order by order by usual Feynman diagrams. For example, the second order in λ term is

$$-\frac{\lambda^2}{2} \int dt dt' T(S^a(t)S^b(t')) \cdot T \left[\psi^\dagger(t) \frac{\sigma^a}{2} \psi(t) \psi^\dagger(t') \frac{\sigma^b}{2} \psi(t') \right] \quad (4)$$

where T is time ordering. Using the Wick's theorem, we could reduce expression (4) into

$$\begin{aligned} & -\frac{\lambda^2}{2} \int dt dt' \psi^\dagger \left[\frac{\sigma^a}{2}, \frac{\sigma^b}{2} \right] \psi T \langle \psi(t) \psi^\dagger(t') \rangle \left(\theta(t-t') S^a S^b + \theta(t'-t) S^b S^a \right) \\ = & \frac{\lambda^2}{2} \int dt dt' \psi^\dagger \frac{\vec{\sigma}}{2} \psi \cdot \vec{S} \text{sign}(t-t') \langle \psi(t) \psi^\dagger(t') \rangle . \end{aligned} \quad (5)$$

The corresponding Feynman diagrams contributing to renormalization of the Kondo coupling constant are shown in Fig(1).

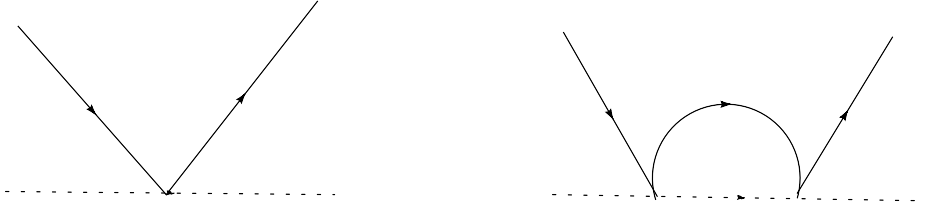


Figure 1: Feynman diagrams to Kondo problem up to second order.

Applying renormalization group method, we need integrate out the momentum shell $D' < k < D$. The easiest way to work out the integral is to write it in the momentum space instead of real space:

$$\begin{aligned} & \int \frac{d^3k}{(2\pi)^3} \int \frac{d\omega}{2\pi} \left[\frac{1}{i\omega + \delta} + \frac{1}{i\omega - \delta} \right] \frac{i}{\omega - \epsilon_k + i\delta \text{sign}(\epsilon_k)} \\ & \int \frac{d^3k}{(2\pi)^3} \frac{1}{|\epsilon_k|} \approx 2\nu \int_D^{D'} \frac{d\epsilon}{\epsilon} = 2\nu \ln \frac{D}{D'} . \end{aligned} \quad (6)$$

Hence we can get RG recursion relation equation:

$$\delta\lambda = v\lambda^2 \ln \frac{D}{D'}, \quad (7)$$

equivalently, it can be written as

$$\frac{d\lambda}{d\ln D} = -v\lambda^2. \quad (8)$$

To see how Kondo coupling depends on the band width D , we can integrate the equation (8):

$$\lambda_{eff}(D) = \frac{\lambda_0}{1 - v\lambda_0 \ln \frac{D_0}{D}}. \quad (9)$$

Let us look at physics of equation (9). We find there is a fixed point in Kondo problem : $\lambda = 0$, which separates two physical phases. For $\lambda_0 > 0$ (antiferromagnetic phase), the effective Kondo coupling $\lambda_{eff}(D)$ diverges at $D \sim T_k \sim D_0 e^{-\frac{1}{v\lambda_0}}$. In this case, as we discussed above, the perturbation theory fails at low temperature. For $\lambda_0 < 0$ (ferromagnetic phase), effective coupling constant $\lambda_{eff} \rightarrow 0$. We should notice that the physical behavior at temperature T is determined by effective Kondo coupling $\lambda_{eff}(T)$ rather than bare coupling. Thereby it is trivial for ferromagnetic case since $\rho(T) \rightarrow 0$ as $T \rightarrow 0$. It is interesting to ask what happens for antiferromagnetic case?

3 Low T Behavior of Antiferromagnetic Kondo Model

From last section, we find that $\lambda_{eff} \rightarrow \infty$ as $T \rightarrow 0$ for antiferromagnetic case. This case was first studied in detail by Nozières in 1975. We could consider the strong coupling limit of a lattice model. For simplicity, we only consider the model in spatial dimension $D = 1$. The Hamiltonian is

$$H = t \sum_i (\psi_i^\dagger \psi_{i+1} + \psi_{i+1}^\dagger \psi_i) + \lambda \vec{S} \cdot \psi_0^\dagger \frac{\vec{\sigma}}{2} \psi_0. \quad (10)$$

Strong coupling limit means $\lambda \gg |t|$. Hence we can do perturbation theory in t instead of λ . Let us look at physics picture in general before doing any

serious calculation. What is the ground state configuration of Hamiltonian (10) in strong coupling limit. At site 0, one electron must form a singlet with impurity: $|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$. (We assume spin of impurity is half). Electrons can hop on all sites on the lattice except site-0, since it would destroy the singlet state and hence cost an energy $\Delta E \sim \lambda \gg t$. Therefore we can simply form free electron Bloch states with boundary condition $\phi(0) = 0$, where $\phi(i)$ is the single-electron wavefunction. At zero Kondo coupling, this model can be solved exactly: one parity even single particle wavefunctions $\phi(i) = \cos ki$ and one parity odd single particle wavefunctions $\phi(i) = \sin ki$. However, in the strong coupling limit, since the boundary condition $\phi(0) = 0$, we find parity even wavefunctions become $\phi(i) = |\sin ki|$, while the parity odd ones do not change.

The parity even channel in strong coupling limit corresponds to a $\pi/2$ phase shift to the s-wave channel:

$$\phi_j \sim e^{-ik|j|} + e^{+2i\delta} e^{ik|j|}, \quad \delta = \pi/2. \quad (11)$$

This shows that Kondo impurity effect can be replaced by free electron theory with a non-magnetic s-wave scattering with $\pi/2$ phase shift. How could we understand this statement physically? This is because of screening effect as explained below.

We can linearize the spectrum near Fermi surface. If particle-hole symmetry, the Fermi surface lies midway between levels or on a level as shown in Figure (2). Two pictures only differ by a phase shift.

Wilson used numerical RG method to calculate the low-lying spectrum numerically. The result indicates that λ renormalizes to ∞ even if it is initially small as we expect. However, in real system, electron screening effect should be taken into account, which gives a length scale in the problem

$$\xi \sim \frac{v_F}{T_K} \sim \frac{v_F}{D} e^{1/\nu\lambda}. \quad (12)$$

That means wavefunctions of screening electrons are no longer extended to whole space. It should have a length scale ξ . We get low energy Bloch states of free electrons only for $|k - k_F| \ll 1/\xi$, i.e. $l \gg \xi$. The free electron theory with a phase shift picture corresponds to an universal stable low energy fixed point for the Kondo problem. Kondo impurity problem is equivalent to a non-magnetic s-wave scatter with a $\pi/2$ phase shift at Fermi energy.

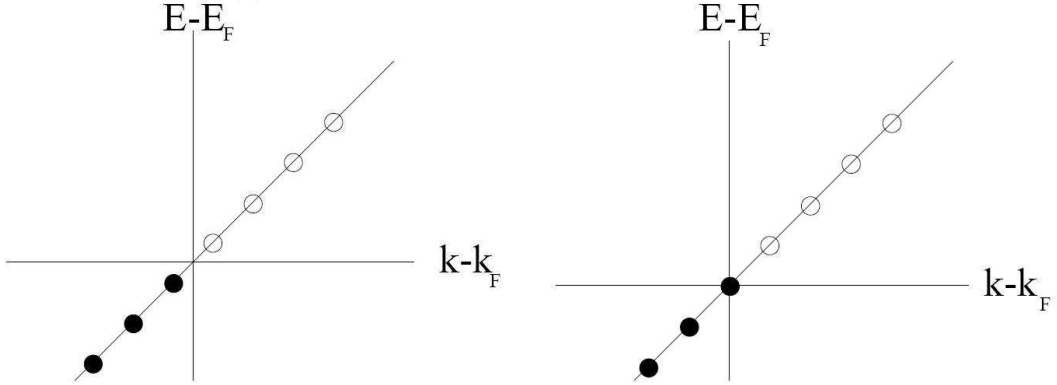


Figure 2: Free fermion energy level

More interesting low-T behavior comes from the leading irrelevant operator. Although we find that impurity spin has been screened from the description of the low-T physics, a certain interaction between electrons are generated at impurity site only in the process of eliminating the impurity spin. How could we write these effective interaction between electrons? One way is to start from microscopic theory, however it is fairly complicated. Following the spirit of Landau, we can determine these terms by simply writing the lowest dimension operators allowed by symmetry.

For simplicity, we only work with left-movers in 1D case. Hence the interaction can be written in terms of ψ_L . The dimension analysis determines the various dimension of operators in 1D field theory

$$H = \int dx \psi_L^\dagger i \frac{d}{dx} \psi_L + \dots \quad (13)$$

The length and time dimensions are same (we convert them with v_F), the dimension of ψ field is

$$[H] = E = 1 \Rightarrow [\psi] = E^{\frac{1}{2}} = 1/2. \quad (14)$$

If we assume the interactions are local, then they can be expanded by some local operators

$$\delta H = \sum_i \lambda_i O_i(x=0), \quad (15)$$

with dimension $[\lambda_i] + [O_i] = 1$. Hence λ_i had negative energy dimension, i.e. irrelevant, if $[O_i] > 1$. One usually defines a dimensionless coupling constant in RG theory. If $[\lambda_i] = E^{-a}$, then the dimensionless coupling constant can be defined as

$$\tilde{\lambda}_i \equiv \lambda_i D^a. \quad (16)$$

From RG recursion relation

$$\frac{d\tilde{\lambda}_i}{d \ln D} = a \tilde{\lambda}_i, \quad (17)$$

$\tilde{\lambda}_i$ decreases as lowering D . So what are the lowest dimension operators allowed by symmetry? For $d = 1$ case, we might consider operator $\psi^{\dagger\alpha}(0)\psi_\alpha(0)$. However this operator is not allowed because it breaks the particle-hole symmetry. This term actually contributes to a potential for scattering, which adds a term to the phase shift. Next, for $d = 2$, there are two operators allowed: one is $i\psi^{\dagger\alpha}\frac{d}{dx}\psi_\alpha(0) - i\frac{d}{dx}\psi^{\dagger\alpha}\psi_\alpha(0)$, which produces a k -dependent phase shift; another term is $\psi^{\dagger\uparrow}\psi_\uparrow\psi^{\dagger\downarrow}\psi_\downarrow$. This term represents the interaction between electrons induced by impurity spin flip. It turns out these are the only two operators allowed with dimension $d \leq 2$. No $d \leq 1$ operators allowed implies that the low energy fixed point is stable.

Using Wilson's numerical method or Bethe ansatz, one can calculate these two coupling constants. However, both of these two methods are quite complicated. Dimensional analysis is helpful to understand the problem qualitatively. Both of these two coupling constants have dimension E^{-1} , hence we expect them to be $O(1/T_K)$ by a standard scaling argument. For $T_K \ll D$ ($\lambda \ll 1$), Nozières argued that these two irrelevant coupling constants have a universal ratio, thereby there is only one parameter (Wilson number) describing the whole theory. This irrelevant coupling constant governs all low temperature behavior. We can do perturbation theory in the irrelevant coupling constant $\sim 1/T_K$.

For the specific heat, we find

$$C \sim \frac{\pi}{3v_F}lT + a\frac{T}{T_K}. \quad (18)$$

This is the specific heat of one-dimension system with a single magnetic impurity located at origin. Physically, this expression is very easy to be understood. The first term is just usual specific heat for the free electron system. It is bulk property, hence it should be proportional to the size of the system l . The second term is independent of the size of system and is due to impurity at origin. Why is this impurity specific term proportional to T ? That is the result of first order perturbation theory in the irrelevant coupling constant of order $O(1/T_K)$. The linearity of T is fixed by simple dimensional analysis. To generate one dimensional result to three dimension, we need only simply multiply the first term by the ratio $vV/(l/2\pi v_F)$, i.e. the ratio of densities of states per unit energy, and second term by the number of impurities.

Supposing the spin of impurity is $1/2$, then impurity of the system at high T is

$$S(T) = \frac{\pi l}{3v_F}T + ln2. \quad (19)$$

The system entropy at low T can be expressed as

$$S(T) = \frac{\pi l}{3v_F}T + \frac{aT}{T_K}. \quad (20)$$

The first term is propotional to the size of system, which is the entropy background for free system. What we are interested in is the entropy for the impurity, hence we can subtract this entropy background, we write

$$S_{imp} \equiv S(T) - \frac{\pi l}{3v_F}T = g(T/T_K), \quad (21)$$

where g is an universal scaling function for weak bare coupling. The behavior of $g(T/T_K)$ of small T/T_K can be determined by RG-improved weak coupling perturbation theory. However, the knowledge of the behavior of g for whole range T/T_K is a property of the universal crossover between fixed points and is found by Bethe ansatz. The qualitative behavior of the impurity entropy is shown in Figure. 3.

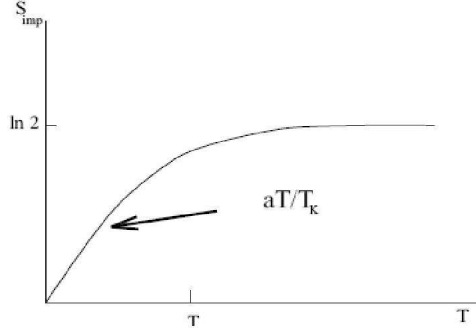


Figure 3: Qualitative behavior of the impurity entropy.

We could also calculate the susceptibility. At high T , we expect our result should be approximately like a free spin:

$$\xi \sim \frac{l}{2\pi v_F} + \frac{1}{4T}. \quad (22)$$

At low T , the susceptibility can be computed by the RG improved perturbation theory:

$$\xi \sim \frac{l}{2\pi v_F} + \frac{1}{4T} \left[1 - \frac{1}{\ln(T/T_K)} + \dots \right]. \quad (23)$$

Hence the impurity susceptibility reads

$$\xi_{imp} \equiv \xi - \frac{l}{2\pi v_F} = \frac{1}{T} f(T/T_K), \quad (24)$$

where $f(T/T_K)$ is another universal scaling function. See Figure (4).

The low T resistivity for the dilute impurities can be computed by RG group method up to second order,

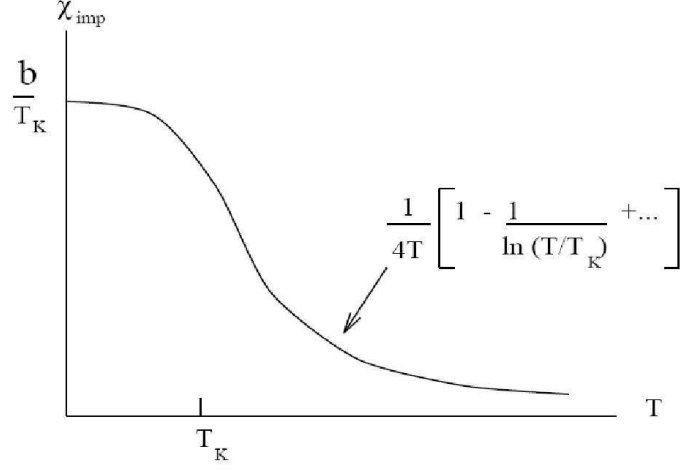


Figure 4: Qualitative behavior of the impurity susceptibility.

$$\rho \sim \rho_u [1 - d(T/T_K)^2], \quad (25)$$

where $\rho_u = \frac{3n_i}{\pi v^2 v_F^2 e^2}$ is unitary limit resistivity and d is some dimensionless constant. Second order perturbation theory in the irrelevant coupling constant gives the contribution of the second term in expression (25).

At high T , as we state at the beginning, the usual naive perturbation theory still holds, hence the result is just given by equation (2):

$$\rho(T) \sim n_i [\lambda + \lambda^2 \ln(D/T) + \dots]^2. \quad (26)$$

The scaling behavior of resistivity is sketched in Figure (5).

4 Summary

We discuss the Kondo effect based on renormalization group method in this essay. We derive the RG recursion relation and find that there have two separate phases: antiferromagnetic phase and ferromagnetic phase in Kondo problem. Detail discussion of low T behavior of the antiferromagnetic Kondo problem is given. An

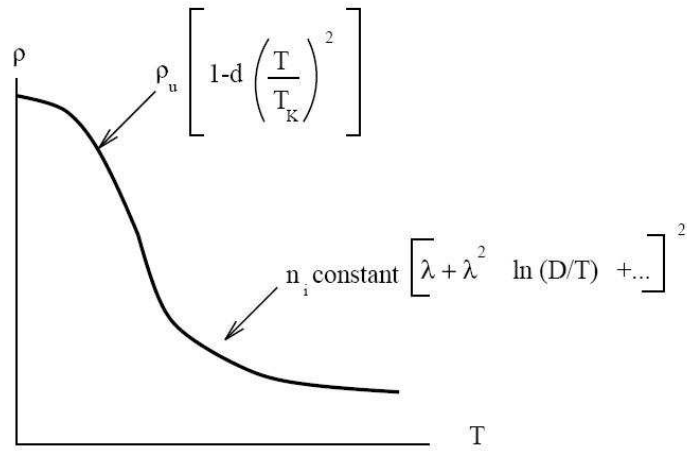


Figure 5: Qualitative behavior of the resistivity.

universal scaling behavior of impurity specific heat, impurity entropy, impurity susceptibility and resistivity is shown at the end of the essay.

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