

A Perturbative Calculation of the Low- Temperature Resistivity of a Metal Having Magnetic Impurities

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Abstract: In this paper, a microscopic theory of low temperature resistivity of a metal containing localized magnetic impurities is presented utilizing the method of second quantization and the time-dependent perturbation theory up to second order in the spin-exchange Hamiltonian. The transition rate of scattering is calculated both in the first and second order approximations considering non-spin-flip and spin-flip processes. The Kondo effect is revealed in the second-order spin-flip calculation. The results are in very good agreement with the experimental observations.

Keywords: Second quantization, Fermi's golden rate, transition rate of scattering, spin-exchange interaction

I. Introduction

The study of the anomalous behavior of the low temperature resistivity of a metal containing trace of magnetic impurities has been of profound interest both for experimental and theoretical physicists. Since 1930's [1,2], it has been observed that the resistivity of a host metal such as copper or gold with traces of magnetic impurities like iron, shows a minimum as temperature is lowered and then increases logarithmically with further lowering of temperature. The physics of the mechanism involved in such cases, was first correctly proposed in 1964 by Kondo [3]. According to Kondo, the anomalous behavior of resistivity is due to an exchange interaction between the spins of local impurity d-electrons and the itinerant electrons. Since then the phenomenon of this resistivity minimum has been named as the Kondo effect. Although discovered long back, the Kondo effect has continued to be a very active field of research in condensed matter physics. Recently the Kondo effect has been observed in unusual materials. The formation of heavy fermions in inter-metallic compounds, those involving rare-earth elements like cerium, praseodymium and ytterbium is now thought to be a manifestation of the Kondo effect extended to a lattice of magnetic impurities.

Sengupta and Baskaran [4] have recently made theoretical prediction of unconventional Kondo effect in graphene that can be tuned by a controlled gate voltage. In graphene a mass-less Dirac like spectrum for electrons is exhibited. The experimental works in this correction have been also reported [5, 6]. Even in quantum dots tunable Kondo effect has been observed [7, 8]. After the original suggestions of Kondo, various theoretical works have been reported to understand the Kondo effect in special materials. In this connection the work by Wehling et.al. [9] is worth mentioning, where the first-principle theory of resonant impurities and density functioned calculations have been used. In the present work we exploit the original Kondo Hamiltonian to perform a second-quantized calculation of spin-spin interactions involving the impurity and conduction electrons. We then use the Fermi golden rule extended to the second order in the perturbation Hamiltonian, to derive expressions for the scattering rate and hence the resistivity of a metal having traces of magnetic impurities. We find that the Kondo effect is not a first order perturbation effect but arises only in second order perturbation calculations involving spin-flip scattering processes.

II. Kondo Hamiltonian in the second quantized form

The Kondo effect arises due to the interaction of impurity spins (d-electrons) with those of the conduction electrons of the host metal. The simplest Hamiltonian for this interaction can be written as,

$$H_k = \sum_{k,\sigma} E_k c_{k\sigma}^+ c_{k\sigma} - \sum_{k,k'} \frac{J_{kk'}}{\hbar^2} (\Psi_{k'}^+ \vec{s} \Psi_k) \cdot (\Psi_d^+ \vec{S} \Psi_d) \quad (1)$$

The first term in (1) is the unperturbed energy of the conduction electrons and the second term represents the perturbation Hamiltonian responsible for scattering of conduction electrons from \vec{k} to \vec{k}' , caused by the localized d-electrons. The quantity $n_{k\sigma} = c_{k\sigma}^+ c_{k\sigma}$ is the number operator for conduction electrons with spin index σ , each having kinetic energy E_k . The operators Ψ_d and Ψ_k are the two components of spinors that remove electrons from impurity and conduction states respectively. \vec{S} and \vec{s} denote the spin operators for

impurity and conduction electrons respectively. The interaction $J_{kk'}$ has the unit of energy and is the analogue of the famous Heisenberg spin-exchange interaction.

As is known, the Kondo effect is due to anti-ferromagnetic interaction and hence $J_{kk'} < 0$. To rewrite (1) in a more convenient form, we shall introduce the relevant creation and annihilation operators for electrons which are fermions.

The two component spinors in (1) will be written as,

$$\Psi_k = \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \end{pmatrix} ; \quad \Psi_d = \begin{pmatrix} c_{d\uparrow} \\ c_{d\downarrow} \end{pmatrix} \quad (2)$$

The non-vanishing anti-commutation relations for the creation and annihilation operators corresponding to conduction and impurity electrons follow from,

$$\begin{aligned} [c_{k'\sigma'}, c_{k\sigma}^\dagger]_+ &= \delta_{kk'} \delta_{\sigma\sigma'} \\ [c_{d\sigma'}, c_{d\sigma}^\dagger]_+ &= \delta_{\sigma\sigma'} \end{aligned} \quad (3)$$

We shall employ the spin-raising operators (s_+ and S_+) and the spin-lowering operators (s_- and S_-) which increases or decreases the z-component of electron spins. These are given by,

$$\begin{aligned} \hbar\sigma_+ &= s_x + is_y = s_+ ; & \hbar\Sigma_+ &= S_x + iS_y = S_+ \\ \hbar\sigma_- &= s_x - is_y = s_- ; & \hbar\Sigma_- &= S_x - iS_y = S_- \end{aligned} \quad (4)$$

where σ and Σ denote the corresponding Pauli spin matrices.

Now, we have

$$\vec{s} \cdot \vec{S} = s_x S_x + s_y S_y + s_z S_z \quad (5)$$

Using (4), we can rewrite (5) as,

$$\vec{s} \cdot \vec{S} = s_z S_z + \frac{1}{2}(s_- S_+ + s_+ S_-) \quad (6)$$

It will be convenient to write (6) in terms of the Pauli spin operators of the conduction electrons. Thus,

$$\vec{s} \cdot \vec{S} = \frac{\hbar}{2} \sigma_z \cdot S_z + \frac{\hbar}{2} (\sigma_- S_+ + S_- \sigma_+) \quad (7)$$

where (4) has been used.

To make calculations easier, we now find a simplified expression for the coupling constant $J_{kk'}$ for the spin-spin interaction. In the position space, the exchange interaction is a short-range point-like interaction. Hence, this can be represented by a Dirac delta-function. Thus,

$$J(\vec{r} - \vec{r}') = J_0 \delta(\vec{r} - \vec{r}') \quad (8)$$

where J_0 is a negative constant.

In that case, $J_{kk'}$ is the Fourier transform of (8). Using the integral representations of the Dirac delta-function,

$$\delta(\vec{r} - \vec{r}') = \frac{1}{(2\pi)^3} \int e^{i\vec{k} \cdot (\vec{r} - \vec{r}')} d\vec{k} \quad (9)$$

And the Fourier transform integral,

$$f(\vec{r}) = \frac{1}{(2\pi)^{3/2}} \int g(\vec{k}) e^{i\vec{k} \cdot \vec{r}} d\vec{k} \quad (10)$$

We easily find that

$$\begin{aligned} J_{kk'} &= \text{Fourier transform of } J(\vec{r} - \vec{r}') \\ &= \frac{J_0}{(2\pi)^{3/2}} \end{aligned} \quad (11)$$

For convenience, the constant $(2\pi)^{3/2}$ can be replaced by the constant volume V . Thus

$$J_{kk'} = \frac{J_0}{V} \quad (12)$$

Substituting (7) and (12) in the perturbation part of the Hamiltonian given in (1), we have

$$H_{\text{exch}} = -\left(\frac{J_0}{2\hbar V}\right) \sum_{k,k'} [(\Psi_k^+ \sigma_z \Psi_k) S_z + (\Psi_k^+ \sigma_- \Psi_k) S_+ + S_- (\Psi_k^+ \sigma_+ \Psi_k)] \quad (13)$$

Equ.(13) can be further simplified by expressing it in terms of the creation and annihilation operators of the conduction electron. Using the matrices for the Pauli operator we have from (4),

$$\sigma_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad ; \quad \sigma_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad (14)$$

In that case, we obtain,

$$\begin{aligned} \Psi_k^+ \sigma_z \Psi_k &= (c_{k\uparrow}^+ c_{k\downarrow}^+) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \end{pmatrix} \\ &= c_{k\uparrow}^+ c_{k\uparrow} - c_{k\downarrow}^+ c_{k\downarrow} \end{aligned} \quad (15)$$

$$\begin{aligned} \Psi_k^+ \sigma_+ \Psi_k &= (c_{k\uparrow}^+ c_{k\downarrow}^+) \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \end{pmatrix} \\ &= c_{k\uparrow}^+ c_{k\downarrow} \end{aligned} \quad (16)$$

and

$$\begin{aligned} (\Psi_k^+ \sigma_- \Psi_k) &= (c_{k\uparrow}^+ c_{k\downarrow}^+) \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} c_{k\uparrow} \\ c_{k\downarrow} \end{pmatrix} \\ &= c_{k\downarrow}^+ c_{k\uparrow} \end{aligned} \quad (17)$$

Substituting (15), (16), and (17) in (13), we then have

$$H_{\text{exch}} = -\left(\frac{J_0}{2\hbar V}\right) \sum_{k,k'} [(c_{k\uparrow}^+ c_{k\uparrow} - c_{k\downarrow}^+ c_{k\downarrow}) S_z + S_+ c_{k\downarrow}^+ c_{k\uparrow} + S_- c_{k\uparrow}^+ c_{k\downarrow}] \quad (18)$$

III. Calculation Of Rate Of Scattering

Our object is to calculate the resistivity arising due to the perturbation Hamiltonian given by (18), when a conduction electron in a given state \vec{k} gets scattered by a localized impurity d-electron into any of the final state \vec{k}' . We shall separately consider both non-spin-flip and spin-flip scattering processes. The transition rate of scattering due to first order and second order perturbation, is given by the famous Fermi's golden rule [10],

$$W_{k \rightarrow k'} = \left(\frac{2\pi}{\hbar}\right) \sum_{k'} \delta(E_k - E_{k'}) \left| T_{k'k} + \sum_{q \neq k} \frac{T_{k'q} T_{qk}}{E_k - E_q} \right|^2 \quad (19)$$

Where,

$$T_{k'k} = \langle \vec{k}' ; spin | H_{\text{exch}} | \vec{k} ; spin \rangle \quad (20)$$

is the relevant matrix element.

In (20), spin refers to impurity spin. The quantity $\sum_{k'} \delta(E_k - E_{k'})$ in (19), represents the sum over the final group of states \vec{k}' . Using the well-known equivalence,

$$\sum_{k'} = \int \frac{(4\pi k'^2 dk') V}{(2\pi\hbar)^3} \quad (21)$$

We have,

$$\begin{aligned} \sum_{k'} \delta(E_k - E_{k'}) &= \frac{4\pi V}{(2\pi\hbar)^3} \int_0^{+\infty} k'^2 dk' \delta(E - E') \\ \text{or } \sum_{k'} \delta(E_k - E_{k'}) &= \frac{V}{2\pi^2 \hbar^3} \int m \sqrt{2m} E'^{1/2} \delta(E - E') dE' \\ &= \frac{Vm}{2\pi^2 \hbar^3} \sqrt{2m} E^{1/2} \end{aligned} \quad (22)$$

Since, we are interested in states near the Fermi surface, we can write

$$E = E_F = \frac{K_F^2}{2m}$$

so that (22) reduces to

$$\sum_{k'} \delta(E_k - E_{k'}) = \left(\frac{mK_F}{2\pi^2\hbar^3}\right)V \tag{23}$$

Since (23) represents the total number of single-spin electron states, hence

$$\left(\frac{1}{V} \sum_{k'} \delta(E_k - E_{k'})\right) = \left(\frac{mK_F}{2\pi^2\hbar^3}\right) = N(0) \tag{24}$$

gives the density of such states. Thus, we can write

$$\sum_{k'} \delta(E_k - E_{k'}) = N(0)V \tag{25}$$

Using (25) in (19), we have,

$$W_{k \rightarrow k'} = \left(\frac{2\pi N(0)V}{\hbar}\right) |T_{K'K}^{(1)} + T_{K'K}^{(2)}|^2 \tag{26}$$

Where $T_{K'K}^{(1)}$ = first-order matrix element

$T_{K'K}^{(2)}$ = Second-order matrix element.

Such that

$$T_{k'k} = \langle \vec{k}'; spin | H_{exch} | \vec{k}; spin \rangle \tag{27}$$

where ‘spin’ refers to impurity spin and H_{exch} is given by (18).

(A) First Order Scattering Processes

To determine the rate of scattering of a conduction electron by the impurity electrons in the first order approximation, we have to calculate the transition amplitude $T_{K'K}^{(1)}$ appearing in (26).

The relevant diagrams for the two possible processes corresponding to the non-spin-flip and the spin-flip of the conduction electron are shown in Fig1.

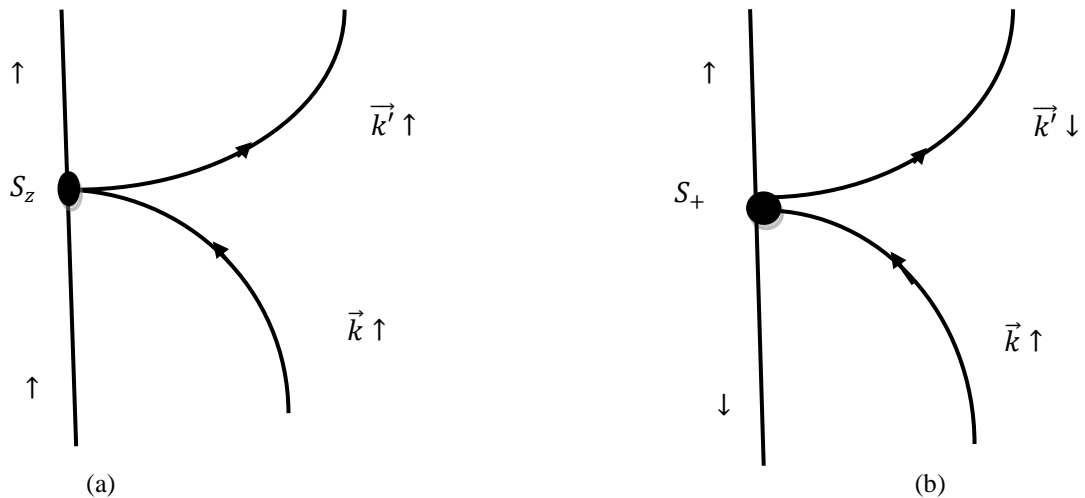


Figure 1: (a) non-spin-flip and (b) spin-flip first order scattering processes.

For the non-spin flip process shown in Fig.1a, only the first term in (18) will contribute.

We write the composite state vector of the conduction and the impurity electrons as

$$|k(\sigma_z); S, m_s\rangle = |k(\sigma_z)\rangle |S, m_s\rangle \tag{28}$$

In (28), S is the total spin of the impurity electron and $(\hbar m_s)$ is the eigen value of S_z . Using (28) and (18) in (27), we then get,

$$T_{K'K}^{(1)} = \left(-\frac{J_0}{2\hbar V}\right) \langle k'_\uparrow | c_{k'_\uparrow}^\dagger c_{k_\uparrow} | k_\uparrow \rangle \langle S, m_s | S_z | S, m_s \rangle \quad (29)$$

Since,

$$\langle k'_\uparrow | c_{k'_\uparrow}^\dagger c_{k_\uparrow} | k_\uparrow \rangle = \langle k'_\uparrow | k'_\uparrow \rangle = 1$$

and

$$\langle S, m_s | S_z | S, m_s \rangle = \hbar m_s \langle S, m_s | S, m_s \rangle = \hbar m_s \quad (30)$$

we can reduce (29) to,

$$T_{K'K}^{(1)} = -\left(\frac{J_0}{2V}\right) m_s \quad (31)$$

Substituting (31) in (26), we have for the first-order scattering,

$$W_{k \rightarrow k'}^{(1)}(\text{non-flip}) = \left(\frac{\pi}{2\hbar V}\right) N(0) J_0^2 m_s^2 \quad (32)$$

Next, we consider the spin-flip process shown in Fig.1b. As the spin of the conduction electron flips, the spin of the impurity changes as, $m_s \rightarrow m_s + 1$. Taking into account the second term in (18), we can write,

$$T_{k_\uparrow \rightarrow k'_\downarrow}^{(1)} = \left(-\frac{J_0}{2\hbar V}\right) \langle k'_\downarrow | c_{k'_\downarrow}^\dagger c_{k_\uparrow} | k_\uparrow \rangle \langle S, m_s + 1 | S_z | S, m_s \rangle \quad (33)$$

Using the well-known result [11],

$$\langle j', m' | J_\pm | j, m \rangle = \hbar [j(j+1) - m(m \pm 1)]^{1/2} \delta_{jj'} \delta_{m', m \pm 1} \quad (34)$$

We have

$$\langle S, m_s + 1 | S_z | S, m_s \rangle = \hbar \sqrt{S(S+1) - m_s(m_s + 1)} \quad (35)$$

Also

$$\langle k'_\downarrow | c_{k'_\downarrow}^\dagger c_{k_\uparrow} | k_\uparrow \rangle = \langle k'_\downarrow | k'_\downarrow \rangle = 1 \quad (36)$$

Hence, we can simplify (33) as,

$$T_{k_\uparrow \rightarrow k'_\downarrow}^{(1)} = -\left(\frac{J_0}{2V}\right) \sqrt{S(S+1) - m_s(m_s + 1)} \quad (37)$$

The corresponding transition rate of scattering is, therefore, given by

$$W_{k \rightarrow k'}^{(1)}(\text{flip}) = \left(\frac{\pi}{2\hbar V}\right) N(0) J_0^2 [S(S+1) - m_s(m_s + 1)] \quad (38)$$

The total rate of scattering is the sum of (32) and (38). Thus,

$$W_{k \rightarrow k'}^{(1)} = \left(\frac{\pi}{2\hbar V}\right) N(0) J_0^2 [S(S+1) - m_s] \quad (39)$$

When we sum over all impurities, the m_s -term in (39) vanishes. If N_i is the number of impurity electrons in V, then due to scattering by them, we shall have

$$W_{k \rightarrow k'}^{(1)} = \left(\frac{\pi}{2\hbar}\right) S(S+1) n_i J_0^2 N(0) \quad (40)$$

where n_i the density of impurities.

Now, the density of conduction electrons at $T = 0$, is given by [12],

$$n_e = \frac{K_F^3}{3\pi^2 \hbar^3} \quad (41)$$

Also, as shown earlier,

$$N(0) = \left(\frac{m K_F}{2\pi^2 \hbar^3}\right) \quad (42)$$

Hence,

$$n_e = N(0) \left(\frac{4E_F}{3}\right) \quad (43)$$

Writing the fractional concentration of impurities as

$$c = \frac{n_i}{n_e} \tag{44}$$

we can now, because of (43), rewrite (40) as

$$W_{k \rightarrow k'}^{(1)} = \left(\frac{2\pi c E_F}{3\hbar} \right) S(S+1) (J_0 N(0))^2 \tag{45}$$

The resistivity ρ is given by the well-known relation [12],

$$\rho = \left(\frac{m}{e^2 n_e} \right) W_{k \rightarrow k'} \tag{46}$$

Because of (45), it is clear from (46), that the resistivity is temperature independent in the first-order perturbation calculation. Hence Kondo effect cannot be a first-order effect.

(B) Second-Order Scattering Processes

We now calculate the second order transition amplitude $T_{K'K}^{(2)}$ in the expression for the scattering rate given in (26). This involves double scattering process as in the second Born approximation and hence we have,

$$T_{K'K}^{(2)} = \sum_{q \neq k} \frac{\langle k'(\sigma_z); S, S_z | H_{exc} | q(\sigma_z); S, S_z \rangle \langle q(\sigma_z); S, S_z | H_{exc} | k(\sigma_z); S, S_z \rangle}{E_k - E_q} \tag{47}$$

The relevant diagrams are shown in Fig.2.

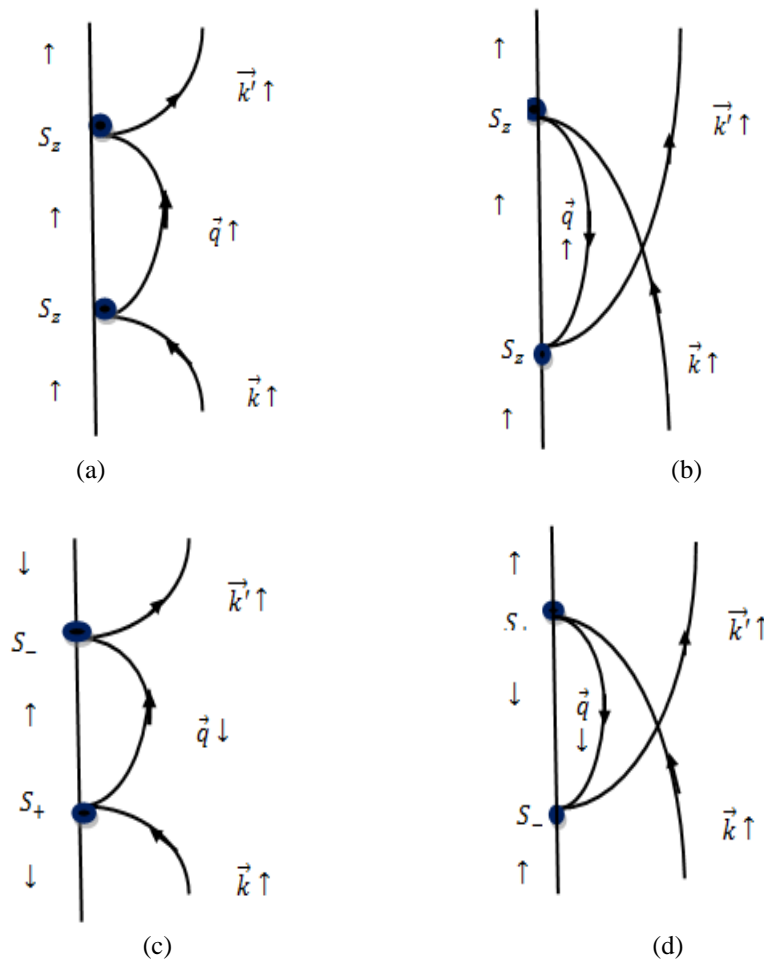


Figure 2: Second order scattering processes: (a) and (b) for non-spin-flip and (c) and (d) for spin-flip scatterings.

We first calculate $T_{K'K}^{(2)}$ for the non-spin-flip cases in (a) and (b) in Fig.2. In Fig. (2a), the initial electron $\vec{k} \uparrow$ gets scattered into an unoccupied intermediate state $\vec{q} \uparrow$, and then finally into the state $\vec{k}' \uparrow$.

We have to consider only the first term in H_{exch} . given in (18). Again, since electrons are fermions, we must use the Fermi distribution function f_q while evaluating $T_{K'K}^{(2)}$. Now, we know that

$$f_q = \text{Probability that the state } q \text{ is occupied.}$$

$$\text{And } (1 - f_q) = \text{probability that the state } q \text{ is unoccupied.}$$

Taking analogy from (29) and (30), we have from (47),

$$T_{K'K}^{(2)}(non - flip) = \left(-\frac{J_0}{2\hbar V}\right)^2 \sum_q |\langle S, m_s | S_z | S, m_s \rangle|^2 \frac{(1 - f_q)}{E_k - E_q}$$

$$= \left(-\frac{J_0}{2\hbar V}\right)^2 (\hbar m_s)^2 \sum_q \frac{(1 - f_q)}{E_k - E_q} \quad (48)$$

We have multiplied by the factor $(1 - f_q)$ to emphasized that the state $\vec{q} \uparrow$, is unoccupied.

Defining

$$p(k) = \frac{1}{V} \sum_q \frac{1 - f_q}{E_k - E_q} \quad (49)$$

We rewrite (48) as,

$$T_{K'K}^{(2)}(non - flip) = \left(-\frac{J_0 m_s}{2}\right)^2 \left(\frac{p(k)}{V}\right) \quad (50)$$

Fig.(2b) corresponds to the case where the intermediate state \vec{q} is occupied. The transition amplitude, in this case is the same as in (50), except that $p(k)$ must be replaced by

$$h(k) = \frac{1}{V} \sum_q \frac{f_q}{E_k - E_q} \quad (51)$$

Hence, for Fig. (2b), we have

$$T_{K'K}^{(2)}(non - flip) = -\left(\frac{J_0 m_s}{2}\right)^2 \left(\frac{h(k)}{V}\right) \quad (52)$$

The total transition amplitude is the sum of (50) and (52), and is given by

$$T_{non-flip}^{(2)}(\vec{k} \uparrow \rightarrow \vec{k}' \uparrow) = \left(-\frac{J_0 m_s}{2V}\right)^2 \sum_q \left(\frac{1}{E_k - E_q}\right) \quad (53)$$

In (53), the Fermi-distribution functions get cancelled. Thus, the transition amplitude given by (53) is independent of temperature and hence the resulting resistivity. We, therefore, conclude that the second-order scattering involving no-spin-flip process cannot give rise to Kondo effect.

To get temperature-dependent resistivity, it is necessary to consider the scattering processes in Fig.(2(c) and (2d)), where spin-flip occurs in the intermediate state for both the conduction and the impurity electrons.

In this spin-flip case, the second and the third terms in (18) will contribute. Substituting these in (47) and referring to Fig. (2c), we have

$$T_{K'K}^{(2)} = \left(-\frac{J_0}{2\hbar V}\right)^2 \sum_q \langle S, m_s | S_- | S, m_s + 1 \rangle \langle S, m_s + 1 | S_+ | S, m_s \rangle \times \left(\frac{1 - f_q}{E_k - E_q}\right) \quad (54)$$

But $\langle S, m_s | S_- | S, m_s + 1 \rangle = \langle S, m_s + 1 | S_+ | S, m_s \rangle^*$

Using this result in (54), we obtain

$$T_{K'K}^{(2)} = \left(\frac{J_0}{2\hbar V}\right)^2 \sum_q |\langle S, m_s + 1 | S_+ | S, m_s \rangle|^2 \left(\frac{1 - f_q}{E_k - E_q}\right) \quad (55)$$

Making use of (34) and (49) in (55), we then get

$$T_{KK}^{(2)} = \left(\frac{J_0}{2}\right)^2 \left(\frac{1}{V}\right) [S(S+1) - m_s(m_s+1)]p(k) \tag{56}$$

In the same way the contribution from Fig.(2d) will be given by

$$T_{KK}^{(2)} = \left(\frac{J_0}{2}\right)^2 \left(\frac{1}{V}\right) [S(S+1) - m_s(m_s-1)]h(k) \tag{57}$$

where $h(k)$ is given by (51).

We rewrite (57) as

$$T_{KK}^{(2)} = \left(\frac{J_0}{2}\right)^2 \left(\frac{1}{V}\right) [S(S+1) - m_s(m_s+1) + 2m_s]h(k) \tag{58}$$

The total contribution from the two spin-flip processes is given by the sum of (56) and (58). We thus get,

$$T_{flip}^{(2)} (\vec{k} \uparrow \rightarrow \vec{k}' \uparrow) = \left(\frac{J_0}{2}\right)^2 \left(\frac{1}{V}\right) [2m_s h(k) + \{S(S+1) - m_s(m_s+1)\} \times (p(k) + h(k))] \tag{59}$$

In (59), the second term involving $(p(k) + h(k))$ will be temperature-independent and hence it will be ignored. However, the first term in (59) containing $h(k)$ will be temperature-dependent. Retaining this term, we have,

$$T_{flip}^{(2)} (\vec{k} \uparrow \rightarrow \vec{k}' \uparrow) = \left(\frac{J_0}{2}\right)^2 \left(\frac{1}{V}\right) (2m_s h(k)) = \left(\frac{J_0^2 m_s}{2V}\right) h(k) \tag{60}$$

To calculate $h(k)$ in (60), we convert the summation over q into an integral and we write,

$$h(k) = \frac{1}{V} \int_0^{k_F} \frac{(4\pi q^2 dq)V}{(2\pi\hbar)^3} \left(\frac{1}{\frac{k^2}{2m} - \frac{q^2}{2m}}\right) \tag{61}$$

where we have used the fact that $f_q = 1$, at $T=0$.

Equ.(61) can be expressed in terms of $N(0)$ as,

$$h(k) = \frac{2N(0)}{k_F} \int_0^{k_F} \left(\frac{q^2}{k^2 - q^2}\right) dq \tag{62}$$

The integral in (62) can be evaluated as,

$$\begin{aligned} \int_0^{k_F} \left(\frac{q^2}{k^2 - q^2}\right) dq &= - \int_0^{k_F} dq + \frac{k}{2} \int_0^{k_F} \left(\frac{1}{k+q} + \frac{1}{k-q}\right) dq \\ &= -k_F - \frac{k}{2} \ln \left| \frac{k - k_F}{k + k_F} \right| \end{aligned} \tag{63}$$

Now, for $T \neq 0$, but $T \ll T_F$, the range of k -values for the thermally excited electrons is determined by,

$$\left| \frac{k^2}{2m} - \frac{k_F^2}{2m} \right| \approx k_B T \quad (k_B \text{ is the Boltzmann constant})$$

This gives,

$$|k - k_F|(k + k_F) \approx 2mk_B T$$

and hence,

$$\left| \frac{k - k_F}{k + k_F} \right| \approx \frac{mk_B T}{2k_F^2} = \frac{mk_B T}{4mE_F} = \frac{1}{4} \left(\frac{T}{T_F}\right) \tag{64}$$

where we have used the results,

$$k_F^2 = 2mE_F \quad \text{and} \quad E_F = k_B T_F$$

Substituting (64) in (63), we obtain

$$\int_0^{k_F} \left(\frac{q^2}{k^2 - q^2}\right) dq = -k_F - \frac{k}{2} \left[\ln \left(\frac{1}{4}\right) + \ln \left(\frac{T}{T_F}\right) \right]$$

Writing $k \approx k_F$ and ignoring the constant terms, and then substituting the result in (62), we get

$$h(k) = N(0) \ln \left(\frac{T_F}{T} \right) \tag{65}$$

Using (65) in (60), we have

$$T_{flip}^{(2)}(\vec{k} \uparrow \rightarrow \vec{k}' \uparrow) = \left(\frac{J_0^2 m_s}{2V} \right) N(0) \ln \left(\frac{T_F}{T} \right) \tag{66}$$

To get the total transition amplitude, we have to add $T^{(1)}(\vec{k} \uparrow \rightarrow \vec{k}' \uparrow)$ given by (31) to (66). We arrive at the result,

$$T(\vec{k} \uparrow \rightarrow \vec{k}' \uparrow) = \left(-\frac{m_s}{2V} \right) J_0 \left[1 - J_0 N(0) \ln \left(\frac{T_F}{T} \right) \right] \tag{67}$$

If we compare (67) with (31), we see that in the second-order corrections, we should replace J_0 by the temperature-dependant term, as follows,

$$J_0 \Rightarrow J_0 \left[1 - J_0 N(0) \ln \left(\frac{T_F}{T} \right) \right]$$

Using this replacement in (45), we then get,

$$W_{k \rightarrow k'} = \left(\frac{2\pi E_F}{3\hbar} \right) c S(S+1) N(0)^2 J_0^2 \left[1 - 2J_0 N(0) \ln \left(\frac{T_F}{T} \right) \right] \tag{68}$$

In writing (68), we have retained terms up to third power in J_0 .

To compare our results with experiments, it will be convenient to rewrite (68) as,

$$W_{k \rightarrow k'} = W(0) \left[c - 2cJ_0 N(0) \ln \left(\frac{T_F}{T} \right) \right] \tag{69}$$

Where $W(0) = \left(\frac{2\pi E_F}{3\hbar} \right) S(S+1) N_0^2 J_0^2$ is clearly independent of temperature and impurity concentration, and hence a constant for a given host metal.

Using the expressions for ρ given by (46), we have,

$$\frac{\rho_{imp}(T)}{\rho(0)} = c - 2J_0 N(0) c \ln \left(\frac{T_F}{T} \right) \tag{70}$$

Ignoring the first term in (70), we have the following expression for the variation of $\rho_{imp}(T)$ with temperature and concentration of impurities.

$$\frac{\rho_{imp}(T)}{\rho(0)} = -2J_0 N(0) c \ln \left(\frac{T_F}{T} \right) \tag{71}$$

At very low temperatures, there is also a contribution to $\rho(T)$, due to only electron-phonon scattering. This is given by [12],

$$\frac{\rho_{ph}(T)}{\rho(0)} = aT^5 \tag{72}$$

The sum of (71) and (72) gives the total resistivity of a host metal containing magnetic impurities. Thus we have

$$\frac{\rho(T)}{\rho(0)} = aT^5 - 2J_0 N(0) c \ln \left(\frac{T_F}{T} \right) \tag{73}$$

It is the quantity given by (73) which is measured experimentally. For comparison with experiment, we note that the second term in (73) is positive since J_0 is negative for anti-ferromagnetic coupling of spins. We now consider the following representative values of the parameters in (73), taken from [13],

$$\begin{aligned} N(0) &\approx n_e \approx 10^{22} \text{m}^{-3} \\ |J_0| &\approx 0.02 \text{eV} = 3.2 \times 10^{-21} \text{J} \end{aligned} \tag{74}$$

$$\begin{aligned} T_F &\approx 10^4 \text{K} \\ a &\approx 10^{-10} \text{K}^{-5} \end{aligned}$$

Using (74) in (73) and taking two values of c corresponding to 0.05% and 0.1% impurity, we present the theoretical results in Fig.3.

The corresponding experimental results for Cu with Fe impurities are shown in Fig.4.

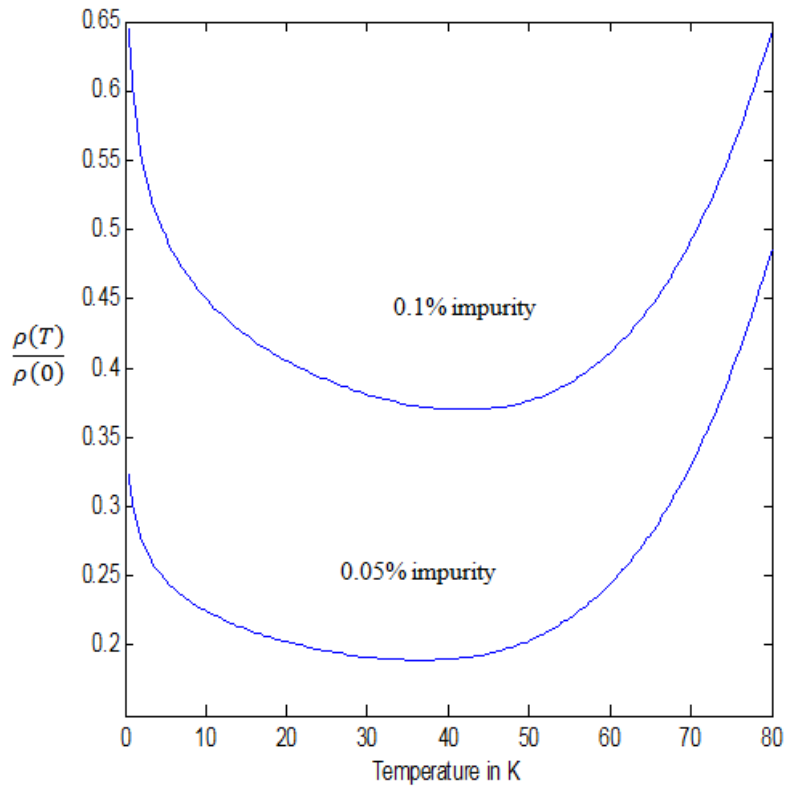


Figure 3: Temperature variation of resistivity, $\frac{\rho(T)}{\rho(0)}$, showing clearly the appearance of resistivity minimum.

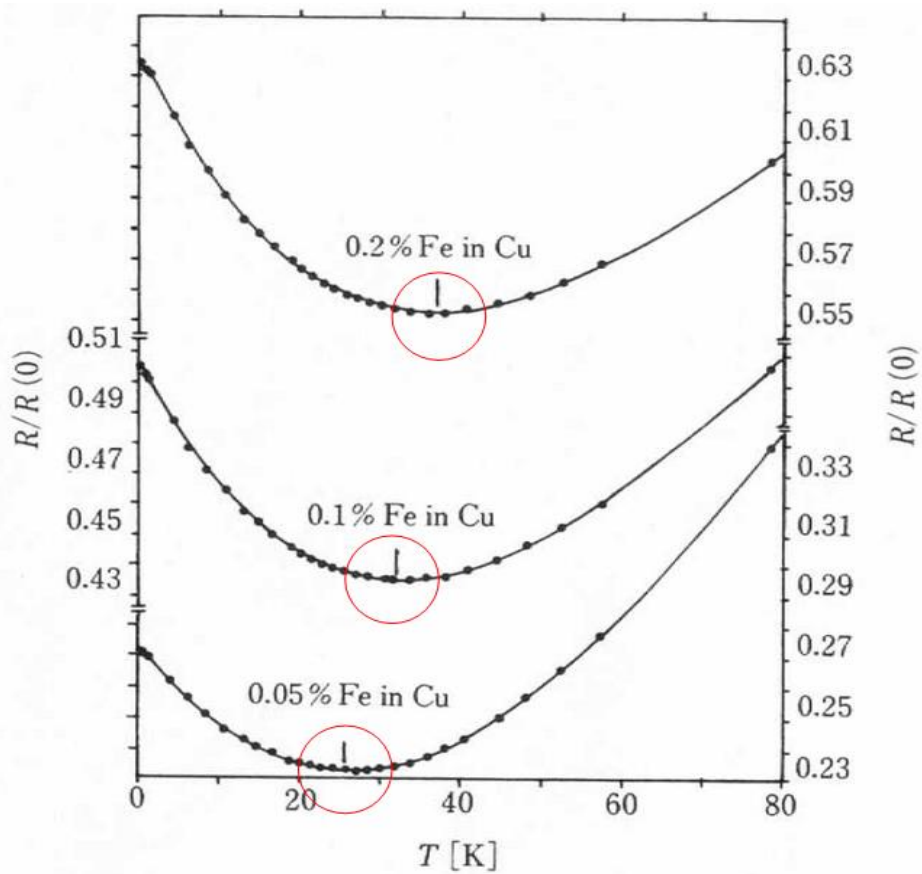


Figure 4: Resistances at low temperatures for Cu with 0.05%, 0.1% and 0.2% of Fe impurities.

The theoretical curves in Fig.3. Indicate how for a general host metal containing magnetic impurities, the low-temperature resistivity behaves, showing clearly the logarithmic increase and the existence of a resistivity minimum. The theoretically predicted trend is in agreement with the experimental observations shown in Fig.4. It should be emphasized that experimentally one determines resistivity for a specified alloy of a non-magnetic metal and magnetic impurities. The results from alloy to alloy differ in specific details but still retaining similar trends.

IV. Conclusion

In this work, we have presented a quantum mechanical formulation of the anomalous behavior of the low-temperature resistivity of a metal in the presence of magnetic impurities. The results indicate that the Kondo effect is a very subtle physical phenomenon which manifests itself only as a second order perturbation in the spin-exchange interaction Hamiltonian. The existence of a resistivity minimum and the logarithmic increase in resistivity are clearly brought out. The theory presented is quite impressive and successful, considering the high level of complexities of physical mechanisms involved in the Kondo effect

References

- [1]. W. J. De Hass, De Boer, and G. J. Van Den Berg, *Physica*, vol. 1, 1934, p 1115-1124.
- [2]. H. Shiba, *Kofainodenshiron Marazen*, vol. 82, 1996, p 852- 870.
- [3]. J. Kondo, *Progress of Theoretical Physics*, vol. 32, 1964, p 37-49.
- [4]. K. Sengupta and G. Baskaran, *Phys. Rev. B*, vol. 77, 2008, p045417.
- [5]. Jian-Hao Chen, Liang Li, Williams G.Cullen and Michael S.Fuhrer, *Nature Physics*, vol. 7, 2011, p 535-538.
- [6]. M. Vojta, L. Fritz and R. Bulla, *Europhys. Lett.*, vol. 90, 2010, p 27006.
- [7]. H. Jeong, A. M. Chang, and M. R. Melloch, *Science*, vol. 293, 2001, p 2221-2223.
- [8]. Sara M. Cronewett, T. H. Oostervamp, and X.P. Kouwenhoven, *Science*, vol.281, 1998, p 540 -544
- [9]. T. O. Wehling, S. Yuan, A. I. Lichtenstein, A. K. Gein and M. I. Katsnelson, *Phys. Rev. Lett.*, vol. 105, 2010, p 056802.
- [10]. J. J. Sakurai, *Modern Quantum Mechanics*, 1993, Revised Ed., Boston: Addison Wesley.
- [11]. B. H. Bransden and C. J. Joachain, *Quantum Mechanics*, 2000, Pearson Ed. Ltd., England, p 296-297.
- [12]. N. W. Ashcroft and N. D. Mermin, *Solid State physics*, 1976, Suanders College, New York.
- [13]. H. J. Noh, T. U. Nahm, J. Y. Kim, W. Q. Park and C. O. Kim, *Solid State Communicatins*, vol. 116, 2000, p 134-141.