

**THE ANOMALOUS LOW TEMPERATURE
ELECTRICAL
RESISTIVITY PROPERTIES
OF DILUTE MAGNETIC ALLOYS**

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BY

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To my parents.....

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ABSTRACT

The existence of localized magnetic moments in dilute magnetic alloys that couple to the conduction electrons has important consequences for the electrical resistivity. The magnetic impurities act as scattering centers, and if they are the predominant type of impurity then at low enough temperature the scattering causes the electrical resistivity. The exchange interaction between the conduction and the localized moments leads to scattering events in which the electron spin is flipped. Calculating the transition probabilities of the conduction electrons to the third order of interaction it is shown that the transition probability has a logarithmic anomaly at the Fermi-surface and that in the resistivity there appears a term proportional to $\ln T$ and diverges as the temperature approaches zero.

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CHAPTER-ONE

INTRODUCTION

The electrical resistivity can be considered as a sum of two independent parts, one of which is a function of purity of the metal and the other a function of temperature characteristics [*Mathiessen's rule*] of the pure metals $\rho(T) = \rho_i + \rho_0(T)$. The addition of further impurities to the metal is then predicted to displace the curve of $\rho(T)$. At low temperatures, much lower than the *Debye* temperature the resistivity of a metal should be given by an expression of the form $\rho_{(T)} = \rho_0 + AT^5$. Here, the electron- phonon scattering contributes T^5 behavior while the impurities in the metal give rise to the constant term ρ_0 , provided that the impurity scattering is elastic. If the scattering is inelastic, then variety of interesting phenomena may occur.

When a metal such as copper is doped with magnetic impurities, whose spin states introduce an extra degree of freedom in to scattering problem, interaction between the spins of the conduction electron and those of the impurities then provides mechanisms for inelastic scattering of the conduction electrons. That is why considerable attention has been directed towards understanding of localized magnetic states in magnetic alloys.

The magnetic impurities can be found in three classes. They are the transition metals (i.e. iron and manganese), the rare earth's such as cerium, and actinides (the most important is uranium). The origin of the magnetic character of these groups is partially filled inner d – or f – shells. For transition metals $3d$ -shell and for rare earth's the $4f$ – shell that remains only partially filled even though the outer valance states (i.e. $4s$ and $5s$ respectively) also contains electrons. According to [1] this situation appears because the centripetal force experienced by the electron in the state of the higher orbital angular momentum like a $3d(4f)$ states, causes its wave function to vanish at the nucleus, and so it resides in a region where the coulomb potential of the nucleus is partially screened. Although the $5s$ state extends much further from the nucleus than that of the more localized $4f$ – state, it suffers no centripetal force.

The process where charge is transported is under the influence of the existence of forces or fields are known as transport phenomena. The scattering of electron is determined by various mechanisms in electron-lattice system, which disturbs the periodicity (impurity, thermal vibration, etc). It turns out that the magnetic properties, the degenerate statistics of current carriers and the existence of the Fermi surface are crucial for transport phenomena.

The theoretical description of transport phenomena includes a number of parameters such as concentration (n) and charge sign of current carriers (e), parameters of various interactions (electron-lattice, electron-impurity, electron-spin, electron-electron). The interactions influence the mean free path and relaxation time. The simplest expression for the electrical resistivity is given in equation (2.5).

For most materials, the situation given in equation (2.5) is more complicated due to the presence of several current carriers and different scattering mechanisms. The main problem of the microscopic theory in such a situation is separating these

factors and determining their contributions. This problem is important for transition metal and their alloys that demonstrate a great variety of transport phenomena.

There are some special situations, which occurs in comparison to simple metals. For instance existence of current carriers with strongly different characteristics ("s" and "d" electrons); even though 4f – electrons usually do not take part in the conductivity they may influence the current carriers due to s – f hybridization in rare earth compounds [2]. In addition to these, presence of internal partially filled d – shell may be subsidiary scattering source (due to s – d transition). Because of occurrence of additional scattering mechanisms by d – and f – shells magnetic moments may induce anomalous transport phenomena which are connected with the magnetization of d(f) ions rather than with the external magnetic field.

In the case of transition metal based alloys, it is probable that the s-d scattering provides an important contribution to the resistivity. This means that the coupling of the s-electrons to the impurity spin should be taken in-to account [3]. At high temperatures, the spin of an isolated magnetic impurity flips about freely, presenting a small isotropic scattering potential to incoming electrons. At low temperatures by pointing in definite direction, the magnetic impurity becomes more effective in scattering electron [4].

The thesis is organized as follows. The second chapter explores metals containing a dilute concentration of magnetic impurities; and look at the consequence of increasing the concentration and the criteria of low concentration limit. The electrical resistivity of different scattering mechanisms is described theoretically. The third chapter deals with conduction and transport phenomenon, which is beginning with the general formulation of this transport phenomena, investigation of electrical conductivity is shown in the chapter. Scattering aspects and interaction of conduction electrons with the magnetic ions are discussed in the fourth chapter. In

addition to this, Born approximations to scattering processes are described. Finally, in the fifth chapter the anomalous electrical resistivity contributed from scattering of conduction electrons by magnetic impurity at low temperature are presented using Born approximation. Chapter six is discussion and conclusion and the last part is the references.

CHAPTER –TWO

REVIEW OF LITERATURE

2.1 Transition Metals

The transition metals lying in columns 3-8 of periodic table are not described by the nearly free electron model. That is the three rows of the periodic table extending from the alkali earths (Ca, Sr, Ba) to the noble metals (Cu, Ag, and Au) each contain nine transition metals, in which the d –shell that is empty in the alkali earths and completely filled in the noble metals, is gradually filled in. All are metals but their properties are to considerable degree dominated by d –electrons. Band calculations have shown that the d – band not only lies high up the conduction band (as in the noble metals) but also in general (unlike the noble metals) extends through the Fermi energy.

The d - bands are narrower than nearly free electron conduction band, and can accommodate ten-electron levels. Because of having more levels in the narrower energy range, the density of levels is likely to be substantially higher than free electron density of levels. The effect can be observed in the electronic contribution of the low temperature specific heat. Furthermore, studies of transition metals are complicated by the fact that the partially filled d – bands can give raise to striking magnetic properties.

2.1.1 Magnetic Properties of Transition Metals

Many compounds of transition elements are paramagnetic because of unpaired electron spins in the atom. From the transition elements iron, cobalt, and nickel are ferromagnetic. Paramagnetism arises where there is one or more unpaired electrons in the compound. The unpaired electron gives rise to a magnetic field because of its spin, and because of the angular orbital momentum. The general equation for the magnetic moment of the first row of the transition metal ion is [6]

$$\mu_{S+L} = \hbar \sqrt{4S(S+1) + L(L+1)} , \quad (2.1)$$

where S - is the sum of spin quantum number and L is the sum of the orbital momentum quantum number. For an electron, the spin quantum number m has value $\pm 1/2$ hence $S = m.n$ where n is the number of unpaired electrons.

In many compounds including the first row of transition elements, the orbital contribution is quenched out by the electric fields of the surrounding atoms. So that, the magnetic moment may be considered to arise only from unpaired spins.

$$\mu_S = \hbar \sqrt{4S(S+1)} . \quad (2.2)$$

In some second and third row transition elements, the orbital motion is not quenched or prevented, and more complicated formula involving J which is obtained from coupling of L and S quantum numbers is used. That is

$$\mu = g\hbar \sqrt{J(J+1)} , \quad (2.3)$$

where $g = 1 + \frac{S(S+1) - L(L+1) + J(J+1)}{2J(J+1)}$, is lande factor.

2.2 The Rare Earth Metals

The elements between lanthanum and hafnium are rare earth elements, and are chemically very similar due to an almost identical outer electron arrangement [5]. Their electronic configurations are characterized by partially filled $4f$ – shells. The $4f$ –electrons shell are very effectively screened from effects at the outside of the atom by the $5s$ and $5p$ electrons.

The atomic $4f$ – orbital in the rare earth elements are much localized than the highest occupied atomic d –levels in the transition metal elements. Electron-electron interactions among the $4f$ –electrons at each atomic site are strong enough to yield local magnetic moments. The $4f$ – band in the rare earths splits in to two narrow parts; one fully occupied well below the Fermi level, and the other completely empty.

The rare earths do however have different occupation numbers on the shallow inner $4f$ - shell ranging from zero to 14 through the series La to Lu. This changing $4f$ - occupation means that the rare earth elements and their compounds have wide range of different magnetic properties and electronic structures.

2.2.1 Magnetism in Rare Earth Metals

The magnetic properties are the fundamentally different from those of transition elements. Since the $4f$ – electrons are well shielded from external fields by the

overlying $5s$ and $5p$ electrons, the magnetic effect of the motion of the electron in its orbital is not quenched out, and magnetic moments must be calculated taking in account of both spin and orbital contributions [6]. However, the magnetic moments of the rare earth metals are dominated by the spin contribution from the highly localized $4f$ –electrons, and are thus good examples of local–moment ferromagnetism.

2.3 Metallic Alloys

An alloy is a solid solution. It differs from chemical compounds in that, in a solid solution the range of concentration of the solute relative to the solvent may vary, while in chemical compounds this concentration is fixed [7]. According to [8], the theory of band structure of solids assumes that crystal has translational invariance. However, crystal composed of two elements. A and B that occupies at random regular lattice sites of the structure, is proportional to X and $(1 - X)$ for composition A_XB_{1-X} . The translational symmetry is no longer perfect.

Alloys are conventionally grouped into two classes [9], *ordered* and *disordered*. The former one has translational symmetry of the *Bravais* lattice. An alloy is disordered if the A and B atoms are randomly arranged, which occurs for a general value of X in the composition A_XB_{1-X} .

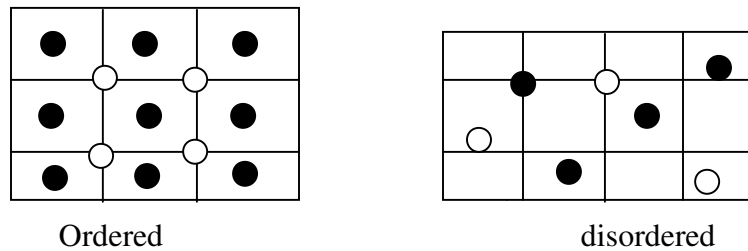


Figure 1: Ordered (a) and disordered (b) arrangements of AB ions in the alloy AB

2.3.1 Alloy and Residual Resistivity

In principle, all kinds of lattice imperfections (impurity atoms, vacancies interstitials, etc) contribute to resistivity. If, however, we speak of the residual resistivity we usually mean the resistivity which is left over at very low temperature, and hence it is known as low temperature predominant resistivity. It is temperature independent constant value [10], and proportional to the density of imperfections that cause it.

The residual resistivity is of great importance for the situation in mixed crystals (alloy). By this we mean crystals in which two or more kinds of atoms are randomly distributed over the lattice positions. The term $X(1-X)$ is the measure of the degree of maximum disorder possible for a given value of X [2]. In this way the residual resistivity is proportional to the total contents of the imperfections, $X(1-X)$. As an example the effect for the alloy made from copper and gold (Cu-Au) as shown bellow.

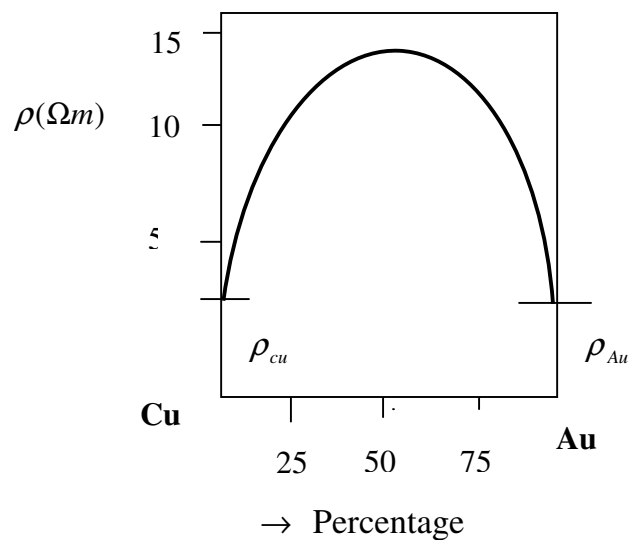


Figure 2: Resistivity of a gold-copper alloy as a function of the mixing ratio [7].

When the specimen is cooled from high temperature, ordered structures are formed at Cu_3Au and CuAu . From this, one can speculate that, residual electrical resistivity can be used to measure the effect of alloying in disordered structure. As an example [7] one atomic percent of copper dissolved in silver (which lies in the same column of periodic table) increases the residual resistivity by $0.077 \mu\Omega\text{cm}$

In transition metals, the availability of the $3d$ -band as a path for the conduction in parallel with the $4s$ -band would increase the conductivity, but this is not the way it works out. The resistivity of the s -electron path is increased by the collisions with the d - electrons; this is a powerful extra scattering mechanism not available when the d - band is filled.

2.4 Localized Moments in Alloys

Localized moments are the origin of magnetism in insulators, and in metals, their interaction with the mobile charge carriers changes the nature of metallic state. Because of this fact, in this section, we will see which conditions are required to have or not to have magnetic moments on the $3d$ – or the $4f$ - impurities, which are dissolved in a metal. When a small amount of transition metal elements are dissolved in a non-magnetic metal the resulting alloy may display a localized moment [12]. Using Hund's rule the moments of the free ion can be determined. Magnetic measurements provide a useful criterion for the localized moment; if the impurity contributes a *Curie Weiss* temperature term to the magnetic susceptibility, then there is a localized moment. If there is no temperature-dependent contribution, there is no localized moment.

$$\chi = N_A \frac{\mu_B^2 g^2 S(S+1)}{3k_B T}. \quad (2.4)$$

The following table is characterized by the equation 2.4

Host	Impurities						
	Ti	V	Cr	Mn	Fe	Co	Ni
Cu	—		×	×	×	—	—
Ag			×	×	×		
Au	—	×	×	×	×	×	—
Zn	—	—	×	×	—	—	—
Al	—	—	—	—	—	—	—

Table 1: Presence “×” or absence “—” of localized moments when transition metal impurities are dissolved in non-magnetic hosts [9].

Here “×” indicates a Curie-Weiss behavior (presence) “—” indicates a temperature independent Pauli like susceptibility.

Many experimental observations indicate that an impurity becomes magnetic if it is embedded in a host metal exhibiting a small electronic density of states at the Fermi energy. In contrast to this, a large electronic density of states causes the vanishing of the Curie-Weiss behavior.

The low concentration limit of the metal in which the conduction electrons interact with impurity atoms, each of which has two localized electron spin states (spin up and spin down states). In this limit (dilute limit) the impurities are far enough apart that the interaction between them can be neglected. The impurities can then be

treated as independent and we can study this system by considering a single magnetic impurity in a non-magnetic metal. In other words the low concentration limit, we can ignore interaction between impurities. With increasing impurity concentration the wave functions start to overlap and the impurity are no longer independent of each other. If the impurities are sufficiently dilute, the potential describing the interaction between electron and a single impurity is sufficiently weak [2]. Sufficiently dilute mean that treating electrons as interacting with one impurity at a time.

2.5 The Indirect Exchange Interaction

Under favorable circumstance [12], an isolated impurity in a simple metal may form a local moment. This is a cooperative effect arising from the interaction of two electrons on a single ion. From this, we may imagine that with many local moments present there might be interaction between these, and a cooperative alignment of these moment occur.

There will of course be a direct magnetic interaction between the magnetic moments on individual impurities but this is always very small. There is also an interaction moments through the electron-electron interaction. Physically this interaction between moments arises from the conduction electron scattering from one impurity, sensing the corresponding local spin, propagating with the spin information to the second impurity, and scattering from the second in a way dependent up on its local spin.

In other world, the conduction electron gas is magnetized in the vicinity of magnetic ion. The magnetization causes an indirect exchange between the magnetic ions, because a second ion perceives the magnetization induced by the first ion. It is this interaction known as indirect interaction.

2.6 The electrical Resistivity

In this section the contributions of electrical resistivity (impurity, ρ_i , phonon, ρ_{ph} , magnetic, ρ_{mag} , Motto s-d scattering, ρ_{sd} , electron-electron, ρ_{ee} , an so on) will be discussed after introducing the general definition of resistivity according to *Drude* formula i.e.:

$$\rho = \frac{m}{ne^2\tau}, \quad (2.5)$$

where e the electron charge and τ is the relaxation time for scattering processes. The relaxation time describes the particular scattering events, which are subject to the conduction electrons. Theoretically, the relaxation time follows from the velocity of the conduction electrons \bar{v} , which are scattered after a certain mean free path. The relaxation time for simple metals is mainly determined by scattering processes of conduction electrons on static lattice imperfections like impurity atoms, grain boundaries, phonon, etc. For independent scattering

$$\frac{1}{\tau} = \sum_i \frac{1}{\tau_i}. \quad (2.6)$$

2.6.1 Resistivity from Electron-Electron Scattering

One of the important scattering mechanism is electron-electron scattering. The scattering probability of this interaction is to be proportional to T^2 . Since the potential energy of the interaction between electrons is of the same order as their kinetic energy, the relaxation time, τ can only be of the form [13]

$$\tau \approx \hbar\mu/T^2. \quad (2.7)$$

The corresponding contribution to the resistivity varies as T^2 .

2.6.2 Resistivity from Scattering by Lattice Vibration

A real scattering process requires a finite momentum and energy transfer from the electron to the lattice and vice versa [13]. Excited states of an electron can be described in terms of the phonon picture (vibrational quanta). A scattering process can therefore be viewed as the emission or absorption of phonon by an electron, so that the process takes place at temperature different from zero. For temperature larger than *Debye* temperature [4] the resistivity varies with T^5 , for much larger temperature the resistivity is linear in temperature. At the lowest temperature, the number of phonons decreases rapidly with lowering temperature as a result the resistivity varies as T^2 for simple metals.

2.6.3 Mott s-d Scattering Mechanisms

An independent mechanism for the resistivity of transition metals is the *s-d* scattering considered by Mott [15]. This mechanism is based on the assumption that an appreciable part of scattering corresponds to transitions of main current carriers (*s-electrons*) to the unoccupied part of *d-band*, the states of which possess much smaller mobility. Such interband transitions may occur due to any scattering mechanism (impurities, phonons, spin excitations etc.), their probability being large because of high density of *d-states* near the Fermi level.

The Mott's model is widely used to explain concentration dependences of resistivity of transition metal alloys. In particular, the resistivity decreases at filling of *d-shells*

of transition metal ions by electrons of another alloy component, which results in prohibition of *s-d* transitions.

2.6.4 Resistivity of Magnetic Metals

If in addition to the already mentioned scattering processes, an interaction of conduction electron with magnetic moments takes place, a further resistivity term has to be considered. Existence of magnetic moments in transition elements results in additional factors which influence the behavior of current carriers in external electric field [15]. First, thermal fluctuations in the system of magnetic moments provide a new scattering mechanism owing to *s-d exchange* interaction. Second, electron spectrum of magnetic crystals depends appreciably on spontaneous magnetization (or sublattice magnetization in antiferromagnets) and, consequently, on temperature.

If only local magnetic moments are considered using perturbation type of calculation in the scope of Heisenberg model give the result for the magnetic resistivity at high temperature (for paramagnetic region) is given by

$$\rho_{mag} = \frac{3\pi}{2} \frac{m}{\hbar e^2} \frac{J^2}{E_F} S(S+1). \quad (2.8)$$

2.6.5 Resistivity of Transition Metal Alloy

Investigation of transport phenomena in alloys as a function of concentration of various components gives a possibility to obtain information on their electron structure. In particular, data on concentration dependence of residual resistivity $\rho(X)$ in transition metal alloys yields important information on change of *d*-states.

In disordered alloys of simple metals with the same valence, (metals with different valence do not form usually the continuous solid solution series), the contribution to residual resistivity [15] is

$$\rho(x) = \rho_o X(1 - X) . \quad (2.9)$$

In transition metal alloys, the symmetry of $\rho(x)$ curve can be is violated due to variation of X. An explanation of this violation can be obtained within the Mott s-d transition model. To demonstrate this we write down the conductivity of the alloy A_xB_{1-x} , with atoms A being a transition metal and B a simple metal, in the form equation (2.10).

Experimentally it is observed that [4] a resistivity minimum appears when local moments develop in materials. For example resistivity data for Mo_xNb_{1-x} alloy shows a local moment develops for $X > 0.4$, and the resistivity develop a minimum beyond this point as shown in the figure 3.

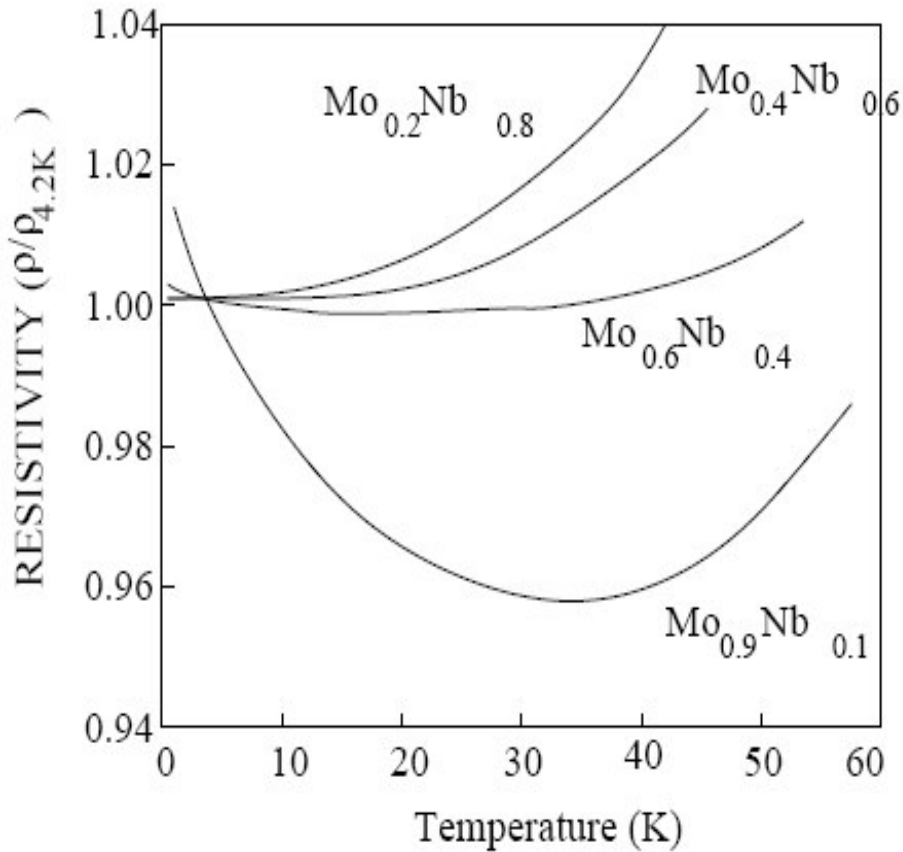


Figure 3: Sketch of resistance minimum in $\text{Mo}_x\text{Nb}_{1-x}$ [4]

It is explained in the literatures [2, 3, 4] that the occurrence of resistivity minimum is said to be Kondo effect. The occurrence of a resistivity minimum is connected with the existence of localized magnetic moments on the impurity atoms.

The resistivity minimum for various dilute alloys of iron and copper was also shown experimentally. The result of the experiment has confirmed that the position of the minima depends on the concentration of iron [9]. Temperature for minimum resistivity of 0.05%Fe in Cu is approximately 26K.

CHAPTER-THREE

TRANSPORT AND CONDUCTION PHENOMENA

Conduction phenomena occur through the motion of electrons, on the one hand, are affected by external fields and, on the other hand, are interacting with the lattice, impurities, etc. In addition to the interaction, the effects of the external field appear afresh therefore [16]. This problem is covered by the transport equation, which gives the deviation of the electron distribution from the equilibrium state, which is essential for the conduction phenomena.

Electronic transport phenomena have played a great role in formulation of principal statements of the quantum solid-state physics. In particular, the classical theory does not explain the finite value of electrical resistivity at absolute zero, which should be determined by cross sections of electron scattering by impurity ions. In quantum theory, electrons in a periodical crystal are described by Bloch states with a definite wavevector \vec{k} and carry current without a loss of energy. The scattering of electrons is determined by various mechanisms in electron-lattice systems that disturb the periodicity (impurities, thermal vibrations etc.).

The theoretical description of transport phenomena includes a number of parameters: concentration, n , and charge sign of current carriers, e , effective mass, m^* , electron velocity at the Fermi level v_F , parameters of various interactions:

electron-lattice, electron-impurity, electron-spin, electron-electron. These interactions influence not only energy spectrum, but also the mean free path, and the relaxation time. The simplest expression for the electrical conductivity derived from equation (2.5) is:

$$\sigma = (\rho)^{-1} = \frac{e^2 n \tau}{m^*}. \quad (3.1)$$

In real substances, the situation is more complicated due to presence of several groups of current carriers, combined influence of different scattering mechanisms and so on. Main problem of the microscopic theory in such a situation is separating these factors and determining their relative contributions. This problem is rather important for transition metals, which demonstrate a great variety of transport phenomena. For our case, we pay especial attention to peculiarities, which occur in comparison with simple metals.

3.1 Calculating the Transport Coefficient

To evaluate transport coefficients (for example *resistivity*) we need to know the scattering probability, which is determined by the values and \vec{k} dependences of interaction matrix elements. The simplest method to solve this problem is consideration of the transport equation for the electron distribution function f in a crystal in the presence of external fields.

For this consider the equation of continuity for the function f , of which can be the probable occupation number of either electrons or phonons. This relates the rate of change of f in the absence of collisions to the number

of particles leaving an element of volume of six- dimensional $k-r$ space. By a simple generalization of the usual three – dimensional version, we find

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial \vec{r}} \cdot \frac{d\vec{r}}{dt} + \frac{\partial f}{\partial \vec{k}} \cdot \frac{d\vec{k}}{dt} = - \left(\frac{\partial f}{\partial t} \right)_{coll} . \quad (3.2)$$

For phonons this is obvious, since $v = \frac{\partial \omega}{\partial \vec{q}}$, and does not depend on position while $\vec{k} = \vec{q}$, the wave number, and is constant. For electrons using the fact $\hbar \vec{v} = \frac{\partial \mathcal{E}}{\partial \vec{k}}$ we insure

$$\frac{\partial \vec{k}}{\partial t} = \frac{e}{\hbar c} (c \vec{E} + \vec{V} \times \vec{H}) . \quad (3.3)$$

We now consider the steady state ($\partial f / \partial t = 0$), but we add to the right - hand side a term to allow for changes in due to collisions. We then have a form of the *Botzamann* equation, which states

$$\left(\frac{\partial f}{\partial t} \right)_{collision} + \vec{v} \cdot \frac{\partial f}{\partial \vec{r}} + \frac{d\vec{k}}{dt} \cdot \frac{\partial f}{\partial \vec{k}} = 0 . \quad (3.4)$$

The spatial variation in f may be attributed solely to variation in temperature, giving

$$\frac{\partial f}{\partial \vec{r}} = \frac{df}{dT} \nabla T .$$

We then have the following equations for the phonon and electron systems respectively:

$$\left(\frac{\partial f}{\partial t}\right)_{collision} = \frac{d\omega}{d\vec{q}} \cdot \nabla T \left(\frac{\partial f}{\partial T}\right). \quad (3.5)$$

$$\left(\frac{\partial f_k}{\partial t}\right)_{collision} = \frac{1}{\hbar} \frac{\partial \varepsilon}{\partial \vec{k}} \cdot \nabla T \left(\frac{\partial f_k}{\partial T}\right) + \frac{e}{\hbar c} (\vec{E}c + \vec{v} \times \vec{H}) \cdot \left(\frac{\partial f}{\partial \vec{k}}\right). \quad (3.6)$$

In general these two equations are coupled since in the presence of the electron - phonon interaction the scattering probability for the electrons depends on the phonon occupation function, and conversely. If one is measuring thermal conductivity, for example, one usually wishes to determine this quantity as a function of temperature. The resulting currents of heat and electricity are consequently linear in \vec{E} and ∇T . This leads to a *linearization* of equation (3.5) and equation (3.6). We expand in powers of \vec{E} and ∇T , and keep only the first two terms so that

$$f \approx f^0 + f^1. \quad (3.7)$$

Here f^0 will represent the distribution in the equilibrium situation, and will be given by the *Bose Einstein function* for phonons and the *Fermi-Dirac function* for electrons. By definition $\left(\frac{\partial f_{\vec{k}}^0}{\partial t}\right)_{collision}$ vanishes. We also note that for electrons $f_{\vec{k}}^0$ depends on \vec{k} only through the function ε_k and so

$$\frac{\partial f_{\vec{k}}^0}{d\vec{k}} = \frac{df_{\vec{k}}^0}{d\epsilon} \frac{\partial \epsilon}{\partial \vec{k}}. \quad (3.8)$$

It thus follows that the term $\vec{v} \times \vec{H} \cdot (\partial f^0 / \partial \vec{k})$ also vanishes. On neglect of terms of second order of smallness we are then left with

$$\left(\frac{\partial f}{\partial t} \right)_{collision} = \vec{v}_{\vec{q}} \cdot \nabla T \left(\frac{\partial f_q^0}{\partial T} \right). \quad (3.9)$$

$$\left(\frac{\partial f_k}{\partial t} \right)_{collision} = \frac{e}{\hbar} \vec{v}_{\vec{k}} \times \vec{H} \cdot \frac{\partial f_k^1}{\partial \vec{k}} + \vec{v}_k \cdot \left(\nabla T \frac{\partial f_{\vec{k}}^0}{\partial T} + e \vec{E} \frac{\partial f_{\vec{k}}^0}{\partial \epsilon} \right). \quad (3.10)$$

This is as far as we can conveniently go in simplifying the *Boltzmann* equations without specializing to a consideration of specific models and situations.

The collision term: the collision term $\left(\frac{\partial f}{\partial t} \right)_{collision}$ is central to the Boltzmann equation. It is treated in relaxation time approximation. The first step in microscope theory of resistivity is the attempt to calculate the relaxation time $\tau(\vec{k})$ treating from the picture of electron-collisions. In relaxation time approximation [4]

$$\left(\frac{\partial f}{\partial t} \right)_{collision} = - \left(\frac{f^1 - f^0}{\tau} \right). \quad (3.11)$$

The collision term can also be written as

$$\left(\frac{\partial f}{\partial t}\right)_{\text{collision}} = \sum_{k'} [f_{\vec{k}'}(1-f_{\vec{k}})P_{\vec{k}' \rightarrow \vec{k}} - f_{\vec{k}}(1-f_{\vec{k}'})P_{\vec{k} \rightarrow \vec{k}'}], \quad (3.12)$$

where $P(\vec{k}, \vec{k}')$ is the probability per unit time for an electron scattered from an occupied state \vec{k} to an unoccupied state \vec{k}' .

3.2 Calculating the Conductivity of Metals

Let now consider the electrical conductivity of a metal in which the electrons are scattered *elastically* by a random array of impurities. If the positions of the scattering centers are not correlated in any way, then we can neglect *coherent scattering* by the array of impurities as a whole, and assume that the scattering probability between Bloch states is just the scattering probability due to a single impurity multiplied by n . This argument will be valid if the density of the impurities is low, as we can then consider our calculation as finding the first term of an expansion of the resistivity in powers of the impurity density n . For small enough n the scattering probability [1]

$$P_{\vec{k} \rightarrow \vec{k}'} = n \frac{2\pi}{\hbar} \left| \langle \phi_{\vec{k}'} | V | \phi_{\vec{k}} \rangle \right|^2 \delta(\epsilon_{\vec{k}} - \epsilon_{\vec{k}'}). \quad (3.13)$$

The rate of change of $f_{\vec{k}}$ will be the average net number of electrons entering state \vec{k} from all other states \vec{k}' . Making allowances for the *Exclusion Principle*, which will prevent an electron from entering the state \vec{k} if it is already occupied, we find

$$\left(\frac{\partial f_k}{\partial t}\right)_{collusion} = \sum_{k'} [f_{k'} P_{\bar{k} \rightarrow \bar{k}'} (1 - f_{\bar{k}}) - f_{\bar{k}} P_{\bar{k}' \rightarrow \bar{k}} (1 - f_{\bar{k}'})]. \quad (3.14)$$

Since for elastic scattering $P_{\bar{k} \rightarrow \bar{k}'} = P_{\bar{k}' \rightarrow \bar{k}}$ then we can have

$$\left(\frac{\partial f_k}{\partial t}\right)_{collusion} = \sum_{k'} P_{\bar{k} \rightarrow \bar{k}'} (f_{\bar{k}'} - f_{\bar{k}}). \quad (3.15)$$

Because energy is conserved $P_{\bar{k} \rightarrow \bar{k}'}$ vanishes unless $\varepsilon_{\bar{k}} = \varepsilon_{\bar{k}'}$ and as $f_{\bar{k}}^0$ depends only on $\varepsilon_{\bar{k}}$. We immediately verify that

$$\sum_{k'} P_{\bar{k} \rightarrow \bar{k}'} (f_{\bar{k}'}^0 - f_{\bar{k}}^0) = 0.$$

We may thus write

$$\left(\frac{\partial f_k}{\partial t}\right)_{collusion} = \left(\frac{\partial f_k^1}{\partial t}\right)_{collusion} = \sum_{k'} P_{\bar{k} \rightarrow \bar{k}'} (f_{\bar{k}'}^1 - f_{\bar{k}}^1). \quad (3.16)$$

Therefore, we obtain the integral equation for the function f_k^1 depending on the scattering situations. After its solution, the electron conductivity can be calculated. The quantity $P_{\bar{k} \rightarrow \bar{k}'}$ can be calculated for each scattering mechanism (like non-magnetic impurity and spin). In the case of independent mechanism the total resistivity

$$\rho = \rho_i + \rho_s + \dots. \quad (3.17)$$

The additivity of various mechanism contributions is called *Mathiesson rule*. We should notice that deviation from this rule occurs which are connected with interference of different process.

3.3 Inelastic Scattering and the Temperature Dependence of Resistivity

In section 3.2 the theory of electrical conductivity was presented based on the assumption that only elastic scattering occurred between the Bloch states. At temperature different from zero, this assumption will not be valid since then the electron-phonon interaction will cause electrons to be scattered between Bloch states with the emission or absorption of phonons.

The matrix element that appear in expression for the scattering probability will be those of electron-phonon interaction, are function of the occupation of the phonon states as well as the Bloch states.

The scattering probability between two states to the first order is given by:

$$P_{1 \rightarrow 2} = \frac{2\pi}{\hbar} \left| \langle 1 | H_{e-p} | 2 \rangle \right|^2 \delta(\varepsilon_1 - \varepsilon_2), \quad (3.18)$$

where $|1\rangle$ and $|2\rangle$ are the descriptions of all the particles and phonons, ε_1 and ε_2 are the corresponding energies and H_{e-p} is the interaction energy between electron and phonon. When both impurities and phonon are present the total probability of scattering is approximately the sum of the two scattering probabilities taken separately. This is so because the inelastic scattering by phonon connects the

initial state to the final state, which is different from those entered by the elastic scattering.

CHAPTER-FOUR

EXCHANGE INTERACTION AND SOME ASPECTS OF SCATTERING

In this chapter, we will see some aspects and mechanisms of scattering that causes electrical resistivity, and the interaction between conduction electrons and magnetic ions.

4.1 Scattering by a Potential Center

Consider a particle, scattered by a certain scattering center that can be represented by a potential $V(r)$ having a spherical symmetries. In terms of quantum theory, we describe the incident beam of free particles by a plane wave of frequency $\omega = E/h$ and wave number $k = p/h$. If we suppose that the particles are traveling in the positive x -direction, they are represented by the wave function

$$\varphi = \exp i(kx - \omega t) . \quad (4.1)$$

This has been normalized to represent a beam of particles with one particle per unit volume since $\int \varphi^* \varphi d^3 r = 1$. For elastic scattering, the frequency factor remains unchanged and will be dropped. We thus write the wave function of incident particles

$$\varphi = \exp i(kx) . \quad (4.2)$$

Let see how we represent the particles when they are scattered from a potential $V(r)$ of limited range, i.e. $V(r) = \text{zero}$ at points distant from scattering centre, the wave function of the electrons must have the form [17]

$$\varphi = \exp i(kx) + \frac{\exp i(kx)}{r} f(\theta) + O\left(\frac{1}{r^2}\right) . \quad (4.3)$$

The first term represents the incident wave and the second term a spherical wave function radiating from the scattering centre and representing the scattered particles, the remaining terms can be neglected at large distances. $f(\theta)$ - describes the angular distribution of the scattered wave and is known as the scattering amplitude. The number of particles per unit volume so scattered is given by $f(\theta)/r^2$ at a distance r from the scattering center.

4.2 Scattering by Impurities

The two most important mechanisms that limit the magnitude of the current attains in particular field are scattering by *lattice vibration (Phonon)* and *scattering by impurities*. The interaction of the Bloch electrons with phonons is a major part of the theory of solids [1]. Let consider an electron in the Bloch state, $\phi_{\vec{k}}$, and then apply the perturbation potential, V . The wave function then will be transformed in to some new function, $\varphi_{\vec{k}}$ as given in equation (4.3).

The scattering probability of the two Bloch states, $\phi_{\vec{k}}$ and $\phi_{\vec{k}'}$ is proportional to the amount of $\phi_{\vec{k}'}$ contained in $\varphi_{\vec{k}}$. To measure the amplitude that tells us how much the

state the wave originally ϕ_k has been transformed to ϕ_k we form the integral $\langle \phi_{\vec{k}'} | \phi_{\vec{k}} \rangle$. The square of the modulus of this quantity is proportional to the probability $P_{\vec{k} \rightarrow \vec{k}'}$ that in unit time an electron is scattered between these states, i.e.

$$P_{\vec{k} \rightarrow \vec{k}'} \propto \left| \langle \phi_{\vec{k}'} | V | \phi_{\vec{k}} \rangle \right|^2. \quad (4.4)$$

We suppose the electron (scattering particle) in the presence of the scattering centre has a wave function $\phi_{\vec{k}}(\vec{r})$ as described by equation (4.3) and in order to know the probability that it is scattered into the state $\phi_{\vec{k}'}$ in which we are interested. The scattering probability per unit time according to *Golden rule* for weak scatterer is as given in equation (3.13) is:

$$P_{\vec{k} \rightarrow \vec{k}'} = \frac{2\pi}{h} \left| \langle \phi_{\vec{k}'} | V | \phi_{\vec{k}} \rangle \right|^2 \delta(\epsilon_{\vec{k}} - \epsilon_{\vec{k}'}). \quad (4.5)$$

For weak, potential $\phi_{\vec{k}}$ may be replaced by $\phi_{\vec{k}}$, and if the electron is scattered near the scatterer of energy $\epsilon_{\vec{k}} = \epsilon_0$ the scattering probability is

$$P_{\vec{k} \rightarrow \vec{k}'} = \frac{2\pi}{h} \left| \langle \phi_{\vec{k}'} | V | \phi_{\vec{k}} \rangle \right|^2 N(\epsilon_0) \quad (4.6)$$

where $\langle \phi_{\vec{k}'} | V | \phi_{\vec{k}} \rangle$ is called scattering amplitude for transition from \vec{k} to \vec{k}' . $N(\epsilon_0)$ -is the density of states at $\epsilon_{\vec{k}} = \epsilon_0$ into which the particles are scattered.

In general solving the *Schrödinger equation* for the particle in the field of the scattering potential, the solution can be written in the form [19]:

$$\phi_{\vec{k}}^- = \phi_{\vec{k}}^- + \sum_q \frac{\langle \phi_{\vec{q}}^- | V | \phi_{\vec{k}}^- \rangle}{\epsilon_{\vec{k}}^- - \epsilon_{\vec{q}}^-} \phi_{\vec{q}}^- . \quad (4.7)$$

The scattering amplitude equation (4.4) cannot be evaluated unless we know $\phi_{\vec{k}}^-$ in the first place. Equation (4.7) is not an explicit solution since $\phi_{\vec{k}}^-$ appears on the right-hand side of the equation does allow successive and systematic approximations to $\phi_{\vec{k}}^-$ through iteration. Let think about the two *Born approximations* in the following section.

4.3 First and Second Born Approximations

4.3.1 The First Born Approximation

The first approximation in using equation 4.6 is to replace $\phi_{\vec{k}}^-$ in the matrix element by $\phi_{\vec{k}}^-$ the wave function of the particles in absence of the scattering centre; in equation 4.6 this involves taking just the first term and neglecting any terms due to scattering. This approximation can be shown to be valid the interaction energy is treated as small perturbation. From this, the *Born* approximation is useful for relatively high energy particles (for example for high kinetic energy particle).

As an illustration, if treating electrons as free particles the wave functions corresponding to \vec{k} and \vec{k}' are $\exp(i\vec{k}\cdot\vec{r})$ and $\exp(i\vec{k}'\cdot\vec{r})$ respectively. Thus, the matrix element of equation (4.6) becomes

$$V_{\vec{k}\vec{k}'} = \left| \langle \phi_{\vec{k}} | V | \phi_{\vec{k}'} \rangle \right|^2 = \int V(\vec{r}) \exp i(\vec{k} - \vec{k}')\vec{r} d\vec{r}, \quad (4.8)$$

which is just the *Fourier transform* of $V(\vec{r})$.

4.3.2 Second Born Approximation

In this approximation, the wave function of the initial state of the electron $\phi_{\vec{k}}$ is taken as the perturbed wave function $\phi_{\vec{k}}$. It is perturbed by the potential V taken to first order in V . Which means that to iterate once by putting $\phi_{\vec{k}} = \phi_{\vec{k}'}^i$ in the matrix element on the right hand side of equation 4.6 and take for $\phi_{\vec{k}}$ the following:

$$\begin{aligned} \phi_{\vec{k}} &= \phi_{\vec{k}} + \sum_q \frac{\langle \phi_{\vec{q}} | V | \phi_{\vec{k}} \rangle}{\epsilon_{\vec{k}} - \epsilon_{\vec{q}}} \phi_{\vec{q}} \\ &= \phi_{\vec{k}} + \sum_q \frac{\langle \phi_{\vec{q}} | V | \phi_{\vec{k}} \rangle}{\epsilon_{\vec{k}} - \epsilon_{\vec{q}}} \phi_{\vec{q}} \\ &= \phi_{\vec{k}} + \sum_q \frac{V_{\vec{q}\vec{k}} \phi_{\vec{q}}}{\epsilon_{\vec{k}} - \epsilon_{\vec{q}}}. \end{aligned} \quad (4.9)$$

Here $V_{\vec{q}\vec{k}}$ is the matrix element $\langle \phi_{\vec{q}} | V | \phi_{\vec{k}} \rangle$ of the scattering potential V between the unperturbed states \vec{k} and \vec{q} . The modulus square of the matrix element $\langle \phi_{\vec{k}'} | V | \phi_{\vec{k}} \rangle$ of equation (4.9) is evaluated as follows

$$\begin{aligned}
\left| \langle \phi_{\bar{k}'} | V | \phi_{\bar{k}} \rangle \right|^2 &= \left| \left\langle \phi_{\bar{k}'} | V \left| \phi_{\bar{k}} + \sum_q \frac{V_{\bar{q}\bar{k}} \phi_{\bar{q}}}{\epsilon_{\bar{k}} - \epsilon_{\bar{q}}} \right. \right\rangle \right|^2 = \\
&= \left(\langle \phi_{\bar{k}'} | V | \phi_{\bar{k}} \rangle + \sum_q \frac{V_{\bar{q}\bar{k}}}{\epsilon_{\bar{k}} - \epsilon_{\bar{q}}} \langle \phi_{\bar{k}'} | V | \phi_{\bar{q}} \rangle \right)^2 \\
&= \left(\langle \phi_{\bar{k}'} | V | \phi_{\bar{k}} \rangle + \sum_q \frac{V_{\bar{q}\bar{k}}}{\epsilon_{\bar{k}} - \epsilon_{\bar{q}}} \langle \phi_{\bar{k}'} | V | \phi_{\bar{q}} \rangle \right) \times \\
&\quad \left(\langle \phi_{\bar{k}} | V^* | \phi_{\bar{k}'} \rangle + \sum_p \frac{V_{\bar{p}\bar{k}}}{\epsilon_{\bar{k}} - \epsilon_{\bar{p}}} \langle \phi_{\bar{p}} | V^* | \phi_{\bar{k}'} \rangle \right). \quad (4.10)
\end{aligned}$$

This can be simplified using the following facts: $\langle \phi_{\bar{k}'} | V | \phi_{\bar{k}} \rangle = V_{\bar{k}'\bar{k}}$, $\langle \phi_{\bar{q}} | V | \phi_{\bar{k}'} \rangle = V_{\bar{q}\bar{k}'}$, $V_{\bar{k}'\bar{k}} = V_{\bar{k}\bar{k}'}$ and $\left| \langle \phi_{\bar{k}'} | V | \phi_{\bar{k}} \rangle \right|^2 = \langle \phi_{\bar{k}} | V | \phi_{\bar{k}'} \rangle \langle \phi_{\bar{k}'} | V^* | \phi_{\bar{k}} \rangle$. Then the square of the matrix element becomes:

$$\begin{aligned}
\left| \langle \phi_{\bar{k}'} | V | \phi_{\bar{k}} \rangle \right|^2 &= \\
&\quad \left((V_{\bar{k}'\bar{k}} + \sum_q \frac{V_{\bar{k}'\bar{q}} V_{\bar{q}\bar{k}}}{\epsilon_{\bar{k}} - \epsilon_{\bar{q}}}) (V_{\bar{k}\bar{k}'} + \sum_p \frac{V_{\bar{k}\bar{p}} V_{\bar{p}\bar{k}'}}{\epsilon_{\bar{k}} - \epsilon_{\bar{p}}}) \right) \\
&= |V_{\bar{k}'\bar{k}}|^2 + \left(V_{\bar{k}\bar{k}'} \sum_q \frac{V_{\bar{k}'\bar{q}} V_{\bar{q}\bar{k}}}{\epsilon_{\bar{k}} - \epsilon_{\bar{q}}} \right) + \\
&\quad V_{\bar{k}'\bar{k}} \sum_p \frac{V_{\bar{k}\bar{p}} V_{\bar{p}\bar{k}'}}{\epsilon_{\bar{k}} - \epsilon_{\bar{p}}} + O(V^4). \quad (4.11)
\end{aligned}$$

Then the probability of scattering from initial state \vec{k} to final state \vec{k}' to the third order of interaction can be written as

$$P_{\vec{k} \rightarrow \vec{k}'} = \frac{2\pi}{\hbar} \left(V_{\vec{k}\vec{k}'} V_{\vec{k}'\vec{k}} + \sum_{q \neq k} \frac{V_{k\vec{k}'} V_{\vec{k}'\vec{q}} V_{\vec{q}\vec{k}}}{\mathcal{E}_{\vec{k}} - \mathcal{E}_{\vec{q}}} + \sum_p \frac{V_{\vec{k}'\vec{k}} V_{\vec{k}\vec{p}} V_{\vec{p}\vec{k}'}}{\mathcal{E}_{\vec{k}} - \mathcal{E}_{\vec{p}}} \right) N(\mathcal{E}_0). \quad (4.12)$$

The probability equation (4.12) is interpreted as total scattering probability, a probability of going directly from state \vec{k} to state \vec{k}' together with the sum of probabilities of going from \vec{k} to \vec{k}' indirectly via the intermediate states. For our problem, equation (4.12) has great utility that will be applicable in the next chapter.

4.4 Interaction of Conduction Electrons with Magnetic Ions

The interaction of a conduction electron characterized by its “spin coordinate” $\vec{\sigma}$ with a magnetic ion \vec{S} is determined by two different contributions. The *spin-independent* part may be represented by a potential $V(\vec{r})$ in a usual way and may well resemble a screened *Coulomb* potential centered on the magnetic ion. The spin-dependent part is due to an exchange interaction; its contribution to the total energy of the metal can be represented using *Heisenberg exchange* model as

$$H = -J(\vec{r}) \vec{\sigma} \cdot \vec{S}, \quad (4.13)$$

where $J(\vec{r})$ is the exchange coupling parameter, which falls rapidly with \vec{r} . This coupling has only appreciable values on the site of the localized ion. Its value is positive for ferromagnetic exchange and negative for antiferromagnetic exchange.

The spin state of the conduction electron is described by σ having only two permissible values spin up and spin down ($\sigma = \pm 1$). The spin angular momentum of the electron is quantized in such a way that in a particular direction (that of the magnetic field in which the electron moves and conventionally chosen as the z -direction of coordinate axes). The value of the components parallel and anti parallel to Z -direction are $S^Z = \pm \frac{1}{2} \hbar$. Therefore we associate the state in which $S^Z = \pm \frac{1}{2} \hbar$ with $\sigma = \pm 1$. Thus, $\sigma = \frac{2S^Z}{\hbar}$.

For the magnetic quantum number m , we have $-S \leq m \leq S$. Since for the $s - d$ model [12] the orbital contribution is neglected (due to the quenching by the crystalline electric field) the total angular momentum follows from simply adding up the spins.

4.4.1 Elastic Scattering of Conduction Electrons on Magnetic Impurities

The electron in a spin state $\vec{\sigma}$ may feel a potential of which the non-magnetic part is described by $V(\vec{r})$ and the magnetic part $H = -J(\vec{r})\vec{\sigma} \cdot \vec{S}$. Suppose that the ion is in a state whose magnetic quantum number is m . Then if say, $\sigma = +1$ the exchange part of the potential has the value $-mJ(\vec{r})$ and the total potential for conduction electrons with this spin is

$$V = V(\vec{r}) - mJ(\vec{r}). \quad (4.14)$$

In elastic collisions the spin up electrons are scattered without change of energy and without a spin-flip. Under these conditions [17], the magnitude of the scattering is determined as in the non-magnetic scattering by suitable matrix elements of the scattering potential. Suppose $\phi_{\vec{k}}$ and $\phi_{\vec{k}'}$ are the initial and the final states of the conduction electron, the scattering probability is

$$\begin{aligned}
P_{\vec{k} \rightarrow \vec{k}'} &\propto \left(\int \phi_{\vec{k}'}^* (V(\vec{r}) + mJ(\vec{r})) \phi_{\vec{k}} d^3 r \right)^2 \\
&= \left(\int \phi_{\vec{k}'}^* V(\vec{r}) \phi_{\vec{k}} d^3 r - m \int \phi_{\vec{k}'}^* J(\vec{r}) \phi_{\vec{k}} d^3 r \right)^2 . \quad (4.15)
\end{aligned}$$

If $\phi_{\vec{k}}$ and $\phi_{\vec{k}'}$ are plane waves the above two integrals are just the Fourier transforms of $J(\vec{r})$ and $V(\vec{r})$. Denoting them by V_{FT} and J_{FT} the transition probability be

$$P_{\vec{k} \rightarrow \vec{k}'} \propto V_{FT}^2 + m^2 J_{FT}^2 - 2mJ_{FT} V_{FT} . \quad (4.16)$$

The *spin down* electrons by contrast sees the potential

$$V = V(\vec{r}) + mJ(\vec{r}) . \quad (4.17)$$

By similar argument and approximations done for spin up electron, the elastic scattering probability of the spin down electrons is proportional to

$$P_{\vec{k} \rightarrow \vec{k}'} \propto V_{FT}^2 + m^2 J_{FT}^2 + 2mJ_{FT} V_{FT} . \quad (4.18)$$

We have to notice here is that from the two equations (4.16) and (4.18) the scattering probability for elastic scattering of conduction electrons on the impurity depends only on the magnetic ion parameter, m , and coupling integral, J .

4.4.2 Inelastic Collisions of Conduction Electrons on Magnetic Impurities

Let see now the case in which scattering by magnetic impurities may induce transitions in which the spin state of the conduction electron changes, that is an electron with spin up may be scattered to spin down and vice versa. The magnetic quantum number of the impurity spin changes accordingly (i.e. $\Delta m = \pm 1$) [14]. Since the energy of the ion is given by $-mg\mu_B H$ its energy changes to a lower value when $\Delta m = +1$, and to a higher value when $\Delta m = -1$. The change in energy is thus

$$\Delta E_{ion} = \mp g\mu_B H. \quad (4.19)$$

In inelastic transitions, the total Z -component of spin and the total energy are conserved. However, we should notice that the spin up electrons always have their energy increased whereas the spin down electrons always have their energy decreased.

CHAPTER-FIVE

APPROXIMATE CALCULATION OF THE ELECTRICAL RESISTIVITY

We are now targeted to the problem, studying the low temperatures electrical resistivity of dilute magnetic alloys. The experience of the preceding chapters is very vital ground to approximate electrical resistivity of the lesson.

5.1 Scattering of an Electron by an Isolated Magnetic Ion

To study the behavior of low temperature electrical resistivity of dilute magnetic alloys we begin from the interaction of conduction electron with the magnetic impurity as given by the *s-d model*. In this model, the conduction electrons spin \vec{s} is coupled to the local moment of the impurity with angular momentum \vec{S} by the effective exchange coupling $J(\vec{r})$ as

$$H = -J(\vec{r})\vec{s}\cdot\vec{S}, \quad (5.1)$$

where $J(\vec{r})$ is the exchange integral and it is treated as constant.

To treat the scattering problem in the second order there are two scattering processes.

- a. In the *first stage*, an electron is scattered into an intermediate state by the magnetic impurity that likewise makes a transition into its intermediate state.
- b. In the *second stage*, the impurity is restored to its original state and the conduction electron is scattered into its final state.

For an electron scattered from initial state $|\vec{k} \sigma\rangle$ to final state $|\vec{k}' \sigma'\rangle$ the scattering probability as given in equation (4.12) can be used:

$$P_{\vec{k} \rightarrow \vec{k}'} = \frac{2\pi}{\hbar} \left(V_{\vec{k}\vec{k}'} V_{\vec{k}'\vec{k}} + \sum_q \frac{V_{\vec{k}\vec{k}'} V_{\vec{k}'\vec{q}} V_{\vec{q}\vec{k}}}{\epsilon_{\vec{k}} - \epsilon_{\vec{q}}} + \sum_p \frac{V_{\vec{k}\vec{k}'} V_{\vec{k}\vec{p}} V_{\vec{p}\vec{k}'}}{\epsilon_{\vec{k}} - \epsilon_{\vec{p}}} \right). \quad (5.2)$$

For a time being let leave the density of state, $N(\epsilon_0)$.

Here we should note that the sum is over all possible intermediate states; $V_{\vec{k}\vec{k}'} V_{\vec{k}'\vec{k}}$ represents the *first Born approximation*, yielding a temperature independent scattering, and the second part (the sum part) is temperature-dependent. Thus, we will focus on this second part especially in case of inelastic scattering during spin flip.

While an electron is scattered in the second order it is important to consider the following possible happenings:

- I. The energies $\epsilon_{\vec{k}}$ and $\epsilon_{\vec{k}'}$ are assumed to be equal but $\epsilon_{\vec{q}}$ is different.
- II. The scattering to the intermediate state by the impurity may entail a spin flip of the conduction electron and [14] a compensating spin of change in the impurity. This situation may be illustrated as if an electron in state $|\vec{k} \uparrow\rangle$ is changed to state $|\vec{q} \downarrow\rangle$ an impurity

state $|S, m\rangle$ is changed to $|S, m+1\rangle$.

- III.** In going to the final state, the impurity reverts to its initial state and the conduction electron reverts to its initial spin direction. An electron in state $|\bar{q} \downarrow\rangle$ is scattered to state $|\bar{k}' \uparrow\rangle$ while an impurity make a compensation, that is its state $|S, m+1\rangle$ is changed to $|S, m\rangle$.

In the process involving *spin flip*, we should note that there are two *coherent* second order scattering process:

1. In the first order, an electron is scattered by the impurity to intermediate state and then scattered to its final state:
 - a. An electron from state $|\bar{k} \uparrow\rangle$ is scattered to state $|\bar{q} \downarrow\rangle$ as a result an impurity make a compensation, $m \rightarrow m+1$
 - b. The intermediate state $|\bar{q} \downarrow\rangle$ is changed to final $|\bar{k}' \uparrow\rangle$ thus an impurity $m+1 \rightarrow m$
2. In the second order, an electron is scattered to its final state and then another electron is scattered into this unoccupied intermediate state so created
 - I. An electron state $|\bar{q} \downarrow\rangle$ is scattered to state $|\bar{k}' \uparrow\rangle$ as a result an impurity $m \rightarrow m-1$
 - II. Another electron in the intermediate state $|\bar{q} \downarrow\rangle$ is scattered to final $|\bar{k}' \uparrow\rangle$ thus an impurity $m-1 \rightarrow m$

In general, in the second order perturbation theory, two types of scattering process contribute to the matrix element of equation (4.4). The sign of the contribution is

opposite to that of the first contribution because of antisymmetry of the many electron function.

5.2 Transition Probabilities of Inelastic Scattering of Electron

In the preceding chapter, we noticed that the scattering by the magnetic impurities cause transitions in which the spin state of an electron changes (i.e. $\sigma = \pm 1 \rightarrow \sigma = \mp 1$).

The following table shows the possible fluctuations (change) in spin in both conduction and magnetic ion in the interaction.

Spin change in conduction electron	Spin change in the magnetic ion	Transition probability $ \langle \phi_f V \phi_i \rangle ^2$
+1/2 \rightarrow -1/2	m \rightarrow m+1	W_{m+1}
-1/2 \rightarrow +1/2	m \rightarrow m - 1	W_{m-1}

Table 2: The change in spin of both conduction electron and magnetic spin due to interaction

For the scattering process taking place from $|\vec{k} \uparrow\rangle$ to state $|\vec{q} \downarrow\rangle$ the initial state of the electron plus the magnetic ion can be put as

$$|\phi_i\rangle = \left| S; m; +\frac{1}{2} \right\rangle. \quad (5.3)$$

And the final state

$$|\phi_f\rangle = \left| S; m+1; -\frac{1}{2} \right\rangle. \quad (5.4)$$

From this, the matrix operator can have the form:

$$\langle \phi_f | V | \phi_i \rangle = \left\langle S; m+1; -\frac{1}{2} \left| -J \vec{s} \cdot \vec{S} \right| S; m; +\frac{1}{2} \right\rangle. \quad (5.5)$$

The product $\vec{s} \cdot \vec{S}$ can be put using *rising* and *lowering* operator s^- , s^+ , S^- , and S^+ for both Bloch and localized electrons respectively as

$$\vec{s} \cdot \vec{S} = \frac{1}{2} (s^+ S^- + s^- S^+) + s^z S^z. \quad (5.6)$$

Replacing (5.6) in to (5.5)

$$\begin{aligned} \langle \phi_f | V | \phi_i \rangle = & -J \left[\left\langle S; m+1; -\frac{1}{2} \left| \frac{s^+ S^-}{2} \right| S; m; +\frac{1}{2} \right\rangle + \right. \\ & \left. \left\langle S; m+1; -\frac{1}{2} \left| \frac{s^- S^+}{2} \right| S; m; \frac{1}{2} \right\rangle + \right. \\ & \left. \left\langle S; m+1; -\frac{1}{2} \left| s^z S^z \right| S; m; +\frac{1}{2} \right\rangle \right]. \quad (5.7) \end{aligned}$$

Using the fact in [18] we have $\left\langle -\frac{1}{2} \left| s^+ \left| \frac{1}{2} \right\rangle = \left\langle -\frac{1}{2} \left| s^z \left| \frac{1}{2} \right\rangle = 0 \right.$ and

$\left\langle -\frac{1}{2} \left| s^- \left| \frac{1}{2} \right\rangle = 1 \right.$ the second and the third term of the right hand side of equation (5.7) vanish. The matrix element then becomes

$$\langle \phi_f | V | \phi_i \rangle = \langle S; m+1 | S^+ | S; m \rangle J.$$

Finally, since $S^+ | S; m \rangle = [(S - m)(S + m + 1)]^{\frac{1}{2}} | S; m + 1 \rangle$, the operation of S^+ yields the following

$$\langle \phi_f | V | \phi_i \rangle = J[(S - m)(S + m + 1)]^{\frac{1}{2}}. \quad (5.8)$$

For the second process in which a conduction electron is scattered from the intermediate state $|\bar{q} \downarrow\rangle$ to $|\bar{k}' \uparrow\rangle$ while the ion makes a compensation transition from $m \rightarrow m - 1$. The combined initial and final states respectively are

$$|\phi_i\rangle = \left| S; m; -\frac{1}{2} \right\rangle,$$

$$\phi_f = \left| S; m - 1; +\frac{1}{2} \right\rangle. \quad (5.9)$$

The matrix element for this transition is

$$\langle \phi_f | V | \phi_i \rangle = \left\langle S; m-1; +\frac{1}{2} \left| -J \vec{s} \cdot \vec{S} \right| S; m; -\frac{1}{2} \right\rangle. \quad (5.10)$$

Here again using equation (5.6) and the same facts in [18] the matrix element becomes

$$\langle \phi_f | V | \phi_i \rangle = J[(S+m)(S-m+1)]^{\frac{1}{2}}. \quad (5.11)$$

Now from equation (5.6) and (5.10) the *transition probabilities* for each case are

$$W_{m+1} = \left| \langle \phi_f | V | \phi_i \rangle \right|^2 = J^2 (S-m)(S+m+1) \quad (5.12)$$

and

$$W_{m-1} = \left| \langle \phi_f | V | \phi_i \rangle \right|^2 = J^2 (S+m)(S-m+1). \quad (5.13)$$

For the first process to be possible, the intermediate state \bar{q} must be empty. The probability of this is $1-f^0(q)$ where $f^0(q)$ is the Fermi functions. For the second process, the intermediate state \bar{q} must be occupied. The probability of this is $f^0(q)$. For low impurity concentrations, the scattering events on different impurities are independent and their contributions add incoherently. So that their respective probabilities become (from here then for simplicity we use $\varepsilon_{\bar{k}} = \varepsilon_k$ $\varepsilon_{\bar{q}} = \varepsilon_q$ and $\varepsilon_{\bar{k}'} = \varepsilon_{k'}$).

$$P_{\bar{k} \rightarrow \bar{q}} = \sum_q \frac{\beta(1-f^0(q))}{\varepsilon_k - \varepsilon_q} W_{m+1} \quad (5.14)$$

is the total probability for the compensation transition of the ion from $m \rightarrow m + 1$, and

$$P_{\bar{q} \rightarrow \bar{k}'} = - \sum_q \frac{\beta f^0(q)}{\epsilon_q - \epsilon_{k'}} W_{m-1} \quad (5.15)$$

is the total probability for the transition from $m \rightarrow m - 1$.

The (-) sign in equation (5.15) comes from antisymmetrical character of the electrons wave function with respect to particle exchange [13]. β is constant in

both equations (i.e. $\beta \propto \frac{2\pi}{\hbar} V_{\bar{k}\bar{k}'} \propto \frac{2\pi}{\hbar} J^2$)

The total probability for this particular transition is the sum of the two, i.e.

$$\begin{aligned} P_{\bar{k} \rightarrow \bar{k}'} &= P_{\bar{k} \rightarrow \bar{q}} + P_{\bar{q} \rightarrow \bar{k}'} \\ &= \sum_q \frac{\beta(1 - f^0(q))}{\epsilon_k - \epsilon_q} W_{m+1} - \sum_q \frac{\beta f^0(q)}{\epsilon_q - \epsilon_{k'}} W_{m-1}. \end{aligned} \quad (5.16)$$

Putting $\epsilon_k = \epsilon_{k'}$ the total probability becomes:

$$P_{\bar{k} \rightarrow \bar{k}'} = \sum_q \beta \frac{W_{m+1}}{\epsilon_k - \epsilon_q} - \sum_q \frac{\beta f^0(q) (W_{m+1} - W_{m-1})}{\epsilon_k - \epsilon_q}. \quad (5.17)$$

It is the $f^0(q)$ that produces the temperature dependent scattering. Therefore, if we observe equation (5.17) the temperature-dependent part could be

$$P_{\bar{k} \rightarrow \bar{k}'}(T) = - \sum_q \frac{\beta f^0(q) (W_{m+1} - W_{m-1})}{\epsilon_q - \epsilon_{k'}}. \quad (5.18)$$

To evaluate this, we assume $T = \text{zero}$,

$$f^0(q) = \begin{cases} 1 & \text{for } q < q_0 \\ 0 & \text{for } q > q_0 \end{cases}, \quad (5.19)$$

where q_0 is the Fermi wave number.

The second supposition for simplicity of equation (5.18) is that the conduction electrons are free then:

$$\epsilon_q = \frac{h^2 q^2}{2m}, \quad \epsilon_k = \frac{h^2 k^2}{2m}.$$

Using the previous assumptions the important factor is the sum, and let it be $g(\epsilon_k)$

$$g(\epsilon_k) = - \sum_q \frac{f_o(q)}{\epsilon_k - \epsilon_q} = - \sum_{q < q_0} \frac{1}{\epsilon_k - \epsilon_q}. \quad (5.20)$$

To convert this sum in to integral in k -space, let have N atoms in the metal with Z conduction electrons per atom; these require $ZN/2$ k -states since each state can hold two electrons of opposite spin. From this, it follows that

- The volume enclosed by the Fermi sphere is, $\frac{4}{3} \pi q_0^3$
- The number of states per unit volume in k -space is, $n(q) = \frac{2}{3} ZN / \pi q_0^3$
- The number of states lying between wavevectors \vec{q} and $\vec{q} + d\vec{q}$ is $d^3 \vec{q} = (4\pi^3 q^2 dq) n(q)$.

So that, it easy to transform equation (5.20) in to the integral as:

$$g(\epsilon_k) = - \int_0^{q_0} \frac{d^3 \vec{q}}{\epsilon_k - \epsilon_q}.$$

Using the facts given on top of we write for $g(\epsilon_k)$ as

$$\begin{aligned} g(\epsilon_k) &= - \frac{3ZNm}{q_o^3 \hbar^2} \int_0^{q_0} \frac{q^2 dq}{k^2 - q^2} \\ &= \frac{3ZNm}{q_o^3 \hbar^2} \int_0^{q_0} \left[1 - \frac{k}{2(k - q_0)} - \frac{k}{2(k + q_0)} \right] dq. \end{aligned}$$

Carrying out the integral yields

$$\begin{aligned} g(\epsilon_k) &= \frac{3ZNm}{q_o^3 \hbar^2} \left[q_0 + \frac{k}{2} \ln \left| \frac{k - q_0}{k + q_0} \right| \right] \\ &= \frac{3ZN}{2E_F} \left[1 + \frac{k}{2q_0} \ln \left| \frac{k - q_0}{k + q_0} \right| \right]. \end{aligned} \quad (5.21)$$

Neglecting the first part of equation (5.21) and replacing the remaining part to equation (5.18), to the expression of the temperature-dependent part gives:

$$P_{\vec{k} \rightarrow \vec{k}'} = \frac{3ZN\beta}{2E_F} \left[(W_{m+1} - W_{m-1}) \frac{k}{2q_0} \ln \left| \frac{k - q_0}{k + q_0} \right| \right]. \quad (5.22)$$

For small temperature $T \ll T_F$, $(k - q_o)$ for thermally excited electrons is on average $(k_B T / E_F) q_o$. Setting $k \approx q_o$ so that $k + q_o = 2q_o$ and substituting this in to equation (5.22) we have for the *temperature-dependent* part

$$P_{\vec{k} \rightarrow \vec{k}'} = \frac{3ZN\beta}{2E_F} \left[(W_{m+1} - W_{m-1}) \ln \left| \frac{k_B T}{2E_F} \right| \right]. \quad (5.23)$$

We should note that this equation is derived only for one particular transition case (i.e. for the state change from $|\vec{k} \uparrow\rangle$ to $|\vec{k}' \uparrow\rangle$). In addition to this, we have to consider the remaining three possible scattering conduction.

These are transitions from $|\vec{k} \downarrow\rangle$ to $|\vec{k}' \downarrow\rangle$, $|\vec{k} \downarrow\rangle$ to $|\vec{k}' \uparrow\rangle$, and $|\vec{k} \uparrow\rangle$ to $|\vec{k}' \downarrow\rangle$. It is expected that these transitions may involve $\ln T$ terms of similar structures like equation (5.23). Following the same techniques that we did for the first case

- a.** The total transition probability for a transition from $|\vec{k} \downarrow\rangle \rightarrow |\vec{k}' \downarrow\rangle$ yields

$$P_{\vec{k} \rightarrow \vec{k}'}(T) = \frac{3ZN\beta}{2E_F} \ln \left| \frac{k_B T}{2E_F} \right| (W_{m+1} + W_{m-1}). \quad (5.24)$$

- b.** For the third transition, $|\vec{k} \downarrow\rangle \rightarrow |\vec{k}' \uparrow\rangle$ an electron first scattered to the intermediate state $|\vec{q} \uparrow\rangle$ and then to final state $|\vec{k}' \uparrow\rangle$. Here we can observe that in the former case, there is spin flip and hence the transition is inelastic. The latter one is elastic. Calculating the total probabilities for the inelastic one gives

$$P_{\bar{k} \rightarrow \bar{q}'}(T) = \frac{3ZN\beta}{2E_F} \ln \left| \frac{k_B T}{2E_F} \right| W_{m-1}. \quad (5.25)$$

- c. With the same argument performed for equation (5.25) the total probability for the scattering (inelastic case) from $|\bar{k} \uparrow\rangle \rightarrow |\bar{k}' \downarrow\rangle$ will provide

$$P_{\bar{k} \rightarrow \bar{q}'}(T) = \frac{3ZN\beta}{2E_F} \ln \left| \frac{k_B T}{2E_F} \right| W_{m+1}. \quad (5.26)$$

The two temperature-independent parts contributed from the elastic scattering of b and c is

$$P_{\bar{q} \rightarrow \bar{k}'} = \frac{3\pi n}{2\hbar E_F} J^2 S(S+1). \quad (5.27)$$

Now we are in the right position to calculate the total probability contributed from each scattering mechanisms (i.e. the sum of equations from (5.23) to (5.26), the temperature dependent total scattering probability let say it is $P_T(T)$ and found to be

$$P_T(T) = \frac{3ZN\beta}{2E_F} \ln \left| \frac{k_B T}{2E_F} \right| (3W_{m+1} + W_{m-1}). \quad (5.28)$$

Replacing equation (5.12) and (5.13) results

$$P_T(T) = \frac{3ZN\beta}{2E_F} \ln \left| \frac{k_B T}{2E_F} \right| J^2 (4S(S+1) - 4m^2 - 2m). \quad (5.29)$$

The localized spin can have a total spin different from $\frac{1}{2}$, we here for simplicity consider localized spin $m = -1/2$ states. Therefore (5.29) reduces to

$$P_T(T) = \frac{3ZN\beta}{2E_F} \ln \left| \frac{k_B T}{2E_F} \right| J^2 4S(S+1). \quad (5.30)$$

Applying the definition i.e. equation (3.1) the electrical resistivity contributed from this magnetic impurity scattering of spin flip can be computed as

$$\rho_{imp}(T) = \frac{3\pi m J^2 S(S+1)}{2e^2 \hbar E_F} \left[4JN(E_F) \ln \left(\frac{k_B T}{2E_F} \right) \right] \quad (5.31)$$

Here note that m is mass of an electron.

Including the temperature independent part (5.27) to equation (5.31) we find

$$\rho_{imp}(T) = \frac{3\pi m J^2 S(S+1)}{2e^2 \hbar E_F} \left[1 + 4JN(E_F) \ln \left(\frac{k_B T}{2E_F} \right) \right]. \quad (5.32)$$

Putting the constant, $a = \frac{3\pi m}{2e^2 \hbar E_F}$ and $D = 2T_F$ is the cut of parameter (width of the conduction band).

$$\rho_{imp}(T) = aJ^2(S(S+1)) \left[1 + 4JN(E_F) \ln \left(\frac{T}{D} \right) \right], \quad (5.33)$$

Finally including the residual resistivity, and the phonon contribution the resistivity has to be written in the form

$$\rho(T) = \rho_i + bT^5 + aJ^2(S(S+1)) \left[1 + 4JN(E_F) \ln\left(\frac{T}{D}\right) \right]. \quad (5.34)$$

Here, the first term is the non-magnetic impurity contribution; the second one is the phonon term while the third one describes the magnetic scattering processes.

The treatment to equation (5.34) yields a convincing explanation of the temperature dependent resistivity of diluted magnetic systems; depending on sign of coupling parameter J we deduce the behavior of spin resistivity and the resistivity at all.

CHAPTER – SIX

DISCUSSION AND CONCLUSION

6.1 Properties of Electrical Resistivity

At this moment, we can say most mechanisms contributing to the electrical resistivity $\rho(T)$, give either $\rho(T)$ decreasing to zero at temperatures approaching zero (phonon or electron–electron interaction), or $\rho(T) = \text{constant}$ as $T \rightarrow 0$ (non-magnetic impurity). However, metals containing magnetic impurities show *anomalous electrical resistivity* behavior as the temperature lowers.

If we examine the low temperature properties of electrical resistivity of our case, from equation (5.34), it is dominated by scattering of magnetic impurity. So that we describe its low temperature dependence based on methods discussed in the preceding chapter. Taking this prevailing (the most dominating) part from it and putting like

$$\frac{\rho_{imp}(T)}{\rho_0} = \left[1 + 4JN(E_F) \ln\left(\frac{T}{D}\right) \right], \quad (6.1)$$

Where $\rho_0 = \frac{3\pi mJ^2 S(S+1)}{2e^2 \hbar E_F}$, is constant for a fixed value of S .

Using equation (6.1) we can generate the following figure, it will ensure the approximate behavior of electrical resistivity of dilute magnetic alloys at low temperature.

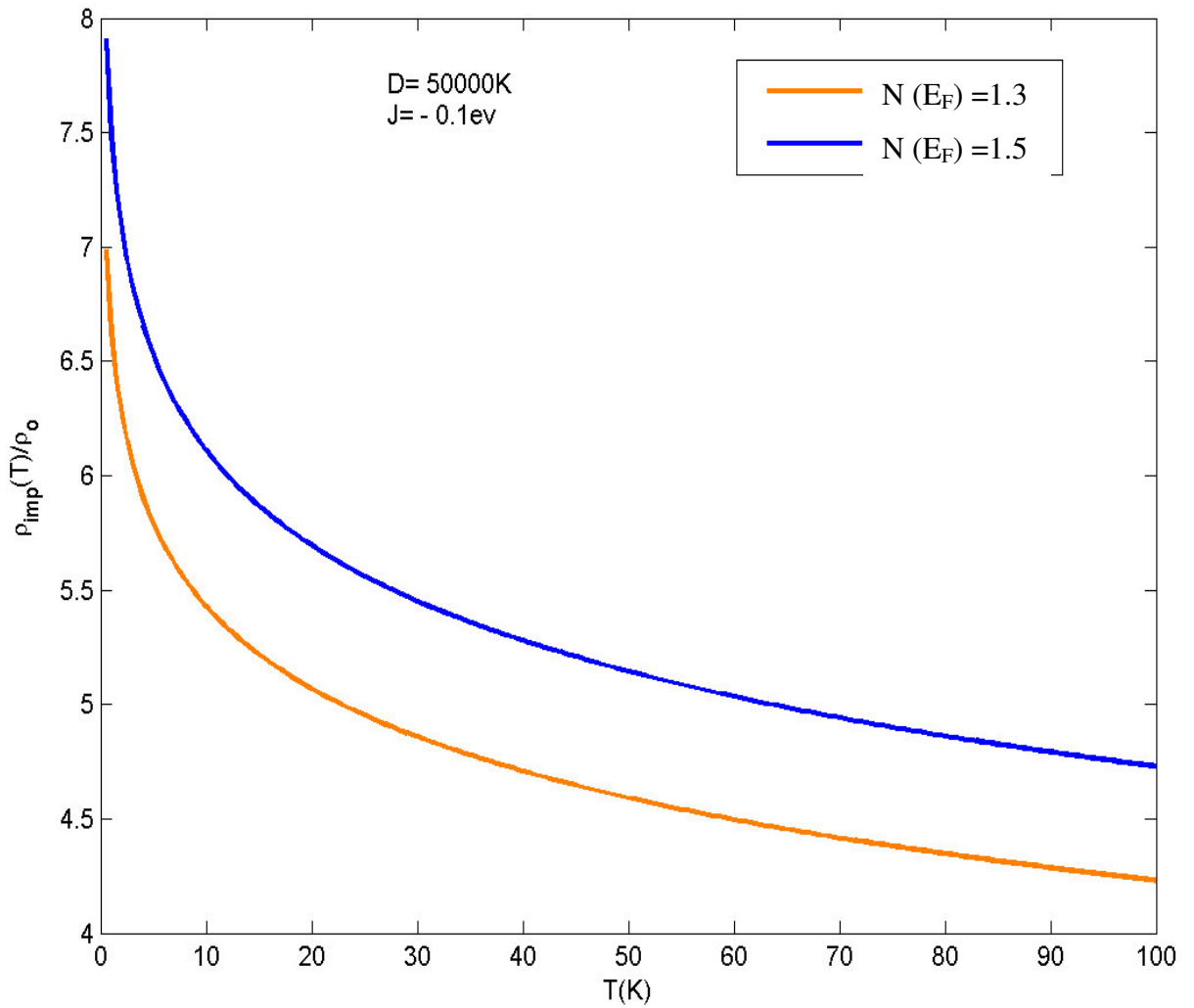


Figure 4: Temperature dependence of the electrical resistivity plotted in a normalized representation according to equation (6.1) for two values of $N(E_F)$ in the temperature range between zero to 100K

From figure 4, we can deduce that, if the coupling constant, J is negative (antiferromagnetic) the electrical resistivity increases with decreasing temperature. In other word due to the divergence of the logarithmic term, the resistivity diverges as temperature approaches zero.

The experimental results shown in section 2.6 particularly for an alloy of copper and iron indicate that there is a temperature corresponding to the minimum resistivity. In our case the resistivity minima can be found if phonon contribution is taken in to account. For the resistivity increase at high temperature is mainly due to scattering of electrons by thermal phonons.

6.2 Conclusion

Most scattering mechanisms lead one to conclude that the resistivity of metals fall with decreasing temperature and become constant at low temperature. However, for some materials like the magnetic alloys the resistivity some times goes through a minimum and then rises as the temperature decreases. The effect is due to the presence of impurity with unfilled inner shells, and net spin in the host metal. Transition metal atoms such as Mn, Cr, Fe, and Co are typical magnetic impurities. The potential describing the interaction of electron with such impurities contains an additional spin-dependent contribution.

A simple s - d model was used based on the supposition that a magnetic moment is formed at the impurity. Once the moment is formed, the approximation is that, its interaction with the conduction electron could be treated separately. In the interaction the conduction electron with spin, is coupled to the total angular momentum of the impurity by an effective exchange integral J .

By assuming that an antiferromagnetic J exchange coupling, the calculation of the s - d model Hamiltonians is presented to the third order perturbation theory (the second Born approximation) of conduction electron scattering on magnetic impurity electrons. It is the spin flips of the conduction /magnetic impurity electrons during their interaction, which makes the conduction electrons Fermi-Dirac energy distribution (and therefore the temperature) dominant in calculation of the scattering probability.

The basic physical idea here is that during the scattering the spin angular momentum of the electron of the impurity fluctuates (i.e. it changes its projection along the main quantization axis direction) and the fluctuation depends on the different scattering channels with the conduction electrons of the Fermi-sea, whose occupation are determined by the Fermi distribution. In calculating the transition probability of the conduction electrons to the third order of interaction it is shown

that the transition probability has *logarithmic anomaly* at the Fermi-surface and that in the resistivity there appears a term proportional to $\ln T$.

In general, for an antiferromagnetic coupling (negative J) the contribution to the electrical resistivity from the s - d interaction decreases with increases temperature; at low temperatures a logarithmic term in the expression of resistivity dominates; and then as the temperature approaches zero the logarithmic term diverges.

It will be interesting to consider alloys incorporating rare earth elements in my future studies.

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DECLARATION

I hereby declare that this thesis is my original work and has not been presented for a degree in any other university. All sources of material used for the thesis have been duly acknowledged.

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