Chapter

Temperature Dependence of Electrical Resistivity of $(III, Mn)V$ Diluted Magnetic Semiconductors

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Abstract

In this work, a theory of temperature dependence of electrical resistivity is developed, with a particular emphasis on dilute magnetic semiconductors (DMSs). The approach is based on the equation of motion of the Ruderman-Kittel-Kasuya-Yosida (RKKY) exchange interaction and considers both spin and charge disorder. The formalism is applied to the specific case of $Ga_{1-x}Mn_xAs$. Using the RKKY exchange interaction, the relaxation time τ and the exchange interaction J are calculated. Then using spin-dependent relaxation time, electrical resistivity of the material is calculated. The electrical resistivity of Mn-doped III—V DMS is decreased with increasing temperature and magnetic impurity concentration.

Keywords: RKKY interactions, electrical resistivity, spin-dependent relaxation time

1. Introduction

The motivation for this study has been to better understand semiconductors, which could be the building block for the next generation of computers. Semiconductors have been the subject of very extensive research over recent decades, because of ever more numerous and powerful applications. As conventional electronics, semiconductors are more appropriate than normal metals, since metal devices do not amplify current. Because of the complementary properties of semiconductor and ferromagnetic material systems, a growing effort is directed toward studies of semiconductor-magnetic nanostructures [1, 2].

Semiconductors and magnetic materials both play essential roles in modern electronic industry. Since the applications of semiconductors and magnetic have evolved independently, it appears logical to combine their properties for possible spin-electronic applications with increased functionalities [3]. This is known as spintronics, which utilizes both charge and spin of the electrons to process and store data. This is to control the spin degree of freedom of electrons in semiconductors. The direct method to introduce spin degrees of freedom in semiconductors is to introduce magnetic ions into semiconductors. Such semiconductors are referred to as diluted magnetic semiconductors (DMSs) [4]. The curie temperature of the DMS material and whether the ferromagnetism in the DMS material originates from free carrier mediation or purely from localized magnetic dopants limit DMS practical applications for devices [5].

For practical applications, increasing T_C beyond room temperature is a necessity. Thus, exploring various roots of raising the value of T_C is a great fundamental and practical significance. Carrier-mediated ferromagnetism in p-type II-VI DMS hetero-structures occurs only at very low temperatures T_C typically below $2.0K$. Therefore, very significant strides have been made in developing ferromagnetic-based $III-V$ semiconductors containing $Mn,$ which remaining ferromagnetic to much higher T_C [3, 6]. A discovery of ferromagnetic ordering in III–V DMSs with critical temperatures of annealed $Ga_{1-x}Mn_xAs$ could exceed 110 k; reaching ~191 K has renewed and greatly intensified an interest in those materials, but still too low for actual applications. This was, at least partially, related to expectations that their Curie temperatures can be relatively easily brought to room temperature range through a clearly delineated path [7–9].

For the ferromagnetic transition to occur in $Ga_{1-x}Mn_xAs$, the concentration of Mn impurities should be relatively high, x = 0.01–0.05. Such high concentration of impurities makes the study of the DMS more challenging. Moreover, the issue of solubility of the magnetic ions into the regular semiconductor was a major challenge to fabricate high-quality DMSs. In recent years, Molecular Beam Epitaxy techniques have led to the successful growth of various DMS including $(Ga, Mn)As$. In order to prevent phase separation order, magnetic $Ga_{1-x}Mn_xAs$ should be grown at low temperatures (T; 200–300°C). These problems are not specific to $Ga_{1-x}Mn_xAs$, in fact, all presently known DMS materials suffer from the same problems. As a result, theoretical study of DMS electrical properties such as resistivity is very difficult. Since these properties are influenced by the exchange interaction between the carriers and the localized moments, it must be taken into account non-perturbatively [10, 11]. Due to these influences, spin fluctuation scattering contributes to the resistivity. The experimentally measured dc resistivity in the DMS materials shows interesting behavior strongly depending on the concentration of the magnetic impurity and temperature. In (Ga,Mn)As, there is a metal–insulator transition between insulating samples with small manganese concentration and metallic samples with larger concentration. In and with low concentration (x < 0.03), only an insulating behavior has been observed in transport measurements. Insulating behavior is here characterized by a diverging resistivity for T → 0, indicating localization of carriers. However, near-optimal doping x = 0.05, where the highest value of is reported, the nonmonotonic behavior of insulator–metal–insulator of the resistivity as a function of temperature is observed. A resistivity peak appears near the critical temperature, and the resistivity shows metallic behavior below and insulating behavior at higher temperatures. In metallic samples, the resistivity decreases and eventually saturates for T → 0. The peak has been understood as the critical scattering effects of spin fluctuations [11–13]. In this paper, a Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction was used for the calculation of the resistivity. This paper focuses on the group $III-Mn-V$ ferromagnetic semiconductors, more specifically $Ga_{1-x}Mn_xAs$. Even though we focus on III–V compound based DMS such as $Ga_{1-x}Mn_xAs$, the results presented in this paper are general for all DMS materials.

2. Theoretical formalism

2.1 RKKY interaction approaches to p-d exchange interaction

The carrier-mediated spin–spin coupling is usually described in terms of the Ruderman-Kittel-Kasuya-Yosida (RKKY) model, which provides the energy J_{ij} of exchange coupling. When magnetic impurity Mn is introduced into semiconductors,

spin flip processes become possible. The spin of the scattered electron and the spin of magnetic impurities are flipped simultaneously while the component of the total spin along the quantization axis is conserved. The interaction of the impurity with conduction electron is described as p-d or s-d interaction. The spin density of electrons determines this interaction at the localized moment. Like in the Heisenberg model, the scalar product of two spins is taking with the exchange coupling J [14, 15]. Writing the spin density of electrons in terms of the field operators, the interaction between the spin S_j at r_j and the conduction electron is

$$H_{p-d} = -2JS_j.S_i(r_j) = -J\sum_{\alpha\beta}S_j.\sigma_{\alpha\beta}(\hat{\psi}^+{}_\alpha(r_j)\hat{\psi}_\beta(r_j)) \tag{1}$$

Where $\hat{\psi}$ is the field operator states expanded in terms of the block states. Using the field operators, the Fourier transform of number density operator $n(r)$ becomes

$$n(q) = \int n(r)e^{-q.r}dr = \frac{1}{V}\sum_{kk'\sigma}\int e^{-i(k+q-k').r}u_k^*(r)u_{k'}(r)c_{k\sigma}^+ c_{k'\sigma}dr \tag{2}$$

Where $c_{k\sigma}$ and $c_{k\sigma}^+$ are the annihilation and creation operators of electrons, respectively. The integral in Eq. (2) is vanished unless $k' = k + q + G$ due to the lattice periodicity of the function s $u_k(r)$. Where G is the reciprocal lattice vectors. The coupling strength depends on state k', the state in which the electron of wave vector k is scattered. If we express Eq. (2) in terms of the spin density and the system contains N_i localized spins, the interaction with conduction electrons is determined by

$$H_{p-d} = -\frac{J}{V}\sum_{l=1}^{N_i}\sum_{k,k'}\sum_{k,k'}e^{i(k-k').r}\left\{S_l^+ c_{k'\downarrow}^+ c_{k\uparrow} + S_l^- c_{k'\uparrow}^+ c_{k\downarrow} + S_l^z\left(c_{k'\uparrow}^+ c_{k\uparrow} + c_{k'\downarrow}^+ c_{k\downarrow}\right)\right\} \tag{3}$$

The interaction of localized spin *Mn* ions with electron gives rise to the creation or annihilation of an electron–hole pair. By considering elastic transitions and the common energy $E_k = E_{k'}$ denoted by E_0, the Hamiltonian is written as

$$\langle k'|H_{eff}|k\rangle = -\sum_j \frac{\langle k'|\lambda H_{eff}|j\rangle\langle j|\lambda H_{eff}|k\rangle}{E_j - E_0} \tag{4}$$

Where $|k\rangle$ is ground state, $|k'\rangle$ is the state of the scattering of electron, λ is the coupling constant, and H_{eff} is the effective Hamiltonian, which is equal to H_{p-d}. Since the flip of the impurity spin is accompanied by the flip of an electron spin, the collision term of distribution function of spin-up and spin-down electrons is

$$\left(\frac{\partial f(k)}{\partial t}\right)_{coll} = \sum_{k'}W_{k\uparrow,k'\uparrow}\left\{f_\uparrow(k')\left[1 - f_\uparrow(k)\right] - f_\uparrow(k)\left[1 - f_\uparrow(k')\right]\right\}$$
$$+ \sum_{k'}W_{k\uparrow,k'\downarrow}\left\{f_\downarrow(k')\left[1 - f_\uparrow(k)\right] - f_\uparrow(k)\left[1 - f_\downarrow(k')\right]\right\} \tag{5}$$

Where $W_{k,k'}$ is the transition probability, $f(k)$ and $f(k')$ are the distribution functions of the initial states and the scattered states, respectively. The transition probability between two states α and β is given by

$$W_{\alpha\beta} = \frac{2\pi}{\hbar} \left| \langle \alpha | H_{p-d} | \beta \rangle \right|^2 \delta \left(E_\alpha - E_\beta \right) \tag{6}$$

Where $|\alpha\rangle$ is the eigen state of the initial system, and E_α is the corresponding eigen values, $|\beta\rangle$ is the final eigen states, and E_β is the corresponding eigen values, respectively. If the spin is flipped in the intermediate state, an electron of quantum numbers M_l'' appears in the first process, and the impurity spin goes over from the initial state $S^z = M$ to $S^z = M + 1$. Where the electron–hole pair is composed of a spin-up electron and spin-down hole, the impurity spin has to flip down, to the state $S^z = M - 1$. Then by substituting state α and β and using the distribution function for the spin of the electron–hole pair, the total contribution is

$$\langle f | H_{eff} | i \rangle = - \left(\frac{J}{N} \right)^2 \sum_{ij} \frac{f_0(E_k)\left[1 - f_0(E_{k'})\right]}{E_{k'} - E_k} e^{i(k-k') \cdot (r_j - r_i)} \left\{ 2 \langle \{M_l'\} | S_i^z S_j^z + \frac{1}{2} \left(S_i^+ S_j^- + S_i^- S_j^+ \right) |M_l\rangle \right. \tag{7}$$

Where $|\{M_l''\}\rangle$ is the state of the spins of the z-component of the intermediate states, and M_l'' is the corresponding eigen values, $|\{M_l'\}\rangle$ is the state of the spins of the z-component of the scattered states, and M_l' is the corresponding eigen value, and $|\{M_l\}\rangle$ is the state of the spins of initial state, and M_l is the corresponding eigen value.

Eq. (7) can be considered as the matrix element of the operator H, when we write the exchange energy between S_i and S_j, which is written as

$$H = - \sum_{ij} J \left(r_i - r_j \right) S_i . S_j \tag{8}$$

To determine the exchange coupling strength $J \left(r_i - r_j \right)$, we introduce $\boldsymbol{r} = \boldsymbol{r_i} - \boldsymbol{r_j}$ where **r** is the displacement vector between the ions i and j, and using the following integral notation I as

$$I = (1/V)^2 \sum_{kk'} \frac{f_0(E_k)\left[1 - f_0(E_{k'})\right]}{E_{k'} - E_k} e^{i(k-k') \cdot r} \tag{9}$$

Replacing the sum in Eq. (9) by an integral, using the quadratic dispersion relation valid for free electrons and the notations $\kappa = kr, \kappa' = k'r$, the parabolic energy $E_k = \frac{\hbar^2 k^2}{2m^*}$, in which m^* is the effective mass, and trigonometric identity $sin \, \kappa' = \frac{e^{i\kappa'} - e^{-i\kappa'}}{2i}$ and the complex variable $\kappa' + i\eta$ instead of κ', where η is an infinitesimal quantity, the angular integral becomes

$$I = - \frac{m_e k_F^4 {}_{J^2}}{\hbar^2 \pi^3} \frac{sin \, 2k_F r - 2k_F r cos 2k_F r}{(2k_F r)^4} \tag{10}$$

Then the effective exchange interaction or the coupling exchange interaction constant between magnetic impurities and delocalized charge carriers is given by

$$J(r) = \frac{m_e J^2 k_F^4}{\hbar^2 \pi^3} F(2k_F r) \tag{11}$$

Where k_F is the Fermi wave vector and the function $F(x) = \frac{x\cos x - \sin x}{x}$, $x = 2k_F r$. Eq. (11) gives the well-known RKKY interaction. As the value of the oscillatory function $F(2k_F r)$ varies, the value of the exchange interaction is either positive or negative, and hence, the interaction in the system can be ferromagnetic or antiferromagnetic.

By using Eq. (11), we can determine the relaxation time τ of the impurity spin of electrons. For spin conserving scattering, the matrix element of Eqs. (7) and (8) is

$$\langle k'|H_{eff}|k \rangle = -\frac{J}{V}S^z \tag{12}$$

A better approximation can be obtained for the transition probability by replacing the matrix element of the scattering matrix T in Eq. (6). Then Eq. (6) is rewritten as

$$W_{\alpha\beta} = \frac{2\pi}{\hbar}|\langle \alpha|T|\beta \rangle|^2 \delta(E_\alpha - E_\beta) \tag{13}$$

The scattering (transition) probability in Eq. (13) can be expressed in terms of the interaction Hamiltonian up to third order in the coupling constant. Then using the second-order correction to the T matrix, the Fermi-Dirac distribution function, which is expressed by $f_0(k) = \langle c_k^+ c_k \rangle$ and if the z-component of the impurity spin is unchanged by the scattering, the combined contribution is

$$\left(-\frac{J}{V}\right)^2 \sum_{k''} (S^z)^2 \frac{(1 - f_0(k''))}{E_k - E_{k''}} - \frac{f_0(k'')}{E_{k''} - E_{k'}} = \left(-\frac{J}{N}\right)^2 (S^z)^2 \sum_{k''} \frac{1}{E_k - E_{k'}} \tag{14}$$

If the impurity spin goes over from the initial state $S^z = M$ to $S^z = M + 1$, the electron–hole pair is composed of a spin-up electron and a spin-down hole (i.e., the impurity spin has to flip down) to the state $S^z = M$ to $S^z = M - 1$, and on the account of conservation of energy $E_k = E_{k'}$, then the combined contribution of these processes gives

$$\left(-\frac{J}{V}\right)^2 \sum_{k''} \left\{ [S(S+1) - M^2] \frac{1}{E_k - E_{k''}} - M \frac{1 - 2f_0(k'')}{E_k - E_{k''}} \right\} \tag{15}$$

The first term in Eq. (15) is negligible since it is small; however, the second term is no longer small. The second term diverges logarithmically. Using this form, the transition probability Eq. (13) in J by summing over the possible spin orientations is given by

$$W(k\uparrow, k'\uparrow) = W(k\uparrow, k'\downarrow) = \frac{N_i 2\pi J^2 S(S+1)}{3\hbar}[1 + 4Jg(E_k)]\delta(E_k - E_{k''}) \tag{16}$$

Where N_i is the concentration of magnetic impurities, which is $N_i = 4x/a_{lc}^3$ where x is the concentrations of the impurity added to the semiconductors, a_{lc} is lattice constant, and the singular function in the third order correction is

$$g(E_k) = \frac{1}{V} \sum_{k''} \frac{f_0(k'')}{E_k - E_{k''}} \tag{17}$$

We shall investigate the dependence of Eq. (16) on the energy of the initial state E_K, which is entirely involved in the function $g(E_k)$. At the absolute zero of temperature, $f_0(k'')$ can be replaced by a step function, which is unity when $k'' < k_0$ and zero when $k'' > k_0$, where k_0 is the magnitude of the Fermi momentum.

By using Fermi-Dirac distribution, $E_k = \frac{\hbar^2 k^2}{2m^*}$ and for electron close to the Fermi surface at low temperature, the singular function becomes

$$g(E_k) = \left(\frac{3z}{2E_F}\right)\{1 + (k/2k_0)\log|(k - k_0)/(k - k_0)|\} \tag{18}$$

Where z is the number of conduction electrons per atom. Since at $T \neq 0$, the average of $|k - k_0|$ for thermally excited electrons is proportional to T, even at this stage of calculation we can expect a term proportional to $\log T$ in the expression of the resistivity. It is true that $g(E_k)$ diverges when E_k approaches to E_F. Eq. (18) makes the calculation easier to retain the definition of $g(E_k)$ here and to carry out the summation after we get the expression for the resistivity.

Then substituting Eq. (16) into collision integral, the relaxation time τ is the inverse of the transition probability. Therefore, the spin-dependent relaxation time is

$$\frac{1}{\tau} = \frac{N_i 2\pi J^2 S(S + 1)}{3\hbar E_F}[1 + 4Jg(E_k)] \tag{19}$$

The Fermi energy E_F is given by $E_F = \frac{\hbar^2 k^2}{2m^*} = \frac{\hbar^2}{2m^*}\left(3\pi^2\left(\frac{N}{V}\right)\right)^{\frac{2}{3}}$. In $III - V$ semiconductors, it is found that the maximum and minimum energy locations of the Fermi level typically do not deviate by more than 1ev. In the specific case of $GaAs$, the conduction band is located at $E_{FS} + 0.9eV$ and the valence band at $E_{FS} - 0.5eV$ [3]. Where E_{FS} is the Fermi-level stabilization energy, and it is found to be located at $\sim 4.9eV$ below the vacuum level and is the same for all III-V and II-VI SCs. since Mn-doped $GaAs$ is a p-type, we use Fermi level energy of the valence band. By using this value of Fermi energy and the values of other constant, we can calculate τ_0.

In the presence of external perturbation due to the electric field or temperature gradient, there is a variation in the function $f_k^{\pm}$. Supposing the electric field lies along the z-direction, then using Eq. (19), the rate change of the probability $f_k^{\pm}$ with which the state $K_{\pm}$ is occupied due to the collision with the localized spins becomes

$$\left(\frac{\partial f_k^{\pm}}{\partial t}\right)_{coll} = -\frac{(f_k^{\pm} - f_k^0)}{\tau} \tag{20}$$

Then from standard theory, we can easily obtain the resistivity as

$$\rho_{spin} = x\rho_0\left\{1 - \left(\frac{\hbar^2 j}{\pi m_h^* k_0}\right)\int g(E_k)\left(\frac{df^0}{dE_k}\right)d^3k\right\} \tag{21}$$

Where ρ_0 is defined by

$$\rho_0 = 3\pi m_h^* J^2 S(S + 1)(V/N)/2e^2\hbar E_F \tag{22}$$

Where V is the volume of the crystal. Then using some techniques, the total electrical resistivity becomes

$$\rho_{spin} = x\rho_0\{1 - (3zJ/E_F)\log T\} \qquad (23)$$

Since substitutional *Mn* ions in *GaAs* (i.e., $Ga_{1-x}Mn_xAs$) are a p-type semiconductor, we use the hole concentration $p = \frac{N}{V}$, instead of n. The hole concentration p would ideally to be given by $p = xN_0$ where $N_0 = 2.2x10^{22}cm^{-3}$ is the concentration of *Ga* sites in *GaAs* and x is the concentration of impurity [3]. For $(Ga, Mn)As$, the hole effective mass $m_h^* = 0.5m_0$, where $m_0 = m_e$ is the electron mass [16].

3. Results and discussion

As mentioned in Section 2, the temperature dependence of electrical resistivity is calculated. The electrical resistivity of p-type *Mn*-doped *GaAs* has been investigated theoretically. This theoretical calculation is done using RKKY interaction models. This theoretical calculation is somewhat similar to experimental work, which is done on this material. In this paper, we use RKKY to calculate the exchange interaction constant and spin-dependent relaxation time approximation. Using these exchange interaction constant and spin-dependent relaxation time, the electrical resistivity of this material is calculated.

Electrical resistivity is the inverse of electrical conductivity of the material. The electrical resistivity of semiconductors decreases exponentially with increasing temperature in contrast to that of pure metals. The electrical resistivity of extrinsic semiconductor is decreased with increasing both the concentration of magnetic impurity and the temperature. From this concept the electrical resistivity of DMSs, in
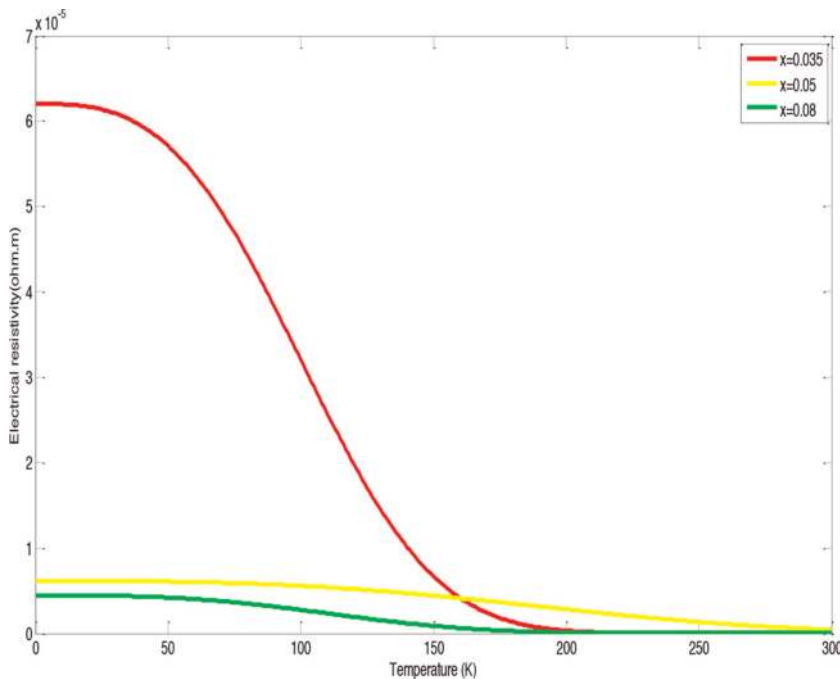

Figure 1.
Electrical resistivity of $Ga_{0.92}Mn_{0.08}As$ versus temperature.

which magnetic impurities are incorporated into standard semiconductors, is decreased with temperature and concentration of magnetic ions. The temperature dependence of resistivity in $Ga_{1-x}Mn_xAs$ for $0.08 \leq x \geq 0.01$ is shown in **Figure 1**. From Eq. (23) the electrical resistivity is inversely proportional to the hole density or hole concentration (i.e., $\rho \propto \frac{1}{p}$). Since $Ga_{1-x}Mn_xAs$ is an extrinsic semiconductor, its hole concentration is increased with adding the impurity. Then the electrical resistivity decreases with increasing concentration. From **Figure 1** the electrical resistivity of $Ga_{1-x}Mn_xAs$ for x = 0.035, x = 0.05, and x = 0.08 is drawn. From the graph as the magnetic impurity concentration is increased, its resistivity decreases. As the temperature and hole concentration increase, the electrical resistivity is decreased. At x = 0.08 or at high concentration, there is low resistivity and at x = 0.035, the resistivity is high.

4. Conclusion

In this paper, we studied the theoretical temperature dependence of electrical resistivity of DMS specifically $Ga_{1-x}Mn_xAs.Ga_{1-x}Mn_xAs$ has become the most understood and extensively studied $III_{1-x}Mn_xV$ ferromagnetic semiconductor. DMSs show interesting electrical properties, which strongly depend on the concentration of magnetic dopants and temperature. These properties of $Ga_{1-x}Mn_xAs$ is affected by concentration and temperature. Since the electrical properties are dependent on the density of states, the impurity added to the semiconductor increases this density of state and decreases energy gap. The electrical resistivity of $Ga_{1-x}Mn_xAs$ is exponentially decreased with an increase of temperature from $0K - 300K$ and concentration of magnetic ions in the range of $0.08 \leq x \geq 0.01$. In general, if T_C of the DMSs can be increased, there is a possibility of utilizing the system under consideration for the spintronic purpose at room temperature.

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Conflicts of interest

The authors declare no conflicts of interest.

Data availability

No data were used to support this study.

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