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On the Scattering of Conduction Electrons by Magnetic Impurities in Semiconductors of InSb-Type and HgTe-Type Band Structure

By

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The relaxation time and the mobility are calculated for the case of the conduction electrons scattered by impurities possessing localized magnetic moments. The Kane model is used to describe the energy bands. The perturbing potential is assumed to be of a short range. The numerical estimations are made for two special forms of perturbation: delta-like and square-well form. The estimations show that the contribution of the considered mechanism to the mobility is small compared to that of other scattering mechanisms. However, there exist transport phenomena which seem to be strongly influenced by magnetic impurity scattering.

Производится расчет времени релаксации и подвижности электронов проводимости для случая рассеяния на примесях с локализованным магнитным моментом. Для описания зонной структуры исплользуется модель Кейна. Возмущающий потециал рассматрывается как потенциал короткодействующий. Численные расчеты выполнены для двух частных видов возмущениий: для контактного взаимодействия и для прямоугольной потенцальной ямы. Численные оценки указывают, что влияние рассматриваемого механизма на подвижность мало по сравнению с влиянием других механизмов рассеяния. Существуют однако эффекты, на которые рассеяние на магнитных примесях имеет по-видимому существенное влияние.

1. Introduction

The relaxation time for various charge carrier scattering mechanisms in semiconductors is a basic quantity for any further transport phenomena considerations. In this paper we shall be interested in narrow- and zero-gap semiconductors. There are several papers treating the problem of the relaxation time in n-type InSb (e.g. [1, 2]) as well as in n-HgTe (e.g. [3, 4]) for different scattering mechanisms.

When paramagnetic impurities are present in a semiconductor (such as manganese replacing mercury atoms in $\mathrm{Hg}_{1-x}\mathrm{Mn}_x\mathrm{Te}$, or germanium atoms in $\mathrm{Ge}_{1-x}\mathrm{Mn}_x\mathrm{Te}$), one may think of a scattering mechanism which was not considered till now in narrow- and zero-gap semiconductors, namely the scattering of electrons by magnetic impurities. This problem was already considered in the case of magnetic semiconductors with large energy gap (e.g. [5]). In this paper we shall calculate the relaxation time for such a process. The calculation is based on the localized magnetic moment approximation. The scope of our considerations will be limited to weak external magnetic fields and to low concentrations of magnetic impurities ($H(\mathrm{G}) < 1.0 \times 10^2 T$, T being absolute temperature in K; concentration of e.g. Mn in HgTe: $N < 5\,\mathrm{at\%}$). For stronger magnetic

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fields one has to take into account the Landau splitting of the conduction band. This problem will be dealt with in another paper. For weak magnetic field the scattering may be regarded as an elastic process. Therefore one can introduce a single relaxation time.

In Section 2 we describe in detail the considered system which consists of semiconductor and magnetic impurities. Also specified is the interaction of these two subsystems. Section 3 is devoted to the derivation of formulas for the relaxation time of the considered scattering mechanism. The numerical estimations of electron mobility resulting from the relaxation time calculated in the previous section are presented in Section 4. The mobility was computed in the limit of high degeneracy for two simple models of short-range perturbations: contact potential and square-well potential.

2. Specification of the System

We shall consider the following system: narrow- or zero-gap semiconductor with InSb-type or HgTe-type energy band structure, containing a small amount of paramagnetic impurities which substitute Hg or In atoms of the host crystal. Such impurities possess magnetic moments which, as we assume, are well localized. A direct interaction between two magnetic moments will be neglected. This is justified for low concentration of impurities when the mean distance between two impurities is large compared to the spatial extension of the wave functions of the electrons producing the magnetic moments. Hence the overlap of these functions of two neighbouring impurities is small, which makes direct interaction negligible. We assume a random spatial distribution of impurities in the crystal.

We do not consider eventual clusters of impurities. These clusters can have a pronounced influence on magnetic susceptibility of the crystal [6], but they should not affect significantly the transport phenomena. We shall also neglect the indirect (via conduction electrons) coupling of magnetic moments of the impurities [6]. Therefore we are dealing with a kind of paramagnetic system of magnetic moments.

The Hamiltonian of the entire system can be written in the following form:

$$\mathcal{H} = \mathcal{H}_\mathrm{e} + \mathcal{H}_\mathrm{m} + \mathcal{H}_\mathrm{i}\,, \tag{1}$$

$\mathcal{H}_\mathrm{e}$ is the conduction electron Hamiltonian. According to Kane's theory it gives (e.g. [2, 4]) the following eigenfunctions of conduction electrons:

$$\Phi_{j_z,\boldsymbol{k}} = V^{-1/2} \exp\,[i\boldsymbol{k}\cdot\boldsymbol{r}]\, u_{j_z}(\boldsymbol{r})\,. \tag{2}$$

V is the crystal volume, j_z is the projection of the electronic total momentum on z-axis, and $u_{jz}(\boldsymbol{r})$ is a lattice periodic function equal to ([2, 4])

$$\left.\begin{aligned} u_{1/2} &= \left(iaS + \frac{b - c\sqrt{2}}{2}\,\frac{k_+}{k}\,R_- - \frac{b + c\sqrt{2}}{2}\,\frac{k_-}{k}\,R_+ - c\,\frac{k_z}{k}\,Z\right)\uparrow + \\ &\quad + b\left(\frac{k_z}{k}\,R_+ - \frac{k_+}{k}\,\frac{Z}{\sqrt{2}}\right)\downarrow\,, \\ u_{-1/2} &= \left(iaS - \frac{b + c\sqrt{2}}{2}\,\frac{k_+}{k}\,R_- + \frac{b - c\sqrt{2}}{2}\,\frac{k_-}{k}\,R_+ - c\,\frac{k_z}{k}\,Z\right)\downarrow - \\ &\quad - \left(b\,\frac{k_z}{k}\,R_- - \frac{k_-}{k}\,\frac{Z}{\sqrt{2}}\right)\uparrow\,. \end{aligned}\right\} \tag{3}$$

Here $k_\pm = k_x \pm ik_y$, $R_\pm = 1/\sqrt{2}(X \pm iY)$ and X, Y, Z, S are Luttinger-Kohn amplitudes possessing the symmetry properties as x, y, z, s functions under operations of the tetrahedral group. The coefficients a, b, c are given in the limit of $E \ll \Delta$ by

$$a^2 = \frac{E_g + E}{E_g + 2E}, \qquad b^2 = \frac{E}{3(E_g + 2E)}, \qquad c^2 = \frac{2E}{3(E_g + 2E)} \tag{4}$$

for InSb-type band structure and

$$a^2 = \frac{E}{E_g + 2E}, \qquad b^2 = \frac{E + E_g}{3(E_g + 2E)}, \qquad c^2 = \frac{2}{3}\frac{E + E_g}{E_g + 2E} \tag{5}$$

for HgTe-type band structure.

Δ is the spin–orbit splitting, E_g the energy distance between Γ_6 and Γ_8 levels, and E denotes the energy of the electron in question. $\downarrow$ and $\uparrow$ in (3) denote Pauli's spinors for electron spin down and up, respectively.

The eigenvalues of $\mathcal{H}_e$ depend on the wave vector of the electron in the following way (free electron mass term omitted):

$$E = -\frac{E_g}{2} + \left[\left(\frac{E_g}{2}\right)^2 + E_g \frac{\hbar^2 k^2}{2m_e^*}\right]^{1/2}, \tag{6}$$

m_e^* being the effective mass of the electron at the bottom of the conduction band.

The $\mathcal{H}_m$ term in (1) describes the system of magnetic impurities. As it was already said before, we assume that the impurities do not interact with each other, so $\mathcal{H}_m$ is simply the sum of Hamiltonians $\mathcal{H}_m^n$, each describing a single impurity in the n-th lattice site:

$$\mathcal{H}_m = \sum_n \mathcal{H}_m^n \,. \tag{7}$$

It is fair to assume that the wave function χ_n of a single magnetic impurity in the n-th lattice site is characterized by two quantum numbers: $S_n(S_n + 1)$ and M_n: the square of impurity spin and its projection on z-axis, respectively. In other words $[\mathcal{H}_m^n, S_n^2] = 0$ and $[\mathcal{H}_m^n, S_n^z] = 0$. We shall assume also that for different M_n values eigenfunctions of (7), $\chi_n(M_n)$, form an orthonormal set. If all impurities are identical, S_n has the same value for all n and it will be denoted by S. In such a case the following equations hold:

$$\left.\begin{aligned} S_n^z \chi_n(M_n) &= M_n \chi_n(M_n)\,, \\ S_n^2 \chi_n(M_n) &= S(S+1)\,\chi_n(M_n)\,. \end{aligned}\right\} \tag{8}$$

In consequence of (7) the full wave function of the whole magnetic impurity system is a product $\prod_n \chi_n(M_n)$. If the external magnetic field H parallel to z-axis is applied to the crystal, one has to add two further terms to the Hamiltonian (1). These are

$$g\,\beta \sum_n S_n^z H \quad \text{and} \quad g'\beta\sigma_z H\,, \tag{9}$$

where $\beta = e\hbar/2mc$, σ is conduction electron spin operator, and g, g' are g-factors of the magnetic impurity and conduction electron, respectively.

The interaction term $\mathcal{H}_i$ in (1) describing the coupling of conduction electrons and magnetic impurities will be adopted in the simple form

$$\mathcal{H}_i = \sum_n V(\boldsymbol{r} - \boldsymbol{R}_n) - \sum_n I(\boldsymbol{r} - \boldsymbol{R}_n)\,\boldsymbol{\sigma} \cdot \boldsymbol{S}_n\,, \tag{10}$$

where $\boldsymbol{R}_n$ denotes the position of the magnetic impurity, $V(\boldsymbol{r} - \boldsymbol{R}_n)$ describes the spin-independent part of the interaction, and $I(\boldsymbol{r} - \boldsymbol{R}_n)$ is an exchange term. One can easily show that $[\mathcal{H}_\text{i}, \boldsymbol{S}_n] = 0$, so the value of S is conserved in the process of interaction. The scattering caused by the exchange part of $\mathcal{H}_\text{i}$ is an elastic process, provided there is no external magnetic field. Of course, $V(\boldsymbol{r} - \boldsymbol{R}_n)$ leads also to elastic scattering.

When the magnetic field is applied to the system there is an energy exchange between the scattering electron in the conduction band and the localized magnetic moment in the magnetic field. For sufficiently weak fields this energy exchange is negligible and the scattering is almost elastic. The following condition for the magnetic field can thus be established: $g\beta H < k_\text{B}T$. In case of Mn impurities this is equivalent to $H(\text{G}) < 0.7 \times 10^4 T(\text{K})$.

If the magnetic field fulfills the above condition, the process of scattering can be regarded as elastic. This condition, however, is weaker than the similar magnetic field limitation

$$\hbar\omega_\text{c} = \hbar \frac{e}{m^* c} H < k_\text{B}T$$

ensuing from the requirement that there should be no Landau splitting of the conduction band. This latter condition reads $H(\text{G}) < 7.4 \times 10^3 Tm^*$, which gives $H(\text{G}) < 1.0 \times 10^2 T(\text{K})$ for InSb and $H(\text{G}) < 1.7 \times 10^2 T(\text{K})$ for HgTe.

We have therefore three regions of magnetic field (it is more appropriate to speak about the H/T ratio here). In the first region we have a simple, non-split conduction band and the scattering is elastic. In the second region we have a ladder of Landau levels, but the scattering is still elastic, and in the third region the non-elasticity cannot be neglected. In this paper we consider only the first region. In this region one can treat the problem of scattering within the relaxation time approximation.

3. The Relaxation Time

To perform the task of calculation of the relaxation time one has to compute the matrix elements $\langle \varphi_{\frac{1}{2}k'} \chi' | \mathcal{H}_\text{i} | \varphi_{\frac{1}{2}k} \chi \rangle$, $\langle \varphi_{-\frac{1}{2}k'} \chi' | \mathcal{H}_\text{i} | \varphi_{-\frac{1}{2}k} \chi \rangle$, and $\langle \varphi_{-\frac{1}{2}k'} \chi' | \mathcal{H}_\text{i} | \varphi_{\frac{1}{2}k} \chi \rangle$. The latter of these matrix elements describes the transition with conduction electron spin flip. In this problem the spin flip transitions have two causes:

1. The electron wave function is not a pure spin function but a mixture of spin up and spin down functions. This leads to spin flip transitions even for the spin independent perturbing potential.
2. The interaction Hamiltonian depends on electronic spin. The second cause can lead to spin flip transitions even if the electron wave function is a pure spin function (which is the case for the InSb structure in parabolic approximation suitable for very small E values). The calculation of the above-mentioned matrix elements gives the following results:

$$\langle \varphi_{\pm\frac{1}{2}k'} \chi' | \mathcal{H}_\text{i} | \varphi_{\pm\frac{1}{2}k} \chi \rangle = \frac{1}{V} \sum_n \Bigg\{ \Big[\langle \chi' | \chi \rangle v_1^\pm + \frac{1}{2} (\pm I_1^\pm \langle \chi' | S_n^z | \chi \rangle + \\ + I_2^\pm \langle \chi' | S_n^\mp | \chi \rangle + I_3^\pm \langle \chi' | S_n^\pm | \chi \rangle) \Big] \exp\left[-i(\boldsymbol{k} - \boldsymbol{k}') \boldsymbol{R}_n\right] \Bigg\}, \qquad (11)$$

where

$$\begin{aligned}
&S_n^{\pm} = S_n^x \pm iS_n^y\,,\\
&\left.\begin{aligned}
I_1^{\pm} &= \int \exp\,[i(\boldsymbol{k}-\boldsymbol{k}')\,\boldsymbol{r}]\; I(\boldsymbol{r})\,(A^*_{\pm k'}A_{\pm k} - B^*_{\pm k'}B_{\pm k})\,\mathrm{d}^3\boldsymbol{r}\,,\\
I_2^{\pm} &= \int \exp\,[i(\boldsymbol{k}-\boldsymbol{k}')\,\boldsymbol{r}]\, I(\boldsymbol{r})\, A^*_{\pm k'}B_{\pm k}\,\mathrm{d}^3\boldsymbol{r}\,,\\
I_3^{\pm} &= \int \exp\,[i(\boldsymbol{k}-\boldsymbol{k}')\,\boldsymbol{r}]\, I(\boldsymbol{r})\, B^*_{\pm k'}A_{\pm k}\mathrm{d}^3\boldsymbol{r}\,,\\
v_1^{\pm} &= \int \exp\,[i(\boldsymbol{k}-\boldsymbol{k}')\,\boldsymbol{r}]\, V(\boldsymbol{r})\,(A^*_{\pm k'}A_{\pm k} + B^*_{\pm k'}B_{\pm k})\,\mathrm{d}^3\boldsymbol{r}\,.
\end{aligned}\right\}
\end{aligned} \tag{12}$$

In (12) we use the notation

$$\left.\begin{aligned}
A_{\pm k} &= iaS \pm \frac{b \mp c\sqrt{2}}{2}\,\frac{k_+}{k}\,R_- \mp \frac{b \pm c\sqrt{2}}{2}\,\frac{k_-}{k}\,R_+ - c\,\frac{k_z}{k}\,Z\,,\\
B_{\pm k} &= \pm\, b\left(\frac{k_z}{k}\,R_\pm - \frac{k_\pm}{k}\,\frac{Z}{\sqrt{2}}\right).
\end{aligned}\right\} \tag{13}$$

The spin flip matrix element is equal to

$$\begin{aligned}
\langle\varphi_{\frac{1}{2}k'}\chi'|\,\mathcal{H}_1\,|\varphi_{\frac{1}{2}k}\chi\rangle = \frac{1}{V}\sum_n \Bigg\{\Bigg[\frac{1}{2}\,(\mathcal{L}\,\langle\chi'|\,S_n^z\,|\chi\rangle + K_1\langle\chi'|\,S_n^-\,|\chi\rangle\,+\\
+\,K_2\langle\chi'|\,S_n^+\,|\chi\rangle) + v_2\langle\chi'|\chi\rangle\Bigg]\exp\,[-i(\boldsymbol{k}-\boldsymbol{k}')\,\boldsymbol{R}_n]\Bigg\},
\end{aligned} \tag{14}$$

where

$$\left.\begin{aligned}
\mathcal{L} &= \int \exp\,[i(\boldsymbol{k}-\boldsymbol{k}')\,\boldsymbol{r}]\, I(\boldsymbol{r})\,(A^*_{+k'}B_{-k} - B^*_{+k'}A_{-k})\,\mathrm{d}^3\boldsymbol{r}\,,\\
K_1 &= \int \exp\,[i(\boldsymbol{k}-\boldsymbol{k}')\,\boldsymbol{r}]\, I(\boldsymbol{r})\, A^*_{+k'}A_{-k}\,\mathrm{d}^3\boldsymbol{r}\,,\\
K_2 &= \int \exp\,[i(\boldsymbol{k}-\boldsymbol{k}')\,\boldsymbol{r}]\, I(\boldsymbol{r})\, B^*_{+k'}B_{-k}\,\mathrm{d}^3\boldsymbol{r}\,,\\
v_2 &= \int \exp\,[i(\boldsymbol{k}-\boldsymbol{k}')\,\boldsymbol{r}]\, V(\boldsymbol{r})\,(A^*_{+k'}B_{-k} + B^*_{+k'}A_{-k})\,\mathrm{d}^3\boldsymbol{r}\,.
\end{aligned}\right\} \tag{15}$$

Having calculated the transition matrix elements one can obtain the transition probabilities according to

$$P(j_z, \boldsymbol{k}, \chi \to j_z', \boldsymbol{k}', \chi') = \frac{2\pi}{\hbar}\,\delta(E_{k'} - E_k)\,|\langle\varphi_{j_z'k'}\chi'|\,\mathcal{H}_1\,|\varphi_{j_zk}\chi\rangle|^2. \tag{16}$$

We shall take an average value of these probabilities over all possible initial states, χ, of magnetic impurities:

$$\sum_\chi w_\chi P(j_z, \boldsymbol{k}, \chi \to j_z', \boldsymbol{k}', \chi') \equiv \bar{P}(j_z, \boldsymbol{k} \to j_z', \boldsymbol{k}', \chi')\,, \tag{17}$$

where

$$w_\chi = \prod_n w_\chi^n$$

and

$$w_\chi^n = \frac{1}{Z}\exp\left[-\frac{g\beta H M_n}{k_{\mathrm{B}}T}\right], \tag{18}$$

$$Z = \sum_{M_n=-S}^{S} \exp\left[-\frac{g\beta H M_n}{k_{\mathrm{B}}T}\right]. \tag{19}$$

The inverse relaxation time is to be calculated according to

$$\frac{1}{\tau_{\boldsymbol{k}}} = \frac{1}{2}\sum_{\boldsymbol{k}'}\sum_{\chi'}\sum_{j_z, j_z'} P(j_z, \boldsymbol{k} \to j_z', \boldsymbol{k}', \chi')\,(1 - \cos\vartheta)\,, \tag{20}$$

ϑ is the angle between $\boldsymbol{k}$ and $\boldsymbol{k}'$.

We shall proceed now to the calculation of integrals (12) and (15). If, as we expect, $V(\boldsymbol{r})$ and $I(\boldsymbol{r})$ are a short-range functions (their range being the measure of magnetic impurity localization), rapidly decreasing for $\boldsymbol{r}$ larger than the unit cell dimensions, one can put $\exp\left[-i(\boldsymbol{k}-\boldsymbol{k}')\,\boldsymbol{r}\right]$ equal to unity within the region of non-vanishing $V(\boldsymbol{r})$, $I(\boldsymbol{r})$. The group theoretical consideration yields that the only non-vanishing matrix elements are (compare [7])

$$\left.\begin{aligned} C &= \langle S|\, I(\boldsymbol{r})\,|S\rangle \equiv \int_{\Omega_0} S^*(\boldsymbol{r})\, I(\boldsymbol{r})\, S(\boldsymbol{r})\, \mathrm{d}^3\boldsymbol{r}\,, \\ D &= \langle S|\, V(\boldsymbol{r})\,|S\rangle \equiv \int_{\Omega_0} S^*(\boldsymbol{r})\, V(\boldsymbol{r}) S(\boldsymbol{r})\, \mathrm{d}^3\boldsymbol{r}\,, \\ C' &= \langle X|\, I(\boldsymbol{r})\,|X\rangle\,, \\ D' &= \langle X|\, V(\boldsymbol{r})\,|X\rangle \end{aligned}\right\} \tag{21}$$

and equivalent e.g. $\langle Y|\, V\,|Y\rangle$. Then it is possible to express (12) and (15) in the form

$$\left.\begin{aligned} v_1^{\pm} &= D[a^2 + (c^2 + b^2)\cos\vartheta x]\,, \\ I_1^{\pm} &= C[a^2 + (c^2 - b^2)\cos\vartheta y]\,, \\ I_2^{\pm} &= \mp\, Cy\frac{b}{2}\left(b + c\sqrt{2}\right)\sin\vartheta\, \mathrm{e}^{\pm i\varphi}\,, \\ I_3^{\pm} &= \pm\, Cy\; bc\frac{1}{\sqrt{2}}\sin\vartheta\, \mathrm{e}^{\mp i\varphi}\,, \\ \mathscr{L} &= -\frac{1}{2}Cyb^2\, \mathrm{e}^{-i\varphi}\sin\vartheta\,, \\ K_1 &= C(a^2 + c^2 y\cos\vartheta)\,, \\ K_2 &= 0\,, \\ v_2 &= -\,Dxb\left(\frac{b}{2} - c\sqrt{2}\right)\mathrm{e}^{-i\varphi}\sin\vartheta\,, \end{aligned}\right\} \tag{22}$$

where $x = D'/D$ and $y = C'/C$.

From (16), (17), and (20) we obtain

$$\begin{aligned} \frac{1}{\tau_k} = \frac{1}{\pi\hbar}\, Nk^2\frac{\mathrm{d}k}{\mathrm{d}E}\, \Bigg\{ & D^2\left[L^2 - \frac{2}{3}L(1-L)\,x + \frac{1}{2}(1-L)^2\,x^2\right] + \\ & + \frac{1}{4}\langle S_z^2\rangle_{\mathrm{av}}\, C^2\left[L^2 - \frac{2}{9}L(1-L)\,y + \frac{1}{18}y^2\,(1-L)^2\right] + \\ & + \frac{1}{4}\langle S^+S^-\rangle_{\mathrm{av}}\, C^2\left[L^2 - \frac{4}{9}L(1-L)\,y + \frac{21}{54}\,y^2(1-L)^2\right] + \\ & - \frac{1}{9}\langle S_z\rangle_{\mathrm{av}}\, DC\; xy(1-L)^2 \Bigg\} \end{aligned} \tag{23}$$

for the HgTe-type band structure and

$$\begin{aligned}\frac{1}{\tau_k} = \frac{1}{\pi\hbar} N k^2 \frac{\mathrm{d}k}{\mathrm{d}E} \Bigg\{ & D^2 \left[(1-L)^2 - \frac{2}{3} L(1-L)\, x + \frac{1}{2} L^2 x^2\right] + \\ & + \frac{1}{4} \langle S_z^2\rangle_{\mathrm{av}} C^2 \left[(1-L)^2 - \frac{2}{9} L(1-L)\, y + \frac{1}{18} L^2 y^2\right] + \\ & \frac{1}{4} \langle S^+ S^-\rangle_{\mathrm{av}} C^2 \left[(1-L)^2 - \frac{4}{9} L(1-L)\, y + \frac{21}{54} y^2\, (1-L)^2\right] - \\ & - \frac{1}{9} \langle S_z\rangle_{\mathrm{av}}\, DC\, xyL^2 \Bigg\} \end{aligned} \tag{23'}$$

for the InSb-type band structure.

In (23), (23′) N denotes the concentration of magnetic impurities (it was obtained by means of averaging over possible $\boldsymbol{R}_n - \boldsymbol{R}_m$ distances), $\langle \cdots \rangle_{\mathrm{av}}$ denotes the thermal average value specified by (18), (19), and $L = E/(E_{\mathrm{g}} + 2E)$. The short-range potentials $V(\boldsymbol{r})$ and $I(\boldsymbol{r})$ can be approximated by contact interactions in the form

$$V(\boldsymbol{r}) = V_0 \delta(\boldsymbol{r}) \qquad \text{and} \qquad I(\boldsymbol{r}) = I_0 \delta(\boldsymbol{r})\,.$$

This approximation corresponds to $x = y = 0$.

Then (23) and (23′) simplify to

$$\frac{1}{\tau_k} = \frac{N k^2}{\pi\hbar} \frac{\mathrm{d}k}{\mathrm{d}E} \left[D^2 a^4 + \frac{1}{4} \langle S_z^2 + S^+ S^-\rangle_{\mathrm{av}}\, C^2 a^4\right]. \tag{24}$$

The other, often used, form of short-range potential is the "square-well" form, i.e.

$$V(\boldsymbol{r}),\, I(\boldsymbol{r}) = \begin{cases} \tilde{V},\, \tilde{I} = & \text{const in the unit cell,} \\ 0 & \text{otherwise.} \end{cases}$$

This approximation corresponds to $x = y = 1$.

The k-dependent electron mobility can be calculated now according to the formula $\mu_k = e\tau_k/m^*$, m^* being the energy dependent effective mass. It is worth noting that the energy dependence of μ_k is exactly the same as in the case of acoustic phonon scattering, i.e. it can be expressed in the form

$$\mu_k = \mu_0 \frac{1}{F} \left(\frac{\mathrm{d}E}{\mathrm{d}k}\right)^2 k^{-3}\,, \tag{25}$$

where F and μ_0 can be easily deduced from (23) and (23′).

4. The Numerical Estimations

In order to estimate the numerical values of the mobility calculated in Section 3, one has to compute first the thermal averages $\langle S_z^2\rangle_{\mathrm{av}}$, $\langle S^+ S^-\rangle_{\mathrm{av}}$, $\langle S_z\rangle_{\mathrm{av}}$. We did that for Mn impurities, i.e. for $S = \frac{5}{2}$ [8]. In the absence of external magnetic field, $\langle S_z\rangle_{\mathrm{av}} = 0$, as we are treating the problem in the paramagnetic region. The non-vanishing average values are almost independent of T and H in the first H/T region. The masses, energy gap, and other material constants of InSb and HgTe were used in the calculation (see Table 1). The value of C was chosen to be 0.4×10^{-22} eVcm³ [9, 10], and the value of D was chosen to be 2.5×10^{-22} eVcm³ [11].

Table 1

	m_e^*	E_g (eV)	$\frac{dE_g}{dT}$ $\left(\frac{eV}{K}\right)$	$\frac{dE_g}{dx}$ $\left(\frac{eV}{\%}\right)$
InSb	$0.0145m_e$	0.23	-9.6×10^{-5}	—
HgTe	$0.025m_e$	0.303	-4.2×10^{-4}	0.027

The calculation took into account the dependence of E_g on manganese concentration [12] (see Table 1). The calculations were carried out for two cases: $x = y = 1$, i.e. for delta-like and square-well forms of $I(\boldsymbol{r})$ and $V(\boldsymbol{r})$.

The resulting mobility proved to be only slightly dependent on the actual x and y values. In case of InSb-type band structure the mobilities for $x = y = 0$ are slightly smaller than for $x = y = 1$. Quite an opposite situation occurs in case of inverted band structure: mobility for $x = y = 0$ is slightly larger than for $x = y = 1$. This can be understood if we have in mind that the HgTe electron wave function consists mainly of a p-like part which is not "felt" by δ-like perturbation. So the probability of scattering is greater (mobility is smaller) in the case of the smeared out potential. The same arguments help to understand qualitatively the difference between $x = y = 0$ and $x = y = 1$ cases in the InSb-type structure. The calculations were performed in the regime of strong degeneracy. As an example we present the results of these calculations in case of InSb-type with 5% Mn (see Fig. 1) with δ-like potential. For comparison the mobility curve resulting from ionized impurities, acoustic and optical phonon scattering taken from [1] is plotted also. Fig. 1 shows that the mobility is, even for the highest concentrations of Mn ions considered here, always greater by a factor of at least two than the mobility corresponding to acoustic phonon + optical phonon + charged centre scattering mechanisms. Therefore, the magnetic impuritiy scattering up to 5% Mn is of small importance when one has in mind its contribution to electronic mobility. This mechanism can, however, affect strongly other transport phenomena, e.g. Hall effect [10, 13]. Because of the strong electron energy dependence of relaxation time (similar to that for acoustic phonon scattering), the magnetic impurity scattering may influence strongly the thermoelectric power at low temperatures.

Since $\langle S_z^2 \rangle_{av}$, $\langle S^+S^- \rangle_{av}$ do not depend significantly on the external magnetic field in the first H/T region, one can expect a very weak magnetoresistance due to this terms. However, when a magnetic field is applied $\langle S_z \rangle_{av}$ does not vanish

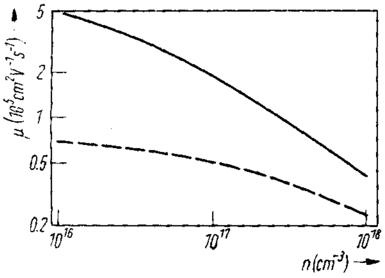

Fig. 1. Mobility of a hypothetical semiconductor with InSb-band structure parameters, containing 5% of Mn at $T = 300$ K. The broken curve represents the mobility resulting from other scattering mechanisms taken from [1]

and its strong magnetic field dependence may cause a significant magnetoresistance via the crossed *CD* term in (23) and (23′). These problems will be treated in papers to follow.

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