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Role of the spin–orbit interaction in elastic scattering of electrons in quantum wells

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Abstract

We present a theoretical study of the spin-dependent electron scattering from screened impurities in III–V semiconductor quantum wells. The effective one band Hamiltonian and the Rashba spin-orbit interaction are used. We calculated the Mott scattering cross-section and the Sherman function for two-dimensional electrons spin-polarized parallel to the z-axis (direction of structure growth). We have found a large spin-dependent asymmetry in the elastic cross-section for electrons scattered from impurities in CdTe/InSb/CdTe symmetrical semiconductor quantum wells. The Sherman function amplitude for repulsive impurities in CdTe/InSb/CdTe quantum wells is predicted to be about 0.01

Keywords: Quantum wells; Sherman function; Spin-polarized

Transport of spin-polarized electrons in two-dimensional (2D) semiconductor structures attracts a great interest since a new branch of semiconductor electronics (so called spintronics) starts to utilize electron spin in semiconductors [1]. The extra degree of freedom provided by the electron spin opens up a new field for device research. Yet, electron spin dynamics in semiconductor heterostructures is best studied by optical experiments. There is much to be done to develop a proper understanding of spin dependent electron transport in nano-scopic semiconductor systems.

In this paper, we investigate the spin-dependent elastic scattering in semiconductor quantum wells in the presence of the spin–orbit interaction. In the absence of magnetic impurities, the main source of the spin-dependent scattering processes at low temperatures is the spin–orbit coupling to local defects. Unlike most of the theoretical simulations of 2D electron scattering processes from the impurities that have been conducted in the first Born approximation, we calculate the electron elastic cross section exactly by means of partial waves method. Our results demonstrate a large left-right scattering asymmetry for different location of the impurities in a narrow gap semiconductor symmetric quantum wells.

We consider electrons in semiconductor heterostructures and use the approximate one electron band effective Hamiltonian for the electron envelop wave functions [2,3]

$$\hat{H} = \hat{H}_0 + \hat{V}_{\mathrm{im}}(\mathbf{r}) \tag{1}$$

In Eq. (1) H_0 is the Hamiltonian of the system without impurities

$$\hat{H}_0 = -\frac{\hbar^2}{2}\nabla_{\mathbf{r}}\left(\frac{1}{m(E,\mathbf{r})}\right)\nabla_{\mathbf{r}} + V(\mathbf{r}) - \mathrm{i}\nabla_{\mathbf{r}}\beta(\mathbf{r})\cdot[\sigma\times\nabla_{\mathbf{r}}],$$

and $\hat{V}_{im}(\mathbf{r})$ is the scattering potential, $\nabla_{\mathbf{r}}$ stands for the spatial gradient, $m(E,\mathbf{r})$ is the energy and position dependent electron effective mass E is the electron energy, $V(\mathbf{r})$ is the confinement potential of the well, and $\beta(\mathbf{r})$ is the spin-orbit coupling parameter in the Rashba spin–orbit interaction [2–4].

The impurity potential consists of two parts

$$V_{\mathrm{im}}(\mathbf{r}) = V_{\mathrm{c}}(\mathbf{r}) + V_{\mathrm{so}}(\mathbf{r}),$$

where $V_{\mathrm{c}}(\mathbf{r})$ is the Coulomb potential of the charged impurity and $V_{\mathrm{so}}(\mathbf{r})$ describes the spin–orbit interaction with the impurity

$$V_{\mathrm{so}}(\mathbf{r}) = \mathrm{i}\alpha(E,\mathbf{r})\nabla V_{\mathrm{c}}(\mathbf{r})\cdot[\hat{\sigma}\times\nabla_{\mathbf{r}}],$$

where $\alpha(E,\mathbf{r})$ is taken from Ref. [2].

In a semiconductor quantum well we denote by z the direction perpendicular to the well interface and $\rho = (x, y)$ is

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the position vector parallel to the interface. Here we consider III–V semiconductor symmetric quantum wells of thickness L and assume that an isolated impurity is located with a distance d from the center of the well ($z = 0$) and the unscreened Coulomb potential of the impurity is given by

$$V_c 0(\mathbf{r}) = \frac{Ze2}{4\pi\varepsilon_s[\rho^2 + (z-d)^2]^{1/2}}, \tag{2}$$

where ε_s is the permittivity of the system and Z is the charge of the impurity. For most of III–V quantum wells we can neglect the image potential.

For systems with a sharp discontinuity in the conduction band edge between the quantum well (material 1) and the barrier region (material 2) the potential can be presented as

$$V(\mathbf{r}) = \begin{cases} 0, & -\dfrac{L}{2} \le z \le \dfrac{L}{2}; \\ V_0, & |z| > \dfrac{L}{2}; \end{cases} \tag{3}$$

Following Ref. [5] we present the solution of the confinement problem with the Hamiltonian $\hat{H}_0$ as

$$\Psi(\boldsymbol{\rho}, z) = \psi^s(\rho)\varphi_n(z),$$

where n labels the eigen-energies E_n in the normal direction, and $s = \pm 1$ is the quantum number related to the spin states.

In this work, we consider only the intrasubband elastic scattering for the electrons in the first subband of the quantum well. First we consider the ground state (the first sub-band with $n = 1$) of z-direction. The wave function of this ground state has the form

$$\varphi_1(z) = \begin{cases} A\cos\kappa z, & |z| \le \dfrac{L}{2}; \\ B\exp(-\mu z), & |z| > \dfrac{L}{2}; \end{cases} \tag{4}$$

where

$$\kappa = \sqrt{2m_1(E)E_1}/\hbar,$$

$$\mu = \sqrt{2m_2(E)(V_0 - E_1)}/\hbar,$$

and $E = E_\rho + E_1$ consists of the ρ and z direction motion energies correspondingly. Due to the symmetry of the well spin-spliting of the electron spectrum does not occur [2,3] and from the Ben Daniel–Duke boundary conditions [6] in z-direction we obtain a spinless transcendental equation

$$\tan[\kappa(E_\rho, E_1)L/2] = \frac{m_1(E)\mu(E_\rho, E_1)}{m_2(E)\kappa(E_\rho, E_1)}. \tag{5}$$

Eq. (5) gives us the eigen-energy in z-direction in an implicit form. The wave function $\varphi_1(z)$ (after proper normalization), we substitute in the three-dimensional Schrödinger equation with the Hamiltonian (1) and integrate out the z coordinate by taking the average

$$\hat{H}_\rho = \int_{-\infty}^{+\infty} \mathrm{d}z\varphi_1^*(z)\hat{H}\varphi_1(z).$$

After the averaging the quasi 2D Schrödinger equation in the polar coordinates $\rho = (\rho, \phi)$ is given by the form

$$\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right) - \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2} - \tilde{V}_c(\rho) - is\tilde{W}(\rho)\frac{\partial}{\partial\phi} + k^2\right]\psi^s(\rho) = 0 \tag{6}$$

where

$$\tilde{V}_c(\rho) = \frac{Ze^2\tilde{m}(E)}{2\pi\varepsilon_s\hbar^2} \times \int_0^\infty \frac{\mathrm{d}q}{\varepsilon(q)} J_0(q\rho) \int_{-\infty}^{+\infty} \mathrm{d}z|\varphi_1(z)|^2 \mathrm{e}^{-q|z-d|},$$

$$\tilde{W}(\rho) = -\frac{Ze^2\tilde{m}(E)}{2\pi\varepsilon_s\rho\hbar^2} \int_0^\infty \frac{q\,\mathrm{d}q}{\varepsilon(q)} J_1(q\rho) \times \left[\alpha_1(E)\int_{z\le|L/2|} \mathrm{d}z|\varphi_1(z)|^2\mathrm{e}^{-q|z-d|} + \alpha_2(E)\int_{z\ge|L/2|} \mathrm{d}z|\varphi_1(z)|^2\mathrm{e}^{-q|z-d|}\right],$$

$$k^2 = \frac{2\tilde{m}(E)E\rho}{\hbar^2},$$

$$\frac{1}{\tilde{m}(E)} = \frac{1}{m_1(E)}\int_{z\le\left|\frac{L}{2}\right|} \mathrm{d}z|\varphi_1(z)|^2 + \frac{1}{m_2(E)}\int_{z\ge\left|\frac{L}{2}\right|} \mathrm{d}z|\varphi_1(z)|^2,$$

$J_n(x)$ is the Bessel function,

$$\varepsilon(q) = 1 + \frac{q_f}{q}$$

is the 2D dielectric function, and

$$q_f = \frac{e^2 m_1(E_f)}{2\pi\hbar^2\varepsilon_s}\left\{1 + E_f\frac{\mathrm{d}}{\mathrm{d}E}\ln[m_1(E)]\Big|_{E_f}\right\}$$

is the 2D Thomas–Fermi screening constant, and E_f is the Fermi energy of the system. Due to the radial symmetry of the potentials $\tilde{V}_c(\rho)$ and $\tilde{W}(\rho)$ the method of partial waves is convenient for our description and we can present the wave function as the following [7]

$$\psi^s(\rho) = \sum_{l=-\infty}^{l=+\infty} R_l^s(\rho)\mathrm{e}^{\mathrm{i}l\phi}\chi^s.$$

where l is the orbital momentum number and χ^s is a spin function upon which the Pauli matrix vector operates. The Schrödinger equation for the radial wave function becomes

$$\left[\frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho}\left(\rho\frac{\mathrm{d}}{\mathrm{d}\rho}\right) - \frac{l^2}{\rho^2} - \tilde{V}_c(\rho) + sl\tilde{W}(\rho) + k^2\right]R_l^s(\rho) = 0.$$

In the variable phase approach [7] the phase function $\delta_l^s(\rho)$ at the point ρ determines the phase shift produced by the part of the potential contained within the cycle of a radius ρ. The scattering phase shift for the total potential is equal to

the asymptotic value

$$\delta_l^s = \lim_{\rho\to\infty} \delta_l^s(\rho).$$

The phase function satisfies the following differential equation

$$\frac{d\delta_l^s(\rho)}{d\rho} = -\frac{\pi}{2}\rho[\tilde{V}_c(\rho) - sl\tilde{W}(\rho)] \times [\cos\delta_l^s(\rho) J_l(k\rho) - \sin\delta_l^s(\rho) N_l(k\rho)]^2 \quad (7)$$

with the boundary condition

$$\delta_l^s(0) = 0. \quad (8)$$

The Mott scattering cross-section for electrons spin-polarized parallel to the z-axis can be expressed in terms of the incident electron spin-polarization P_i as

$$\sigma(\theta) = I(\theta)[1 + S(\theta)P_i], \quad (9)$$

where $I(\theta)$ is the differential cross-section for an unpolarized incident electron

$$I(\theta) = |f(\theta)|^2 + |g(\theta)|^2,$$

where θ is the scattering angle between initial ($\mathbf{k}_i$) and final ($\mathbf{k}_f$) wave vectors and

$$S(\theta) = \frac{f^*(\theta)g(\theta) + f(\theta)g^*(\theta)}{|f(\theta)|^2 + |g(\theta)|} \quad (10)$$

is the Scherman function for 2D electrons.

The complex 2D scattering amplitude

$$\mathbf{F}^s(\theta) = [f(\theta) + \sigma_z g(\theta)]\chi^s,$$

is discussed in Ref. [4] in terms of the scattering phase shifts. The Sherman function is an important characteristic of the spin-dependent scattering [8]. It presents the left-right asymmetry in the scattering cross-section for initially polarized electron beams and the average polarization of unpolarized electrons after scattering and, for instance, in the anomalous Hall effect the Hall angle is proportional to the Sherman function at the Fermi energy shell [9]. The phase shifts were obtained by the numerical solution of Eq. (7) with the initial condition Eq. (8) and used in Eqs. (9) and (10) to calculate the cross-section and the Sherman function. Our calculation shows that the convergence criteria on the cross-section (the maximum net error is less than 10^{-4}) can be reached by taking the necessary number $|l| \leq 70$ of partial waves.

Fig. 1 shows the example of angle dependencies of the elastic scattering cross-section for 2D electrons scattered from an impurity in different locations for the symmetrical CdTe/InSb/CdTe quantum well. The results demonstrate the fast declination of the cross section at large angle with the increasing distance between the well center and the impurity. The exact numerical solution allows as to calculate the spin-polarization effects and the Sherman function of CdTe/InSb/CdTe quantum well with impurities.

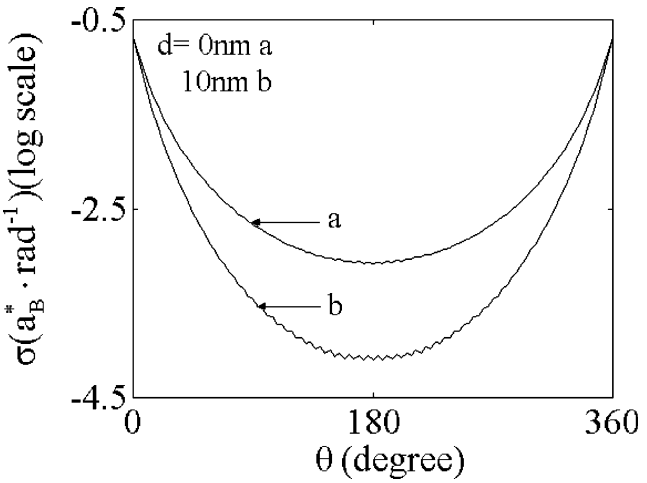

Fig. 1. The scattering cross-sections for a screened repulsive ($Z = 1$) impurity located in the center and well edge of a 20 nm wide CdTe/InSb/CdTe quantum well with $E_\rho = 0.04$ eV. The structure parameters are from: Refs. [10,11].

In Fig. 2 we present the Sherman function obtained. The insert presents the maximum amplitude with different impurity location. The left-right asymmetry in the Sherman function indicates that the spin–orbit interaction can provide a recognizable spin-dependent scattering in the system. The asymmetry differs in the magnitude for impurities with opposite charges (smaller for attractive impurity) and it is significantly lager than it was calculated for the spin-dependent elastic scattering in the bulk [9]. This difference is attributed to the influence of the 2D confinement and screening on the elastic scattering processes in quantum wells [5,12].

In conclusion we have presented the theoretical study of the spin-dependent elastic scattering of 2D electrons from the screened Coulomb centers in semiconductor quantum

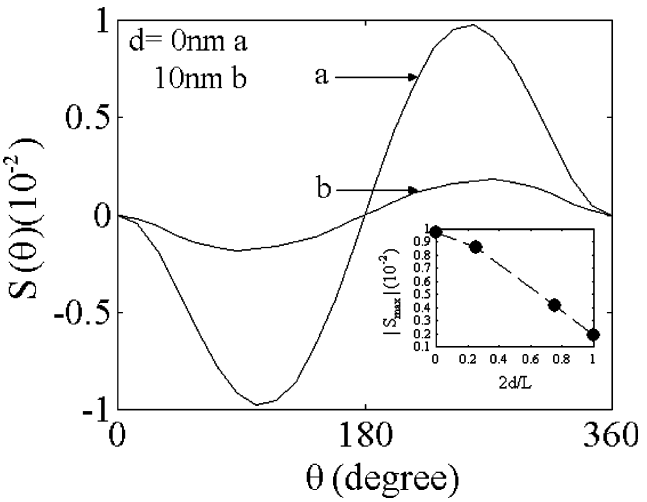

Fig. 2. The Sherman function for a screened repulsive ($Z = 1$) impurity located in the center and well edge of a 20 nm wide CdTe/InSb/CdTe quantum well with $E_\rho = 0.04$ eV.

wells. The one electron band effective Hamiltonian and the Rashba model of the spin-orbit interaction allowed us to calculate the left-right asymmetry in the electron scattering cross-section. We have calculated the Sherman function with different locations of doped impurities centers in CdTe/InSb/CdTe symmetrical quantum wells. The amplitude of the Sherman function for CdTe/InSb/CdTe quantum well is predicted to reach about 0.01 that is possible to detect with the anomalous Hall effect measurement at zero magnetic field. This effect is potentially useful in integrated electron spin-polarization devices based on semiconductor heterostructures. It also can be used as a tool of determination of spin coupling parameters in III–V narrow gap semiconductor heterostructures. Our model can be used as the starting point for more detailed calculations. Experimental investigations should be conducted to verify our theory predictions.

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