Spin-orbit interaction and electron elastic scattering from impurities in quantum wells

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We present a theoretical study of the spin-dependent scattering of electrons from screened impurities in III-V semiconductor quantum wells. Our calculation is based on the effective one-electronic-band Hamiltonian and the spin-orbit coupling with the Coulombic potential of the impurities. We demonstrate that the spin-orbit interaction can lead to recognizable magnitudes of spin asymmetry in the elastic-scattering cross section. Fairly large values of the Sherman function (about 0.01) are obtained for repulsive and attractive impurities in quantum wells of narrow gap semiconductors.

I. INTRODUCTION

A large number of studies of the electron transport in two-dimensional (2-D) semiconductor systems has been carried out over the past 40 years (see, for instance, Refs. 1–8). This is especially important for electronic applications. Progress in modern semiconductor technologies has allowed us to experimentally and theoretically model the various scattering mechanisms in 2-D semiconductor structures within a wide range of material parameters.4–8 It is commonly accepted now that the electron mobility of a semiconductor 2-D heterostructure is determined by impurity scattering at low temperatures and by the phonon scattering at high temperatures.

Recently there has been renewed interest in spin-dependent scattering and transport phenomena in semiconductor heterostructures because a branch of semiconductor electronics so called spintronics, has become a focus of interest (see Refs. 9–12, and references therein). The extra degree of freedom provided by the electron spin opens a new field for the development of semiconductor devices. In principle, one can use the semiconductor approach to generate, control, and detect electron-spin polarization.11,13 This approach has the advantage of being compatible with conventional semiconductor technology.

In the absence of magnetic impurities, the main source of spin-dependent scattering processes at low temperatures is spin-orbit coupling to local defects. The effect of spin-orbit interaction on spin relaxation for semiconductor 2-D systems also has been studied for a long time.14–17 Recently coherent spin transport has been demonstrated in homogeneous semiconductors and heterostructures.19,18 Unfortunately, the theory of spin-dependent transport for semiconductor 2-D systems is still far from being complete. For this reason we recently investigated spin-dependent elastic-scattering processes in semiconductors in the presence of spin-orbit interaction.20,21 In 2-D quantum wells,20 this effect is expected to be stronger than that in the bulk21 because of the localization of electronic wave functions in the conductive channel. It should be noted that the problem remains complicated even for the simplest models of 2-D electron motion because, in general, spin-orbit interaction should be described by a three-dimensional model.

Using the delta-doping technique, Coulomb attractive and repulsive impurities can be precisely placed in heterostructures. Using this fact one can model theoretically the scattering from the impurities located inside8 or outside22 the conductive channel. Most of the theoretical simulations of 2-D electron elastic-scattering processes from the impurities were conducted in detail in the first Born approximation.2,4 However, it is well known that when perturbation theory is used, the dependence on spin in the elastic cross section appears only in the approximation that follows the first Born approximation.23–27 For this reason, one should use other approaches in calculations of the spin-dependent scattering cross section. In particular, this is the partial-wave approach,25,27 which was also used in some simulations of the spin-independent elastic-scattering cross section when the first Born approximation is not applicable.28–30

In this paper we calculate the spin-dependent elastic-scattering cross section for electrons scattered by impurities in 2-D heterostructures of III-V semiconductors. We use the effective one-electronic-band Hamiltonian with Ben-Daniel-Duke boundary conditions for electronic envelope functions to calculate the spin-dependent cross section for electrons scattered by repulsive and attractive isolated impurities with spin-orbit coupling.24–26 The impurities are located inside the quantum well. For narrow gap semiconductor quantum wells (systems with large spin-orbit coupling parameters) we found a large spin-related asymmetry in the cross section.

The paper is organized as follows: Section II begins with an introduction to the effective one-electronic-band 2-D Hamiltonian with impurities located inside semiconductor quantum wells. Section III gives details of the variable phase approach to spin-dependent elastic scattering in 2-D systems. The calculation results are presented in Sec. IV and conclusions are given in Sec. V.

II. BASIC EQUATIONS

We consider electrons in semiconductor heterostructures with charged impurities and use the approximate one-electronic-band effective Hamiltonian for the electron envelope wave functions

\[ \hat{H} = \hat{H}_0 + \hat{V}_{im}(\textbf{r}). \]
In Eq. (1) \( \hat{H}_0 \) is the Hamiltonian of the system without impurities,31–34

\[
\hat{H}_0 = -\frac{\hbar^2}{2m(E, r)} \nabla + V(r),
\]

where \( \nabla \) stands for the spatial gradient; \( m(E, r) \) is the energy and position-dependent electron effective mass,

\[
\frac{1}{m(E, r)} = \frac{2\rho^2}{\hbar^2} \left[ \frac{2}{E + E_g(r)} - \frac{1}{E + E_g(r) + \Delta(r) - V(r)} \right],
\]

where \( V(r) \) is the confinement potential of the well; \( E \) is the electron energy; \( E_g(r) \) and \( \Delta(r) \) stand for the position-dependent band gap and the spin-orbit splitting in the valence band; \( \rho \) is the momentum matrix element; and \( \hat{V}_{im}(r) \) is the scattering potential of the impurity.

The impurity scattering potential consists of two parts,

\[
V_i(r) = V_{ic}(r) + V_{iso}(r),
\]

where \( V_{ic}(r) \) is the Coulomb potential of the charged impurity and \( V_{iso}(r) \) describes the spin-orbit interaction of electrons with the impurity

\[
V_{iso}(r) = -i \gamma(E, r) \nabla V_{ic}(r) \cdot [\hat{\sigma} \times \nabla],
\]

where \( \gamma(E, r) = \frac{\rho^2}{3} \left[ \frac{1}{E + E_g(r) - V(r)} \right] - \frac{1}{E + E_g(r) + \Delta(r) - V(r)} \right].
\]

The spin-orbit interaction in the form of Eq. (2) is the generalization of the well-known Rashba spin-orbit interaction,33 which comes from system inversion asymmetry.32,34 In semiconductor structures with the average uniform electric field \( \mathbf{F} \) one can consider

\[
\mathbf{F} = -\frac{1}{e} \nabla \mathbf{V}_p(r),
\]

where \( e \) is the electron charge and \( \mathbf{V}_p(r) \) is the average space-charge electric potential. When the electron with the wave vector \( \mathbf{k} \) in the field \( \mathbf{F} \) is moving in the field, one can readily obtain from Eq. (2) the well-known Rashba interaction

\[
V_{iso}(r) = \alpha \mathbf{n} \cdot [\hat{\sigma} \times \mathbf{k}],
\]

where \( \alpha = -e \gamma F \) and \( \mathbf{n} \) is the unit vector parallel to the field.33

Here we consider III-V semiconductor symmetrical quantum wells of thickness \( L \). In the structure we denote by \( z \) the direction perpendicular to the well interfaces, and \( \mathbf{r} = (x, y) \) is the position vector parallel to the interfaces (\( z = 0 \) is the center of the well). For systems with 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

\[
V(r) = \begin{cases} 
0, & \frac{L}{2} \leq z \leq \frac{L}{2}; \\
V_0, & |z| > \frac{L}{2}; 
\end{cases} \quad (r \in 1),
\]

\[
V(r) = \begin{cases} 
0, & \frac{L}{2} \leq z \leq \frac{L}{2}; \\
V_0, & |z| > \frac{L}{2}; 
\end{cases} \quad (r \in 2).
\]

We assume that an isolated impurity is located at \( z = d \) and the unscreened Coulomb potential of the impurity is given as

\[
V_{ic}(r) = \frac{Ze^2}{|r|^2},
\]

where \( \varepsilon_r \) is the relative permittivity of the system and \( Z \) is the charge of the impurity. For most III-V quantum wells we can neglect the image potential and use for simplicity \( V_{ic} = (e_1 + e_2)/2 \) (\( e_1 \) and \( e_2 \) are the dielectric constants of materials 1 and 2, correspondingly).

Following Refs. 1, 2, and 31 we present the solution of the confinement problem with the Hamiltonian \( \hat{H}_0 \) as

\[
\Psi_{n,s}(\mathbf{r}, z) = \psi_n(\mathbf{r}) \varphi_s(z),
\]

where \( n \) labels the eigenenergies in the normal direction \( (E_n) \), and \( s = \pm 1 \) is the quantum number related to the spin polarization along the \( z \) direction.

As is shown in Ref. 32, due to the reflection symmetry of the well in the \( z \) direction (there are no built-in electric fields) the Rashba spin splitting in the electron spectrum does not occur and one can use the conventional Ben-Daniel-Duke boundary conditions31 for the wave function \( \varphi_s(z) \),

\[
\varphi_s(z), \quad \frac{1}{m(E, z)} \frac{d}{dz} \varphi_s(z)
\]

continuous at

\[
z = \pm \frac{L}{2}.
\]

Considering for simplification only the first subband as being populated we describe only intrasubband elastic-scattering processes. First we obtain the ground state (the first subband with \( n = 1 \)). The wave function of this ground state has the well-known form

\[
\varphi_1(z) = \begin{cases} 
A \cos \kappa z, & |z| \leq \frac{L}{2}; \\
B \exp(-\mu z), & |z| > \frac{L}{2}; 
\end{cases}
\]

where

\[
\kappa = \sqrt{2m_1(E) \frac{E_1}{\hbar}}, \quad \mu = \sqrt{2m_2(E)(V_0 - E_1)}/\hbar,
\]

\[n=1\]
and $E = E_\rho + E_1$ consists of the energies of the $\rho$ and $z$ directions of motion, correspondingly. From the Ben-Daniel-Duke boundary conditions \((6)\) we obtain the spinless transcendental equation

$$\tan[\kappa(E_\rho,E_1)L/2] = \frac{m_1(E)\mu(E_\rho,E_1)}{m_2(E)\kappa(E_\rho,E_1)}.$$ \(8\)

Equation \((8)\) gives us the eigenenergy in the $z$ direction in an implicit form.

The wave function \((7)\) (after proper normalization), we substitute into the three-dimensional Schrödinger equation with the Hamiltonian \((1)\) and integrate out the $z$ coordinate by taking the average,

$$\hat{H}_\rho = \int_{-\infty}^{+\infty} dz \varphi_\rho^*(z) \hat{H} \varphi_\rho(z).$$

After the averaging and introducing the screening of the impurity at low temperatures by means of Refs. 1 and 23 the quasi-2-D Schrödinger equation in the polar coordinates $\rho=(\rho,\phi)$ is given by

$$\left[ \frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial}{\partial \rho} \right) - \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} - \tilde{V}(\rho) + i\hbar \tilde{W}(\rho) \frac{\partial}{\partial \phi} + k^2 \right] \psi^J(\rho) = 0,$$ \(9\)

where

$$\tilde{V}(\rho) = \frac{2Z}{a_\hbar^2} \frac{\tilde{m}(E)}{m_1(0)} \int_{-\infty}^{+\infty} dq \frac{d}{e(q)} J_0(q\rho) \int_{-\infty}^{+\infty} dz |\varphi_\rho(z)|^2 e^{-q|z|d}$$

is the statically screened Coulomb potential in the quantum well plane,

$$\tilde{W}(\rho) = \frac{2Z}{a_\hbar^2} \frac{\tilde{m}(E)}{m_1(0)} \int_{-\infty}^{+\infty} dq \frac{d}{e(q)} J_1(q\rho)$$

$$\times \left[ \alpha_1(E) \int_{z<|L/2|} dz |\varphi_\rho(z)|^2 e^{-q|z|d} + \alpha_2(E) \int_{z>|L/2|} dz |\varphi_\rho(z)|^2 e^{-q|z|d} \right]$$

is the screened spin-orbit interaction, $a_\hbar^2 = \hbar^2/e^2m_1(0)$ is the effective Bohr radius in the well,

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

$$\frac{1}{\tilde{m}(E)} = \frac{1}{m_1(E)} \int_{z<|L/2|} dz |\varphi_\rho(z)|^2$$

$$+ \frac{1}{m_2(E)} \int_{z>|L/2|} dz |\varphi_\rho(z)|^2.$$  

$J_\mu(x)$ is the Bessel function.
\[
\frac{d \delta_\ell}{d \rho} = -\frac{\pi}{2} \rho [\mathcal{V}(\rho) + s l \mathbb{W}(\rho)] [\cos \delta_\ell J_\ell(k \rho) - \sin \delta_\ell N_\ell(k \rho)]^2
\]

with the boundary condition
\[
\delta_\ell(0) = 0.
\]

The complex 2-D scattering amplitude can be expressed as \[20,24,25\]
\[
F^\ell(\theta) = [f(\theta) + \sigma g(\theta)] \chi',
\]

where \(f(\theta)\) and \(g(\theta)\) describe scattering without and with electron-spin reorientation, and they are determined by the expressions
\[
f(\theta) = \sum_{l=0}^{\infty} f_l \cos(l \theta),
\]
\[
g(\theta) = \sum_{l=1}^{\infty} g_l \sin(l \theta),
\]

where
\[
f_l = \sqrt{\frac{1}{2 \pi k}} \left\{ \exp(2i \delta_l) - 1; \quad l = 0; \right. \left. \exp(i2 \delta_l) + \exp(i2 \delta_l) - 2; \quad l \geq 1; \right. \]
\[
g_l = i \sqrt{\frac{1}{2 \pi k}} [\exp(i2 \delta_l) - \exp(i2 \delta_l)],
\]

where \(\theta\) is the scattering angle between initial \((k_i)\) and final \((k_f)\) wave vectors.

The Mott scattering \[24\] cross section for electrons spin polarized parallel to the \(z\) axis can be expressed in terms of the incident electron-beam spin polarization \(P_i\) along the \(z\) direction as the following:
\[
\sigma(\theta) = I(\theta) [1 + S(\theta) P_i],
\]

where \(I(\theta)\) is the differential cross section for unpolarized incident electrons,
\[
I(\theta) = |f(\theta)|^2 + |g(\theta)|^2,
\]

and
\[
S(\theta) = \frac{F^*(\theta) g(\theta) + f(\theta) g^*(\theta)}{|f(\theta)|^2 + |g(\theta)|^2}
\]

is the Sherman function for 2-D electrons. The Sherman function is an important characteristic of the spin-dependent scattering (see Refs. 37 and 38, and references therein). It presents the left-right asymmetry in the scattering cross section for initially polarized electron beams and the average polarization of unpolarized electrons after the scattering. This characteristic is important in the evaluations of the anomalous Hall effect in different materials and structures.

For degenerated electronic systems, for instance, the Hall angle is proportional to the Sherman function at the Fermi energy shell. \[26,39-41\]

IV. CALCULATION RESULTS

To present the realistic estimation of the effect of the spin-orbit coupling on the electron elastic cross section we choose two types of symmetrical quantum well structures: type I is \(\text{Al}_{0.48}\text{In}_{0.52}\text{As}/\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{Al}_{0.48}\text{In}_{0.52}\text{As}\) (where \(E_g^1 = 0.813\) eV, \(E_g^2 = 1.508\) eV, \(\Delta_1 = 0.361\) eV, \(\Delta_2 = 0.332\) eV, \(m_1(0) = 0.041 m_0\), \(m_2(0) = 0.075 m_0\), \(e_1 = 14\), \(e_2 = 12.5\), \(V_0 = 0.504\) eV, \(\mu_{0j}\) is the free-electron mass) and type II is \(\text{CdTe/InSb/CdTe}\) (where \(E_g^1 = 0.24\) eV, \(E_g^2 = 1.59\) eV, \(\Delta_1 = 0.81\) eV, \(\Delta_2 = 0.8\) eV, \(m_1(0) = 0.015 m_0\), \(m_2(0) = 0.08 m_0\), \(e_1 = 16.8\), \(e_2 = 10.2\), \(V_0 = 0.55\) eV). While type I presents quantum well structures with well-developed growth technology, type II demonstrates

FIG. 1. The scattering cross section for the screened impurities in the type-I structure \((L = 20\) nm): (a) repulsive \((Z = +1)\) impurity; (b) attractive \((Z = -1)\) impurity; (c) the ratio between the complete numerical result \((\sigma_{\text{exact}})\) and the first Born approximation \((\sigma_{\text{Born}})\) for the repulsive impurity when \(ka_B^* = 1.8\) \((E_p = 0.01\) eV).
the largest spin-coupling effects. In all calculations we assure the validity of the one-subband scattering model, when the intersubband gap is larger than the energy of the \( \rho \)-direction motion: \( E_\rho < E_2 - E_1 \). This allows us to consider scattering of electrons with the following wave vectors: for type-I structures with \( L \leq 30 \text{ nm} \), \( k \approx k_F^1 = 2.5(a_B^1)^{-1} \) (the electron concentration \( n_s = 3.5 \times 10^{11} \text{ cm}^{-2} \)); for type-II structures with \( L \leq 30 \text{ nm} \), \( k \approx k_F^2 = 6.6(a_B^2)^{-1} \) (\( n_s = 3 \times 10^{11} \text{ cm}^{-2} \)). Notice that \( a_B^2 \) is taken to be different according to the definitions for the different types of the systems.

The phase shifts were obtained by the numerical solution of Eq. (10) with the initial condition of Eq. (11) and then used in Eqs. (12)–(17) to calculate the elastic-scattering cross section. From our calculation experience 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 the partial waves included Eqs. (13) and (14). Figure 1 shows energy and angle dependencies of the elastic-scattering cross section for 2-D electrons scattered from attractive \((Z = +1)\) and repulsive \((Z = -1)\) impurities located in the center of the type-I structure. The cross sections demonstrate the well-known logarithmic divergence at zero energy \((E_\rho \rightarrow 0)\) for both types of impurities (repulsive and attractive).\(^{28}\) In Fig. 1(c) we compare our results with the cross sections obtained within the first Born approximation\(^{27,28}\)

\[
f_i \approx - \sqrt{\frac{\pi}{2k}} \int_0^\infty J_0^2(k\rho) \bar{V}(\rho) \rho d\rho \times \begin{cases} 1, & l = 0; \\ 2, & l \geq 1; \end{cases}
\]

When \( ka_B^\rho \gg 1 \).

It is known\(^{1,44}\) that the first Born approximation is valid for 2-D elastic scattering when

\[
ka_B^\rho \gg 1.
\]

It is worth noting that the numerically calculated cross section for the 2-D screened Coulomb potential is different from that obtained in the first Born approximation near the edge of the approximation validity \((ka_B^\rho = 1.8)\). In addition, it can be seen from Eqs. (18) and (19) that in the first Born approximation all spin-polarization effects in the elastic cross section vanish.\(^{25,24,26}\)

\[
S(\theta) \sim f^s(\theta)g(\theta) + f(\theta)g^s(\theta) = 0.
\]

Thus, the Sherman function should be calculated only by going beyond the first Born approximation and taking into consideration the higher partial waves \((|l| > 0)\). The complete numerical solution allows us to do that.

Figure 2 shows the Sherman functions for the type-I structure, when the repulsive [Fig. 1(a)] and attractive [Fig. 1(b)] impurities are located in the center of the well with the width \( L = 20 \text{ nm} \). We first note that, in the energy range considered, the effect is slightly larger for the repulsive scattering center. Since \( S(\theta) \) is closely connected to the cross sect-
tion curves, the high values of the Sherman function occur where the cross-section is small and vice versa. The change of the impurity sign leads to inversion in the three-dimensional plots. This is a direct and clear consequence of sign altering in the potentials $V_\tilde{1}(r)$ and $W_\tilde{2}(r)$, see Eq. ~10!. It can be seen that with suitable electron energies and the large scattering angles one can reach polarizations of more than 0.1%.

In our simulation we found a decrease in the polarization effect when well width increases. The dependence of the Sherman function on the well width $L$ for the type-I structure is presented in Figs. 3~a! and 3~b! (the impurity is located in the center of the well: $d=0$). This decrease is obviously connected to the form of the averaged effective potentials $V_\tilde{1}(r)$ and $W_\tilde{2}(r)$. The various potentials for different well widths are shown in Fig. 4. The curves represent the absolute value of the potentials [$V_\tilde{1}(r)$ is positive and $W_\tilde{2}(r)$ is negative; for the attractive center $V_\tilde{1}(r)$ is negative and $W_\tilde{2}(r)$ is positive] and demonstrate the influence of the 2-D confinement and screening on the elastic scattering processes in quantum wells.\textsuperscript{2,3,28} The figure shows that the spin-orbit coupling potential becomes stronger near the impurity site when the well width decreases. Electrons that are scattered at large angles (where the polarization effects are expected to be higher) pass through the relatively strong fields at fairly small distances from the impurity site. This causes the stronger polarization effects for the relatively narrow wells (as is shown in the insets of the Fig. 3). This result suggests the possibility of controlling Sherman function by means of the well size.

The spin-orbit interaction is known to be larger in small gap semiconductors. Based on this fact, we show in Fig. 5, as an example, the calculation results for the type-II structures. The asymmetry effect in the scattering cross section for those structures can reach about 1% for electrons with moderate energy, when the impurity is located in the center of the well. The insets show the dependencies of the amplitude of the Sherman function on the position of the impurity in the wells. Obviously, the magnitude of the Sherman function decreases when $d$ increases. But the effect remains valuable even for the impurities located at the edge of the well ($d=L/2$).

In addition, we notice that the spin-dependent asymmetry for the elastic-scattering cross section for the impurities located in the wells (2-D systems) is significantly larger than calculated for 3-D spin-dependent elastic scattering from impurities in the bulk. To demonstrate the difference we present in Table I our results for the type-II structure and results obtained in Ref. 26 and 39, when all parameters of the systems are chosen the same (the systems differ only in the dimensionality). In the table, $\delta_0$ is the phase shift for $l=0$ and $\delta_1^{spin}$ is the correction to the phase shift of the partial wave with $l=1$ when the spin-orbit coupling is included.
TABLE I. The ratio $\nu = \delta/E_0$ for InSb structures $(L = 5 \text{ nm})$.

<table>
<thead>
<tr>
<th>Impurity type</th>
<th>$\nu$ for 3-D system $^a$</th>
<th>$\nu$ for 2-D system</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Z = -1$</td>
<td>$3.7 \times 10^{-5}$</td>
<td>$2.8 \times 10^{-2}$</td>
</tr>
<tr>
<td>$Z = +1$</td>
<td>$2.3 \times 10^{-6}$</td>
<td>$2.7 \times 10^{-2}$</td>
</tr>
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</table>

$^a$Reference 26.

This result suggests that the spin-orbit coupling with the charged impurities in 2-D systems can provide sufficiently larger spin-dependent effects than those in the bulk.

V. CONCLUSIONS

We have presented a theoretical study of the elastic spin-dependent scattering of 2-D electrons from the screened Coulomb centers located in quantum wells. The one-electronic-band effective Hamiltonian and spin-orbit coupling potential of the impurities allow us to calculate the left-right asymmetry in the electron elastic-scattering cross section. We have found a large spin-dependent asymmetry in the cross section for electrons scattered from impurities in AlInAs/InGaAsAs/AlInAs and CdTe/InSb/CdTe symmetrical quantum wells.

For the CdTe/InSb/CdTe quantum well we found that the spin-orbit coupling in the two-dimensional systems leads to larger spin-dependent asymmetry in the scattering cross section than that in the bulk. The calculated amplitude of the Sherman function for this structure is more than 0.01. This could be detected in the measurements of the Hall effect at low temperatures$^{26,39,40,45}$ and this is potentially useful in integrated electron-spin polarization devices based on semiconductor heterostructures. It also can be used as a tool to determine spins coupling parameters in III-V narrow gap semiconductor heterostructures.

Finally, we would like to point out that the described effect is a clear analog of the well-known effect of spin-dependent scattering in magnetic materials (see Ref. 37), but it can also be realized in nonmagnetic semiconductor structures. Our model can be used as the starting point for more detailed calculations. Experimental investigations need to be conducted to verify our theory predictions.

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