Two-dimensional electron scattering in regions of nonuniform spin-orbit coupling

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We present a theoretical study of elastic spin-dependent electron scattering caused by a nonuniform Rashba spin-orbit coupling strength. Using the spin-generalized method of partial waves the scattering amplitude is exactly derived for the case of a circular shape of scattering region. We found that the polarization of the scattered waves are strongly anisotropic functions of the scattering angle. This feature can be utilized to design a good all-electric spin-polarizer. General properties of the scattering process are also investigated in the high and low energy limits.

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The presence of the spin-orbit interaction (SOI) destroys the spin-rotational symmetry, therefore the properties of the scattering get influenced by the spin state of the incident particle[1]. The SOI may lead to the asymmetry of the differential scattering cross section (skew-scattering), and it may affect the polarization vector of the incident beam[1,2,3]. In nuclear physics, this property has been utilized to generate spin-polarized neutrons from an unpolarized beam by scattering it on a zero-spin nucleus[4]. In low-dimensional semiconductors, significant spin-splitting in the absence of a magnetic field is observed, which is mostly attributed to the SOI of the Rashba type arising from the structural inversion asymmetry of the hosting heterostructure[5]. Promising spin transistor application has been proposed exploiting the tunability of the strength of the Rashba coupling by an external electrostatic field[6], and initiated an intensive research in the field of spintronics[7]. To generate spin-polarized electron beams, which is a fundamental problem in spintronics, several mechanisms have been proposed[8].

Recently, all-electrical (without externally applied magnetic fields) spin-polarizer devices have been suggested[9] utilizing the properly designed spatial modulation of the Rashba SOI strength α. The spatial variation of the Rashba strength, which is proportional to the magnitude of the electric field applied perpendicular to the two-dimensional electron gas (2DES) systems, can be achieved by small biased electrodes on the top of the heterostructure.

In this work we show that the polarization of the elastically scattered wave caused by a nonuniform Rashba strength becomes strongly anisotropic, ie depends on the angle (called scattering angle) between the directions of the incident electron beam and that of the scattering wave. We also demonstrate that (i) the differential scattering cross section has a skew-scattering feature[1,2,3] for polarized incoming electron beams, (ii) using experimentally relevant material parameters[10] an almost full polarization of unpolarized incident electron beams can be observed in a narrow window of scattering angles. Moreover, our analytical calculations allows us to derive universal properties for the scattering amplitude and the polarization $\mathbf{P}^{\rm sc}$ in the high and low energy limits.

To this end, we consider a system in which the Rashba SOI strength $\alpha(\mathbf{r})$ varies on the plane of the 2DES as $\alpha(\mathbf{r}) = \alpha_1\Theta(a-|\mathbf{r}|)+\alpha_2\Theta(|\mathbf{r}|-a)$, where a is the radius of the scattering center, Θ is the Heaviside function and $\mathbf{r}=(x,y)$ defines the position on the plane (see Fig. 1). The Hamiltonian of the system in the one-band effective-mass approximation is given by

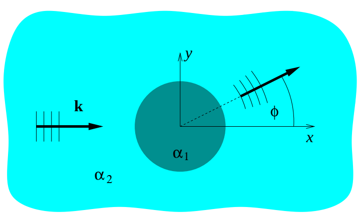

FIG. 1: (Color online) The plane wave of an incident electron with wave vector $\mathbf{k}$ gets scattered by a scattering region defined by a nonuniform Rashba coupling strength $\alpha(\mathbf{r})$ (see the text), and its portion propagates along the direction given by the scattering angle φ.

$$\mathcal{H} = \frac{\mathbf{p}^2}{2m^*} + \frac{\alpha(\mathbf{r})}{2\hbar}(\sigma_x p_y - \sigma_y p_x) + (\sigma_x p_y - \sigma_y p_x)\frac{\alpha(\mathbf{r})}{2\hbar}, \quad (1)$$

where $\mathbf{p}=(p_x,p_y)$ is the momentum operator, m^* is the effective mass of the electron, σ_x, σ_y are the Pauli matrices. Note that this Hamiltonian is symmetrized to make it Hermitian. For simplicity, we set $\alpha_2 = 0$, and α_1 is a constant value throughout this paper (our analysis can easily be extended to the case $\alpha_2 \neq 0$). Recently, similar scattering problems have been studied with uniform $\alpha(\mathbf{r})$ and an electrostatic potential varying in the plane of the 2DES[11,12].

The spin-density matrix[2,3] is proved to be useful for treating the coupled spin-charge quantum transport in spintronic devices[13]. Employing this formalism allows us to derive explicit formulas for the differential and the total scattering cross section, and the polarization $\mathbf{P}^{\rm sc}$ of the scattered wave in terms of the polarization $\mathbf{P}^{\rm inc}$ of the incident electron beam.

As can be seen below, the physics of the scattering of electrons shown in Fig. 1 is fundamentally different from the Mott scattering originating from the spin-dependent scattering potential[1,2,3,4] and the spin-dependent two-dimensional electron scattering from quantum dots and antidots studied in Ref. 14. In these scattering problems the polarization $\mathbf{P}^{\rm sc}$ of the scattered wave is always perpendicular to the scattering plane for unpolarized ($\mathbf{P}^{\rm inc}=0$) incident particles of spin 1/2, while in our scattering problem this is not the case in general.

First, we briefly outline the spin-density matrix approach of our spin-dependent scattering problem. The incident plane wave with wave number $\mathbf{k}$ has the form $\psi^{\rm inc}(\mathbf{r}) = e^{i\mathbf{kr}}\,|\gamma\rangle$, where $|\gamma\rangle$ denotes the spin state. In two dimensions the form of the scattered wave asymptotically far from the scattering center is

$$\psi^{\rm sc}(r,\varphi) \sim \frac{e^{ikr}}{\sqrt{r}}\,\mathbf{f}(\varphi)\,|\gamma\rangle, \tag{2}$$

where $\mathbf{f}(\varphi)$ is the scattering amplitude (2×2 matrix in spin space), and depends on the scattering angle φ and $\mathbf{k}$. The scattering amplitude $\mathbf{f}(\varphi)$ can be expanded in terms of the unit matrix σ_0 and the vector $\boldsymbol{\sigma}=(\sigma_1,\sigma_2,\sigma_3)$ formed from the three Pauli matrices (for convenience, we use $\sigma_1\equiv\sigma_x, \sigma_2\equiv\sigma_y, \sigma_3\equiv\sigma_z$ notations for the three Pauli matrices):

$$\mathbf{f}(\varphi) = \sum_{k=0}^{3} u_k(\varphi)\,\sigma_k = u_0(\varphi)\sigma_0 + \mathbf{u}(\varphi)\cdot\boldsymbol{\sigma}, \tag{3}$$

where u_0 and $\mathbf{u}=(u_1,u_2,u_3)$ can only be obtained by solving the Schrödinger equation for the scattering problem.

The spin-density matrix $\rho^{\rm inc} = \frac{1}{2}\left(\sigma_0 + \boldsymbol{\sigma}\cdot\mathbf{P}^{\rm inc}\right)$ of the incident wave for a given polarization $\mathbf{P}^{\rm inc} = \langle\boldsymbol{\sigma}\rangle_{\rm inc} = \mathrm{Tr}\left(\rho^{\rm inc}\,\boldsymbol{\sigma}\right)$ is related to the spin-density matrix $\rho^{\rm sc}$ of the scattered wave as[2]

$$\rho^{\rm sc} = \frac{\mathbf{f}\rho^{\rm inc}\mathbf{f}^\dagger}{\mathrm{Tr}\left(\mathbf{f}\rho^{\rm inc}\mathbf{f}^\dagger\right)}, \tag{4}$$

where Tr denotes the trace in the spin states. Then using (3) the differential scattering cross section reads as

$$\frac{d\sigma}{d\varphi} \;=\; \mathrm{Tr}\left(\mathbf{f}\rho^{\rm inc}\mathbf{f}^\dagger\right) = c + \mathbf{v}\cdot\mathbf{P}^{\rm inc}, \text{ where} \tag{5a}$$

$$c \;=\; \sum_{k=0}^{3}|u_k|^2 \;\text{ and }\; \mathbf{v} = 2\mathrm{Re}(u_0^*\mathbf{u}) - i(\mathbf{u}\times\mathbf{u}^*). \tag{5b}$$

Here $\mathrm{Re}(\cdot)$ denotes the real part of the argument, and the star stands for the complex conjugation. Note that, in general, $\mathbf{u}\times\mathbf{u}^*$ is not zero but it is always a purely imaginary vector.

Similarly, we found for the polarization vector $\mathbf{P}^{\rm sc}$ of the scattered beam

$$\mathbf{P}^{\rm sc} \;=\; \langle\boldsymbol{\sigma}\rangle_{\rm sc} = \mathrm{Tr}\left(\rho^{\rm sc}\,\boldsymbol{\sigma}\right) = \frac{\mathbf{w} + \boldsymbol{\mathcal{M}}\mathbf{P}^{\rm inc}}{c + \mathbf{v}\cdot\mathbf{P}^{\rm inc}}, \tag{6a}$$

where $\mathbf{w} = 2\mathrm{Re}(u_0^*\mathbf{u}) + i(\mathbf{u}\times\mathbf{u}^*)$ and the components of the matrix $\boldsymbol{\mathcal{M}}$:

$$\begin{aligned}\mathcal{M}_{ij} \;&=\; \left(|u_0|^2 - |\mathbf{u}|^2\right)\delta_{ij} + 2\,\mathrm{Re}\left(u_i^* u_j\right) \\ &+\; 2\sum_{k=1}^{3}\varepsilon_{ijk}\,\mathrm{Im}\left(u_0^* u_k\right),\end{aligned} \tag{6b}$$

with $i,j=1,2,3$, and δ_{ij} and ε_{ijk} denote the Kronecker delta and the Levi-Civita symbol, respectively. Here $\mathrm{Im}(\cdot)$ stands for the imaginary part of the argument. The components of $\boldsymbol{\mathcal{M}}$ are real numbers.

The spin-dependent form of the optical theorem can be derived by considering the scattering time-evolution of Gaussian wave packets, and we obtain:

$$\sigma_{\rm tot} \;=\; \sqrt{\frac{8\pi}{k}}\,\mathrm{Im}\left\{e^{-i\frac{\pi}{4}}\,\left[u_0(0) + \mathbf{u}(0)\cdot\mathbf{P}^{\rm inc}\right]\right\}, \tag{7}$$

where $\sigma_{\rm tot}$ is the total scattering cross section.

As can be seen, all physical quantities are expressed in terms of the coefficients $u_k(\varphi)$ which define the scattering amplitude $\mathbf{f}(\varphi)$ in Eq. (3). To calculate these unknown coefficients $u_k(\varphi)$ for our scattering problem we apply the method of partial waves, similarly as in Ref. 11. Choosing the spin quantization axis along the z axis, the eigenspinors (the eigenvectors of the Pauli matrix σ_z) are γ_σ, where $\gamma_+ = (1,0)^T$ for $\sigma=+1$, and $\gamma_- = (0,1)^T$ for $\sigma=-1$ (T stands for the transposed of vectors). Hereafter, we write $\pm$ for the spin quantum number $\sigma=\pm1$. Since the Hamiltonian $\mathcal{H}$ in Eq. (1) commutes with the total angular momentum operator $J_z = -i\hbar\partial_\varphi + \frac{\hbar}{2}\sigma_z$, any partial wave, which is a solution of the Schrödinger equation can be labeled by the quantum number $j\in\mathbb{J}$ and the spin quantum number σ of the incident electron. Here $\mathbb{J} = \{\cdots,-\frac{3}{2},-\frac{1}{2},\frac{1}{2},\frac{3}{2},\cdots\}$. We chose the direction of the propagation of the incoming plane wave along the x direction. Then, in polar coordinates, the incoming plane wave with spin quantum number σ and energy E can be expanded in terms of partial waves[15]:

$$\phi_\sigma(\mathbf{r}) = e^{ikx}\gamma_\sigma = \frac{1}{2\sqrt{-\sigma}}\sum_{j\in\mathbb{J}} i^{j+1/2}\left[h^{(1)}_{j,\sigma}(\mathbf{r}) + h^{(2)}_{j,\sigma}(\mathbf{r})\right], \tag{8}$$

where $h^{(1,2)}_{j,\sigma}(\mathbf{r}) = H^{(1,2)}_{j-\sigma/2}(kr)e^{i(j-\sigma/2)\varphi}\gamma_\sigma$, are the outgoing (superscript 1) and incoming (superscript 2) waves, and $k=|\mathbf{k}|=\sqrt{2m^*E}/\hbar$ is the magnitude of the wave vector. Here $H^{(1,2)}_m(z)$ are the 1st and 2nd kind of Hankel functions of order m.

First, we consider the individual partial waves. The partial waves outside the scattering region ($r>a$) have the form $\psi^{(\rm N)}_{j,\sigma} = h^{(2)}_{j,\sigma} + S^{(j)}_{\sigma,\sigma}h^{(1)}_{j,\sigma} + S^{(j)}_{-\sigma,\sigma}h^{(1)}_{j,-\sigma}$, while inside the scattering region ($r<a$) they can be written as $\psi^{(\rm R)}_{j,\sigma} = A^{(j)}_{+,\sigma}\chi_{j,+} + A^{(j)}_{-,\sigma}\chi_{j,-}$, where

$$\chi_{j,\tau}(\mathbf{r}) = \begin{pmatrix}\tau J_{j-1/2}(q_\tau r)e^{-i\varphi/2} \\ J_{j+1/2}(q_\tau r)e^{i\varphi/2}\end{pmatrix} e^{ij\varphi}, \tag{9}$$

and $J_m(x)$ is the Bessel function, $q_\tau = \sqrt{k^2 + k_{\rm so}^2} - \tau k_{\rm so}$, $k_{\rm so} = \alpha_1 m^*/\hbar^2$ and $\tau = \pm 1$ is the spin branch index[16]. The coefficients $A^{(j)}_{\pm,\pm}$ and $S^{(j)}_{\pm,\pm}$ can be calculated from the boundary conditions[17]:

$$\psi^{\rm (N)}_{j,\sigma}\Big|_{r=a} = \psi^{\rm (R)}_{j,\sigma}\Big|_{r=a}, \tag{10a}$$

$$\partial_r \psi^{\rm (N)}_{j,\sigma}\Big|_{r=a} = \left(\partial_r - i k_{\rm so}\sigma_\varphi\right)\psi^{\rm (R)}_{j,\sigma}\Big|_{r=a}, \tag{10b}$$

valid for all $j \in \mathbb{J}$ and $\sigma = \pm 1$, and $\sigma_\varphi = -\sin\varphi\,\sigma_x + \cos\varphi\,\sigma_y$. For a given j these equations involving Bessel and Hankel functions result in eight linear inhomogeneous equations for the eight unknown coefficients $A^{(j)}_{\pm,\pm}$ and $S^{(j)}_{\pm,\pm}$. The explicit forms of the equations are independent of the angle φ. These coefficients can easily be calculated numerically. Note that the following exact relations hold $S^{(j)}_{\sigma,\sigma} = S^{(-j)}_{-\sigma,-\sigma}$ and $S^{(j)}_{-\sigma,\sigma} = S^{(j)}_{\sigma,-\sigma} = S^{(-j)}_{-\sigma,\sigma} = S^{(-j)}_{\sigma,-\sigma}$ for all $j \in \mathbb{J}$ and $\sigma = \pm 1$. To proceed further, we assume that the coefficients $S^{(j)}_{\pm,\pm}$ are known from numerical calculations.

Outside the scattering region the complete wave function describing the scattering of the plane wave can be decomposed as $\psi^{\rm (N)}_\sigma = \sum_{j\in\mathbb{J}} \psi^{\rm (N)}_{j,\sigma} = \phi_\sigma + \psi^{\rm (sc)}_\sigma$, where $\psi^{\rm (sc)}_\sigma$ is the scattered wave. It is easy to show that $\psi^{\rm (N)}_\sigma$ and $\psi^{\rm (R)}_\sigma = \sum_{j\in\mathbb{J}} \psi^{\rm (R)}_{j,\sigma}$ satisfy the boundary conditions (10). Using the Hankel's asymptotic expansions[15] we have $h^{(1)}_{j,\sigma}(\mathbf{r}) \sim \sqrt{\frac{2}{i\pi k r}}\, e^{i\left(kr-(j-\sigma/2)\frac{\pi}{2}\right)}\, e^{i(j-\sigma/2)\varphi}\,\gamma_\sigma$ valid for $r \gg a$, and then the asymptotic form of the scattered waves $\psi^{\rm (sc)}_\sigma$ can be calculated. Finally, Eq. (2) yields $\langle\gamma_\sigma|\psi^{\rm (sc)}_{\sigma'}\rangle = \frac{e^{ikr}}{\sqrt{r}} f_{\sigma,\sigma'}$, and using Eq. (3) we obtain

$$u_0(\varphi) = \sum_{j\in\mathbb{J}^+} B_j \cos\left(j-\frac{1}{2}\right)\varphi + C_j \cos\left(j+\frac{1}{2}\right)\varphi, \tag{11a}$$

$$u_1(\varphi) = 2\sin(\varphi/2)\sum_{j\in\mathbb{J}^+} D_j \cos(j\varphi), \tag{11b}$$

$$u_2(\varphi) = -2\cos(\varphi/2)\sum_{j\in\mathbb{J}^+} D_j \cos(j\varphi), \tag{11c}$$

$$u_3(\varphi) = i\sum_{j\in\mathbb{J}^+} B_j \sin\left(j-\frac{1}{2}\right)\varphi + C_j \sin\left(j+\frac{1}{2}\right)\varphi, \tag{11d}$$

where we introduced the notations $B_j = (S^{(j)}_{+,+} - 1)$, $C_j = (S^{(j)}_{-,-} - 1)$, $D_j = S^{(j)}_{-,+}$ and $\mathbb{J}^+ = \{\frac{1}{2}, \frac{3}{2}, \cdots\}$.

In numerical calculations the two dimensionless parameters characterizing the scattering process are ka and $k_{\rm so}a$. Figure 2 shows the asymmetric (skew-scattering) feature of the differential scattering cross section calculated from (5) for different spin polarizations $\mathbf{P}^{\rm inc}$ of the incident electron beam. The scattering cross sections at a given scattering angle φ are different for spin up and spin down polarization of an incident beam, ie for $\mathbf{P}^{\rm inc}$ and $-\mathbf{P}^{\rm inc}$. From Eq. (11) it follows that

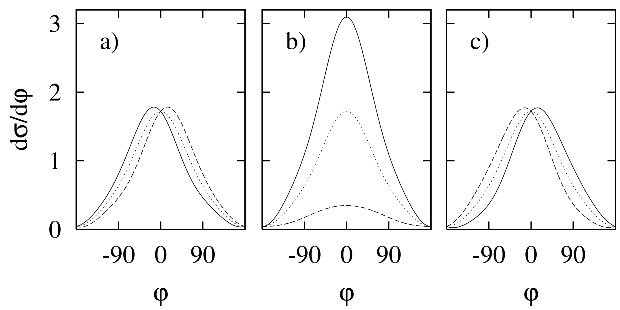

FIG. 2: Differential scattering cross sections (in units of a) as functions of the scattering angle φ (in units of degrees) for spin polarizations $\mathbf{P}^{\rm inc} = 0, (\pm 1, 0, 0)^T$ (a), $\mathbf{P}^{\rm inc} = 0, (0, \pm 1, 0)^T$ (b) and $\mathbf{P}^{\rm inc} = 0, (0, 0, \pm 1)^T$ (c) with dotted, solid and dashed lines, respectively in each figures. The parameters are $ka = 1$ and $k_{\rm so}a = 1$.

$\mathbf{u}(\varphi = 0) \sim (0, 1, 0)^T$, therefore the optical theorem (7) implies that the polarization dependence of the total scattering cross section (the areas under the curves in Fig. 2) takes the form $\sigma_{\rm tot}(\mathbf{P}^{\rm inc}) = c_1 + c_2 P^{\rm inc}_y$, where $P^{\rm inc}_y$ is the y component of the polarization vector of the incident wave, and c_1 and c_2 depend only on ka and $k_{\rm so}a$. Thus, in Fig. 2a and c, and for $\mathbf{P}^{\rm inc} = 0$ the total scattering cross sections are the same.

The magnitude of the polarization $|\mathbf{P}^{\rm sc}|$ of the scattered waves obtained from Eq. (6) and the differential scattering cross section are plotted in Fig. 3 for unpolarized ($\mathbf{P}^{\rm inc} = 0$) incident electron beam using experimentally relevant parameters[10]. As can be seen from the

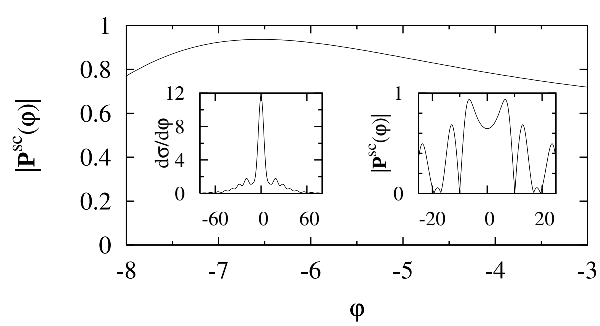

FIG. 3: The magnitude of polarization $|\mathbf{P}^{\rm sc}|$ (main panel) and the differential scattering cross section $d\sigma/d\varphi$ (left inset) as functions of the scattering angle φ (in units of degrees) for unpolarized ($\mathbf{P}^{\rm inc} = 0$) incident waves. The large scale φ (in units of degrees) dependence of $|\mathbf{P}^{\rm sc}|$ is shown in the right inset. The parameters are $ka = 20$ and $k_{\rm so}a = 4$.

figure, the differential cross section is rather high and the scattered beam is almost fully polarized for a narrow window of angles. This result suggests an effective tool for spin-filtering without using magnetic field.

We also studied the high energy limit of the scattering. This is the case, when $ka \gg 1$, ie the Fermi wave length of the electron is much smaller than a. Then one can apply the first Born approximation and it can be shown that the scattering amplitude $\mathbf{f} \sim \sigma_y$. Thus, from (3) we have $u_0 = 0$ and $\mathbf{u} \sim (0,1,0)^T$, while from (6) $\mathbf{w} = 0$. Therefore, for unpolarized incident electron beam ($\mathbf{P}^{\rm inc} = 0$) the polarization of the scattered waves is negligible in the high energy limit. However, a finite spin polarization can arise even in the first Born approximation if an additional electrostatic potential is present beside the spin-orbit interaction, eg, in an imaging experiment[11]. In this case, u_0 and u_2 are finite and it yields a finite value of $\mathbf{P}^{\rm sc}$ for unpolarized incident beams.

In the opposite limit, ie for low energy limit ($ka \ll 1$) it is also possible to derive an analytical result for the scattering amplitude and the polarization $\mathbf{P}^{\rm sc}$ of the scattered waves. Keeping only the first order terms in $k/k_{\rm so}$ of $S^{(j)}_{\pm,\pm}$ resulting from the boundary equations (10) and that of $u_k(\varphi)$ in Eq. (11), it yields

$$\mathbf{P}^{\rm sc}(\varphi) \approx 2\,\frac{k}{k_{\rm so}}\,(-\sin\varphi, 1+\cos\varphi, 0)^T, \qquad (12)$$

valid for $ka \ll 1$ and $k \ll k_{\rm so}$ and for unpolarized incident electron beams. We found an excellent agreement between this result and that obtained from (6) with numerically exact calculations. Similarly, it can be shown that the differential scattering cross section is approximately isotropic (independent of the scattering angle φ) in the low energy limit.

In conclusions, we have shown that for a circular shape of region with non-zero Rashba coupling strength, the scattering properties are strongly anisotropic, and the scattered wave is well polarized in a narrow window of the scattering directions. Such a nonuniform SOI can be utilized to produce spin-polarized electrons in an all-electric realization of spintronic devices.

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