Spin angular impulse due to spin-dependent reflection off a barrier

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The spin-dependent elastic reflection of quasi-two-dimensional electrons from a lateral impenetrable barrier in the presence of band-structure spin-orbit coupling results in a spin angular impulse exerted on the electrons which is proportional to the nontrivial difference between the electrons' momentum and velocity. Even for an unpolarized incoming beam we find that the spin angular impulse is nonzero when averaged over all components of the reflected beam. We present a detailed analysis of the kinematics of this process.

Spin-dependent scattering in confined systems with spin-orbit coupling (SOC) offers fascinating possibilities to manipulate the electrons' spin degree of freedom if the electrons move through an appropriate orbital environment. In the presence of band-structure SOC the elastic reflection of quasi-two-dimensional (2D) electrons from a lateral impenetrable barrier depends on their spin orientation so that such a setup can act like a spin filter.\textsuperscript{2} Also, one can obtain spin accumulation near the barrier.\textsuperscript{2} Scattering off circular barriers was investigated in Refs. \textsuperscript{3,4}. Several groups studied the propagation of electrons in systems where the magnitude of SOC is modulated in space.\textsuperscript{5,6,7,8} A related configuration uses a magnetic field perpendicular to the plane of a quasi-2D system which results in spin-dependent magnetic focusing.\textsuperscript{9,10} The studies of these systems focused on the spatial separation of the trajectories of electrons with different spin orientations, on the generation of a spin polarization, and on interference effects related to the different paths that scattered electrons can take. These phenomena complement the spin precession that characterizes the propagation of electrons moving freely in the effective magnetic field characterizing SOC.\textsuperscript{11,12}

Here we show that scattering off barriers also allows one to manipulate the spin degree of freedom in a conceptually different way as SOC results in an effective spin torque that can change the orientation of the spin vector nonadiabatically during the scattering process. Recently, spin torques have been a subject of significant interest as a tool for reorienting the magnetization direction of magnetic layers.\textsuperscript{13} Spin-dependent scattering off barriers give rise to spin torques in a well-defined setting. The effect is proportional to the nontrivial difference between the electrons' momentum and velocity. When integrated over the duration of the scattering process, the spin torque corresponds to a spin angular impulse. Like the mechanical torque discussed by Mal’shukov et al.,\textsuperscript{14} the spin angular impulse is a manifestation of the fundamental conservation laws characterizing the electron dynamics in the presence of SOC. We show that even for an unpolarized incoming beam the spin angular impulse is nonzero when averaged over all components of the reflected beam. The effect is the largest in magnitude if the angle of the incoming beam relative to the reflecting barrier approaches a critical value. Our findings are relevant for a large variety of transport experiments in confined geometries.\textsuperscript{15}

For this study, we consider the Hamiltonian

\[ H = \frac{1}{2} \mu k^2 + \alpha (k_y \sigma_x - k_x \sigma_y) + V(x), \]

where \( k = (k_x, k_y, 0) \) is the 2D in-plane wave vector and \( \mu \equiv \hbar^2/m^* \) with the effective mass \( m^* \). The second term in Eq. (1) is the Rashba SOC\textsuperscript{16} with Rashba coefficient \( \alpha > 0 \), and \( \sigma_i \) are the Pauli spin matrices. Finally, \( V(x) \) is the potential due to the impenetrable barrier. We assume \( V(x) = 0 \) for \( x < 0 \) and \( V(x) = \infty \) for \( x > 0 \). Previous studies showed that smoother gradients preserve the important physics.\textsuperscript{2,17} While we restrict ourselves for conceptual clarity to Rashba SOC, it is straightforward to include other contributions to SOC such as Dresselhaus SOC.\textsuperscript{18} The spin-split dispersion is

\[ E_{\pm}(k) = \frac{1}{2} \mu k^2 \pm \alpha k. \]

For a given density \( N \) the dispersion results in Fermi wave vectors\textsuperscript{19}

\[ k_\pm = \sqrt{2\pi \left( N + \frac{\alpha}{\pi \mu} \sqrt{2\pi \mu^2 N - \alpha^2} \right)} = \frac{1}{\mu} \sqrt{2\pi E_F} + \alpha^2 + \alpha, \]

where \( E_F = E_+(k_+) = E_-(k_-) \) is the Fermi energy. We note that \( k_- - k_+ = 2\alpha/\mu > 0 \) independent of \( N \) (Ref. \textsuperscript{12} provided that \( k_- > 2\alpha/\mu \), i.e., \( N > N_g \equiv \alpha^2/(\pi \mu^2) \)). As \( N \) is typically much larger than the “quantum density” \( N_g \), the case \( N < N_g \) is ignored in the following.\textsuperscript{20} Yet we note that all formulas developed below give the largest observable effects for small densities, consistent with the fact that the SOC term in Eq. (1) is most important for small densities.

We consider a ballistic electron beam with wave vector \( k_0^\parallel \) that is reflected elastically from the barrier at \( x = 0 \), see Fig. [1] The wave functions are\textsuperscript{21}

\[ \psi_{k_\pm}(r) = \frac{A_0 e^{ik_0^\parallel r}}{\sqrt{2}} \left( \frac{1}{\mp i e^{i\phi_0}} + \frac{A_\pm e^{i(k_\pm - k_0^\parallel) r}}{\sqrt{2}} \right) \left( \frac{1}{\mp i e^{i\phi_0}} + \frac{A_\pm e^{i(k_\pm + k_0^\parallel) r}}{\sqrt{2}} \right), \]

where \( \phi_0 \) is the polar angle of \( k_0^\parallel \). Throughout, the index 0 refers to the incoming beams, 1 (2) denotes the ordinarily (extraordinarily) reflected beam preserving (not
which yields the ordinary reflection law
\[ \phi_1 = \pi - \phi_0, \]
and the extraordinary reflection law
\[ \phi_2^\mp = \pi - \arcsin \left( \frac{k_\pm}{k_\mp} \sin \phi_0 \right). \] (7)

As \( k_- > k_+ \), the equation for \( \phi_2^- \) has a real solution for any \( 0 \leq \phi_0 \leq \pi/2 \). However, a real solution for \( \phi_2^+ \) exists only for \( 0 \leq \phi_0 \leq \phi_c \), where
\[ \phi_c \equiv \arcsin(k_+/k_-). \] (8)

For \( \phi_0 > \phi_c \), Eq. (7) becomes equivalent to
\[ \phi_2^+ = \frac{\pi}{2} + i \ln \left[ \frac{\sin \phi_0}{\sin \phi_c} + \sqrt{\left( \frac{\sin \phi_0}{\sin \phi_c} \right)^2 - 1} \right]. \] (9)

It will become evident below that the critical angle \( \phi_c \) plays an important role for many geometrical aspects of this problem. Note that \( \phi_c \rightarrow 0 \) for \( N \rightarrow N_q \). The difference between the angles of the two reflected beams is
\[ \epsilon_\mp \equiv \phi_2^\mp - \phi_1 = \phi_0 - \arcsin \left( \frac{k_\pm}{k_\mp} \sin \phi_0 \right). \] (10)

The splitting angle \( \epsilon_- \) is positive and its largest value is obtained for \( \phi_0 \rightarrow \pi/2 \) (grazing incidence) giving
\[ |\epsilon_{\text{max}}| = \pi/2 - \phi_c. \] (11)

The angle \( \epsilon_+ \) is negative and its largest value in magnitude is obtained for \( \phi_0 = \phi_c \). Yet the corresponding value \( |\epsilon_{\text{max}}| \) is again given by Eq. (11), see Fig. 2(a).

Conservation of the wave vector component \( k_{x1}^\mp \) implies that \( k_{x1}^\mp \) and \( k_{x2}^\mp \) become functions of \( \phi_1 \) and \( \phi_2^\mp \)
\[ k_{x1}^\pm = k_\pm \cos \phi_1, \quad k_{x2}^\pm = k_\mp \cos \phi_2^\mp. \] (12)

For a complex angle \( \phi_2^+ \) the wave vector \( k_{x2}^+ \) becomes imaginary, i.e., \( \kappa_{x2}^+ \equiv ik_{x2} > 0 \) describes an exponentially decaying solution (for \( x \leq 0 \)).

Continuity of the wave function \( \psi_{kz}(r) \) at the interface \( x = 0 \) yields the conditions
\[ \frac{A_1^\pm}{A_0} = \frac{e^{2i\phi_0} - e^{i\epsilon_\mp}}{1 + e^{i\epsilon_\mp}}, \quad \frac{A_2^\mp}{A_0} = -1 + e^{2i\phi_0}. \] (13)

Here the expression for \( A_1^\mp \) refers to the corresponding two-component spinor in Eq. (4) that is not normalized for \( \phi_0 > \phi_c \). Unlike the probability current discussed below, the probability density \( |\psi|^2 \) is not conserved upon reflection. Indeed (note \( \cos \phi_0 = -\cos \phi_1 \))
\[ |A_0|^2 \cos \phi_0 + |A_1^\mp|^2 \cos \phi_1 + |A_2^\mp|^2 \cos(\phi_2^\mp) = 0, \] (14)
which illustrates the importance of \( \epsilon_\mp \) for our problem.

The Hamiltonian (4) yields the following expression for the velocity operator
\[ v = \frac{i}{\hbar}[H, r] = \frac{1}{\hbar}(\mu \mathbf{k} + \alpha \mathbf{\varepsilon} \times \mathbf{\sigma}), \] (15)
where \( \hat{e}_z \) denotes a unit vector perpendicular to the 2D plane. We see here that SOC gives rise to a nontrivial spin-dependent difference between the electrons’ momentum and velocity that plays a crucial role in our analysis below of the spin angular impulse. Outside the region where the beams interfere and for real angles \( \phi \) we get for the magnitude \( v \) of the velocity
\[
v \equiv (v) = \frac{1}{\hbar} (\mu k_+ + \alpha) = \frac{1}{\hbar} (\mu k_- - \alpha),
\]
i.e., all beams have the same velocity \( v \) (parallel to the corresponding wave vector)\(^{22}\). For complex angles \( \phi^*_\pm \) the velocity is slightly larger than Eq. \((16)\), and it is oriented perfectly parallel to the barrier,
\[
v^*_2 = \frac{\hbar}{\mu} \left[ \mu k^- + \alpha \frac{\sin \phi}{\sin \phi_0} \right].
\]
Similar to Eq. \((15)\), we get for the probability current
\[
j \equiv \langle j \rangle = \frac{1}{\hbar} \mu \Re \langle \psi | k | \psi \rangle + \alpha \langle \psi | \hat{e}_z \times \sigma | \psi \rangle.
\]
We emphasize that unlike \( v = \langle v \rangle \) and \( \langle \sigma \rangle \), the expectation value \( j = \langle j \rangle \) is not normalized with respect to the corresponding wave function. Obviously, this is necessary to obtain the continuity equation
\[
\partial_t \rho + \nabla \cdot j = 0,
\]
where \( \rho = |\psi|^2 \) is the probability density. Of course, in our case \( \partial_t \rho = 0 \). For the region where both the incoming and the reflected beams are present we get \( j_x = 0 \) (as expected for an impenetrable barrier). On the other hand, the current component \( j_y \) in this region depends in an oscillatory fashion on the distance \(|x|\) to the barrier due to the interference of the three terms in Eq. \(15\). We do not give here the lengthy expressions.

Outside the region where both the incoming and the reflected beams are present, we get in the undercritical regime [using Eqs. \(13\) and \(16\)]
\[
\begin{align*}
\langle j^0 \rangle & = |A_0|^2 v_0, \\
\langle j^1 \rangle & = |A_0|^2 \frac{\sin^2(\phi_0 - \epsilon_\pm/2)}{\cos^2(\epsilon_\pm/2)} v_1, \\
\langle j^\mp \rangle & = |A_0|^2 \frac{\cos^2\phi_0}{\cos(\epsilon_\pm/2)} v_2,
\end{align*}
\]
where \( v_0 = v \). In the overcritical regime we have
\[
\begin{align*}
\langle j^0 \rangle & = |A_0|^2 v_0, \\
\langle j^1 \rangle & = |A_0|^2 v_1
\end{align*}
\]
with \( v_0 = v_1 = v \). For the extraordinarily reflected beam we get
\[
\langle j^\pm \rangle (x) = |A_0|^2 \frac{2 \cos^2 \phi_0}{1 + \sin \phi_0} e^{2 \alpha x} v^+_2,
\]
i.e., the current \( j^\pm_2 \) dies off exponentially with increasing distance \(|x|\) from the barrier.

We evaluate the currents reflected from a unit segment of the barrier to get the reflection coefficients
\[
R_{\pm} = \frac{\sin^2(\phi_0 - \epsilon_\pm/2)}{\cos^2(\epsilon_\pm/2)}, \quad R_{\mp} = \frac{\cos(\phi_0 - \epsilon_\pm) \cos \phi_0}{\cos^2(\epsilon_\pm/2)},
\]
where the first (second) sign of \( R_{\pm} \) corresponds to the incoming (reflected) beam [Fig. \(2B\)]. Current conservation implies \( R_{++} + R_{+-} = R_{-+} + R_{--} = 1 \), which is equivalent to Eq. \(14\) because \( v_i = v \). We note that in the overcritical regime we have \( R_{--} = 0 \). At a first glance this appears counterintuitive because the reflected current \( j_{2}^\pm \) is nonzero. However, this current is oriented parallel to the barrier so that it does not enter the reflection coefficient.

It is known for the Rashba model \(\text{1}\) that propagating beams are characterized by a spin orientation in the 2D plane and perpendicular to the corresponding wave vector,\(^{13,22}\) i.e., for a wave vector \( k_\pm \) with polar angle \( \phi \) the orientation of the unit vector \( \langle \sigma \rangle \pm \) is characterized by the angle \( \phi \mp \pi/2 \). In the overcritical regime \( \phi_0 > \phi_c \), we obtain the out-of-plane spin orientation\(^2\)
\[
\langle \sigma \rangle^\mp_2 = \left( \begin{array}{c}
\cos \eta \\
n \sin \eta
\end{array} \right),
\]
where \( \eta = \arccos(\sin \phi_c / \sin \phi_0) \). The largest value of \( \eta \) is obtained in the limit of grazing incidence \( (\phi_0 \rightarrow \pi/2) \) giving \( \eta_{\max} = |\epsilon_{\max}| \) [Fig. \(2A\)] with \( \eta_{\max} \rightarrow \pi/2 \) for low densities \( N \rightarrow N_\eta \).

It is well known that during the elastic reflection of electrons off an impenetrable barrier, the barrier exerts a force \( F \) on the electrons. Yet for such a scattering process only the linear impulse, i.e., \( F \) integrated over the time \( \Delta t \) of the collision process is physically meaningful. Obviously, this linear impulse per electron equals the change \( \hbar \Delta k \) of crystal momentum. This result gets modified by the presence of SOC. Using Eq. \(15\) we get
\[
F \Delta t = m^z \left( \Delta \langle v \rangle - \frac{\alpha}{\hbar} \hat{e}_z \times \Delta \langle \sigma \rangle \right) = \hbar \Delta k.
\]

Furthermore, SOC gives rise to multiple reflected beams as discussed above. When taking into account the conservation of the electron number during the scattering process, one finds using a continuous media approach that \( \hbar \Delta k \) for the components of the reflected beam must be weighted by the corresponding reflection coefficients\(^{23}\).

Equation \(25\) implies that the barrier also exerts an orbital torque that changes the orbital angular momentum of the electrons. In a similar way (while there is no direct effect of the barrier on the electron’s spin), SOC and the barrier exert an effective spin torque on the electrons that changes the spin orientation when the electrons are reflected at the barrier. Using Eq. \(23\) we can write the dimensionless spin angular impulse as
\[
\Delta \langle \sigma \rangle = \frac{\hbar}{\alpha} \hat{e}_z \times \left( \frac{\hbar \Delta k}{m} - \Delta \langle v \rangle \right).
\]
which shows that the change of the spin orientation is a combined effect of SOC and the change in orbital motion characterized by a nontrivial difference between the changes of the electron’s momentum and velocity. When averaging over the components of the reflected beam we get
\[
\Delta \langle \sigma \rangle^\pm = R_{\pm \pm} (\langle \sigma \rangle^{\pm}_{1} - \langle \sigma \rangle^{\pm}_{0}) + R_{\pm \mp} (\langle \sigma \rangle^{\pm}_{2} - \langle \sigma \rangle^{\pm}_{0}).
\] (27)

\(\Delta \langle \sigma \rangle^\pm\) approaches magnitude \(\sim 1\) around \(\phi_0 \approx \pi/4\) when on average the spin orientation of the electrons becomes zero upon reflection. In other words, the spin angular momentum carried by a + or − polarized current is fully absorbed by the barrier around \(\phi_0 \approx \pi/4\). Clearly, this has important consequences for spin-dependent transport in confined geometries.\(^{22}\) Also, it offers interesting perspectives for current-driven domain wall motion and magnetization reversal.\(^{22}\) Even for the electrons in an unpolarized incoming beam the average spin angular impulse
\[
\Delta \langle \sigma \rangle = \frac{1}{2} (\Delta \langle \sigma \rangle^{+} + \Delta \langle \sigma \rangle^{-})
\] (28)
is nonzero. Figure 2(c) shows that \(\Delta \langle \sigma \rangle^{\pm}\) can be quite significant and that it is the largest in magnitude at the critical angle \(\phi_c\). For the parameters of Fig. 2 the maximum of \(\Delta \langle \sigma \rangle\) amounts to 0.09. We note that while \(\langle \sigma \rangle^+_2\) in the overcritical regime is out-of-plane,\(^2\) Eq. (23) does not give rise to an out-of-plane component of \(\Delta \langle \sigma \rangle\) because in this regime we have \(R_{-\pm} = 0\).

Finally, we comment on how our findings depend on the sample geometry. The SOC in Eq. (1) can be interpreted as a Zeeman term with an effective magnetic field \(\omega(k) = (2\alpha/\hbar)(k_y, -k_x)\) giving rise to a precessional motion with frequency \(\omega = |\omega(k)|\). Quite generally, the deflection of electron trajectories in confined geometries implies that the orientation of \(\omega(k)\) changes along these trajectories. If we approximate the deflection by a circular orbit with radius \(R\), we can distinguish two regimes.\(^{13,23}\) If \(\omega \gg \Omega \equiv \hbar k/(m^* R)\), the electron spins follow adiabatically \(\omega(k)\). Here, \(\Delta \langle \sigma \rangle\) is simply given by the change of \(\omega(k)\). Thus \(\Delta \langle \sigma \rangle = 0\) for an unpolarized incoming beam. If, on the other hand, \(\omega \lesssim \Omega\), i.e., \(R \lesssim R_0 = h^2/(2m^* \alpha)\), we are in the nonadiabatic regime, where spin eigenstates are scattered into a superposition of oppositely oriented eigenstates. (The above discussion corresponds to the limiting case \(R = 0\).) For the parameters used in Fig. 2 we have \(R_0 = 270\) nm. In systems with weaker SOC than InSb, \(R_0\) is yet larger. Therefore, taking typical sample dimensions into account, the spin angular impulse discussed here is important for a large variety of spin-dependent transport experiments in confined geometries.\(^{23}\) We note that spin relaxation lengths are usually significantly larger than \(R_0\).

In conclusion, our analysis demonstrates that the spin-dependent reflection provides a new mechanism that changes the spin orientation via the spin angular impulse exerted on the electrons when they are reflected off a barrier in the presence of SOC. While the present work has focused for conceptual clarity on a straight and infinitely high barrier, the underlying physics is relevant for a large variety of transport experiments in confined geometries including soft barriers or sample boundaries with different shapes. The mechanism provides interesting possibilities for current-driven magnetization dynamics. RW appreciates stimulating discussions with J. Heremans and U. Zülicke. Work at Argonne was supported by DOE BES under Contract No. DE-AC02-06CH11357.

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