Polarized electric current in semiclassical transport with spin-orbit interaction

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Semiclassical solutions of two-dimensional Schrödinger equation with spin-orbit interaction and smooth potential are considered. In the leading order, spin polarization is in-plane and follows the evolution of the electron momentum for a given subband. Out-of-plane spin polarization appears as a quantum correction, for which an explicit expression is obtained. We demonstrate how spin-polarized currents can be achieved with the help of a barrier or quantum point contact open for transmission only in the lower subband.

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I. INTRODUCTION

Achieving spin manipulation in nanodevices by means of electric fields (without using less selective magnetic fields) represents the ultimate goal of spintronics. Spin-orbit interaction, which couples electron momentum to its spin, is one of the most promising tools for realizing spin-polarized transport.[1,2] Several schemes leading either to spin accumulation or to polarization of the transmitted current induced by the spin-orbit interaction have been put forward. Predictions of electric field induced spin accumulation at the boundaries of a sample, which originates from asymmetric scattering from impurities[3,4] (extrinsic spin-Hall effect) or from spin-orbit split band structure[5,6] (intrinsic effect), has recently reached a stage of experimental realization.[7] In-plane bulk spin polarization appears in two-dimensional systems with broken inversion symmetry.[8] Spin polarization in quantum wires with low carrier density has been shown to occur due to the interfaces of spin-degenerate and spin-split regions.[9] Interfaces between two-dimensional regions with different spin-orbit splitting have also been used for that purpose, in the case of a sharp[10,11] or an arbitrary[12] interface, as was the scattering from a sample edge.[13,14] Other proposals include polarization due to tunneling through a double-barrier structure[15,16] and tunneling between two quantum wires.[17] Reference 18 suggested a three-terminal device with a spin-orbit split central region as a spin filter, which was numerically tested by Refs. 19 and 20. Reference 21 pointed to a possibility of generating spin-polarized currents by utilizing crossings of spin-orbit-split subbands belonging to different transverse channels. These proposals are still lacking experimental realization.

In the present paper we suggest a way to polarize electric currents by passing them through a region where, by increasing the external electrostatic potential, the upper spin-orbit-split subband is locally positioned *above* the Fermi level. The proposed method utilizes electric gating whose effect is twofold: (i) it completely suppresses transmission via the upper spin-orbit-split subband, and (ii) it allows transmission only in a narrow interval of incident angles in the lower subband. In contrast to the proposals which advocate strong variations of the spin-orbit coupling and, thus, rely on strong gate voltages, our method requires only weak potentials of the order of a few millivolts (which is a typical scale of the Fermi energy). In addition, we predict a specific pinch-off behavior of the conductance, which would allow to detect polarized currents without actual measurement of spin.

We consider ballistic electron transport in gated two-dimensional electron gas with the Hamiltonian

$$H = \frac{p^2}{2m} + \lambda(p_y\sigma_x - p_x\sigma_y) + \frac{m\lambda^2}{2} + V(x,y). \tag{1}$$

For the sake of simplicity we concentrate on the case of the "Rashba" spin-orbit interaction (the same method, however, can be used for more complicated interactions). Construction of semiclassical solutions of the Schrödinger equation with the Hamiltonian (1) follows the reasoning of the conventional WKB approach,[22–25] which is valid for a smooth potential, $\hbar|\nabla V| \ll \min(p^3/m, p^2\lambda)$. The advantages of semiclassics are twofold. First, it allows us to obtain approximate analytical solutions for otherwise complicated problems. Second, as we will see, it turns out to be especially simple to achieve strong polarization of electron transmission in the semiclassical regime.

The Mexican hat shape of the effective kinetic energy in the case of spin-orbit interaction leads to a variety of unusual classical trajectories (see Fig. 2 below), which have never been investigated before. Our approach employs strong spin-orbit interaction (or smooth external potential) sufficient to affect individual electron trajectories, in contrast to previous semiclassical treatments[26,27] which consider spin-orbit interaction as a perturbation. Still we do not require the spin-orbit interaction to be comparable with the bulk value of the Fermi energy. To produce spin-polarized current, it will be sufficient to make spin-orbit interaction comparable with the kinetic energy at some particular area of the system, for example, near the pinch-off of a quantum point contact.

II. SEMICLASSICAL WAVE FUNCTION

Without the external potential V, the electron spectrum consists of the two subbands, $E_\pm(p_x,p_y)=(p\pm m\lambda)^2/2m$. The subbands meet at only one point, $p=0$, and the spin in each subband is always aligned with one of the in-plane directions perpendicular to the momentum $\vec{p}$. The semiclassical electron dynamics[22] naturally captures the essential features of this translationally invariant limit. The classical motion in each subband is determined by the equations of motion which follow from the effective Hamiltonian:

$$H_{\rm eff} = \frac{(p \pm m\lambda)^2}{2m} + V(x,y). \qquad (2)$$

Despite the fact that spin does not appear in this equation, one can easily construct semiclassical wave functions, which have spin pointed within the xy plane perpendicular to the momentum:

$$\psi_0 = u e^{iS/\hbar}, \quad u = \sqrt{\frac{\rho}{2p}} \begin{pmatrix} \sqrt{p_y + ip_x} \\ \pm\sqrt{p_y - ip_x} \end{pmatrix}. \qquad (3)$$

Here the action S is related to the momentum by $\vec{p}=\nabla S$, and $\rho = u^\dagger u$ is the classical density for a family of classical trajectories corresponding to a given energy E. The action S obeys the classical Hamilton-Jacobi equation, $(|\nabla S| \pm m\lambda)^2/2m + V = E$. Application of the Hamiltonian (1) to the approximate wave function ψ_0 gives, after some algebra,

$$H\psi_0 = E\psi_0 - \frac{i\hbar}{2\rho}(\nabla \cdot \rho\vec{v})\psi_0 + \hbar\lambda F\sigma_z\psi_0, \qquad (4)$$

where (summation over repeating indices is assumed)

$$F = \frac{p \mp m\lambda}{2m\lambda p^3}(p_y p_i \partial_i p_x - p_x p_i \partial_i p_y) \pm \frac{p_y \partial_x \rho - p_x \partial_y \rho}{2p\rho}. \qquad (5)$$

The second term in the rhs of Eq. (4) vanishes due to the continuity equation

$$\nabla \cdot \rho\vec{v} = 0, \quad \vec{v} = \vec{p}/m \pm \lambda\vec{p}/p. \qquad (6)$$

The last ($\sim\sigma_z$) term in (4) indicates that the spin of an accelerated electron cannot exactly stay in the plane of propagation and acquires a small $\sim\hbar\nabla V$ projection onto the z axis. To take into account this out-of-plain spin precession one has to go beyond the approximation of Eq. (3), which is done by

$$\psi = (1 + \hbar f\sigma_z)\psi_0. \qquad (7)$$

Since $(H-E)f\sigma_z\psi_0 = \mp 2\lambda p f\sigma_z\psi_0$, to the lowest order in $\hbar$, one can relate the functions F and f

$$f = \pm F/2p, \qquad (8)$$

and find the out-of-plane spin density [F is found from Eq. (5)]

$$\psi^\dagger\sigma_z\psi = \pm\frac{\hbar\rho}{2p}F. \qquad (9)$$

Note that Eq. (9) does not describe the nonadiabatic transitions between subbands. After the electron leaves the region with nonzero potential gradient, $\nabla V \neq 0$, the in-plain spin orientation is restored.

The out-of-plane polarization of the electron flow in the external potential is a subject of the rapidly developing field of the spin-Hall effect.[3–7] Our result, Eqs. (5) and (9), incorporates previous calculations of Ref. 6 which were restricted to the one-dimensional form of the potential, $V(x)$, with p_y being the integral of motion. The validity of Eq. (9), however, is not restricted to a simple one-dimensional case and describes the out-of-plain polarization for *any* smooth two-dimensional potential (including confining potentials which create quantum wires, quantum dots, etc.). In particular, Eq. (9) may serve as a good starting point for an analytical calculation of the edge spin accumulation in ballistic quantum wires.[28,29] We leave further investigation of these interesting effects for subsequent research.

Solutions of the form, Eq. (3), have clear and important consequences. During its motion, an electron changes the momentum p but always remains in the same spin-subband. To change the subband the electron trajectory should pass through the degeneracy point where both components of momentum vanish simultaneously, $\vec{p}=0$, which is generically impossible. Moreover, with the proper use of potential barriers, one may realize a situation where electrons *of only one subband* are transmitted and the others are totally reflected. This leads to strong polarization of the transmitted electron flow.

III. SHARVIN CONDUCTANCE

To give an example of such a spin-polarized current let us consider transmission through a barrier, $V(x)$, varying along the direction of a current propagation. We assume periodic boundary conditions in the perpendicular direction ($y+L \equiv y$). As such a condition makes p_y the integral of motion, mixing of orbital channels, which is strongly suppressed for generic smooth potential (2), is now absent exactly. For a smooth potential $V(x)$ the conduction channels may either be perfectly transmitting or completely closed. The conserved transverse momentum takes the quantized values, $p_y^n = 2\pi\hbar n/L$. Consider the functions

$$E_\pm^n(p_x) = \frac{(p^n \pm m\lambda)^2}{2m}, \quad p^n = \sqrt{p_x^2 + p_y^{n2}}. \qquad (10)$$

For $n \neq 0$ the function $E_\pm^n(p_x)$ splits into two distinct branches. At any point x the equation

$$E_\pm^n(p_x) = E_F - V(x) \qquad (11)$$

yields solutions p_x^L and p_x^R, corresponding to left- and right-moving electrons. Application of a small bias implies, e.g., the excess of right movers over left movers far to the left from the barrier. Particles are transmitted freely above the barrier if Eq. (11) has a solution, p_x^R, for any x. Let $\mu = E_F - V_{\rm max}$ be the difference between the Fermi energy and the maximum of the potential. The nth channel in the upper branch opens when

$$\mu = (2\pi\hbar|n| + m\lambda L)^2/2mL^2. \qquad (12)$$

For the lower branch $E_-^n(p_x)$ Eq. (11) has four solutions (two for right and two for left movers) for $|n| < m\lambda L/2\pi\hbar$ and x close to the top of the barrier. However, far from the barrier (where the excess of right-movers is created) there are still only two crossings described by Eq. (11), one for right and one for left movers. As a result, all the extra electrons injected at $x=-\infty$ follow the evolution of a solution of Eq. (11) with the largest positive p_x. For all $|n| < m\lambda L/2\pi\hbar$ such a solution does exist for any positive μ. Thus, at $\mu=0$ as many

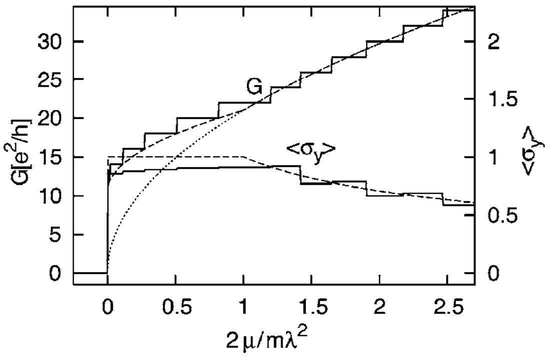

FIG. 1. Conductance (in units of e^2/h), and spin polarization of the current vs gate voltage (in units of $m\lambda^2/2$). Dashed lines show the smoothed curves (14) and (15), solid lines show the quantized values for $m\lambda L/\hbar = 10.5\pi$. Dotted line shows the conductance without spin-orbit interaction.

as $n_0 = m\lambda L/\pi\hbar$ channels *open up simultaneously*. The channels with higher values $|n| > m\lambda L/2\pi\hbar$ in the lower subband E_-^n open when

$$\mu = (2\pi\hbar|n| - m\lambda L)^2/2mL^2. \tag{13}$$

According to the Landauer formula, ballistic conductance is given by the total number of open channels multiplied by the conductance quantum $G_0 = e^2/h$

$$G = G_0 \frac{L}{\pi\hbar} \begin{cases} \sqrt{2\mu m} + m\lambda, & 0 < \mu < m\lambda^2/2 \\ 2\sqrt{2m\mu}, & \mu > m\lambda^2/2. \end{cases} \tag{14}$$

This dependence $G(\mu)$ is shown in Fig. 1. The striking evidence of the presence of spin-orbit interaction is the huge jump of the conductance at the pinch-off point, as opposed to the conventional square-root increase in the absence of spin-orbit coupling. This jump is a consequence of the "Mexican-hat" shape of the spectrum $E_-(p_x, p_y)$. Accuracy of Eqs. (12) and (13) is sufficient to resolve the steps in the conductance due to the discrete values of $|n| = 0, 1, 2, \ldots$, (conductance quantization), as shown in Fig. 1. The steps in $G(\mu)$ are abrupt in the limit $dV/dx \to 0$.

Close to the pinch-off, at $\mu \lesssim m\lambda^2$, the conserved p_y component of the electronic momentum varies for different transmitted channels within the range $|p_y| \lesssim m\lambda$. Therefore, far from the barrier, where the Fermi momentum is large $p_F \gg m\lambda$, we have $p_x \gg p_y$ and transmitted electrons propagate in a very narrow angle interval $|\theta| < \sqrt{m\lambda^2/2E_F} \ll 1$. Since the electron spin is perpendicular to its momentum, we conclude that the current due to electrons from each of the subbands is almost fully polarized. The total polarization of the transmitted current is given by the difference of two currents

$$\langle \sigma_y \rangle = \langle \psi^\dagger \sigma_y v_x \psi \rangle / \langle \psi^\dagger v_x \psi \rangle = \min(1, \sqrt{m\lambda^2/2\mu}), \tag{15}$$

which is also depicted in Fig. 1. This current polarization may also be viewed as a creation of in-plain nonequilibrium spin density, maximal on the barrier.

Vanishing transmission for electrons from the upper band for $0 < \mu < m\lambda^2/2$ (14) resembles the total internal reflection suggested for creation of polarized electron beams in Ref. 12. Unlike the latter case, in our proposal there is no need to collimate incident electron flow, since the upper band electrons are reflected at any angle.

Semiclassical formulas (14) and (15) are valid provided that there are many open transmission channels, and account correctly for the electrons with $p_y^n \neq 0$. The case $n=0$, however, requires special attention. The curve $E_\pm^0(p_x)$ does not split into the lower and upper branches, but instead consists of two crossing parabolas shifted horizontally. Right movers from both parabolas are transmitted or reflected simultaneously. The electron flow due to the channels with $n=0$ is, therefore, unpolarized. For small $n \neq 0$ the crossing of two parabolas is avoided. However, the electrons from the upper subband E_+^n may tunnel into the lower branch E_-^n in the vicinity of the point $p_x = 0$, which results in the decrease of spin-polarization of the current. Let the barrier near the top has a form $V(x) = -m\Omega^2 x^2/2$. Simple estimation shows that classically forbidden transition between the subbands do not change the net polarization of the current as long as $\hbar\Omega \ll m\lambda^2$.

Our results Eqs. (14) and (15) were obtained for the periodic boundary conditions. However, the boundary conditions do not play important role for the conductance ($G \propto L$) if the width of the "wire" is large compared with the width of the barrier, i.e., if $L \gg \sqrt{\hbar/m\Omega} \gg \hbar/m\lambda$. If the transverse confinement in the wide wire is ensured by the smooth potential[30] the semiclassical transmitted scattering states may be constructed explicitly using the method of Ref. 34. However, since the spin-orbit interaction in our approach appears already in the classical Hamiltonian (2), calculation of smoothed conductance (14) requires only a simple counting of classical trajectories.[35] Our next example below demonstrates such semiclassical treatment of realistic boundary conditions.

IV. QUANTUM POINT CONTACT

Let us consider probably the most experimentally relevant example of a quantum point contact, described by the potential

$$V(x,y) = -\frac{m\Omega^2 x^2}{2} + \frac{m\omega^2 y^2}{2}. \tag{16}$$

We will see that even in this simple model the electron flow in the presence of spin-orbit interaction acquires a number of interesting and peculiar features. Classical equations of motion follow in the usual manner from the effective Hamiltonian (2): $\dot{\vec{r}} = \partial H_{\text{eff}}/\partial \vec{p}$, $\dot{\vec{p}} = -\partial H_{\text{eff}}/\partial \vec{r}$. We consider quantum point contact (QPC) close to the opening with only the lower E_- subband contributing to the conductance. A crucial property of the Hamiltonian H_{eff}, Eq. (2), is the existence of a circle of minima of the kinetic energy at $|p| = m\lambda$. Expanding around a point on this circle, $p_{x_0} = m\lambda\cos\alpha$, $p_{y_0} = m\lambda\sin\alpha$, one readily finds the equations of motion for $\mathcal{P} = p_x\cos\alpha + p_y\sin\alpha - m\lambda \ll m\lambda$,

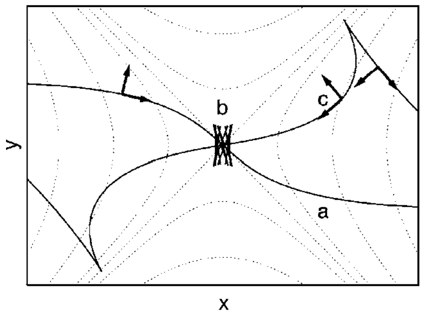

FIG. 2. Three kinds of trajectories in the point contact. *a*, transmitted trajectory whose momentum is always collinear with the velocity. *b*, trajectory bouncing inside the QPC. This trajectory is periodic in the linearized approximation described in the text, while the exact calculation for finite amplitude shows its slow drift. *c*, transmitted trajectory whose momentum inside the contact is opposite to the velocity. Electrons flow from left to right. Arrows show momentum and spin orientations. Few equipotential lines are also shown.

$$\ddot{\mathcal{P}} + (-\Omega^2\cos\alpha^2 + \omega^2\sin\alpha^2)\mathcal{P} = 0, \quad \dot{\alpha} = 0. \tag{17}$$

The trajectory is found from the relations, $\dot{x}=\mathcal{P}\cos\alpha/m$, $\dot{y}=\mathcal{P}\sin\alpha/m$. We observe from Eq. (17) that only the trajectories within the angle

$$\tan|\alpha| < \tan\alpha_0 = \Omega/\omega \tag{18}$$

are transmitted through QPC. Trajectories with larger angles are trapped (oscillate) within the point contact. Examples of both types of trajectories are presented in Fig. 2. Quantization of trapped trajectories would give rise to a set of (extremely) narrow resonances in the conductance, specific for spin-orbit interaction. We leave the detailed investigation of these narrow features for future research. Below we consider only the smoothed conductance.

To calculate the current J through QPC one has to integrate over the phase space of the states which are transmitted from left to right,

$$J = \int dy \int e v_x \frac{d^2p}{(2\pi\hbar)^2} = G\mathcal{V}, \tag{19}$$

and have the energy within the interval $\mu - e\mathcal{V}/2 < E_- < \mu + e\mathcal{V}/2$, with $\mathcal{V}$ standing for the applied voltage. In this section we define μ as the difference between the Fermi energy and the value of the potential at the saddle point $\mu = E_F - V(0,0)$. The integral is most simply evaluated at $x=0$ (with the velocity given by $v_x = \mathcal{P}\cos\alpha/m$). The allowed absolute values of the momentum are

$$2\mu - e\mathcal{V} - m\omega^2y^2 < \mathcal{P}^2/m < 2\mu + e\mathcal{V} - m\omega^2y^2. \tag{20}$$

The angle interval of transmitting trajectories consists of two domains: $|\alpha| < \alpha_0$, $\mathcal{P}>0$, and $|\alpha-\pi| < \alpha_0$, $\mathcal{P}<0$. The appearance of the latter range of integration is highly nontrivial. A simple reasoning shows that the particles with the velocity antiparallel to the momentum ($v_x>0$, $p_x<0$) should not contribute to the conduction in the case of a transition through a one-dimensional barrier $V=V(x)$, see Eq. (14). Despite corresponding to the right-moving electrons, these states *do not originate* in the left lead. Indeed, they exist only in the vicinity of $x=0$, but disappear as $x \to -\infty$ and, thus, cannot be populated by the excess electrons (except due to the tunneling transitions which are irrelevant in the semiclassical regime). Such trajectories, however, *do exist* in QPC, Eq. (16), as demonstrated in Fig. 2. After passing through QPC the trajectory bounces at the wall reversing its velocity. This kind of classical turning points, where both components of the velocity vanish simultaneously, are specific for the effective Hamiltonian (2). The existence of transmitting trajectories with $|\alpha-\pi| < \alpha_0$, $\varrho<0$ results in the doubling of the conductance. Simple calculation yields

$$G = G_0 \frac{4m\lambda\sin\alpha_0}{\pi\hbar\omega}\sqrt{\frac{2\mu}{m}}. \tag{21}$$

The presence of a threshold angle α_0, as well as the square-root dependence of $G(\mu)$, are in a sharp contrast to the well-known result $G=G_0\mu/\pi\hbar\omega$, in the absence of spin-orbit interaction.

Equation (21) is valid in the case of many open channels. Since Eq. (17) describes only the linearized electron dynamics, Eq. (21) is formally valid if $\mu \ll m\lambda^2$. Nevertheless, the current remains totally polarized for $0<\mu<m\lambda^2/2$ [similar to Eq. (15)]

$$\langle\sigma_y\rangle = \langle\psi^\dagger\sigma_y v_x\psi\rangle/\langle\psi^\dagger v_x\psi\rangle = 1. \tag{22}$$

With increasing the chemical potential, $\mu > m\lambda^2/2$, transmission via the upper subband E_+ kicks in and the degree of polarization gradually decreases, similarly to Eq. (15), though with different, more complicated, dependence of spin-polarization on μ. Note that transmission of different orbital channels through QPC is independent as long as the confining potential (16) is smooth over a distance of the characteristic spin-orbit length $\hbar/m\lambda$. It is easy to see that this requirement is equivalent to the condition that $(\omega,\Omega) \ll m\lambda^2/\hbar$. This is also a condition of large conductance $G \gg G_0$.

V. DISCUSSION

In both analyzed systems (of ballistic Sharvin conductance and of QPC) polarization of current is achieved when many channels are transmitting. As a consequence of the Kramers degeneracy, transmission eigenvalues always appear in pairs in the presence of time-reversal symmetry, leading to the prohibition of the spin-current in the lowest ($n=0$) conducting channels (cf. Ref. 18). In the case of higher channels, however, the degenerate transmission eigenvalues belong to the same spin-orbit subband and carry, respectively, the same spin polarization. For example, in the case of the QPC any transmitted trajectory $x(t),y(t)$ (e.g., one of the two shown in Fig. 2) is accompanied by its mirror reflection $x(t),-y(t)$ with identical transmission.

In InAs-based heterostructures, typical value of spin-orbit coupling[36] is $\lambda\hbar = 2\times10^{-11}$ eV m. Characteristic spin-orbit length $l_R = \hbar/m^*\lambda = 100$ nm and energy $m^*\lambda^2/2 = 0.1$ meV. In order to have strongly spin-polarizing QPC, the latter should support many transmitting channels at chemical potential $\mu \sim m^* \lambda^2 / 2 \gg \hbar \omega$. This condition can, equivalently, be written in terms of the width of the point contact Δy, see Eq. (16), as $\Delta y \gg l_R$. This is a realistic condition for typical ballistic constrictions.

To conclude, we have proposed a way to polarize currents in the ballistic regime by means of using electric gates to suppress transmission in the upper spin-orbit-split subband. The polarization is stronger when there are many transmitting channels in the lower subband. This is exactly the condition when the semiclassical expansion in powers of $\hbar$ is applicable. An obvious advantage of our scheme is that we do not require the spatial modulation of the strength of spin-orbit interaction. Neither do we need a restricted angle of incident electrons in order to have a polarized current.

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[30] Once the semiclassical treatment of the Hamiltonian (1) is established, Eqs. (2) and (3), one can use classical trajectories for the calculation of conductance (Ref. 31). Similar calculations would also give the in-plane spin polarization, since in our case spin is completely determined by the "classical" subband index. Thus, even for a wide wire, sufficiently smooth boundaries allow us to avoid a discussion of the chanel mixing, which is crucial for the perturbative treatment of the spin-orbit interaction in ballistic wires (Ref. 32). Numerically, the nonperturbative chanel mixing may be investigated by means of the recursive Green's function method (see e.g. Ref. 33), although this calculation may not be as simple in our case of multichannel wire with many channels having exponentially weak transmission.

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