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Unitarity of scattering and edge spin accumulation

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We consider a two-dimensional (2D) ballistic and quasiballistic structures with spin-orbit-related splitting of the electron spectrum. The ballistic region is attached to the leads with a voltage applied between them. We calculate the edge spin density which arises in the presence of a charge current through the structure. We solve the problem with the use of the method of scattering states and clarify the important role of the unitarity of scattering. In the case of a straight boundary it leads to exact cancellation of long-wavelength oscillations of the spin density. In general, however, the smooth spin oscillations with the spin precession length may arise, as it happens, e.g., for the wiggly boundary. We show that there is no relation between spin current in the bulk and the edge spin density.

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I. INTRODUCTION

Currently, there is a great interest, both experimental and theoretical, in spin currents and spin accumulation in various mesoscopic semiconductor structures. 1,2 Both phenomena are due to spin-orbit (s-o) coupling and are of great importance for the future of spin electronics. The edge electron spindensity accumulation, related to the Mott asymmetry in electron scattering off impurities, has been recently measured.³ Moreover, the edge spin density in the two-dimensional (2D) hole system, which is due to the intrinsic mechanism⁴ of the s-o interaction, has also been observed.⁵ It is well known² that in the diffusive regime (and when a spin diffusion length is much larger than a mean-free path), the spin density appearing near the boundary is entirely determined by the spin flux coming from the bulk. In the case of the Rashba Hamiltonian, depending on boundary conditions either the spin current and the spin-density component perpendicular to the plane is zero everywhere down to the sample boundary,⁶ or there is net spin flux within spin precession length near the boundary which is directed towards the boundary and is precisely the source of the finite S_z component at the edge.⁷ This spin flux is caused by the electric field existing in the bulk.

In an opposite case, when the spin precession length is much shorter than the mean-free path, the situation is much less clear. An example of such a system is a mesoscopic structure with s-o-related splitting of the electron spectrum Δ_R , in the limit $\Delta_R \tau_p \gg 1$, where τ_p is the mean-free time. It includes the case of finite size ballistic structures, when the mean-free path is much larger than the sample size (a mesoscopic spin Hall effect). The existing literature for the ballistic case includes several papers^{8,9} where the problem is treated numerically, but the system size is comparable or less than the spin precession length. The quasiballistic case is treated in Ref. 10. It is hard to find in these papers clear answers to the following important questions: What is the characteristic scale in the problem? Is it Fermi wavelength or spin precession length? How do the results depend on the boundary conditions, etc.? On the other hand, most authors, if not all, believe that the edge spin density in a mesoscopic spin Hall effect is a result of the spin current flowing towards the boundaries. We show below that this is not true in the ballistic case, in contrast to the diffusive limit. Moreover, there is an apparent discrepancy between the analytical results obtained in Ref. 11, where only edge spin oscillations with $2k_F$ were found, and numerical results of Ref. 8, where obviously some smooth spin density S_z component is present.

In order to answer questions formulated above, we solve analytically the problem of edge spin accumulation in purely ballistic regime and when the size of the structure is much larger than the spin precession length. The boundary conditions are *arbitrary*, they include specular scattering for the straight boundary or diffusive scattering for the wiggly one. The obtained exact results allow us to clarify the meaning of the results obtained in Ref. 8.

In the presence of the s-o interaction, the boundary scattering itself is the source of appearance of the spin density. It is obvious that the characteristic length near a boundary, where the spin density arises, is the spin precession length $L_s = \hbar v_F/\Delta_R$, with v_F being the Fermi velocity. This mechanism of the spin-density generation is the subject of our paper. We show that various situations may arise, depending on the form of the s-o Hamiltonians.

We start with a 2D system described by the Rashba Hamiltonian in the *ballistic* limit, where a mean-free path is much larger than the sample sizes. The ballistic region is attached to the leads, and a voltage *V* applied between the leads causes a charge current through the structure, as shown in Fig. 1. Since the electric field is absent inside an ideal ballistic conductor, the edge spin polarization appears not as a result of the acceleration of electrons by an electric field, but rather due to the difference in populations of left-moving and right-moving electrons. The combined effect of boundary scattering and spin precession leads to oscillations of the edge spin polarization.

The problem of the spin-density accumulation in a ballistic system and for a straight boundary has been considered analytically earlier in Ref. 11 with the help of the Green's functions method. Surprisingly, in this case the final result contains only Friedel-like oscillations with the momentum $2k_F$. This effect may be interpreted as s-o splitting of the Friedel oscillations in the charge density: two charge oscillations corresponding to spin-up and spin-down orientations get shifted with respect to each other in the presence of the s-o interaction. Therefore, strictly speaking, this phenomenon is

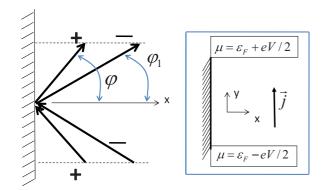


FIG. 1. (Color online) (Left) Schematics of the boundary specular scattering in the presence of spin-orbit coupling. Plus and minus modes are shown for the same energy and the same wave vectors along the boundary. (Right) Geometry of system.

different from a s-o-related accumulation of the spin density upon boundary scattering. Besides, the method used in Ref. 11 does not allow us to understand the reason for the cancellation of long-wavelength oscillations of the spin density.

We solve the problem of edge spin accumulation by using scattering theory, with scattering states coming from different leads of the structure and, therefore, having different occupations. The simplicity of the method allows us to gain an insight into the underlaying physics. We show that it is the unitarity of scattering that leads to the exact cancellation of long-wavelength oscillations of the spin density with the period L_s in the case of a straight boundary. It should be also mentioned that the observed behavior is closely related to the effective one-dimensional character of scattering, arising from the translational invariance along the boundary. However, the case of a straight boundary appears to be a rather exceptional one. In general, smooth spin oscillations with the spin precession length L_s arise, as it happens for example, for the wiggly boundary or for scattering off a circular impurity in a 2D electron system. 12-14 This is a consequence of the fact that in higher dimensions the conditions of the unitarity of scattering take a different form, as explained below. In all these situations, the spin density decays as a power law of the distance from the scatterer.

II. STRAIGHT BOUNDARY

The Rashba s-o Hamiltonian in the bulk of a ballistic 2D electron system takes the following form:

$$\hat{\mathcal{H}}(\mathbf{p}) = \frac{p^2}{2m} + \frac{\alpha}{2}\vec{n}[\vec{\sigma} \times \mathbf{p}],\tag{1}$$

where \vec{n} is the normal to the plane, $\vec{\sigma}$ are the Pauli matrices, and $\bf p$ is the 2D momentum. The solutions of this Hamiltonian corresponding to the helicity values $M=\pm$ have the form $\exp(i{\bf pr}/\hbar)\chi_M({\bf p})$, where ${\bf r}=x,y$. The explicit form of the spinors and their eigenenergies are

$$\chi_{\pm}(\varphi) = rac{1}{\sqrt{2}} \left(rac{1}{\mp i e^{i \varphi}}
ight), \quad \epsilon_M(p) = rac{p^2}{2m} + rac{M}{2} \alpha p,$$

with φ being the angle between the momentum **p** and the positive direction of the x axis.

We consider the semi-infinite system and choose the x axis to be directed perpendicular to the boundary (x = 0) of the 2D system (see Fig. 1). The wave functions, which obey zero boundary conditions at x = 0, are obviously the *scattering states*, which constitute the complete set of the orthonormal functions. Two scattering states corresponding to incident plus and minus modes with given wave vector along the boundary and the same energy are

$$\hat{\Psi}_{+}^{(0)}(x,y) = e^{ik_y y} [\chi_{+}(\pi - \varphi)e^{-ikx} + F_{+}^{+}\chi_{+}(\varphi)e^{ikx} + F_{-}^{+}\chi_{-}(\varphi_1)e^{ik_1 x}], \quad \hat{\Psi}_{+}^{(0)}(0,y) = 0, \quad (2)$$

$$\hat{\Psi}_{-}^{(0)}(x,y) = e^{ik_y y} [\chi_{-}(\pi - \varphi_1)e^{-ik_1 x} + F_{-}^{+}\chi_{+}(\varphi)e^{ikx} + F_{-}^{-}\chi_{-}(\varphi_1)e^{ik_1 x}], \quad \hat{\Psi}_{-}^{(0)}(0,y) = 0.$$
 (3)

Here, the wave vectors are defined as follows:

$$k^2 = k_+^2 - k_y^2$$
, $k_1^2 = k_-^2 - k_y^2$, $\hbar k_{\pm} = m \left(v_F \mp \frac{\alpha}{2} \right)$, (4)

where $p_{\pm} = \hbar k_{\pm}$ are the momenta at the Fermi energy in the plus and minus modes. The angles φ , φ_1 may be expressed as $\sin(\varphi) = k_{\nu}/k_{+}$ and $\sin(\varphi_1) = k_{\nu}/k_{-}$ (see Fig. 1).

From Eqs. (2) and (3), one finds the scattering amplitudes F_+^+ and F_-^- :

$$F_{+}^{+} = -\frac{(e^{i\varphi_{1}} - e^{-i\varphi})}{(e^{i\varphi_{1}} + e^{i\varphi})}, \quad F_{+}^{-} = -\frac{2\cos\varphi}{(e^{i\varphi_{1}} + e^{i\varphi})}.$$
 (5)

One can check that the amplitudes F_{-}^{-} and F_{-}^{+} for the incident minus mode with the same k_{y} and the same energy are obtained from F_{+}^{+} and F_{+}^{-} by replacing $\varphi \leftrightarrow \varphi_{1}$. Then, the components of the unitary scattering matrix \hat{S} acquire the following form:

$$S_{+}^{+} = F_{+}^{+}, \quad S_{-}^{-} = F_{-}^{-}, \quad S_{+}^{-} = S_{-}^{+} = F_{+}^{-} \sqrt{\frac{v_{x,-}}{v_{x,+}}},$$
 (6)

where $v_{x,i} = \partial \epsilon_i / \partial p_x$ are the group velocities. For the Rashba model one has $v_{x,-}/v_{x,+} = \cos \varphi_1 / \cos \varphi$.

A. Spin density

The wave functions (2) and (3) may now be used to calculate the average z component of the spin as a function of coordinates:

$$\langle S_z(x) \rangle = \sum_{i=\pm} \int \frac{dk_y}{(2\pi)^2} \frac{d\epsilon}{v_{x,i}} f_F(\epsilon, k_y) \langle \hat{\Psi}_i^{(0)}(x) | \hat{S}_z | \hat{\Psi}_i^{(0)}(x) \rangle, \tag{7}$$

where $f_F(\epsilon,k_y)$ is the Fermi distribution function, which takes either of two values: $f_F(\epsilon - \mu - eV/2)$ or $f_F(\epsilon - \mu + eV/2)$, depending on the sign of k_y . We find that one may distinguish various contributions to $\langle S_z(x) \rangle$ with different oscillation periods, which originate from an interference of different terms in Eqs. (2) and (3). The smooth part of $\langle S_z(x) \rangle_s$, which involves the interference of the outgoing waves [two last terms in Eqs. (2) and (3)], reads

$$\langle S_z(x) \rangle_s \propto \int dk_y d\epsilon f_F(\epsilon, k_y) \frac{1}{\sqrt{v_{x,-}v_{x,+}}} \times [A\langle \chi_-(\varphi_1) | \hat{S}_z | \chi_+(\varphi) \rangle e^{i(k-k_1)x} + \text{c.c.}],$$
(8)

where

$$A = S_{+}^{+} \cdot (S_{+}^{-})^{\star} + S_{-}^{+} \cdot (S_{-}^{-})^{\star}.$$

Here we used the fact that the distribution function $f_F(\epsilon,k_y)$, describing a particular lead, has the same value at given energy for the plus and minus modes. Note that the period of oscillations of the exponential factor $e^{i(k-k_1)x}$ in Eq. (8) is of the order of the spin precession length. However, the term (8) vanishes because the expression A is nothing but a nondiagonal component of the identity matrix $\hat{S}\hat{S}^{\dagger}$. Thus, we obtain the interesting result that the only reason for the cancellation of the long-wave length oscillations with the period L_s in $\langle S_z(x) \rangle$ is the unitarity of scattering.

By taking into account in Eq. (7) the terms responsible for the interference between incoming and the outgoing waves [for example, between the first and second terms in Eq. (2)] and adding the contribution from the evanescent modes, ¹⁵ we reproduce Eq. (16) of Ref. 11. It can be written in the form $\langle S_z(x) \rangle = [eV/(8\pi^2 m v_F^2)] \text{Im } I$, where

$$I = \int_0^{k_-} dk_y \frac{k_+ k_- + k_y^2 - kk_1}{k_y} (e^{ikx} - e^{ik_1x})^2.$$

Note that in the interval $k_+ < k_y < k_-$, the quantity k has purely imaginary value, which corresponds to the evanescent modes. From this of the presentation, we can immediately see that $\langle S_z(x) \rangle$ contains only the $2k_F$ component, while all the long-wavelength oscillations cancel exactly. Indeed, with the branch cut along the real k_y axis between the points $-k_-$ and $+k_-$ (see Fig. 2), the integrand function in I is an analytical function of the variable k_y in the right half plane $\operatorname{Re} k_y > 0$ (for positive x). Since we need the imaginary part of I, the integration is going along the upper edge of the branch cut from 0 up to $+k_-$ and then back along the lower edge of the branch cut. Because of the analyticity mentioned above, this integral is equal to the one taken along the imaginary axis of $k_y = i\kappa$. Then, for $x \gg \lambda_F$ the latter integral is determined by small $\kappa \ll k_F$:

$$I \simeq -2(e^{ik_{-}x} - e^{ik_{+}x})^{2} \int_{0}^{\infty} d\kappa \kappa e^{i\kappa\kappa^{2}/k_{F}},$$

which gives for the spin density $\langle S_z(x) \rangle \approx [eV/(2\pi^2 v_F x)] \cos(2mv_F x) \sin^2(\alpha mx/2)$, coinciding with the result of Ref. 11. Therefore, the total spin per unit length along the boundary scales as $\int_0^\infty dx \langle S_z(x) \rangle \propto \alpha^2$. Note that the main

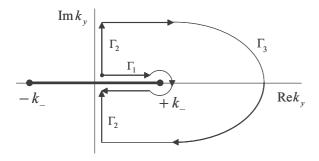


FIG. 2. The original contour Γ_1 along the real axis can be deformed into the part Γ_2 going along the imaginary axis and the part Γ_3 going far from the origin.

contribution to this integral comes from small distances from the boundary, $x \simeq \lambda_F$.

B. Spin current

It is important to note that the spin flux incoming from the bulk to the boundary is simply zero, since only diagonal components of the spin-density matrix are supplied by the leads. By no means the edge spin density can be considered as a result of this flux. The spin current, which is finite only due to the evanescent modes, is

$$\langle q_{xz}(x)\rangle \approx \frac{eV}{4\pi^2 m v_F} \int_{k_{\perp}}^{k_{-}} dk_y \eta e^{-\eta x} \cos k_1 x, \quad \eta = \sqrt{k_y^2 - k_+^2}.$$

The spin current density oscillates with $\xi = (k_-^2 - k_+^2)^{-1/2}$ period and is localized basically over this length near the boundary, $\lambda_F \ll \xi \ll L_s$. At distances larger than ξ from the boundary it has the form $[eV/(4\pi^2\epsilon_F)]\cos(x/\xi)(\hbar/mx^3)$, where at $x \simeq L_s$ its magnitude is parametrically smaller $(\alpha^2/v_F^2 \ll 1)$ than the quantity $v_F \langle S_z(x) \rangle$. The latter quantity follows from naive considerations. Therefore, spin and spin current densities are not related to each other in the purely ballistic case, in strong contrast with the diffusive limit.

C. Quasiballistic case

The cancellation of smooth spin-density oscillations in case of the Rashba Hamiltonian and straight boundary occurs also in the quasiballistic situation: $L \gg l \gg L_s$, where L is the sample size, and l is the mean-free path. In this case, the electric field in the bulk of the sample is finite. Therefore, the distribution functions for the plus and minus modes, $f_{++}(\vec{k}_+)$ and $f_{--}(k_{-})$, are determined by the electric field and by scattering off the impurities in the bulk of a system. 16 The wave vectors \vec{k}_+ and \vec{k}_- , shown in Fig. 1, correspond to a given energy and a given wave vector along the boundary. In the quasiballistic case considered here, these functions are equal, i.e., $f_{++}(\vec{k}_+) = f_{--}(\vec{k}_-)$, similar to a ballistic situation. Under such a condition, the unitarity of scattering, see Eq. (8), leads to the cancellation of smooth edge spin-density oscillations, in contrast to what has been stated in the literature. ¹⁷ Indeed, when the electric field is parallel to the boundary, the distribution functions in questions are $f_{++}(\vec{k}_+) = f_{++}(k_+)\sin\varphi$, and $f_{--}(k_{-}) = f_{--}(k_{-})\sin\varphi_1$ [see Eq. (9) of Ref. 16]. For the case of the Rashba Hamiltonian, the following relation has been obtained: $k_{+}f_{--}(k_{-}) = k_{-}f_{++}(k_{+})^{18}$ Then, the ratio is $f_{++}(\vec{k}_+)/f_{--}(\vec{k}_-) = k_+ \sin \varphi/k_- \sin \varphi_1 = k_v/k_v = 1.$

D. Cubic Hamiltonian

Depending on the form of the s-o Hamiltonian, the unitarity may show up in totally different ways, leading, in general, to different patterns of the edge spin density. Let us consider 2D holes for the case of a normal incidence, where the cubic (in 2D momentum) s-o Hamiltonian has the form $p_x^2/(2m) + \alpha \hat{\sigma}_x p_x^3$. We consider the ballistic case and an abrupt straight boundary. For the plus incident mode and zero boundary conditions one obtains $F_+^+ = 0$, $F_-^- = i$, i.e., the helicity value changes sign. For the charge flux to be conserved, one needs the equality of the group velocities v_+ and v_- , corresponding to the plus

and minus modes at the same energy. In contrast to the case of the Rashba Hamiltonian, those velocities are not equal for the cubic Hamiltonian: $v_+ - v_- = \alpha(p_+ + p_-)^2$. The formal way to resolve the trouble is to note that the cubic Hamiltonian has three solutions for a given energy, one of them corresponding to a fast mode with a momentum larger than k_F (for small spinorbit coupling). Thus, in general, the unitarity of scattering in slow plus and minus channels is violated, and smooth spindensity oscillations occur.

III. SCATTERING BY WIGGLY BOUNDARY

Let us consider now scattering off a wiggly boundary, shown in Fig. 3, for the case of the Rashba Hamiltonian. In this case the translational invariance is broken, therefore the condition of the unitarity of scattering takes a different form as compared to the case of a straight boundary. As a result, the cancellation of the smooth spin-density oscillations does not take place, leading to the total spin that is not small in the parameter α . In order to demonstrate this effect, we consider the mathematically simple case of the abrupt impenetrable boundary described by the equation $x = \zeta(y) \equiv W \sin(2\pi y/\lambda)$. To the lowest order in W, the boundary condition reads

$$\hat{\Psi}(0,y) + \zeta(y) \frac{d\hat{\Psi}(0,y)}{dx} = 0.$$
 (9)

We are looking for the solution in the perturbative form $\hat{\Psi}_{\pm}(x,y) = \hat{\Psi}_{\pm}^{(0)}(x,y) + \hat{\Psi}_{\pm}^{(1)}(x,y)$, where the zeroth-order functions are given by Eqs. (2) and (3). The first-order correction, proportional to W, is the superposition of scattering waves with the wave vectors along the boundary shifted by $\pm 2\pi/\lambda$ (see Fig. 3), and with the k vectors in the x direction given by

$$k^{\frac{2}{5}} = \sqrt{k_+^2 - \left(k_y \pm \frac{2\pi}{\lambda}\right)^2}, \quad k_1^{\frac{2}{5}} = \sqrt{k_-^2 - \left(k_y \pm \frac{2\pi}{\lambda}\right)^2}.$$

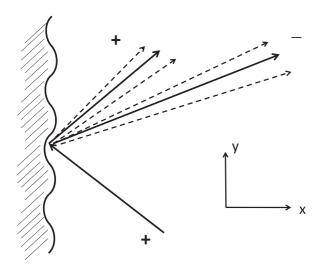


FIG. 3. Schematics of scattering of plus incident mode by a wiggly boundary, $x = W \sin(2\pi y/\lambda)$. Apart from the main scattering channels (solid lines), there are additional scattering waves with the wave vectors along the boundary shifted by $\pm 2\pi/\lambda$ (dashed lines).

From now on, we assume $\lambda_F \ll L_s \ll \lambda$. In addition, in order to obtain an analytical expression for the spin density, we consider the case $x/\sqrt{\lambda\lambda_F} \ll 1$. In contrast to the case of the straight boundary, there are oscillations with three different periods: $2k_F$ - oscillations, and the oscillations with two long periods, ξ and L_s . Here $\xi = (k_-^2 - k_+^2)^{-1/2}$ is the new length scale. Under the conditions considered in the paper we obtain the set of inequalities $\lambda_F \ll \xi \ll L_s$, where $L_s = 1/(k_- - k_+) = \hbar/(m\alpha)$ is the spin precession length. If $k_y \to k_+$ (i.e., $k \to 0$), then k_1 tends to $1/\xi$, which clarifies the physical meaning of ξ .

For the contribution of the long-wavelength oscillations, we obtain²¹

$$\langle S_{z}(x,y)\rangle = \frac{eV}{(2\pi)^{2}\hbar v_{F}} \left(\frac{2\pi W}{\lambda}\right) \cos\left(\frac{2\pi y}{\lambda}\right) I_{\text{long}}(x),$$

$$I_{\text{long}}(x) = \frac{2\sin(\frac{x}{\xi})}{\xi} + \frac{2\cos(\frac{x}{\xi})}{x} + \frac{\pi}{2L_{s}} N_{1}\left(\frac{x}{L_{s}}\right) - \frac{1}{x}$$

$$+ \frac{2x}{\xi} \frac{\partial}{\partial x} \int_{0}^{1} dz e^{-(x/\xi)z} \cos\frac{x\sqrt{1-z^{2}}}{\xi}, \quad (10)$$

where the last term is the contribution of the evanescent modes, and $N_1(x)$ is a Bessel function of the second kind. At the distances $x \ll \xi$, we obtain the following dependence: $I_{\text{long}} = -2x^2/(3\xi^3) + [x/(2L_s^2)]\{\gamma + \ln[x/(2L_s)]\}$. In the opposite limit, $x \gg \xi$, we find $I_{\text{long}} = \frac{\pi}{2L_s}N_1(x/L_s) - \frac{1}{x} + \frac{2}{x}\cos(x/\xi)$. At even larger distances $x \gg L_s$, one obtains smooth oscillations with the period of the order of L_s , with the amplitude being proportional to $\sqrt{\alpha}$. Note that the total spin per unit length along the boundary is proportional to the integral

$$\int dx I_{\text{long}}(x) \simeq (\pi/2L_s) \int_{\xi}^{\infty} dx N_1(x/L_s) - \int_{\xi}^{\sqrt{\lambda \lambda_F}} dx/x$$
$$\simeq -\ln(L_s/\xi) - \ln(\sqrt{\lambda \lambda_F}/\xi)$$
$$\simeq -(1/2) \ln(\lambda/\lambda_F),$$

i.e., it is not small in s-o coupling, in contrast with the case of a straight boundary.

In conclusion, we have considered the problem of the edge spin accumulation in mesoscopic structures with spin-orbitrelated splitting of the energy spectrum, when the associated spin precession length is much smaller than the mean-free path. In the presence of the charge current, the spin density develops oscillations near an edge in the direction transverse to the boundary. The result crucially depends on the form of s-o Hamiltonian and the boundary conditions. The unitarity of scattering in the case of a straight boundary and Rashba Hamiltonian leads to the cancellation of long-wavelength spindensity oscillations. On the contrary, the spin density in the case of wiggly boundary oscillates with a large period of the order of the spin precession length. The results obtained in our work clarify the meaning of the results obtained previously by other authors for related problems. The point is that the geometry of the structure plays crucial role for the form of the unitarity conditions. In particular, the finite length of the structures studied, for example, in Ref. 8 (with the scattering at the interface between the s-o region and the longitudinal lead), and presence of the transverse Hall leads change the form of the unitarity conditions, and are the most probable reasons for an appearance of the observed smooth S_z spin density component. On the other hand, it seems that the finite width of the structure itself in the case of translational invariance along the structure cannot cause the appearance of the smooth spin density.

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- ¹⁹Note that Ref. 20 considers the case of a straight boundary, which is smooth in the transverse direction, instead of an abrupt one. We stress that the physics discussed in Ref. 20 is different from that we consider here. Since the boundary is still straight, the unitarity of scattering leads to the cancellation of smooth oscillations with the period L_s . As a result, the total spin, found in Ref. 20, is small and proportional to α^2 .
- ²⁰P. G. Silvestrov, V. A. Zyuzin, and E. G. Mishchenko, Phys. Rev. Lett. **102**, 196802 (2009).
- ²¹For details, see A. Khaetskii and E. Sukhorukov, JETP Lett. **92**, 244 (2010).