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RESEARCH ARTICLE

Semiclassical Boltzmann theory of spin Hall effects in giant Rashba systems

Cong Xiao

Department of Physics, The University of Texas at Austin, Austin, TX 78712-0264, USA
Corresponding author. E-mail: xc1989@pku.edu.cn
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For the spin Hall effect arising from strong band-structure spin–orbit coupling, a semiclassical Boltzmann theory reasonably addressing the intriguing disorder effect called side-jump has not yet been developed. This paper describes such a theory in which the key ingredient is the spin-current counterpart of the semiclassical side-jump velocity (introduced in the context of the anomalous Hall effect). Applying this theory to spin Hall effects in a two-dimensional electron gas with giant Rashba spin–orbit coupling, largely enhanced spin Hall angle is found in the presence of magnetic impurities when only the lower Rashba band is partially occupied.

Keywords spin Hall effect, semiclassical Boltzmann theory, side jump, Rashba spin–obit coupling

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1 Introduction

It is now generally accepted that three mechanisms — intrinsic, side-jump, and skew scattering — contribute to both the spin Hall effect (SHE) and the anomalous Hall effect (AHE) [1, 2]. Among the three mechanisms, the side-jump mechanism is of special interest because it originates from scattering but can, in some simple cases [1–5], be independent of both the disorder density and the scattering strength. In particular, when the SHE or AHE arises from strong spin–orbit coupling in the band structure, the side-jump belongs to the category of the disorder-induced interband-coherence effect, which has recently been an important topic in condensed matter physics [1–3, 6–9].

In investigating transport phenomena in solids, the semiclassical Boltzmann approach is appealing owing to its intuitive concept [10]. In the study of the SHE and the AHE, incorporation of side-jump effects into the semiclassical formalism is an attractive theoretical issue [2]. In the study of AHE, the renewed semiclassical theory addressing this issue has proven useful in yielding physical pictures [6]. In such a theory, the quantum mechanical information on the side-jump is coded into the expressions of gauge-invariant classical concepts such as the coordinate shift and side-jump velocity [6]. In contrast, in the field of SHE when the spin is not conserved owing to strong spin–orbit coupling in the band structure, such as in a Rashba two-dimensional electron gas (2DEG), a semiclassical description of the side-jump SHE is still absent [11, 12]. Although the modified Boltzmann equation [6] developed in studying the AHE can be directly applied to the SHE, the spin-current counterpart of the side-jump velocity in this case has not been addressed before.

In the present paper, we formulate a semiclassical Boltzmann framework of the SHE when the spin is not conserved owing to strong band-structure spin-orbit coupling. This semiclassical theory takes into account interband-coherence effects induced by both the dc uniform electric field and weak static disorder. We derive the spin-current counterpart of the side-jump velocity based on scattering-induced modifications of conduction-electron states. When the electric field turns on, this quantity contributes one part of the side-jump SHE.

As an application, we consider the SHE in a 2DEG with giant Rashba spin–orbit coupling and short-range impurities. We focus on the enhancement of the spin Hall angle when the Fermi energy is tuned downward toward and below the band crossing point in giant Rashba 2DEGs with magnetic disorder. The spin Hall angle, which measures the generation efficiency of the trans-

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verse spin current from the longitudinal electric current, is the figure of merit of the SHE. Giant Rashba spin–orbit coupling energy comparable to or even larger than the Fermi energy is possible in the polar semiconductor BiTeX (where X = Cl, Br, and I) family and related surfaces and interfaces [13–15]. Thus these systems are promising for realizing efficient conversion of charge current into spin current.

The paper is organized as follows. In Section 2, we outline the semiclassical formulation of the SHE. Section 3 introduces the Rashba model and the SHE is calculated. Section 4 concludes the paper.

2 Semiclassical formulation

Considering the linear response of the spin current polarized in one particular direction (where the z direction is chosen in the following) to a weak dc uniform electric field $\boldsymbol{E}$ in nondegenerate multiband electron systems in the weak-disorder regime, one has the semiclassical formula

$$\boldsymbol{j}^z = \sum_l f_l \boldsymbol{j}_l^z, \tag{1}$$

where $\boldsymbol{j}_l^z$ is the amount of spin current carried by the conduction-electron state denoted by l and f_l is the semiclassical distribution function.

The conduction-electron state may be modified by the electric field and static impurity scattering; $\boldsymbol{j}_l^z$ can thus deviate from the customary pure-band value [10, 11]: $(\boldsymbol{j}_l^z)^0 \equiv \langle l|\hat{\boldsymbol{j}}^z|l\rangle$ with $\hat{\boldsymbol{j}}^z$ as the spin-current operator. Here $|l\rangle = |\eta\boldsymbol{k}\rangle = |\boldsymbol{k}\rangle|u_{\boldsymbol{k}}^\eta\rangle$ is the Bloch state, η is the band index, $\boldsymbol{k}$ is the crystal momentum, and $|\boldsymbol{k}\rangle$ and $|u_{\boldsymbol{k}}^\eta\rangle$ are the plane-wave and periodic parts of $|\eta\boldsymbol{k}\rangle$, respectively. Based on quantum-mechanical perturbation theory for the electric-field-modified Bloch state and the Lippmann–Schwinger equation for the scattering-modified conduction-electron state in Ref. [9], in the weak-disorder regime nontrivial corrections caused by interband-coherence effects to $(\boldsymbol{j}_l^z)^0$ read

$$\boldsymbol{j}_l^z = (\boldsymbol{j}_l^z)^0 + \delta^{in}\boldsymbol{j}_l^z + \delta^{ex}\boldsymbol{j}_l^z. \tag{2}$$

The intrinsic correction $\delta^{in}\boldsymbol{j}_l^z = 2\mathrm{Re}\langle l|\hat{\boldsymbol{j}}^z|\delta^{\boldsymbol{E}} l\rangle$ arises from the interband virtual transition $|\delta^{\boldsymbol{E}} l\rangle = -i\hbar e\boldsymbol{E}\cdot\sum_{\eta'\neq\eta}|\eta'\boldsymbol{k}\rangle\langle u_{\boldsymbol{k}}^{\eta'}|\hat{\boldsymbol{v}}|u_{\boldsymbol{k}}^\eta\rangle/(\epsilon_{\boldsymbol{k}}^\eta-\epsilon_{\boldsymbol{k}}^{\eta'})^2$ (where e is the electron charge) induced by the electric field [11], with $\epsilon_l \equiv \epsilon_{\boldsymbol{k}}^\eta$ the energy of Bloch state $|\eta\boldsymbol{k}\rangle$ and $\hat{\boldsymbol{v}}$ the velocity operator. Thus

$$\delta^{in}\boldsymbol{j}_l^z = \hbar e\sum_{\eta'\neq\eta}\frac{2\mathrm{Im}\langle\eta\boldsymbol{k}|\hat{\boldsymbol{j}}^z|\eta'\boldsymbol{k}\rangle\langle u_{\boldsymbol{k}}^{\eta'}|\hat{\boldsymbol{v}}\cdot\boldsymbol{E}|u_{\boldsymbol{k}}^\eta\rangle}{(\epsilon_{\boldsymbol{k}}^\eta-\epsilon_{\boldsymbol{k}}^{\eta'})^2} \tag{3}$$

is an electric-field-induced interband-coherence effect.

The extrinsic correction $\delta^{ex}\boldsymbol{j}_l^z$ originates from the interband coherence during the elastic electron–impurity scattering process. The scattering-induced modification to conduction-electron states is captured by the Lippmann–Schwinger equation describing the scattering state $|l^s\rangle = |l\rangle + (\epsilon_l - \hat{H}_0 + \mathrm{i}\epsilon)^{-1}\hat{T}|l\rangle$ with the T matrix $\hat{T}|l\rangle = \hat{V}|l^s\rangle$ related to the disorder potential $\hat{V}$ and disorder-free Hamiltonian $\hat{H}_0$. $|\delta l^s\rangle \equiv |l^s\rangle - |l\rangle$ denotes the scattering-induced modification to the Bloch state. Thus $\delta^{ex}\boldsymbol{j}_l^z$ is related to the values of $2\mathrm{Re}\langle\langle l|\hat{\boldsymbol{j}}^z|\delta l^s\rangle\rangle_c$ and $\langle\langle\delta l^s|\hat{\boldsymbol{j}}^z|\delta l^s\rangle\rangle_c$ in the lowest nonzero order in the disorder potential. Here $\langle\ldots\rangle_c$ denotes the average over disorder configurations and we assume that the statistical average of the disorder potential is zero (and a nonzero value only shifts the origin of the total energy), i.e., $\langle V\rangle_c = 0$. Only the terms containing interband matrix elements of $\hat{\boldsymbol{j}}^z$ represent the disorder-induced interband-coherence effects; therefore [16],

$$\delta^{ex}\boldsymbol{j}_l^z = \sum_{\eta''\neq\eta'}\sum_{\eta'\boldsymbol{k}'}\frac{\langle\langle\eta\boldsymbol{k}|\hat{V}|\eta'\boldsymbol{k}'\rangle\langle\eta''\boldsymbol{k}'|\hat{V}|\eta\boldsymbol{k}\rangle\rangle_c\langle\eta'\boldsymbol{k}'|\hat{\boldsymbol{j}}^z|\eta''\boldsymbol{k}'\rangle}{(\epsilon_{\boldsymbol{k}}^\eta-\epsilon_{\boldsymbol{k}'}^{\eta'}-\mathrm{i}0^+)(\epsilon_{\boldsymbol{k}}^\eta-\epsilon_{\boldsymbol{k}'}^{\eta''}+\mathrm{i}0^+)} + 2\mathrm{Re}\sum_{\eta'\neq\eta}\sum_{\eta''\boldsymbol{k}''}\frac{\langle\langle\eta'\boldsymbol{k}|\hat{V}|\eta''\boldsymbol{k}''\rangle\langle\eta''\boldsymbol{k}''|\hat{V}|\eta\boldsymbol{k}\rangle\rangle_c\langle\eta\boldsymbol{k}|\hat{\boldsymbol{j}}^z|\eta'\boldsymbol{k}\rangle}{(\epsilon_{\boldsymbol{k}}^\eta-\epsilon_{\boldsymbol{k}}^{\eta'}+\mathrm{i}0^+)(\epsilon_{\boldsymbol{k}}^\eta-\epsilon_{\boldsymbol{k}''}^{\eta''}+\mathrm{i}0^+)}. \tag{4}$$

It has been shown [9] that the side-jump velocity $\boldsymbol{v}_l^{sj}$, which is an important ingredient in the semiclassical theory of the AHE [6] can also be obtained in this way ($\delta^{ex}\boldsymbol{v}_l = \boldsymbol{v}_l^{sj}$) and thus shares the same origin. $\delta^{ex}\boldsymbol{j}_l^z$ can therefore be deemed as the spin-current counterpart of the side-jump velocity in the case of band-structure spin–orbit coupling.

The properly modified steady-state linearized Boltzmann equation in the presence of weak static disorder has been proposed as [6]

$$e\boldsymbol{E}\cdot\boldsymbol{v}_l^0\frac{\partial f^0}{\partial\epsilon_l} = -\sum_{l'}\omega_{l,l'}\left(f_l - f_{l'} - \frac{\partial f^0}{\partial\epsilon_l}e\boldsymbol{E}\cdot\delta\boldsymbol{r}_{l',l}\right), \tag{5}$$

where $\boldsymbol{v}_l^0 = \partial\epsilon_l/\hbar\partial\boldsymbol{k}$ is the band velocity, f^0 is the Fermi distribution function, $\delta \boldsymbol{r}_{l',l}$ is the coordinate shift in the scattering process ($l \to l'$) [6], and $\omega_{l,l'}$ is the semiclassical scattering rate ($l' \to l$). Up to linear order of the electric field one has the decomposition [6, 17]

$$f_l = f_l^0 + g_l^n + g_l^a, \tag{6}$$

with g_l^n the normal part of the out-of-equilibrium distribution function satisfying the Boltzmann equation in the absence of $\delta \boldsymbol{r}_{l',l}$ and g_l^a the anomalous distribution function related to $\delta \boldsymbol{r}_{l',l}$. It is now clear [6] that $\delta r_{l',l}$ is a disorder-induced interband-coherence effect and so is g_l^a.

Given that the semiclassical formulation is relevant in the weak-disorder regime, Eq. (1) reduces to [9]

$$\boldsymbol{j}^z = \sum_l f_l (\boldsymbol{j}_l^z)^0 + \sum_l g_l^{2s} \delta^{ex} \boldsymbol{j}_l^z + \sum_l f_l^0 \delta^{in} \boldsymbol{j}_l^z, \tag{7}$$

up to the zeroth order of the total impurity density and scattering strength. g_l^{2s} represents the value of g_l^n in the lowest Born order [6]. In higher Born orders, some additional contributions to g_l^n appear and are responsible for the transverse transport owing to the breakdown of the principle of microscopic detailed balance. The analysis of these higher-Born-order contributions under the non-crossing approximation has been detailed in Ref. [17]. Here we only mention that there is an interband-coherence scattering effect called "intrinsic skew-scattering-induced side-jump" appearing in the third Born order under Gaussian disorder. In the following, we set $\boldsymbol{j}^{z,in} = \sum_l f_l^0 \delta^{in} \boldsymbol{j}_l^z$, which is just the intrinsic contribution to the spin current independent of the disorder [11], and $\boldsymbol{j}^{z,sj} = \sum_l g_l^{2s} \delta^{ex} \boldsymbol{j}_l^z$ because it is related to the spin-current counterpart of the side-jump velocity. In the general case of the SHE induced by strong band-structure spin–orbit coupling, $\boldsymbol{j}^{z,sj}$ is just one part of the side-jump SHE arising from disorder-induced interband-coherence effects. Two other semiclassical contributions to the side-jump SHE (from the anomalous distribution function g_l^a and the intrinsic skew-scattering-induced side-jump) [18] and the skew scattering SHE arising from non-Gaussian disorder are all included in the first term of Eq. (7) [6, 17].

To be more clear, we can consider the case of randomly distributed scalar pointlike Gaussian disorder with density n_0 and average strength V_0. Then $g_l^{2s} \sim n_0^{-1} V_0^{-2}$, $\delta^{ex} j_l^z \sim n_0 V_0^2$, $g_l^a \sim n_0^0 V_0^0$, and the third-Born-order contribution to g_l^n behaves as $\sim n_0^0 V_0^0$ (thus is called the intrinsic skew scattering [6, 17]). In this case, the side-jump SHE may consist of three semiclassical contributions in the zeroth order of both the impurity density and scattering strength: $j^{z,sj}$, $\sum_l g_l^a (\boldsymbol{j}_l^z)^0$, and the intrinsic skew-scattering-induced side-jump.

3 Model calculation

3.1 Model

The model Hamiltonian of a Rashba 2DEG is $H_0 = \frac{\hbar^2 \boldsymbol{k}^2}{2m} + \alpha_R \hat{\boldsymbol{\sigma}} \cdot (\boldsymbol{k} \times \hat{\boldsymbol{z}})$, where $\boldsymbol{k}$ is the 2D wave vector, m is the effective mass, $\hat{\boldsymbol{\sigma}}$ is the vector of Pauli matrices, and α_R the Rashba coefficient. The internal eigenstates read $|u_{\boldsymbol{k}}^\eta\rangle = \frac{1}{\sqrt{2}}[1, -i\eta \exp(i\phi)]^T$, where $\eta = \pm$ label the two bands $\epsilon_k^\eta = \hbar^2 k^2/(2m) + \eta \alpha_R k$, and $\tan\phi = k_y/k_x$.

For $\epsilon > 0$, the corresponding wave number in the η band is given as $k_\eta(\epsilon) = -\eta k_R + k_0(\epsilon)$. Here $k_R = m\alpha_R/\hbar^2 = \frac{1}{2}[k_-(\epsilon) - k_+(\epsilon)]$ measures the momentum splitting of two Rashba bands, whereas $k_0(\epsilon) \equiv \alpha_R^{-1}\sqrt{\epsilon_R^2 + 2\epsilon_R \epsilon} = \frac{1}{2}\sum_\eta k_\eta(\epsilon)$. The density of states of the η band takes the form $D_\eta(\epsilon) = D_0 \frac{k_\eta(\epsilon)}{k_0(\epsilon)}$, with $D_0 = m/2\pi\hbar^2$.

For $0 > \epsilon > -\epsilon_R/2$, the iso-energy surface slices the spectrum into two rings of radii $k_{-\nu}(\epsilon) = k_R + (-1)^{\nu-1} k_0(\epsilon)$, where $\nu = 1, 2$ denote the two monotonic segments (Fig. 1), with $k_0(\epsilon) \equiv \alpha_R^{-1}\sqrt{\epsilon_R^2 + 2\epsilon_R \epsilon} = \frac{1}{2}[k_{-1}(\epsilon) - k_{-2}(\epsilon)]$. The density of states of the $-\nu$ branch reads $D_{-\nu}(\epsilon) = D_0 \frac{k_{-\nu}(\epsilon)}{k_0(\epsilon)}$.

The conventional definition of the spin current as an anticommutator of velocity and spin is employed: $\hat{\boldsymbol{j}}^z = \frac{\hbar}{2}\frac{1}{2}\{\hat{\sigma}_z, \hat{\boldsymbol{v}}\} = \frac{\hbar}{2}\frac{\hbar \boldsymbol{k}}{m}\hat{\sigma}_z$. It is purely off-diagonal in band-index space in this model: $(\boldsymbol{j}_l^z)^0 = 0$. Therefore, the SHE in Eq. (7) is determined only by

$$\boldsymbol{j}^z = \boldsymbol{j}^{z,in} + \boldsymbol{j}^{z,sj}. \tag{8}$$

The Boltzmann equation can be conveniently solved by using variables $l = (\epsilon, \eta, \phi)$ for $\epsilon > 0$ and $l =$

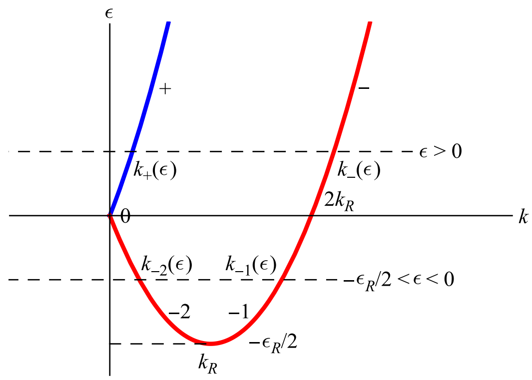

Fig. 1 Band structure of a Rashba 2DEG. The two Rashba bands cross at the zero-momentum point. The minimal energy of the dispersion curve is $-\frac{1}{2}\epsilon_R$. For $\epsilon \geq 0$, the wave number in the $\pm$ band is defined by $k_\pm(\epsilon)$. For $-\frac{1}{2}\epsilon_R < \epsilon \leq 0$, there exist two monotonic branches: The one from $k = k_R$ to $2k_R$ is marked by the -1 branch; the other from $k = 0$ to k_R is marked by the -2 branch. $k_{-\nu}(\epsilon)$ denotes the wave number in the $-\nu$ branch at given ϵ, where $\nu = 1, 2$.

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$(\epsilon,-\nu,\phi)$ for $0>\epsilon>-\epsilon_R/2$. Correspondingly, $\sum_l=\sum_{\eta(\nu)}\int \mathrm{d}\epsilon D_{\eta(-\nu)}(\epsilon)\int\frac{\mathrm{d}\phi}{2\pi}$ for $\epsilon>0$ $(0>\epsilon>-\epsilon_R/2)$. If $\epsilon>0$, in the lowest Born order the energy-integrated elastic scattering rate is $\omega^{\phi,\phi'}_{\eta,\eta'}(\epsilon)=\int \mathrm{d}\epsilon' D_{\eta'}(\epsilon')\omega^{2s}_{l',l}$. However, if $0>\epsilon>-\epsilon_R/2$, there exists elastic scattering between the two branches $\nu=1$ and 2, and one has $\omega^{\phi,\phi'}_{-\nu,-\nu'}(\epsilon)=D_{-\nu'}(\epsilon)\int \mathrm{d}\epsilon_{l'}\omega^{2s}_{l',l}$. Assuming an isotropic disorder potential, transport-time type solutions to g^{2s}_l exist [19]. For $\epsilon>0$, we have

$$g^{2s}_\eta(\epsilon)=(-\partial_\epsilon f^0)e\boldsymbol{E}\cdot\boldsymbol{v}_\eta(\epsilon,\phi)\tau^{tr}_\eta(\epsilon),\tag{9}$$

where the transport time $\tau^{tr}_\eta(\epsilon)$ is determined by

$$1=\sum_{\eta'}\int\frac{\mathrm{d}\phi'}{2\pi}\omega^{\phi,\phi'}_{\eta,\eta'}[\tau^{tr}_\eta-\cos(\phi'-\phi)\tau^{tr}_{\eta'}].\tag{10}$$

For $0>\epsilon>-\epsilon_R/2$, we have

$$g^{2s}_{-\nu}(\epsilon)=(-\partial_\epsilon f^0)e\boldsymbol{E}\cdot\boldsymbol{v}_{-\nu}(\epsilon,\phi)\tau^{tr}_{-\nu}(\epsilon),\tag{11}$$

with the transport time $\tau^{tr}_{-\nu}(\epsilon)$ decided by

$$1=\sum_{\nu'}\int\frac{\mathrm{d}\phi'}{2\pi}\omega^{\phi,\phi'}_{-\nu,-\nu'}[\tau^{tr}_{-\nu}-(-1)^{\nu'-\nu}\cos(\phi'-\phi)\tau^{tr}_{-\nu'}].\tag{12}$$

3.2 Calculations

We consider that the impurity potential is produced by randomly distributed short-range scattering interactions at $\boldsymbol{R}_i$, i.e., $V(\boldsymbol{r})=\sum_{i,\mu}V^i_\mu\sigma_\mu\delta(\boldsymbol{r}-\boldsymbol{R}_i)$ with $\mu=0,1,2,3$ and σ_0 the unity matrix in spin space [20]. Here the short-range potential is approximated by the delta potential. We assume a Gaussian disorder approximation and isotropic magnetic scattering [20, 21]. n_0 and n_m are the concentrations of nonmagnetic and magnetic impurities, respectively. V_0 and V_m are the average strengths for nonmagnetic and magnetic scattering, respectively. The external electric field is applied in the x direction.

3.2.1 Nonmagnetic impurities

When $\epsilon>0$, straightforward calculation leads to the spin-current counterpart of the side-jump velocity:

$$\delta^{ex}(\boldsymbol{j}^z_l)^{nm}_y=-\frac{1}{\tau_0}\frac{\eta}{k_R}\frac{\hbar}{8}\cos\phi,\tag{13}$$

with $\tau_0=(2\pi n_0V_0^2D_0/\hbar)^{-1}$. The transport time reads [19] $\tau^{tr}_\eta(\epsilon)=\tau_0D_\eta(\epsilon)/D_0$, and then the side-jump spin Hall current is

$$j^{z,sj}_y=\sum_l g^{2s}_l\delta^{ex}(\boldsymbol{j}^z_l)^{nm}_y=\frac{e}{8\pi}E_x,\tag{14}$$

which completely cancels out the intrinsic spin Hall current $j^{z,in}_y=\frac{-e}{8\pi}E_x$. This just reproduces the well-known [1] vanishing spin Hall current $j^z_y=0$ in the semiclassical Boltzmann theory for the first time.

When $0>\epsilon_F>-\epsilon_R/2$, the intrinsic spin Hall current is $j^{z,in}_y=\frac{k_0(\epsilon_F)}{k_R}\frac{-e}{8\pi}E_x$. Meanwhile, the spin-current counterpart of the side-jump velocity reads

$$\delta^{ex}(\boldsymbol{j}^z_l)^{nm}_y=\frac{1}{\tau_0}\frac{1}{k_0(\epsilon)}\frac{\hbar}{8}\cos\phi.\tag{15}$$

and thus the side-jump spin Hall current

$$j^{z,sj}_y=\sum_l g^{2s}_l\delta^{ex}(\boldsymbol{j}^z_l)^{nm}_y=\frac{k_0(\epsilon_F)}{k_R}\frac{e}{8\pi}E_x\tag{16}$$

again cancels out the intrinsic one. This also coincides with the zero SHE obtained by using the Kubo formula [22].

3.2.2 Magnetic impurities

For an isotropic delta-like magnetic impurity potential, since the contributions from V^i_x and V^i_y cancel out in Eq. (4), the spin-current counterpart of the side-jump velocity is given by

$$\delta^{ex}(\boldsymbol{j}^z_l)^m_y=-\frac{1}{3}\frac{n_mV_m^2}{n_0V_0^2}\delta^{ex}(\boldsymbol{j}^z_l)^{nm}_y.\tag{17}$$

The transport time is given by

$$\frac{\tau^{tr}_\eta(\epsilon)}{\tau_m}=\frac{8k_0(\epsilon)-k_\eta(\epsilon)}{7k_0(\epsilon)}\tag{18}$$

for $\epsilon>0$ and by

$$\frac{\tau^{tr}_{-\nu}(\epsilon)}{\tau_m}=\frac{k_0(\epsilon)}{k_R}\frac{8k_R-k_{-\nu}(\epsilon)}{7k_R}\tag{19}$$

for $0>\epsilon>-\epsilon_R/2$, with $\tau_m=\left(\frac{2\pi}{\hbar}n_mV_m^2D_0\right)^{-1}$.

When both Rashba bands are partially occupied, the side-jump spin Hall current

$$j^{z,sj}_y=\sum_l g^{2s}_l\delta^{ex}(\boldsymbol{j}^z_l)^m_y=\frac{1}{7}\frac{-e}{8\pi}E_x=\frac{1}{7}j^{z,in}_y\tag{20}$$

enhances the total spin Hall current to $j^z_y=j^{z,in}_y+j^{z,sj}_y=\frac{8}{7}j^{z,in}_y$. This j^z_y is the same as the weak-disorder-limit value of that obtained by Kubo diagrammatic calculations [21, 23]. The longitudinal electric current is $j_x=\frac{e^2}{\pi\hbar^2}\tau_m\frac{3\epsilon_R+7\epsilon_F}{7}E_x$, so the spin Hall angle is therefore

$$\alpha_{sH}=\frac{ej^z_y/\left(\frac{\hbar}{2}\right)}{j_x}=\frac{-2\hbar}{\tau_m\epsilon_R}\frac{1}{3+7\frac{\epsilon_F}{\epsilon_R}}.\tag{21}$$

When only the lower Rashba band is partially occupied, the side-jump and the total spin Hall currents are

$$j_y^{z,sj} = \frac{k_0(\epsilon_F)}{7k_R}\frac{-e}{8\pi}E_x = \frac{1}{7}j_y^{z,in} \tag{22}$$

and $j_y^z = \frac{8}{7}j_y^{z,in}$, respectively. The longitudinal electric current is $j_x = \frac{e^2}{\pi\hbar^2}\tau_m\frac{3\epsilon_R-\epsilon_F}{7}\frac{k_0^2(\epsilon_F)}{k_R^2}E_x$ and thus

$$\alpha_{sH} = \frac{-2\hbar}{\tau_m\epsilon_R}\frac{1}{\left(3-\frac{\epsilon_F}{\epsilon_R}\right)\sqrt{1+2\frac{\epsilon_F}{\epsilon_R}}}. \tag{23}$$

Although $\frac{\hbar}{\tau_m\epsilon_R}$ is a small quantity in giant Rashba systems, the factor $\sqrt{1+2\frac{\epsilon_F}{\epsilon_R}}$ can be very small, leading to a large spin Hall angle when ϵ_F is located close to the band bottom of the lower Rashba band. For instance, if $\frac{\hbar}{\tau_m\epsilon_R}=0.02$, $1+2\frac{\epsilon_F}{\epsilon_R}=0.1$ leads to $\alpha_{sH}\simeq -4\%$, which is quite large [24, 25]. Smaller τ_m and smaller $\sqrt{1+2\frac{\epsilon_F}{\epsilon_R}}$ may lead to larger α_{sH}. However, the quantitative analysis of this possibility is beyond the scope of semiclassical theory, which is valid only in the weak-disorder regime. From the above equation, α_{sH} goes to infinity as ϵ_F goes to the band bottom of the lower Rashba band. However, this low carrier density limit is actually beyond the Boltzmann regime, and more rigorous microscopic treatments are called for.

3.2.3 Both nonmagnetic and magnetic impurities

The coexistence of nonmagnetic and magnetic impurities may be the more realistic case [20, 21]. Only the main results will be given in this case. Since there is no mixing between the nonmagnetic and magnetic scattering as pointed out by Inoue et al. [21], the spin-current counterpart of the side-jump velocity is $\delta^{ex}(\boldsymbol{j}_l^z)_y = \left[1-\frac{1}{3}\frac{\tau_0}{\tau_m}\right]\delta^{ex}(\boldsymbol{j}_l^z)_y^{nm}$. The total spin Hall current reads $j_y^z = \frac{\frac{8}{3}\frac{\tau_0}{\tau_m}}{1+\frac{7}{3}\frac{\tau_0}{\tau_m}}j_y^{z,in}$, depending on the relative weight of different types of scattering [5, 20]. The side-jump effect vanishes when $\tau_0 = 3\tau_m$, the same condition as that for the vanishing of the ladder vertex correction in the Kubo diagrammatic calculation in the spin-σ_z basis for the case $\epsilon_F > 0$ [21, 26].

For Fermi energies above and below the band crossing point, the spin Hall angles are

$$\alpha_{sH} = \frac{-\frac{\hbar}{\tau_S\epsilon_R}\frac{2}{3}\frac{\tau_0}{\tau_m}}{1+\frac{\tau_0}{\tau_m}+\left(1+\frac{7}{3}\frac{\tau_0}{\tau_m}\right)\frac{\epsilon_F}{\epsilon_R}}$$

and

$$\alpha_{sH} = \frac{-\frac{\hbar}{\tau_S\epsilon_R}\frac{2}{3}\frac{\tau_0}{\tau_m}}{1+\frac{\tau_0}{\tau_m}+\left(1-\frac{1}{3}\frac{\tau_0}{\tau_m}\right)\frac{\epsilon_F}{\epsilon_R}}\frac{1}{\sqrt{1+2\frac{\epsilon_F}{\epsilon_R}}},$$

respectively. Here we define $\tau_S^{-1}\equiv\tau_0^{-1}+\tau_m^{-1}$. Tuning the ratio τ_0/τ_m, one can find that α_{sH} changes monotonically and continuously from the scalar-disorder-dominated case to the magnetic-disorder-dominated regime.

4 Discussion and summary

Before concluding this paper, we comment on some important issues not mentioned in the above sections.

First, the simple form of the semiclassical Boltzmann equation (5) is exactly valid only for isotropic bands and isotropic scattering [2, 17]. However, in the presence of anisotropy a more generic and complicated form of the Boltzmann equation may be necessary; the readers are referred to Ref. [27] for detailed discussions.

Second, the recently highlighted "coherent skew scattering" under Gaussian disorder beyond the non-crossing approximation [28] is also included in the first term of Eq. (7). This additional contribution is also in the zeroth order of both the impurity density and scattering strength in the weak-disorder limit in the presence of only one type of disorder, like the side-jump contribution, but is not an interband-coherence scattering effect [18]. Consequently, how to place this contribution into the classification of AHE and SHE mechanisms suggested in Refs. [1, 2] is still an open question. Therefore, in presenting our theory we avoid this issue. Fortunately, in the Rashba model considered in Sec. III the first term of Eq. (7) vanishes. Besides, this so-called "coherent skew scattering" has actually already been proposed sixty years ago by Kohn and Luttinger [27, 29]. We will provide a comprehensive description of a semiclassical Boltzmann theory going beyond the non-crossing approximation in a future publication.

Finally, in the presence of spin–orbit coupling, the electron spin is not conserved and thus the spin current is not uniquely defined. The conventionally defined spin current adopted in this study is not a conserved transport current. A physically attractive definition of the conserved spin current has been suggested by Shi *et al.* [30] by introducing the torque dipole moment. However, disorder effects on the torque dipole spin current [31] in the Bloch representation are difficult to address under a uniform external electric field in Boltzmann theory. We reserve these for future studies.

In summary, we have formulated a semiclassical Boltzmann framework of spin Hall effects induced by strong band-structure spin–orbit coupling in nondegenerate multiband electron systems in the weak-disorder regime. We derived the absent ingredient in previous semiclassical theories, i.e., the spin-current counterpart of the semiclassical side-jump velocity. This gauge-invariant quantity arises from the interband coherence during elastic electron-impurity scattering and contributes one part of the side-jump SHE.

Applying this theory to a 2DEG with giant Rashba spin–orbit coupling, we showed an enhanced spin Hall angle when only the lower Rashba band is partially occupied in the presence of magnetic impurities. We note that this energy regime below the band crossing point in Rashba systems and similar systems is of intense theoretical interest also from the standpoint of enhanced efficiency of spin–orbit torque and the Edelstein effect [32–34], as well as enhanced thermoelectric conversion efficiency [15, 19].

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References and notes

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