Theoretical aspects of the Edelstein effect for anisotropic two-dimensional electron gas and topological insulators

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I. INTRODUCTION

One promising effect providing charge-to-spin conversion in nonmagnetic materials is the Aronov–Lyanda-Geller–Edelstein (ALGE) effect, considered first in 1989 by Aronov and Lyanda-Geller [1] as well as Edelstein [2]. Often, it is called the Edelstein effect or inverse spin-galvanic effect [3]. In systems with broken inversion symmetry, such as surfaces or interfaces, spin-orbit coupling (SOC) lifts the spin degeneracy [4–6]. An in-plane electric current penetrating the system gives rise to a homogeneous in-plane spin polarization perpendicular to the applied electric field. Thus, a nonzero spin polarization is generated in nonmagnetic systems purely electrically.

Because of these promising properties, the ALGE effect has been the subject of numerous theoretical considerations [1–3,7–10]. Experimental evidence for the ALGE effect and its inverse has been given by several experimental methods [11–17].

In this paper we consider the ALGE effect in Rashba systems [4–6] within a two-dimensional free-electron model using the semiclassical Boltzmann transport theory [18]. This approach has been used for the description of the ALGE effect in systems with Rashba, Dresselhaus, and Luttinger SOC in a number of previous works [3,19–22]. However, the isotropic two-dimensional electron gas (2DEG) model addressed in Refs. [1–3,3,7–10,19–22] provides merely a rough approximation to real systems with reduced symmetry, such as surfaces or interfaces, spin-orbit coupling (SOC) lifts the spin degeneracy [4–6]. An in-plane electric current penetrating the system gives rise to a homogeneous in-plane spin polarization perpendicular to the applied electric field. Thus, a nonzero spin polarization is generated in nonmagnetic systems purely electrically.

In addition to the usually considered isotropic 2DEG, we discuss the ALGE effect in anisotropic systems with reduced symmetry. With respect to practical applications our purpose is to maximize the charge-to-spin conversion efficiency. Therefore, we investigate in which direction an external electric field should be applied in systems with C2v symmetry to gain a large ALGE effect. This theoretical consideration is useful for experiments on the ALGE effect. Ast et al. [23] and Premper et al. [24] showed that an enormous Rashba splitting occurs in ordered surface alloys due to an additional in-plane potential gradient, which should be accompanied by a sizable ALGE effect. However, in those systems the in-plane symmetry is broken. We study the influence of this symmetry breaking on the ALGE effect.

Furthermore, the ALGE effect in the surface states of topological insulators (TIs) is examined because TIs are a promising material class for an effective charge-to-spin conversion [25]. We consider the surface states of TIs within a model similar to the Rashba Hamiltonian. Since a Rashba 2DEG and the surface states of TIs differ qualitatively, we discuss similarities and differences in the result for the current-induced spin density. We discuss also the ALGE effect for TIs with C3v symmetry (e.g., Bi2Se3 and Bi2Te3) [26].

This paper is organized as follows. In Sec. II A a general model for the consideration of the ALGE effect in isotropic Rashba systems is introduced. Subsequently, this model is extended to systems with reduced symmetry (Sec. II B). In Sec. II C the ALGE effect in topological insulators is considered. The theoretical results are applied to selected real systems.

II. MODEL AND RESULTS

A. Isotropic systems

A two-dimensional free electron gas within the xy plane with Rashba spin-orbit coupling [5] is described by the Hamiltonian

\[ \hat{H} = \frac{\hbar^2 \vec{k}^2}{2m} + \alpha_R(\vec{e}_z \times \vec{k}) \cdot \vec{\sigma}, \]  

where \( \vec{k} = (k_x, k_y) \) is the in-plane momentum, \( m \) is the effective electron mass, \( \vec{e}_z \) is the unit vector perpendicular to the 2DEG, and \( \vec{\sigma} \) is the Pauli spin vector. The Rashba parameter \( \alpha_R \) is a measure of the strength of the SOC. The energy eigenvalues...
of the Hamiltonian \( \hat{H} \) (1) are

\[
\mathcal{E}(\vec{k}) = \frac{k^2}{2m} \pm \alpha_{\parallel} k, 
\]

(2)

where \( k = |\vec{k}| \). Due to the SOC, the energy parabola of free electrons is split into two parabolas which are shifted by \( \mathcal{E}_{\min} = -\alpha_{\parallel}^2 m / 2\hbar^2 \), \( k_0 = \pm \alpha_{\parallel} m / \hbar^2 \), as shown in Fig. 1. The spin degeneracy is lifted except for the Dirac point \( (k = 0, \mathcal{E} = 0) \).

Corresponding to the \( \pm \) sign of the \( k \) linear term in Eq. (2), two energy branches, \( + \) and \( - \), are defined. The \( + \) branch exists only for \( \mathcal{E} > 0 \). We distinguish two energy regions: region I reaches from the band edge to the Dirac point; region II is above the Dirac point, as shown in Fig. 1. The lines of constant energy consist of two concentric circles in \( \vec{k} \) space.

The eigenfunctions of the Hamiltonian (1) are spinors,

\[
\vec{k}, \pm = \left( \Psi_{\uparrow}(\vec{k}), \Psi_{\downarrow}(\vec{k}) \right),
\]

which are normalized and obey

\[
\Psi_{\uparrow}(\vec{k}) = \pm i e^{i\varphi_{\vec{k}}} \Psi_{\downarrow}(\vec{k}),
\]

(3)

where \( \varphi_{\vec{k}} \) is the azimuth of \( \vec{k} \), \( \cos \varphi_{\vec{k}} = k_x / \sqrt{k^2} \). The spin expectation value \( \langle \vec{\sigma} \rangle_k \) is obtained as

\[
\langle \vec{\sigma} \rangle_k = \frac{1}{4 \pm} \left( \Psi_{\uparrow}(\vec{k}) \Psi_{\downarrow}^*(\vec{k}) \pm \Psi_{\uparrow}^*(\vec{k}) \Psi_{\downarrow}(\vec{k}) \right).
\]

(4)

Due to the inversion asymmetry, spin and orbital momentum are coupled. The \( \vec{k} \)-dependent spin expectation values at the Fermi energy are shown in Fig. 2(a). They are within the plane of the 2DEG, perpendicular to \( \vec{k} \). The spin textures of the branches are clockwise (\( - \) branch) and anticlockwise (\( + \) branch).

For the consideration of the ALGE effect the expectation value of the total spin \( \langle \vec{\sigma} \rangle \) is calculated by summation of the spin expectation values of all occupied states. For reasons of time-inversion symmetry, the total spin polarization vanishes in equilibrium.

Using the semiclassical Boltzmann transport theory [18], the influence of an external electric field \( \vec{E} \) can be interpreted as a shift of the Fermi lines in \( \vec{k} \) space by \( \delta \mathcal{E}_F = -|\vec{e}| |v| \mathcal{E}_F / \hbar \).

Here, \( v \) indicates the \( + \) or \( - \) branch, \( e \) is the elementary charge, and \( v \) is the transport lifetime. The shift of the Fermi lines is shown in Fig. 2(b).

Considering zero absolute temperature, the expectation value of the total spin is obtained as

\[
\langle \vec{\sigma} \rangle = - \sum_{\vec{k},\nu} e |\vec{\sigma}_{\vec{k},\nu} \cdot \vec{E}| \delta |\mathcal{E}_F - \mathcal{E}_{\vec{k}}| \langle \vec{\sigma} \rangle_{\vec{k}}. 
\]

(5)

Here, \( \vec{\sigma}_{\vec{k},\nu} \) is the mean free path, and \( \mathcal{E}_{\vec{k}} \) is the Fermi energy. Only states at the Fermi level contribute. The mean free path is approximated in the relaxation-time approximation, \( \tau_{\nu} = \mathcal{E}_F / \mathcal{E}_{\vec{k},\nu} \), with the transport lifetime \( \tau_{\vec{k}} \) and the group velocity \( \vec{v}_{\vec{k}} = \hbar \nabla_{\vec{k}} \mathcal{E}_{\vec{k}} \).

For the calculation of the transport lifetime we consider scattering processes at \( \delta \)-shaped scattering potentials placed at positions \( \vec{R} \). The perturbation potential is \( \Delta V(\vec{R}) = \sum_{\vec{R}} U(\vec{R} - \vec{R}_j) \), as proposed by Edelstein [2]. The impurity concentration is assumed to be small (dilute limit), so that the scattering potentials do not overlap. Considering a scattering event from an initial state \( |\vec{k},\nu\rangle \) to a final state \( |\vec{k}',\nu'\rangle \), the corresponding transition matrix \( T_{\vec{k}',\nu,\vec{k},\nu} \) is obtained in Born approximation, \( T_{\vec{k}',\nu,\vec{k},\nu} = (\vec{\mathcal{K}},\nu') \Delta V(\vec{k},\nu) \), where \( \vec{\mathcal{K}},\nu) \) are the unperturbed wave functions. The microscopic transition probability is given by Fermi’s golden rule,

\[
P_{\vec{k}',\nu,\vec{k},\nu} = \frac{2\pi}{i \hbar} c_1 |T_{\vec{k}',\nu,\vec{k},\nu}|^2 \delta |\mathcal{E}_{\vec{k}} - \mathcal{E}_{\vec{k}'}| \langle \vec{\sigma} \rangle_{\vec{k}}.
\]

(6)

It is proportional to the impurity concentration \( c_1 \) and the total number of atoms \( N \). The transport lifetime \( \tau_{\vec{k}} \) is obtained by the solution of the linearized Boltzmann equation [18]

\[
\vec{v}_{\vec{k}} = \sum_{\vec{k}',\nu} \left( P_{\vec{k}',\nu,\vec{k},\nu} \vec{v}_{\vec{k}'} - P_{\vec{k}',\nu,\vec{k},\nu} \vec{v}_{\vec{k}} \right).
\]

(7)

With this theoretical background the spin density generated by the electric field \( \vec{E} \) can be calculated. Usually, region II of Fermi energies above the Dirac point, \( \mathcal{E}_F > 0 \), is discussed.
The spin density increases linearly with the Fermi energy \( E_F \). For Fermi energies between the band edge and the Dirac point, \( E_{\text{min}} < E_F < 0 \) (region I), the total spin increases linearly.

\[ \langle \vec{\sigma} \rangle \propto E_F \]

FIG. 3. Expectation value of the total spin \( \langle \sigma \rangle_{\text{total}} \) (gray) versus Fermi energy \( E_F \). The contributions of the + and − branches are shown in blue and red, respectively. Above the Dirac point (region II), the expectation value of the total spin is constant with respect to \( E_F \). For Fermi energies between the band edge and the Dirac point, \( E_{\text{min}} < E_F < 0 \) (region I), the total spin increases linearly.

For those energies, both branches are occupied, and the spin expectation value per area \( A \) of the whole system is

\[
\frac{\langle \vec{\sigma} \rangle}{A} = \frac{|e|}{4\pi \hbar} \left( \tau_F k_F - \tau_b k_F^* \right) \left[ \vec{e}_z \times \vec{E} \right] = \frac{|e|\alpha_R}{\pi c |U|^2 A} \left[ \vec{e}_z \times \vec{E} \right].
\]  

Here, the index \( F \) indicates that the corresponding quantity is at the Fermi level. \( A_0 \) is the area of the unit cell.

The spin expectation values resulting from the two circles of the Fermi line point in opposite directions; thus, their contributions compensate partially. Due to the larger radius of the Fermi line point in opposite directions, their contributions to the total spin compensate partially because the group velocity has opposite signs on the two circles, and therefore, the two Fermi circles are shifted in opposite directions. With decreasing Fermi energy the difference of the radii of the two circles gets smaller, which explains the linear energy dependence (Fig. 3).

In the calculation of the current-induced spin density from Eqs. (8) and (9) the impurity concentration \( c \) and the scattering potential \( U \) appear as parameters. If those quantities are not known, the spin density can be calculated depending on the two-dimensional charge current density \( \vec{j}_c \). Within the Boltzmann transport theory, \( \vec{j}_c \) is given by

\[
\vec{j}_c = \frac{|e|}{A} \sum \delta(\vec{k}) (\vec{k} \cdot \vec{E}) \left[ \vec{e}_z \times \vec{E} \right] v_F^2,
\]

which leads to the relation

\[
\frac{\langle \vec{\sigma} \rangle}{A} = \frac{\alpha_R m \hbar}{|e| (\alpha_R^2 + \hbar^2 \epsilon_F)} \left[ \vec{e}_z \times \vec{J} \right]
\]

for isotropic systems.

In this model, the 2DEG is confined to a plane with zero width (xy plane); hence, the scattering centers are located within that plane. At surfaces, the 2DEG’s wave functions decay exponentially toward the bulk. Therefore, the overlap of these wave functions and the impurities depends on the position of the impurities, more precisely, on the distance from the surface. The less overlap there is, the smaller the scattering is, and the larger the transport lifetimes are [28,29]. This would enhance the ALGE effect. Put differently, our model simulates the maximum overlap of wave functions and scattering potentials. As assumed by Edelstein [2] and in this work, the impurity potentials are \( \delta \) shaped. In real samples, however, the perturbation potentials are extended, or long range [30]. We note in passing that for extended potentials with a Gaussian shape (not reported here) the transition matrices (i.e., the overlap integral of initial and final wave functions with the perturbation potential) are reduced in comparison to \( \delta \)-shaped impurities. As a consequence, the transport lifetime and the ALGE effect are increased. We recall that we take the dilute limit in which scattering potentials do not overlap. The semiclassical Boltzmann approach used here has the advantage that it provides a clear and comprehensive understanding of the physics of the ALGE effect. The number of parameters in the model is small due to the approximations made. For example, long-range potentials would introduce additional parameters, thereby increasing the computational effort but reducing the transparency. In this paper, we restrict ourselves to \( \delta \)-shaped potentials; a treatment of realistic perturbation potentials is left to first-principles calculations [31,32].

In Table I the current-induced spin density for the Au(111) and Ag(111) surface states (sf) for an InGaAs/InAlAs heterostructure (hs) and the ordered \((\sqrt{3} \times \sqrt{3})R30^\circ\) Bi/Ag(111) surface alloy (sfal) is presented, calculated for \( j_c = 10 \text{ A}^{-1} \) within the isotropic model discussed above. Detailed insight into the microscopic origin of the band splitting of surface states is given in Ref. [33]. The Au(111) surface is often considered as a paradigm of a Rashba system [34,35]. However, it has been found that its surface states deviate from those of an ideal Rashba model with respect to the band structure at elevated energies and the spin-flip response to oscillating electric fields [36]. Since we consider energies close to the band crossing and the linear response to a time-independent electric field, these deviations are small, and Au(111) can safely be treated within the isotropic Rashba model.
TABLE I. Current-induced spin density \( \langle \sigma \rangle / A \) for isotropic Rashba systems; sf = surface state, hs = heterostructure, sfal = surface alloy. Here, the two-dimensional current density is set to \( j_x = 10 \, \text{A m}^{-1} \) in the \( x \) direction. The parameters \( m, \alpha_R, \) and \( \xi_F \) are taken from the cited references; \( m_e \) is the electron mass.

<table>
<thead>
<tr>
<th>System</th>
<th>( m ) (units of ( m_e ))</th>
<th>( \alpha_R ) (eV Å)</th>
<th>( \xi_F ) (eV)</th>
<th>( \langle \sigma \rangle / A ) ( \times 10^8 , \text{cm}^{-2} )</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Au(111) sf</td>
<td>0.27</td>
<td>0.33</td>
<td>0.475</td>
<td>10.03</td>
<td>[34], [37]</td>
</tr>
<tr>
<td>Ag(111) sf</td>
<td>0.37</td>
<td>0.03</td>
<td>0.178</td>
<td>3.36</td>
<td>[37], [38]</td>
</tr>
<tr>
<td>InGaAs/InAlAs hs</td>
<td>0.05</td>
<td>0.07</td>
<td>0.092</td>
<td>2.05</td>
<td>[39]</td>
</tr>
<tr>
<td>Bi/Ag(111) sfal</td>
<td>-0.35</td>
<td>3.05</td>
<td>-0.180</td>
<td>94.77</td>
<td>[14], [23]</td>
</tr>
</tbody>
</table>
FIG. 4. (a) Energy dispersion of a Rashba system with $C_2v$ symmetry ($m_x = 0.5m_y, \alpha_{Rx} = \alpha_{Ry}$) in two-dimensional $\vec{k}$ space (schematic). (b) In addition, the energy spectrum is shown for the $k_x$ and $k_y$ directions. At $E_S$ the band minimum in one direction (here, the $k_x$ direction) is reached, and a saddle point occurs. (c)–(f) The Fermi lines for selected energies; the arrows represent the direction of the spin expectation value $\langle \vec{\sigma} \rangle$. (Ref. [41]); $x$ and $y$ correspond to the crystallographic directions [001] and [110], respectively. In Table II the current-induced spin density of Au(110) surface states is presented. The spin density is calculated for an electric field in the directions of the main symmetry axes, [001] and [110]. Here, the absolute value of $\vec{E}$ is set constant and corresponds to a field which produces a two-dimensional charge current density of 10 A m$^{-1}$ if it is applied in the [001] direction. Obviously, the absolute value of the spin density strongly depends on the direction of the electric field. If the electric field is in the [001] direction, $\langle \sigma \rangle$ is enhanced by more than 100% in comparison to the spin density induced by an electric field in the [110] direction.

To gain a better understanding of the influence of the anisotropy of the effective mass and the Rashba parameter we consider the anisotropy of both quantities separately. First, the induced spin density of Au(110) surface states is presented. The spin density is calculated for an electric field in the directions of the main symmetry axes, [001] and [110]. Here, the absolute value of $\vec{E}$ is set constant and corresponds to a field which produces a two-dimensional charge current density of 10 A m$^{-1}$ if it is applied in the [001] direction. Obviously, the absolute value of the spin density strongly depends on the direction of the electric field. If the electric field is in the [001] direction, $\langle \sigma \rangle$ is enhanced by more than 100% in comparison to the spin density induced by an electric field in the [110] direction.

<table>
<thead>
<tr>
<th>Direction of $\vec{E}$</th>
<th>$j_s$(A m$^{-1}$)</th>
<th>$\langle \sigma \rangle/A$ (10$^8$ cm$^{-2}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\vec{E} \parallel [001] \parallel x$</td>
<td>10.00($j_s$)</td>
<td>8.53($\langle \sigma \rangle/A$)</td>
</tr>
<tr>
<td>$\vec{E} \parallel [110] \parallel y$</td>
<td>3.48($j_s$)</td>
<td>$-3.59(\langle \sigma \rangle/A)$</td>
</tr>
</tbody>
</table>

TABLE II. Current-induced spin density of Au(110) surface states. The model parameters $m_x = 0.11m_y, m_y = 0.32m_e, \alpha_{Rx} = 0.80$ eV Å, $\alpha_{Ry} = 0.17$ eV Å, $E_S = 0.370$ eV are taken from Ref. [41].
we assume $a_{Rz} = a_{Rx}$ and $m_z \neq m_x$. The mass anisotropy generates anisotropic Fermi lines. The absolute value of the Fermi vector is largest in the direction of the larger effective mass [for Au(110): [T10] direction]. If the electric field is applied in this direction, the Fermi lines are shifted in the opposite field direction, which implies that, mainly, states at the less extended side of the Fermi line contribute to the spin density. If the electric field is applied in the direction with the smaller effective mass [for Au(110): [001]], the Fermi lines are shifted in such a manner that, mainly, the states at the elongated side of the Fermi line contribute to the spin density. Therefore, in general a larger total spin density is expected if the electric field is applied in the direction of the smaller effective mass.

Now, $m_x = m_y$ and $a_{Rx} \neq a_{Rx}$ are assumed. The anisotropy of the Rashba parameter also affects the symmetry of the Fermi line. In addition, the $k$-dependent spin expectation values on the Fermi lines are rotated in the direction of the smaller Rashba parameter, as expressed by Eq. (14). For reasons of symmetry the total spin polarization in the direction of $\vec{E}$ is always zero, and only a total spin perpendicular to $\vec{E}$ remains. This field-induced spin density is large if $(\vec{\sigma})_k^z$ have large components perpendicular to $\vec{E}$. This means that the total spin density is larger if $\vec{E}$ is applied in the direction with the larger Rashba parameter [for Au(110) surface states: [001] direction].

These considerations explain qualitatively the orientation dependence of the ALGE effect in Au(110) surface states, given in Table II. In general, for systems with $C_{2v}$ symmetry the ALGE effect can be enhanced by an appropriate choice of the direction of $\vec{E}$.

The bulk inversion asymmetry in noncentrosymmetric crystals (e.g., zinc blende) leads to a Dresselhaus SOC contribution which depends on the crystal growth direction [44]. Like the Rashba term, the Dresselhaus term in the Hamiltonian produces spin splitting. Depending on the pointgroup symmetry of the system and the ratio of Rashba and Dresselhaus SOC, unconventional spin textures show up, for example, in systems with a single spin component [45] or showing a persistent spin helix [46].

Due to the symmetry breaking caused by the Dresselhaus SOC, current-induced spin polarization is expected [20,47]. In such systems, the ALGE effect can be analyzed as in Rashba systems. If the Hamiltonian depends only on one spin component [45] the spin expectation values are constant on both energy branches and do not depend on $\vec{k}$. As a result, an electric field does not induce a finite spin density for symmetry reasons. If the Rashba and the linear in-plane Dresselhaus term are of the same strength, a persistent spin helix occurs in real space [46]. The spin expectation values on the Fermi lines are parallel but point in opposite directions within one energy branch [46]. Therefore, a nonvanishing spin density is expected whose orientation does not depend on the direction of $\vec{E}$. Its absolute value reaches a maximum for $\vec{E}$ pointing in the direction of constant spin in real space and is minimized when $\vec{E}$ is oriented perpendicular.

2. $C_{3v}$ symmetry

For systems with $C_{3v}$ symmetry, such as fcc (111) surface states and ordered (111) surface alloys, an additional in-plane potential gradient occurs due to the in-plane structural inversion asymmetry [23]. The corresponding Hamiltonian contains an additional term proportional to $\hat{\sigma}_z$ and third order in $k$ [26],

$$\hat{H} = \frac{\hbar^2 k^2}{2m} + a_R (k_x \hat{\sigma}_x - k_y \hat{\sigma}_y) + \frac{\lambda}{2} (k_x^2 + k_y^2) \hat{\sigma}_z \quad (15)$$

where the parameter $\lambda$ characterizes the strength of the in-plane gradient and $k_\perp = k_x \pm i k_y$. Here, one mirror plane was chosen to be in the $k_x$ direction. Ast et al. [23] and Premper et al. [24] have shown that such an in-plane potential gradient, e.g., in the Ag/Bi($\sqrt{3} \times \sqrt{3}$)R30° surface alloy, results in a strongly enhanced spin splitting. Therefore, those systems are expected to provide a large ALGE effect. The energy eigenvalues of the Hamiltonian (15) are

$$\epsilon^\pm(k) = \frac{\hbar^2 k^2}{2m} \pm \sqrt{\alpha_R^2 k^2 + \lambda^2 k^6 \cos^2(3\psi_F)} \quad (16)$$

This energy spectrum has sixfold rotational symmetry. In the directions of the mirror planes the band structure is unchanged with respect to the isotropic model, whereas the influence of the term $\lambda^2 k^6 \cos^2(3\psi_F)$ is maximal in the directions perpendicular to three mirror planes [48]. The additional third-order Hamiltonian, $\hat{H}_1 = \lambda(2k_x^3 + k_y^3) \hat{\sigma}_x$, also called the warping term, mainly affects the states with large absolute values of $k$, which lie on the $-\text{branch}$. In Fig. 6 the Fermi lines of a system with $C_{3v}$ symmetry are shown. The outer line (—) has a hexagonal warped shape; the inner line (+) is nearly circular.

Due to the in-plane potential gradient the $k$-dependent spin expectation values $(\vec{\sigma})_k^z$ contain an out-of-plane component which increases with $\lambda$. This component is maximal at the regions of the Fermi lines which deviate most from the isotropic case, as sketched in Fig. 6.

The ALGE effect is calculated as for $C_{2v}$ symmetry. In Table III the current-induced spin density for the Bi/Cu(111) and Bi/Ag(111) ($\sqrt{3} \times \sqrt{3}$)R30° surface alloys is shown. To illustrate the influence of the additional warping term of the
The spin density was calculated without (\( \lambda = 0 \)) and with (\( \lambda \neq 0 \)) this term. For both systems the additional third-order term reduces the expectation value of the total spin density in comparison to the isotropic model (\( \lambda = 0 \)).

With increasing \( \lambda \), the \( \mathbf{k} \)-dependent spin expectation values are rotated out of the plane, as shown in Fig. 6; this reduces the in-plane component of \( \langle \hat{\sigma}_y \rangle \), leading to a decreased current-induced in-plane spin density. For symmetry reasons the total spin is completely in plane. In addition, the deviations of the Fermi lines from the circular shape cause a further reduction of the spin density.

C. Topological insulators

Besides the Rashba systems, a current-induced spin polarization is also expected in the surface states of three-dimensional topological insulators [25]. As in Rashba systems, spin and momentum are coupled, and the spin texture is helical. Whereas in Rashba systems the Fermi lines consist of two curves whose contributions to the ALGE effect compensate partially, the surface states of topological insulators provide a single Fermi circle. Therefore, an enhanced ALGE effect is expected in topological insulators.

### Table III. Current-induced spin density \( \langle \sigma \rangle /A \) for Bi/Cu(111) and Bi/Ag(111) \((\sqrt{3} \times \sqrt{3})\overline{R}30^\circ\) surface alloys. The two-dimensional current density is set constant to \( \mathbf{j}_c = 10\, \text{A m}^{-1} \) in the \( x \) direction. The spin density \( \langle \sigma \rangle \) is calculated without (\( \lambda = 0 \)) and with (\( \lambda \neq 0 \)) the warping term. As in Table I, the Fermi energy of the Bi/Ag surface alloy was assumed within the band with strong Rashba SOC.

<table>
<thead>
<tr>
<th>System</th>
<th>( m ) (units of ( m_c ))</th>
<th>( \alpha_R ) (eV ( \mathbf{A} ))</th>
<th>( \lambda ) (eV ( \mathbf{A}^2 ))</th>
<th>( \xi_F ) (eV)</th>
<th>( \langle \sigma \rangle /A ) (10^8 cm(^{-2}))</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bi/Cu(111)</td>
<td>0.29</td>
<td>0.85</td>
<td>0</td>
<td>0.215</td>
<td>54.78</td>
<td>[48–50]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>12</td>
<td>0.215</td>
<td>50.30</td>
<td></td>
</tr>
<tr>
<td>Bi/Ag(111)</td>
<td>0.32</td>
<td>2.95</td>
<td>0</td>
<td>0.180</td>
<td>93.30</td>
<td>[14,23,49,51]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>18</td>
<td>0.180</td>
<td>89.22</td>
<td></td>
</tr>
</tbody>
</table>

### Table IV. Current-induced spin density \( \langle \sigma \rangle /A \) for the surface states of selected topological insulators. The two-dimensional current density is set to \( \mathbf{j}_c = 10\, \text{A m}^{-1} \). Here, results for isotropic systems and for systems with hexagonal warping are presented.

<table>
<thead>
<tr>
<th>System</th>
<th>( v_F ) (10^5 m s(^{-1}))</th>
<th>( \lambda ) (eV ( \mathbf{A}^2 ))</th>
<th>( \xi_F ) (eV)</th>
<th>( \langle \sigma \rangle /A ) (10^8 cm(^{-2}))</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \alpha )-Sn</td>
<td>6.0</td>
<td>0</td>
<td>0.50...0.85</td>
<td>-104.01</td>
<td>[25]</td>
</tr>
<tr>
<td>Bi(_2)Se(_3)</td>
<td>6.2</td>
<td>0</td>
<td>-100.69</td>
<td></td>
<td>[52]</td>
</tr>
<tr>
<td>Bi(_2)Te(_3)</td>
<td>2.9</td>
<td>140</td>
<td>0.45</td>
<td>-22.11</td>
<td>[48]</td>
</tr>
<tr>
<td>Cu doped Bi(_2)Se(_3)</td>
<td>3.9</td>
<td>250</td>
<td>0.28</td>
<td>-71.08</td>
<td>[26]</td>
</tr>
<tr>
<td>Sn doped Bi(_2)Te(_3)</td>
<td>3.9</td>
<td>250</td>
<td>0.28</td>
<td>-71.08</td>
<td>[26]</td>
</tr>
</tbody>
</table>

The Hamiltonian

\[
\hat{H} = \hbar v_F(\mathbf{k}, \hat{\sigma}_y - k_x \hat{\sigma}_x)
\]

yields the linear energy dispersion

\[
\mathcal{E}^{\pm}(k) = \pm \hbar v_F k,
\]

where \( v_F \) is the Fermi velocity. The Dirac point is at \( \mathcal{E} = 0 \); the energy range above (below) the Dirac point is described by the + (−) branch of the energy spectrum (18). The whole energy range is not degenerate except for the Dirac point. The spin density induced by an electric field \( \mathbf{E} \) reads

\[
\langle \hat{\sigma} \rangle /A = \frac{-|e|}{4\pi \hbar} \mathbf{v}_F \times \int \mathbf{E} = \frac{-|e|\hbar v_F}{\pi \epsilon_0 |U|^2 A_0} [\mathbf{E}_x \times \mathbf{E}].
\]
spin density are larger than for the isotropic Rashba systems presented in Table I. For the topological insulators considered here the product $\hbar v_F$ is in the range from 1.91 to 4.08 eV Å, which is large in comparison to the Rashba parameter $\alpha_R$ of the Rashba systems in Table I.

One could argue that the enhanced ALGE effect is caused mainly by the large factor of $\hbar v_F$ in comparison to $\alpha_R$ since the analytical expressions (8) and (19) are very similar. However, the models discussed here describe qualitatively different physical systems. For a comparison between Rashba systems and topological insulators a more detailed consideration is needed.

For small $k$ the Rashba Hamiltonian (1) is approximated in first order in $k$ by the Hamiltonian (17), which is used for topological insulators. Within this approximation, the Fermi circle of a topological insulator corresponds to the inner Fermi circle of a Rashba system. However, the current-induced spin density in a topological insulator is not equivalent to the contribution of the inner Fermi circle of a Rashba system since in topological insulators only scattering events within the single Fermi circle contribute to the transport lifetime, whereas in Rashba systems intercircle scattering is also considered. Therefore, the spin density in topological insulators does not depend on the Fermi energy, while the contribution of the inner Fermi line of Rashba systems shows an energy dependence. Hence, the similarity of the analytic expressions (8) and (19) is by chance rather than of physical origin.

III. CONCLUSION

We provide a complete framework for theoretical consideration of the ALGE effect in common two-dimensional systems. Using the semiclassical Boltzmann transport theory, we present a model for the calculation of the ALGE effect in isotropic and anisotropic Rashba systems as well as in topological insulators. In isotropic systems the total spin generated by an electric field is energy independent for Fermi energies above the Dirac point but increases linearly with the Fermi energy between the band edge and the Dirac point. By introducing anisotropic effective masses and Rashba parameters the isotropic Rashba model can be expanded to anisotropic systems with $C_{2v}$ symmetry. When saddle points of the dispersion occur and the Fermi contours pass through a Lifshitz transition, the total spin of the system vanishes. The ALGE effect can be enhanced by an appropriate choice of the electric field direction (in the direction of smaller effective mass and larger Rashba parameter). For systems with $C_{3v}$ symmetry we include an additional in-plane potential gradient. The consideration of this gradient reduces the calculated spin density slightly; on the other hand, it leads to an enormous Rashba parameter which enhances the ALGE effect. In topological insulators a comparatively large ALGE effect is expected since here only one Fermi circle exists; thus no partial compensation of contributions from other Fermi circles occurs. The sign of the current-induced spin density in topological insulators is determined by the chirality. The ALGE effect provides an opportunity to measure the chirality directly.

Our findings call for experimental verification, especially of the energy dependence, the reduction of the current-induced spin density at the Lifshitz transition, and the influence of the electric field direction. In addition, this work may motivate an ab initio treatment of the ALGE effect.

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APPENDIX: NUMERICAL ASPECTS

If the shape of the Fermi contours deviates from a circle or an ellipse, a parametrization for integration along the Fermi lines is usually not possible. Therefore, we use numerical methods for the determination of the Fermi lines, the integration along the curves, and the solution of the linearized Boltzmann equation (7). In the following, the basic ideas of this numerical procedure are outlined.

First, the $\vec{k}$ points of the Fermi lines need to be determined. We use an adaptive triangle method [53] which is sketched schematically in Fig. 7. The $\vec{k}$ space is divided by a rectangular grid. By connecting the grid points with straight lines, triangles are generated, as shown in Fig. 7(a). Now, for each triangular point (all points of the grid and the center of four grid points), the energy $\mathcal{E}(\vec{k})$ is calculated from Eqs. (13) and (16), respectively. If the Fermi line passes between two triangular points, then the function $\mathcal{E}(\vec{k}) - \mathcal{E}_F$ must change sign in between those points. A triangle which is intersected by the Fermi line is divided into four smaller triangles with the centers of the edges as new points, as shown in Fig. 7(b). This procedure is repeated until the desired precision is reached.

For the summation in $\vec{k}$ space the sums of occupied states in $\vec{k}$ space are converted to integrals along the Fermi line as

$$\sum_{\vec{k}} \delta[\mathcal{E}(\vec{k}) - \mathcal{E}_F] \to \frac{A}{(2\pi)^3 \hbar} \int_{\vec{k} = \vec{k}_F} \frac{1}{v_F} dk_{\vec{k}}.$$  (A1)
Those line integrals are solved numerically according to the trapezoidal rule,
\[
\int_{k_{\max}} f(\vec{k})d\vec{k} \approx \sum_{j=1}^{N_k} \frac{1}{2} [f(\vec{k}_j) + f(\vec{k}_{j+1})]|\vec{k}_j - \vec{k}_{j+1}|, \quad (A2)
\]
where \( f(\vec{k}) \) is an arbitrary function and \( N_k \) is the number of \( \vec{k} \) points which approximate the Fermi line.

The linearized Boltzmann equation (7) is transformed into a matrix equation and solved by LU decomposition [54].