Maximum intrinsic spin-Hall conductivity in two-dimensional systems with $k$-linear spin–orbit interaction

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Abstract

We analytically calculate the intrinsic spin-Hall conductivities (ISHCs) ($\sigma_{xy}^z$ and $\sigma_{yx}^z$) in a clean, two-dimensional system with generic $k$-linear spin–orbit interaction. The coefficients of the product of the momentum and spin components form a spin–orbit matrix $\tilde{\beta}$. We find that the determinant of the spin–orbit matrix $\det \tilde{\beta}$ describes the effective coupling of the spin $s_z$ and orbital motion $L_z$. The decoupling of spin and orbital motion results in a sign change of the ISHC and the band-overlapping phenomenon. Furthermore, we show that the ISHC is in general unsymmetrical ($\sigma_{xy}^z \neq -\sigma_{yx}^z$), and it is governed by the asymmetric response function $\Delta \tilde{\beta}$, which is the difference in band-splitting along two directions: those of the applied electric field and the spin-Hall current. The obtained non-vanishing asymmetric response function also implies that the ISHC can be larger than $e/8\pi$, but has an upper bound value of $e/4\pi$. We will show that the unsymmetrical properties of the ISHC can also be deduced from the manifestation of the Berry curvature in the nearly degenerate area. On the other hand, by investigating the equilibrium spin current, we find that $\det \tilde{\beta}$ determines the field strength of the $SU(2)$ non-Abelian gauge field.

1. Introduction

Within condensed matter physics, spintronics has in itself become a strong field for considerable research, owing to not only its potential applications in electronic technologies but also the many fundamental questions that are raised on the physics of electron spin [1]. In particular, the spin–orbit interaction has recently strongly attracted the attention of theoreticians and experimenters since it opens up the possibility of manipulating electron (or hole) spin in non-magnetic materials by electrical means [2, 3]. Since the theoretical prediction of the spin-Hall effect, the application of spintronics has seen considerable advancement. It has been shown that the Mott-type skew scattering by impurities would result in separation of opposite spin states via the spin–orbit interaction to the impurity atom [3]. This is the extrinsic spin-Hall effect. Nevertheless, it has been found that in p-type [4] (Luttinger model) and n-type [5] (Rashba model) semiconductors, the spin-polarized current (electron or hole) can be generated by the intrinsic spin–orbit interaction in non-magnetic structure in the absence of impurity scattering: this is called the intrinsic spin-Hall effect.

Calculation of the spin-Hall conductivity (SHC) plays a crucial role in studying the spin-Hall effect as it can be compared with experimental results. The extrinsic spin-Hall effect was experimentally discovered in three-dimensional (3D) n-type GaAs by optical means via spin accumulation at the edges of a sample [6, 7] and in two-dimensional (2D) n-type AlGaAs/GaAs [8]. The magnitude of the experimental value of the SHC ($0.5/(em\Omega)$) in [6] agrees with the theoretical value of the SHC ($0.5/(em\Omega)$) in [9]. However, the sign of the theoretical SHC is opposite to the experimental one, and it needs to be further clarified [9]. In 2D p-type AlGaAs/GaAs [10], the experimental value of the SHC ($2.5(e/8\pi)$) also agrees with the theoretical value ($1.9(e/8\pi)$) in order of magnitude [11]. In particular, in [11], the clean limit is considered in the calculation. In 2D n-type InGaN/GaN, the strain-dependent intrinsic spin-Hall effect can be generated by the intrinsic spin–orbit interaction in non-magnetic structure in the absence of impurity scattering: this is called the intrinsic spin-Hall effect.
detected by optical means is explained in terms of SHC in which the strain effect is included [12]. In 3D metal Pt wire, the large ISHC measured electrically through the inverse spin-Hall effect at room temperature is $240\left(\hbar/e\Omega\text{ cm}\right)$ [13, 14]. It was theoretically explained in [15] on the basis of the huge Berry curvature [16] near the Fermi level at the L and X symmetry points in the Pt Brillouin zone; the obtained theoretical value of ISHC is $200\left(\hbar/e\Omega\text{ cm}\right)$ in the absence of impurity scattering. More recently, a large spin-Hall signal has been observed at room temperature in FePt/Au multi-terminal devices [17].

Importantly, both the direction of the applied electric field and the strength of the spin–orbit interactions alter the values of the intrinsic spin-Hall conductivity (ISHC). For the former case, a typical example is the Rashba–Dresselhaus system [18]. When an electric field is applied along the $x$ (i.e., [010]) or $y$ (i.e., [100]) direction, we obtain $\sigma_{yx}^z = -\sigma_{xy}^z$, and these values are equal to the universal constant $e/8\pi r$. However, if an electric field is applied along $x'$ (i.e., [110]) or $y'$, i.e., [110]), we obtain $\sigma_{yx}^z \neq -\sigma_{xy}^z$, and one of these values has a value higher than $e/8\pi$. The latter case requires a systematic investigation because the spin–orbit interaction could be very complicated. For example, it has been proposed that a strained semiconductor results in various kinds of $k$-linear band-splitting [19]. Nevertheless, we find that the strain-induced spin splitting together with the spin–orbit coupling of the host semiconductor can be simplified and expressed in terms of the coefficients of the spin–orbit matrix (see equation (2)). In this study, we focus on generic 2D $k$-linear spin–orbit coupled systems without impurity scattering, and we systematically investigate the effects of spin–orbit interactions and the direction of the applied electric field on the spin-Hall current. We find that the ISHC can be calculated analytically and that its unsymmetrical properties can be described using a unified approach.

We show that $\text{det}\tilde{\beta}$ (see equation (15)) is expressed as the effective coupling of the $z$-component of spin $s_z$ and orbital angular momentum $L_z$. The decoupling of spin and orbital motion associated with the band-overlapping phenomenon results in the vanishing and sign change of the ISHC.

Furthermore, by analytically calculating the ISHCs, we find that the unsymmetrical result for the ISHCs ($\sigma_{zx}^z \neq \sigma_{zy}^z$) is governed by the asymmetric response function $\Delta\tilde{\beta}$ (see equation (30)), which is the difference in band-splitting in two directions: those of the applied electric field and the spin-Hall current. We find that the direction of the applied electric field alters the magnitude of the asymmetric response function. Consequently, we show that there exists a specific direction of the applied electric field such that the asymmetric response function reaches a maximum value. In this case, we show that the ISHC also reaches a maximum value in the range $e/8\pi$ to $e/4\pi$, where $e/4\pi$ is the upper bound value of the ISHC. The unsymmetrical result and the maximum asymmetric response function of the ISHC can also be deduced from the behavior of the Berry curvature in the nearly degenerate area. The nearly degenerate area refers to the area where the inner and outer bands are very close to each other on the Fermi surface.

This paper is organized as follows. In section 2, we define the spin–orbit matrix obtained from the coefficients of the product of momentum and spin. The intrinsic spin-Hall conductivity is shown to be proportional to the determinant of the spin–orbit matrix $\text{det}\beta$. We use the Foldy–Wouthuysen transformation to show that the effective coupling of the spin $z$-component $s_z$ and orbital angular momentum $L_z$ is $-2m(\text{det}\tilde{\beta})/\hbar^4$. In section 3, we analytically calculate the ISHC of the generic 2D $k$-linear spin–orbit coupled system. The asymmetric response function and the upper bound value of the ISHC will be discussed. In section 4, in order to reveal the maximum value of the ISHC, the direction of the applied electric field and its influence on the asymmetric response function are studied. In section 5, we will show that the unsymmetrical properties of the ISHC can be deduced from the variation of the Berry curvature. In section 6, we discuss the relationship between the equilibrium spin current and the spin–orbit matrix. We show that $\text{det}\tilde{\beta}$ plays the role of the color magnetic field strength. Our conclusions are presented in section 7.

2. Intrinsic spin-Hall conductivity

2.1. Spin–orbit matrix and ISHC

The 2D $k$-linear spin–orbit coupled system Hamiltonian in the presence of an applied electric field can be written as

$$H = \varepsilon_k + H_{so} + V(x, y),$$

where

$$H_{so} = \sum_i \beta_{ij}\sigma_i k_j = \begin{pmatrix} \sigma_x & \sigma_y \end{pmatrix} \begin{pmatrix} \beta_{xx} & \beta_{xy} \\ \beta_{yx} & \beta_{yy} \end{pmatrix} \begin{pmatrix} k_x \\ k_y \end{pmatrix}.$$  

The kinetic energy is $\varepsilon_k = \hbar^2 k^2/2m$ and $\sigma_i (i = x, y)$ are the Pauli spin matrices. The external potential $V(x, y) = eE\cdot x$. The generic $k$-linear spin–orbit coupled 2D systems are related to the spin–orbit matrix $\tilde{\beta}$,

$$\tilde{\beta} = \begin{pmatrix} \beta_{xx} & \beta_{xy} \\ \beta_{yx} & \beta_{yy} \end{pmatrix},$$

where the coefficients $\beta_{ij}$ represent the spin–orbit interactions in 2D systems. As examples, consider the Rashba system ($\sigma(x, k_x - \sigma, k_x)$) [20], the pure Dresselhaus system ($-\beta(\sigma, k_x - \sigma, k_x)$) [21] and the Dirac-type system ($g(\sigma, k_x + \sigma, k_x)$) [22, 23]; the corresponding spin–orbit matrices for these systems are

$$\tilde{\beta}_R = \alpha \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad \tilde{\beta}_S = \beta \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \tilde{\beta}_D = g \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

respectively. Another example is the spin splitting in a bulk strained semiconductor [19, 24]. The spin–orbit matrices $\tilde{\beta}_1$ and $\tilde{\beta}_2$ denote, respectively, the system with structure
inversion asymmetry (SIA) strain-induced splitting and the system with bulk inversion asymmetry (BIA) strain-induced splitting. They are given by
\[ \tilde{p}_1^+ = \frac{1}{4} C_3 \xi_{xy} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \]
\[ \tilde{p}_2^+ = D (\xi_{zz} - \xi_{yy}) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \]
where the structure constant \( C_3 > 0 \) and \( D > 0 \) [19].

Thus, in addition to SIA and bulk-inversion-symmetry breaking induced spin-orbit interaction, the strain-induced spin splitting is included in the spin-orbit matrix elements. Accordingly, we do not pose any restrictions on the spin-orbit matrix elements in the following calculations. To calculate the ISHC, we further rewrite equation (1) in the following form:
\[ H = \epsilon_k + d_x \sigma_x + d_y \sigma_y, \]
where
\[ d_x = \beta_x k_x + \beta_y k_y, \quad d_y = \beta_y k_x + \beta_x k_y, \]
The eigenenergy is \( E_{\pm k} = \epsilon_k - nd \) for two branches \( n = \pm \) (\( n = + \) for the outer band and \( n = - \) for the inner band), where the dispersion term \( d = \sqrt{d_x^2 + d_y^2} \) can be written as
\[ d = k \Gamma(\phi), \]
where
\[ \Gamma(\phi)^2 = \left( \beta_{xx}^2 + \beta_{yy}^2 \right) \cos^2 \phi + \left( \beta_{xy}^2 + \beta_{yx}^2 \right) \sin^2 \phi + 2 \beta_{xx} \beta_{xy} \sin(2\phi). \]
The energy dispersion equation (9) satisfies \( \Gamma(\phi) = \Gamma(\phi + \pi) \) because the time-reversal symmetry is preserved. For a positive chemical potential (\( \mu > 0 \)), the Fermi momenta for the two branches satisfy the following condition:
\[ k^+_y - k^-_y = \frac{2m \Gamma(\phi)}{\hbar^2}, \]
which is the band-splitting in the \( \phi \) direction on the Fermi surface. The ISHC can be evaluated by using the Kubo formula [25]
\[ \sigma_{ij}^\gamma(\omega) = \lim_{\omega \to 0} \frac{Q_{ij}^\gamma(\omega)}{-i \omega}. \]

\( Q_{ij}^\gamma(\omega) \) is the spin current–charge current correlation function. The index \( j \) represents the direction of the applied electric field and \( i \) is the direction of the response current. The conventional definition of the spin current is \( J_i^j = \frac{\hbar}{2} \frac{\partial H}{\partial k_i} \sigma_j \) [26], and the charge current is defined as \( J_i^j = \frac{e \partial H}{\partial k_j} \). From the standard approach, it can be shown that [27]
\[ Q_{ij}^\gamma(\omega) = i \hbar \sum_k \frac{\epsilon_k - \epsilon_{k'}}{\omega^2 - 4d^2} \frac{\partial \epsilon_k}{\partial \epsilon_{k'}} \left( d_x \frac{\partial d_x}{\partial k_i} - d_y \frac{\partial d_y}{\partial k_j} \right). \]

1 In constructing the spin–orbit matrix \( \tilde{p}_2 \), we have neglected the term \( Dk_y (\xi_{xx} - \xi_{xy}) \) which exists when \( \xi_{xx} \neq \xi_{xy} \). However, since \( k_z \) is not influenced by the in-plane electric field, \( k_z = 0 \), we can approximately neglect this term (see also [19]).

where \( \hbar k \) represents the Fermi function for the two energy branches. Note that the correlation function contains the kinetic term. Next, we focus on the spin-Hall conductivity in the static case (\( \omega = 0 \)). When an electric field is applied in the \( k_x \) direction and the spin-Hall response in the \( k_y \) direction it is given by
\[ \sigma_{xy}^\gamma = -\frac{e}{V} \sum_k \left( \frac{\hbar k_+ - \hbar k_-}{4d^2} \frac{\partial \epsilon_k}{\partial k_x} \right) \left( d_x \frac{\partial d_y}{\partial k_x} - d_y \frac{\partial d_x}{\partial k_y} \right). \]

Substituting equations (7)–(10) into equation (13) and using the replacement \( (1/\sqrt{V}) \sum_k \int k \, dk \frac{\partial \epsilon_k}{\partial k} / (2\pi)^2 \), after a straightforward calculation, we obtain
\[ \sigma_{xy}^\gamma = \frac{e}{8\pi^2} (\det \tilde{p}) \int_0^{2\pi} d\phi \cos^2 \phi \Gamma(\phi)^2. \]

where \( \det \tilde{p} \) stands for the determinant of the spin–orbit matrix \( \tilde{p} \).

2.2. Effective coupling of spin and orbital motion

We can apply the Foldy–Wouthuysen transformation [28] to the Hamiltonian equation (1), and diagonalize the Hamiltonian up to some order of \( \beta_{ij} \). Because \( \det \tilde{p} \) is of the order of \( \beta_{ij}^0 \), the unitary transformation that can diagonalize equation (1) up to second order is given by (see appendix A)
\[ U = \exp \left\{ -\frac{m}{\hbar^2} D \right\}, \quad D = \sigma_x F_x + \sigma_y F_y, \]
\[ F_x = \beta_{xx} x + \beta_{xy} y, \quad F_y = \beta_{yx} x + \beta_{yy} y, \]
where \( F_x \) and \( F_y \) are obtained by using the replacements \( k_x \to x \) and \( k_y \to y \) in \( d_x \) and \( d_y \). It can be shown that
\[ [D, \epsilon_k] = \frac{\hbar^2}{m} H_{so}. \]

Using the unitary transformation equations (16) and (17), equation (1) becomes (up to the second order of \( \beta_{ij} \))
\[ H' = U^\dagger H U = \epsilon_k + \frac{im}{\hbar^2} \left( 1 - \frac{1}{2!} \right) [D, H_{so}] + V(x, y) + o(\beta_{ij}^3). \]

It can be shown that
\[ [D, H_{so}] = i \sum_j \beta_{ij}^2 + \frac{2i}{\hbar} (\det \tilde{p}) \sigma_z L_z, \]

where \( L_z = h (y k_x - x k_y) \) is the orbital angular momentum. Substituting equation (19) into (18), we obtain
\[ H' = \epsilon_k - \frac{m}{2\hbar^2} \sum_j \beta_{ij}^2 + h_D + V(x, y) + o(\beta_{ij}^3). \]
where

$$h_D = -\frac{m}{\hbar} \left( \det \tilde{\beta} \right) \sigma_z L_z. \quad (21)$$

Equation (21) shows that the coupling between the orbital motion $L_z$ and the spin $z$ component $\sigma_z$ is proportional to $\det \tilde{\beta}$. Therefore, equation (15) together with equations (14) and (21) exhibits a discriminant for a non-vanishing spin-Hall conductivity,

$$\det \tilde{\beta} = 0 \rightarrow \sigma^z_{xy} = 0, \quad \det \tilde{\beta} \neq 0 \rightarrow \sigma^z_{xy} \neq 0. \quad (22)$$

In the Rashba–Dresselhaus system ($\tilde{\beta}_R + \tilde{\beta}_D$), we have $\beta_{xx} = \beta$, $\beta_{xy} = \alpha$, $\beta_{yx} = -\alpha$, $\beta_{yy} = -\beta$ and $\det \tilde{\beta} = \alpha^2 - \beta^2$. It has been shown that the vanishing spin-Hall conductivity in the Rashba–Dresselhaus system results from the fact that the orbital motion is decoupled from the spin $z$-component when $\alpha^2 = \beta^2$ [29].

On the other hand, band degeneracy occurs when $k_F^0(\phi^0) = k_F^0(\tilde{\phi})^0$, namely, the inner band and the outer band overlap for some value $\phi^0$. The solution $\phi^0$ is given by

$$\tan \phi^0 = \frac{-(\beta_{xy} \beta_{yy} + \beta_{yx} \beta_{xy}) \pm \sqrt{-\left(\det \tilde{\beta}^2\right)}}{\beta_{yy}^2 + \beta_{xy}^2}. \quad (23)$$

If $\det \tilde{\beta} \neq 0$, the term $\sqrt{-\left(\det \tilde{\beta}^2\right)}$ is a complex number and the angle $\phi^0$ does not exist. The angle $\phi^0$ exists only when $\det \tilde{\beta} = 0$. The degeneracy could be open upon tuning the spin–orbit interactions such that $\det \tilde{\beta} \neq 0$. Therefore, the decoupling of the spin $s_z$ and orbital motion $L_z$ always accompanies the band-overlapping phenomenon. The decoupling of spin and orbital motion results in a sign change of the ISHC and the band-overlapping phenomenon.

3. Asymmetric and upper bound values of the ISHC

In order to evaluate the integral in equation (14), we transform the integral to the contour integral in a complex plane. If $z$ is defined as $z = e^{i \phi}$, the integral becomes a line integral along a closed loop with unit radius. The function $\Gamma(z)$ can be rewritten as

$$\Gamma(z) \equiv \frac{1}{4\pi^2} \left( \lambda_1 z^2 + \lambda_2 \right)(\lambda^2_2 z^2 + \lambda^2_1), \quad (24)$$

where '*’ symbolizes the complex conjugate and

$$\lambda_1 = (\beta_{xx} + \beta_{yy}) + i(\beta_{yx} - \beta_{xy}), \quad \lambda_2 = (\beta_{xx} - \beta_{yy}) + i(\beta_{yx} + \beta_{xy}). \quad (25)$$

The integral in equation (14) can be evaluated by calculating the residue inside the unit circle $|z| = 1$. The conditions for the poles appearing in the unit circle indicate the boundary of change of ISHC in sign. By using the standard residue theorem [30], the result is derived as

$$\int_{\gamma} d\phi \cos^2 \phi \Gamma(z) \left( \frac{1}{\lambda_1 \lambda_2} \right) \left( \frac{1}{\lambda_1^2 + \lambda_2^2} \right) \left( 1 - \Re \left( \frac{\lambda}{\lambda} \right) \right), \quad (26)$$

where $\Re(\cdot)$ represents the real part of a complex number. $\lambda_>(\lambda_<)$ is taken from the relative maximum (minimum) value of $(|\lambda_1|, |\lambda_2|)$. That is, if $|\lambda_1| > |\lambda_2|$ then $\lambda_> = \lambda_1$ and $\lambda_< = \lambda_2$, and vice versa. Equation (26) can be further simplified. Using equation (25), we find that

$$|\lambda_1|^2 - |\lambda_2|^2 = 4 \det \tilde{\beta}. \quad (27)$$

If $\det \tilde{\beta} \neq 0$ in equation (27), it cancels $\det \tilde{\beta}$ appearing in equation (14). Combining equation (14) together with equations (26) and (27), we have

$$\sigma^z_{xy} = \begin{cases} \begin{array}{ll} 2 & \text{sgn}(\det \tilde{\beta}) \frac{e}{8\pi} \left[ 1 - \Re \left( \frac{\lambda}{\lambda} \right) \right]; \\ 0; \end{array} \end{cases} \quad (28)$$

where $\text{sgn}(\det \tilde{\beta}) = \det \tilde{\beta}/|\det \tilde{\beta}|$ is the sign function. We have $\text{sgn}(\det \tilde{\beta} > 0) = +1$ and $\text{sgn}(\det \tilde{\beta} < 0) = -1$. The real part of $\lambda_>/\lambda_<$ in equation (28) can be written in terms of coefficients of the spin–orbit matrix,

$$\Re \left( \frac{\lambda}{\lambda} \right) = \frac{(\beta_{xx}^2 - \beta_{yy}^2) + (\beta_{yx}^2 - \beta_{xy}^2)}{\sum_{ij} \beta_{ij}^2 + 2|\det \tilde{\beta}|}. \quad (29)$$

Note that in equation (29) there is an absolute value of $\det \tilde{\beta}$. The ISHC generally depends on the spin–orbit interaction (equation (29)), and it is not necessarily a universal constant. We note that the denominator of equation (29) is always positive. Nevertheless, the numerator of equation (29) can be either positive or negative. For convenience in the following discussion, we define the asymmetric response function $\Delta \tilde{\beta}$ as

$$\Delta \tilde{\beta} \equiv (\beta_{xx}^2 - \beta_{yy}^2) + (\beta_{yx}^2 - \beta_{xy}^2) = \Gamma(0)^2 - \Gamma(\pi/2)^2. \quad (30)$$

We find that the asymmetric response function involves two quantities: $2m\Gamma(0)/\hbar^2$ is the band-splitting along the direction of the spin-Hall response and $2m\Gamma(\pi/2)/\hbar^2$ is the band-splitting along the direction of the applied electric field (see equation (10)). The asymmetric response function is the difference of the two specific band-splittings.

For $\Delta \tilde{\beta} > 0$, the ISHC is less than $e/8\pi$. Therefore, the spin-Hall conductivity has an upper bound in magnitude,

$$|\sigma^z_{xy}| \leq \frac{e}{8\pi}, \quad \Delta \tilde{\beta} \geq 0. \quad (31)$$

The equality in equation (31) is valid only when $(\beta_{xx}^2 - \beta_{yy}^2) = (\beta_{yx}^2 - \beta_{xy}^2) = 0$ in the coordinate system $(k_x, k_y)$. If $k_z$ axis is along the $[100]$ direction and the $k_x$ axis is along the $[010]$ direction, then some spin–orbit coupled systems would satisfy this condition, for example, the pure Rashba, the pure Dresselhaus and the Rashba–Dresselhaus systems. This result is in agreement with previous theoretical results [18].

Interestingly, we find that if $\Delta \tilde{\beta} < 0$, then $\Re (\lambda_>/\lambda_>)$ is negative and the spin-Hall conductivity satisfies

$$\frac{e}{8\pi} < |\sigma^z_{xy}| < \frac{e}{4\pi}, \quad \Delta \tilde{\beta} < 0. \quad (32)$$

The ISHC still has an upper bounded value $e/4\pi$; however, it can exceed the value $e/8\pi$. The three conditions are
We find that when \( \sigma \) analytically as follows:

\[
\int e \frac{\Delta \beta}{\pi} \int 0 \Delta \beta = 0 \quad \text{and} \quad \Delta \beta < 0, \quad \text{where} \quad \text{Re} (\lambda_+/\lambda_-) \quad \text{is defined as} \quad N \quad \text{and} \quad |N| < 1.
\]

The integration in equation (33) can also be calculated summarized in figure 1, where we define \( N = \text{Re}(\lambda_+/\lambda_-) \quad \text{and} \quad \text{it has been shown that} \quad |N| < 1. \quad \text{The spin-Hall conductivity} \quad |\sigma_{xy}| = (e/8\pi)(1 − |N|) \quad \text{for} \quad \Delta \beta > 0, \quad |\sigma_{zxy}| = \pi e/8\pi \Delta \beta = 0 \quad \text{and} \quad |\sigma_{zxy}| = (e/8\pi)(1 + |N|) \quad \text{for} \quad \Delta \beta < 0.

When an electric field is applied in the \( k_x \) direction, the spin-Hall response in the \( k_y \) direction is given by

\[
\sigma_{zxy} = e \frac{e}{8\pi} \left( \frac{\Delta \beta}{\pi} \right) \int 0 \frac{2\pi}{\phi} \sin^2 \phi \Gamma(\phi)^2.
\]

The integration in equation (33) can also be calculated analytically as follows:

\[
\sigma_{zxy} = \left\{ \begin{array}{ll}
-\text{sgn}(\Delta \beta) \frac{e}{8\pi} \left[ 1 + \text{Re} \left( \frac{\lambda_-}{\lambda_+} \right) \right] & \text{det} \beta \neq 0, \\
0 & \text{det} \beta = 0.
\end{array} \right.
\]

Unlike the \( \sigma_{xy} \), we have

\[
\frac{e}{8\pi} < |\sigma_{xy}| < \frac{e}{4\pi}, \quad \Delta \beta \leq 0, \quad \Delta \beta > 0.
\]

We find that when \( |\sigma_{xy}| \) is larger than \( e/8\pi \), \( |\sigma_{xy}| \) is less than \( e/4\pi \), and vice versa. In comparison with \( \sigma_{xy} \) (equation (28)), we find that \( \sigma_{xy} \) is in general not equal to \( -\sigma_{xy} \) in the \( k \)-linear system.

The symmetrical result (\( \sigma_{xy} = -\sigma_{xy} \)) is obtained because the electric field is applied in a direction such that the asymmetric response function vanishes. Both the pure Rashba and the pure Dresselhaus systems exhibit circular energy dispersion, and the asymmetric response function always vanishes regardless of the direction of the applied electric field. In the Rashba–Dresselhaus system, if the electric field is applied along the [010] direction and the spin-Hall response occurs along [100], the band-splitting along the direction of the applied electric field is the same as that along the spin-Hall response direction, and thus the asymmetric response function vanishes. However, a small change in the direction of the applied electric field would result in a non-vanishing asymmetric response function in the Rashba–Dresselhaus system. The influence of the applied electric field on the asymmetric response function is discussed in section 4.

4. Maximum value of the ISHC and asymmetric response function

The direction of the applied electric field plays an important role in determining whether the system has a non-vanishing asymmetric response function. We study the asymmetric response function by rotating the coordinate system from \( (k_x, k_y) \) to \( (k_x', k_y') \). Consider counterclockwise rotation of the system along the \( z \) axis by an angle \( \Theta \); the relationship between \( (k_x, k_y) \) and \( (k_x', k_y') \) is given by \( k_x = k_y' \cos \Theta - k_y' \sin \Theta \) and \( k_y = k_y' \sin \Theta + k_y' \cos \Theta \). The terms \( \beta_{ij} \) represent the matrix elements of the spin–orbit matrix in the new coordinates, and they are given by \( \beta_{ij} = \beta_{ix+i} \cos \Theta + \beta_{ix+j} \sin \Theta, \beta_{ij} = \beta_{iy+i} \cos \Theta + \beta_{iy+j} \sin \Theta \). It can be shown that the value of \( \det \beta \) is independent of the choice of coordinates, i.e., \( \det \beta = (\beta_{xy} \beta_{yx} - \beta_{xx} \beta_{yy}) = (\beta_{xy} \beta_{yx} - \beta_{yx} \beta_{xy}) \). Interestingly, it can also be shown that \( \sum_{ij} b_{ij}^2 = \sum_{ij} b_{ij}^2 \), namely, \( \sum_{ij} b_{ij}^2 \) is also independent of the choice of coordinates.

In the coordinate system \( (k'_x, k'_y) \), the term \( \sigma_{xy} \) indicates that the electric field is applied along the \( k'_y \) direction (\( \phi' = \pi/2 \)) and the corresponding spin-Hall response \( J_y' \) is along the \( k'_x \) direction (\( \phi' = 0 \)), where the angle \( \phi' \) is measured from the positive axis of \( k'_x \). On the other hand, the term \( \sigma_{xy} \) indicates that the electric field is applied along the \( k'_y \) direction (\( \phi' = 0 \)) and the corresponding spin-Hall response \( J_y' \) is obtained along the \( k'_x \) direction (\( \phi' = \pi/2 \)). Therefore, in the new coordinate system, equations (28) and (34) are still valid and can be written as

\[
\sigma_{xy} = \text{sgn}(\det \beta) \frac{e}{8\pi} \left[ 1 - \text{Re} \left( \frac{\lambda_-}{\lambda_+} \right) \right],
\]

\[
\sigma_{xy} = -\text{sgn}(\det \beta) \frac{e}{8\pi} \left[ 1 + \text{Re} \left( \frac{\lambda_-}{\lambda_+} \right) \right],
\]

where

\[
\text{Re} \left( \frac{\lambda_-}{\lambda_+} \right) = \frac{\Gamma'(\phi' = 0, \Theta, x) - \Gamma''(\phi' = \pi/2, \Theta, x)}{\sum_{ij} b_{ij}^2 + 2|\det \beta|}.
\]

The energy dispersion in the new coordinate system is

\[
\Gamma'(\phi', \Theta)^2 = (\beta_{xy}^2 + \beta_{yx}^2) \cos^2 \phi' + (\beta_{xx}^2 + \beta_{yy}^2) \sin^2 \phi' + (\beta_{xy} \beta_{yx} + \beta_{yx} \beta_{xy}) \sin 2\phi'.
\]

Equation (37) indicates that the variation in the ISHC is given only by the difference in two band-splittings: the band-splitting along the applied electric field direction and the band-splitting along the spin-Hall response direction.

It can be shown that in the new coordinate system, \( \Gamma'(0, \Theta) \) and \( \Gamma''(\pi/2, \Theta) \) can be written as

\[
\Gamma'(0, \Theta)^2 = \Gamma(0)^2 \cos^2 \Theta + \Gamma(\pi/2)^2 \sin^2 \Theta + (\beta_{xx} \beta_{xy} + \beta_{yx} \beta_{yx}) \sin 2\Theta,
\]

\[
\Gamma''(\pi/2, \Theta)^2 = \Gamma(0)^2 \sin^2 \Theta + \Gamma(\pi/2)^2 \cos^2 \Theta - (\beta_{xx} \beta_{xy} + \beta_{yx} \beta_{yx}) \sin 2\Theta.
\]

\[\text{(38)}\]
where \( \Gamma(0)^{\prime} = \beta_{yx}^{\prime} + \beta_{xy}^{\prime} \) and \( \Gamma(\pi/2)^{\prime} = \beta_{yx}^{\prime} + \beta_{xy}^{\prime} \). Therefore, in general, when \( \Theta \neq 0 \), \( \Gamma(0, \Theta) \) is not equal to \( \Gamma(\pi/2, \Theta) \), even if \( \Gamma(0) = \Gamma(\pi/2) \). A small rotation of the direction of the applied electric field would lead to a non-vanishing asymmetric response function.

According to equations (36) and (37), in order to enhance \( \sigma^{\prime}_{yx} \), i.e., \( |\sigma^{\prime}_{yx}| > e/8\pi \), the band-splitting must satisfy the condition \( \Gamma(0, \Theta) < \Gamma(\pi/2, \Theta) \). This means that the electric field must be applied along the direction with the larger band-splitting in comparison with that in the direction of the spin-Hall response. On the other hand, the corresponding value of \( \sigma^{\prime}_{yx} \) is less than \( e/8\pi \). Conversely, if we want to enhance \( \sigma^{\prime}_{yx} \), i.e., \( |\sigma^{\prime}_{yx}| > e/8\pi \), then we must have \( \Gamma(0, \Theta) > \Gamma(\pi/2, \Theta) \). This means that the electric field must be applied along the direction with larger band-splitting in comparison with that in the direction of the spin-Hall response.

Therefore, we conclude that in order to obtain an ISHC \( \sigma \) with \( \sigma > e/8\pi \), \( \sigma \) still has an upper bound value of \( e/4\pi \). This means that we can further enhance \( \sigma \) by finding the maximum value of the asymmetric response function. In fact, it can be shown that (see appendix B) when all the strengths of the spin–orbit interactions are fixed, the maximum value of \( |\sigma^{\prime}_{yx}| \) exists for a specific direction \( \Theta_{M} \) (see equation (B.1)). This also implies that the direction of the largest band-splitting is always perpendicular to that of the smallest band-splitting on the Fermi surface. Furthermore, the existence of the maximum value of \( |\Gamma(0, \Theta)^{2} - \Gamma(\pi/2, \Theta)^{2}| \) on the Fermi surface provides us with a method to obtain the maximum ISHC with respect to these fixed values of \( \beta_{ij} \).

In section 5, we explain how the enhanced spin-Hall response is a manifestation of Berry curvature in the nearly degenerate area.

5. Berry curvature and the nearly degenerate area

In this section, we analyze the Berry curvature in a system with fixed spin–orbit interactions, and, for convenience, the direction of the electric field is fixed while we rotate the system (see figure 2).

The spin-Hall conductivity \( \sigma^{\prime}_{yx} \) (equation (13)) can be written in terms of the Berry curvature as

\[
\sigma^{\prime}_{yx} = -\frac{e}{\hbar V} \sum_{k} \sum_{n=\pm} f_{kn} \Omega^{(n)}_{yx}(k),
\]

and it can be shown that

\[
\Omega^{(++)}_{yx}(k) = \frac{\hbar^{3}}{4m} \text{det} \beta \frac{\cos^{2} \phi}{k^{2} \Gamma(\phi, \Theta)^{3}},
\]

\[
\Omega^{(--)}_{yx}(k) = -\frac{\hbar^{3}}{4m} \text{det} \beta \frac{\cos^{2} \phi}{k^{2} \Gamma(\phi, \Theta)^{3}}.
\]

The energy dispersion \( \Gamma(\phi, \Theta) \) is given by \( \Gamma(\phi, \Theta)^{2} = A \cos^{2} \phi + B \sin^{2} \phi + C \sin(2\phi) \), where \( A = (\beta_{xx}^{\prime} + \beta_{yy}^{\prime}) \cos^{2} \Theta + (\beta_{xx}^{\prime} + \beta_{yy}^{\prime}) \sin^{2} \Theta + (\beta_{xx}^{\prime} + \beta_{yy}^{\prime}) \cos(2\phi) \). The peak value of \( \Omega^{(++)}_{yx} \) (\( \Omega^{(--)}_{yx} \)) is denoted as \( \Omega^{(++)}_{yx} \) (\( \Omega^{(--)}_{yx} \)). The peak value refers to the value of the Berry curvature in the nearly degenerate area (see figure 4). The ISHCs are \( |\sigma^{\prime}_{yx}| = (e/8\pi)(1 - N) \) and \( |\sigma^{\prime}_{yx}| = (e/8\pi)(1 + N) \), where \( N = (\Gamma_{0}(0, \Theta)^{2} - \Gamma(\pi/2, \Theta)^{2})^{2}/(\sum_{ij} \beta_{ij}^{2} + 2|\text{det} \beta|) \).

We select a system with a non-spherical energy dispersion (a nearly degenerate area exists) and \( \Gamma(0,0) \neq \Gamma(\pi/2,0) \). We use the following coefficients of the spin–orbit matrix: \( \beta_{xx} = 6 \times 10^{-2} \) eV nm, \( \beta_{xy} = 4.14 \times 10^{-2} \) eV nm, \( \beta_{yx} = 4.85 \times 10^{-2} \) eV nm, \( \beta_{yy} = 8.71 \times 10^{-2} \) eV nm. The Fermi energy is 2.67 meV. The particle mass is 0.08 in units of the bare electron mass. The energy dispersion is non-spherical, as shown on the left-hand side of figure 4(a).
Berry curvatures have units of $\text{cm}^2/\text{eV}$ and the peak values of the Berry curvatures (\(\tilde{\sigma}_{xy}^\pm (\phi)\)) have significant values (peak values) in the nearly degenerate area. When the system is rotated, both the positions of the nearly degenerate area and \(\tilde{\sigma}_{xy}^+(\phi)\) and \(\tilde{\sigma}_{xy}^-(\phi)\) change together. Furthermore, \(\tilde{\sigma}_{xy}^+(\phi)\) increases and \(\tilde{\sigma}_{xy}^-(\phi)\) decreases, as seen from figures 4(a)–(d). On the other hand, in figures 4(e)–(h), \(\tilde{\sigma}_{xy}^+(\phi)\) increases and \(\tilde{\sigma}_{xy}^-(\phi)\) decreases (see also figure 3(b)).

The variations in the ISHCs (\(|\sigma_{xy}^\pm|\) and \(|\sigma_{yz}^\pm|\)) corresponding to the Berry curvature variations in figures 4(a)–(h) is shown in figure 5, where \(|\sigma_{xy}^\pm| = (e/8\pi)(1 - N), |\sigma_{yz}^\pm| = (e/8\pi)(1 + N)\) and \(N = [\Gamma(0, \theta)^2 - \Gamma(\pi/2, \theta)^2]/(\sum_{i,j} P_{ij}^2 + 2|\det \vec{P}|)\). The ISHC \(|\sigma_{xy}^\pm|\) decreases in figures 5(a)–(d) and then increases in figures 5(e)–(h). The ISHC \(|\sigma_{yz}^\pm|\) increases in figures 5(a)–(d) and subsequently decreases in figures 5(e)–(h). In the cases shown in figures 5(b) and (f), \(|\sigma_{xy}^\pm| = |\sigma_{yz}^\pm|\) and both the Berry curvatures have the same peak values. The behavior of the Berry curvature in the nearly degenerate area is in agreement with our conclusions in section 4.

In the case of spherical energy dispersion (there is no nearly degenerate area), it can be shown that the Berry curvature \(\tilde{\Omega}_{xy}^\pm(\phi)\) is equivalent to \(\tilde{\Omega}_{xy}^\pm(\phi)\) shifted by \(\pi/2\). As in the non-spherical case, the Berry curvature still exhibits two significant responses along the directions of the spin-Hall current, but the shape and peak value of the Berry curvature do not change when we rotate the system. This means that \(|\sigma_{xy}^\pm| = |\sigma_{yz}^\pm|\) regardless of the orientation of the system. The magnitude of the asymmetric response function always vanishes in this case, and the ISHC is a universal constant \(e/8\pi\).

It must be emphasized that the angle \(\Theta_M\) enables us to find the maximum value of the asymmetric response function for some fixed \(\beta_i\). If we have another set of values \(\beta_i\), the corresponding maximum value of the asymmetric response function is in general different from that with \(\beta_i\). The magnitude of the ISHC may be further enhanced by tuning the spin–orbit interactions to change the maximum value of the magnitude of the asymmetric response function, but it still has an upper bound of \(e/4\pi\).

The measurable responses caused by the spin-Hall effect are very different from those in the present idealized
system, which is infinite in size and does not include impurity scattering. Measurable quantities such as the spin accumulation, however, depend on the boundary conditions. The conserved spin current considered in this paper may correspond to smooth boundaries [26]. However, the presence of impurities can drastically affect clean limit results [31–34]. In [35], it was shown that impurity scattering does not suppress the spin-Hall conductivity in the spatially random Rashba spin–orbit coupled system. In particular, the SU(2) formulation on the extrinsic mechanism of spin-Hall conductivity was recently investigated in [36]. However, the effects of a finite size and impurity scattering are beyond the scope of this paper. Hopefully, our interesting predictions of higher intrinsic ISHC will stimulate measurements in 2D semiconductor systems in the near future.

6. Equilibrium spin current and spin–orbit matrix

We now turn to discussion of the equilibrium spin current in this generic \( k \)-linear spin–orbit coupled system. In [37], it was shown that even in thermodynamic equilibrium, the spin current for the Rashba–Dresselhaus system does not vanish in the absence of external fields. This phenomena has led to many discussions on the definition of the spin current [26, 33, 38–41]. The possibility of detecting equilibrium spin currents has been studied in [39, 42].

We calculate the equilibrium spin current by using the conventional definition of spin current. In the case of a positive chemical potential (\( \mu > 0 \)), two branches are populated. In the absence of external fields, the equilibrium spin current is the sum of the in-plane spin currents of the two branches,

\[
\langle J_{ij}^y \rangle = \frac{1}{V} \sum_{nk} \hbar \mu |\langle n| \frac{1}{2} \left\{ \frac{\partial H}{\partial \hat{k}_i} - \frac{\hbar}{2} \mathbf{\sigma}_j \right\} |n\rangle,
\]

where \( i,j = x,y \) and \( |nk\rangle \) is the eigenstate of Hamiltonian equation (1). From equation (10) and \( k^+_F k^-_F = 2m\mu/\hbar^2 \), a
In agreement with [37]. In the following, we apply this in
The equilibrium spin current obtained from the covariant
The resulting color current satisfies covariant conservation.

−⟨J⟩(see appendix A). Recently, the equilibrium spin current in
fails to explain the physical meaning of det β
−⟨J⟩xy = −⟨J⟩yx = −⟨J⟩yy = −⟨J⟩yx = 0. We have ⟨J⟩yy = −(J)ey and ⟨J⟩ey = (J)ey = 0. In the pure Dresselhaus system, where βxx = −βyy = β and βxx = βyy = 0, we have ⟨J⟩yy = −(J)ey and ⟨J⟩ey = (J)ey = 0. It is interesting to note that the equilibrium spin current ⟨J⟩ey is related to the inverse of the spin–orbit matrix \( \tilde{\beta}^{-1} \) via \( \langle J \rangle_{y} = \beta \tilde{\beta}^{-1} \beta \tilde{\beta} \).

We find that det \( \tilde{\beta} \) also appears in the expression of the equilibrium spin current, equation (45). However, \( J_{y} \) occurs in the third order of \( \beta \). In this sense, equation (20) fails to explain the physical meaning of det \( \tilde{\beta} \) in this case (see appendix A). Recently, the equilibrium spin current in k-linear spin–orbit coupled systems has been found to be linked to the non-Abelian SU(2) gauge theory, where the Pauli spin matrix serves as a color index in the gauge field [43]. The resulting color current satisfies covariant conservation. The equilibrium spin current obtained from the covariant conserved color current in Rashba–Dresselhaus systems is in agreement with [37]. In the following, we apply this formalism to generic k-linear systems.

The Hamiltonian equation (1) can be written in terms of the SU(2) gauge field \( \theta \tilde{A} \), where \( A = A_{i} \hat{e}_{i} \) and \( A_{i} = A_{i}^{a} \sigma_{a} \). We have

\[
A_{i}^{a} = \frac{m}{\hbar^{2}} \beta_{a}, \\
A_{y}^{a} = \frac{m}{\hbar^{2}} \beta_{a},
\]

The equilibrium spin current denoted as \( J_{i}^{a} \) is proportional to \(-i \epsilon_{abc} A_{b}^{a} F_{c}^{y} \), where \( F_{c}^{y} \sigma_{a} = -i[A_{a}, A_{c}] \) is the field strength.

The physical meaning of det \( \tilde{\beta} \) in the equilibrium spin current is now clear. The field strength in the SU(2) non-Abelian gauge field is given by [43]

\[
F_{xy} = -i[A_{x}, A_{y}],
\]

where equation (46) is used. We have \( F_{xy}^{z} = F_{xy}^{z} = 0 \) and \( F_{xy}^{z} = \frac{m}{\hbar^{2}} (\det \tilde{\beta}) \). That is, det \( \tilde{\beta} \) plays the role of the color magnetic field strength \( F_{xy}^{z} \).

7. Conclusions
In conclusion, we have shown that in 2D and k-linear spin–orbit coupled systems, the properties of the intrinsic spin–Hall conductivity are governed by two quantities: the effective coupling of spin and orbital motion (reflected by det \( \tilde{\beta} \)) and the asymmetric response function \( (\Delta \tilde{\beta}) \). The effective coupling of spin and orbital motion is a discriminant for determining whether or not the spin–Hall conductivity vanishes. The decoupling of spin and orbital motion associated with the band-overlapping phenomenon explains the physical origin of the sign change of the intrinsic spin–Hall conductivity. Furthermore, the dependence of the spin–orbit interaction on the spin–Hall effect and the resulting unsymmetrical properties are related to the asymmetric response function, which is determined by the difference in band-splitting along two directions: those of the applied electric field and the spin–Hall current. We varied the orientation of the system and studied the variation in the Berry curvature and the corresponding spin–Hall response. We found that maximum intrinsic spin–Hall conductivity occurs along the direction of the nearly degenerate area, which also leads to maximization of the Berry curvature and the magnitude of the asymmetric response function. The position of the nearly degenerate area can be determined analytically. We also showed that the intrinsic spin–Hall conductivity has an upper bound value of \( e / 4 \pi \).

In addition, we showed that the equilibrium spin current is proportional to \( \tilde{\beta}^{-1} \partial_{y} (\det \tilde{\beta}) \), and det \( \tilde{\beta} \) determines the field strength of the SU(2) non-Abelian gauge field in the equilibrium spin current.
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Appendix A. The Foldy–Wouthuysen transformation

A unitary transformation can be generally written as \( U = e^{-iS} \), where the Hermitian matrix \( S \) can be expanded by the order of \( \beta_i \), i.e. \( S = S^{(1)} + S^{(2)} + S^{(3)} + \ldots \). That is, \( S^{(1)} \) represents the term proportional to the order of \( \beta_i \), \( S^{(2)} \) the order of \( \beta_i^2 \), and so on. Following the approach of the Foldy–Wouthuysen transformation, the Hamiltonian \( H = \varepsilon_k + H_{so} + V(x, y) \) under the unitary transformation \( U = e^{-iS} \) is given by

\[
H' = e^{iS}He^{-iS}
= \varepsilon_k + H^{(1)} + H^{(2)} + H^{(3)} + V(x, y) + \alpha(\beta_i^4),
\]

where

\[
H^{(1)} = H_{so} + [iS^{(1)}, \varepsilon_k],
\]

\[
H^{(2)} = [iS^{(2)}, \varepsilon_k] + [iS^{(1)}, H_{so}] + \frac{1}{2!}[[iS^{(1)}, [iS^{(1)}, \varepsilon_k]],
\]

\[
H^{(3)} = [iS^{(3)}, \varepsilon_k] + [iS^{(2)}, H_{so}] + \frac{1}{2!}[[iS^{(1)}, [iS^{(1)}, \varepsilon_k]],
\]

\[+ \frac{1}{2}[[iS^{(2)}, [iS^{(1)}, \varepsilon_k]], + \frac{1}{2}[[iS^{(1)}, [iS^{(1)}, H_{so}]],
\]

\[
+ \frac{1}{3!}[[iS^{(1)}, [iS^{(1)}, [iS^{(1)}, \varepsilon_k]],]]\]

Because \( H_{so} \) is an odd matrix, we have to find a matrix \( S^{(1)} \) to cancel this term. Namely, we require \( H^{(1)} = 0 \) and

\[
H_{so} + [iS^{(1)}, \varepsilon_k] = 0.
\]

On the other hand, we note that \( H_{so} \) is made up of the linear momenta \( k_i \), i.e., \( H_{so} = \sigma_x(\beta_xk_x + \beta_yk_y) + \sigma_y(\beta_yk_x + \beta_xk_y) \), and \( \varepsilon_k \) is proportional to \( k^2 \); \( S^{(1)} \) is obtained by the replacements \( k_x \to x \) and \( k_y \to y \) in \( H_{so} \). Taking into account the constant \( k^2/m \), we have

\[
ig^{(1)} = \frac{im}{\hbar}\left[\sigma_x(\beta_xx + \beta_yy) + \sigma_y(\beta_yx + \beta_xy)\right].
\]

Substituting equation (A.5) into (H.2), after a straightforward calculation, we find that the last two terms \([iS^{(1)}, H_{so}] + \frac{1}{2!}[iS^{(1)}, [iS^{(1)}, \varepsilon_k]]\) give a diagonalized form \( i\sum \beta_i^2 \) plus \( \frac{2\hbar}{\pi} \left( \det \beta \right) \sigma_xL_z \). This means that (H.2) is already diagonalized, and thus we can choose

\[
ig^{(2)} = 0.
\]

Substituting equations (A.5) and (A.6) into (H.3) (equation (A.3)), we obtain

\[
H^{(3)} = [iS^{(3)}, \varepsilon_k] - \frac{2m^2}{3\hbar} \left( \det \beta \right) \left[ \{x, L_z\}(\sigma_y\beta_{xx} - \sigma_x\beta_{xy}) + \{y, L_z\}(\sigma_y\beta_{xy} - \sigma_x\beta_{yy}) \right].
\]

We find that the term in \( \cdots \) is composed of odd matrices. Therefore, we must require \( H^{(3)} = 0 \). In this sense, the next diagonalized part is of the order of \( \beta_i^4 \).

Appendix B. Maximum and minimum band-splitting

As shown in sections 3 and 4, the value of \( \Gamma'((0, \Theta)^2 - \Gamma'(\pi/2, \Theta)^2 \) determines whether the ISHC is larger than \( e/8\pi \) or equal to \( e/8\pi \). Furthermore, if the magnitude \( |\Gamma'((0, \Theta)^2 - \Gamma'(\pi/2, \Theta)^2| \) increases upon varying \( \Theta \), the ISHC would approach a maximum value with respect to the fixed value of \( \beta_i \). We will show that the maximum value of \( |\Gamma'((0, \Theta)^2 - \Gamma'(\pi/2, \Theta)^2| \) exists for some angle \( \Theta_M \) on the Fermi surface for fixed spin–orbit interactions.

First, we show that when \( \Gamma'((0, \Theta)^2 \) reaches the maximum value for some \( \Theta_M \), \( \Gamma'(\pi/2, \Theta)^2 \) must reach the minimum at \( \Theta_M \), and vice versa. From equation (38), the condition \((d/d\Theta)\Gamma'((0, \Theta)^2 = 0 \) at some \( \Theta_M \) gives

\[
\tan(2\Theta_M) = \frac{2(\beta_x\beta_{xy} + \beta_x\beta_{yy})}{\Gamma(0)^2 - \Gamma(\pi/2)^2},
\]

where \( \Gamma(0) = \Gamma'((0, 0)^2 \) and \( \Gamma(\pi/2) = \Gamma'(\pi/2, 0)^2 \). It can also be shown that \((d/d\Theta)\Gamma'(\pi/2, \Theta)^2 \) is proportional to \( k \). On the other hand, we redefine the parameters \( A, B \) and \( C \) as \( \Gamma(0)^2 = B = \Gamma(\pi/2)^2 \) and \( C = \beta_x\beta_{xy} + \beta_x\beta_{yy} \). The second derivatives give \((d/d\Theta)^2\Gamma'((0, \Theta)^2 = 2(B - A)\cos(2\Theta) - 4C\sin(2\Theta) \) and \((d/d\Theta)^2\Gamma'(\pi/2, \Theta)^2 = 2(A - B)\cos(2\Theta) + 4C\sin(2\Theta) \) to have the form \( \Gamma'(\phi', \Theta)^2 = A^2\cos^2\phi' + B^2\sin^2\phi' \), the coefficient \( \beta'_{x}\beta'_{xy} + \beta'_{y}\beta'_{yy} \) must be zero at some \( \Theta \), and it is obtained from the equation \( \beta'_{x}\beta'_{xy} + \beta'_{y}\beta'_{yy} = 0 \) to have the form \( \Gamma'(\phi', \Theta)^2 = A^2\cos^2\phi' + B^2\sin^2\phi' \), we have

\[
\theta = \Theta_M.
\]

The energy dispersion of the \( \beta_R + \beta_s \) system is of the form \( \Delta(\phi')^2 = A^2\cos^2\phi' + B^2\sin^2\phi' \). Interestingly, it can be shown that for \( \Theta = \Theta_M \), the energy dispersion \( \Delta(\phi', \Theta) \) in general has the same form as that of the \( \beta_R + \beta_s \) system. Because we require \( \Phi'(\phi', \Theta)^2 = (\beta'_{x}\beta'_{xy} + \beta'_{y}\beta'_{yy})\sin^2\phi' + (\beta'_{x}\beta'_{xy} + \beta'_{y}\beta'_{yy})\sin(2\phi') \), we have

\[
\Delta(\phi', \Theta)^2 = A^2\cos^2\phi' + B^2\sin^2\phi',
\]

and \( \beta'_{x}\beta'_{xy} + \beta'_{y}\beta'_{yy} \) must be zero at some \( \Theta \), and it is obtained from the system. Consider the Rashba–Dresselhaus system \( \beta_R + \beta_s \).

If \( k_x \) and \( k_y \) lie along the \([100]\) and \([010]\) directions respectively, then \( \Gamma(0) = \Gamma(\pi/2) \) and \( \beta_{xx}\beta_{xy} + \beta_{yy}\beta_{xx} = 2\alpha \beta \neq 0 \). Equation (B.1) implies that \( \Theta_M = \pi/4, 3\pi/4 \). (See figure B.1.) For \( \Theta_M = \pi/4, 3\pi/4 \), the resulting dispersion in the new coordinate system is given by \( \Gamma'(\phi')^2 = (\alpha + \beta)^2\cos^2\phi' + (\alpha - \beta)^2\sin^2\phi' \) and we have \( \Gamma(0)^2 < \Gamma(\pi/2)^2 \). As a result, in order to obtain a large spin-Hall current \( (\sigma_x > e/8\pi) \), an electric field must be applied along the \( k_i \) direction because the nearly degenerate area is located at \( \Gamma(0) \). For \( \Theta_M = \pi/4, 3\pi/4 \), we have \( \Gamma'(\phi')^2 = (\alpha + \beta)^2\cos^2\phi' + (\alpha - \beta)^2\sin^2\phi', \) and in this case \( \Gamma'(\pi/2)^2 < \Gamma'(\pi/2)^2 \). The electric field must be applied along the
k′_y direction to obtain a large spin-Hall current. As shown in figure B.1, k′_y is obtained as the rotation of k′_x by π/2, and thus it is parallel to k′_z.

In the Rashba–Dresselhaus system, [110] and [110] are nonequivalent axes. The corresponding band-splitting values are 2m(α − β)/ℏ^2 and 2m(α + β)/ℏ^2. We change the coordinate (k_x, k_y) to (k′_x, k′_y) such that k′_y and k′_z are parallel to [110] and [110], respectively. In this case, we have θ_M = π/4. The resulting effective spin–orbit matrix is

$$\frac{1}{\sqrt{2}} (\alpha - \beta) \begin{pmatrix} 1 & 0 \\ -1 & 0 \end{pmatrix} + \frac{1}{\sqrt{2}} (\alpha + \beta) \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix}.$$  \[(B.2)\]  

We have \(\Gamma'(0) = (\alpha - \beta)^2\) and \(\Gamma'(\pi/2) = (\alpha + \beta)^2\). The asymmetric response function \(\Delta\beta'\) corresponding to the spin–orbit matrix in equation (B.2) is \(\Delta\beta' = -4\alpha\beta < 0\). Using equation (37), we can show that

$$\text{Re}(\lambda'_{<}/\lambda'_{>}) = -2\alpha\beta/|\alpha^2 + \beta^2 + |\alpha^2 - \beta^2|].$$  \[(B.3)\]  

For \(\alpha > \beta^2\), the ISHCs are \(\sigma_{x'x'} = (e/8\pi)(1 + \beta/\alpha)\) and \(\sigma_{y'y'} = -(e/8\pi)(1 - \beta/\alpha)\). For \(\alpha^2 < \beta^2\), the ISHCs are \(\sigma_{x'x'} = -(e/8\pi)(1 + \alpha/\beta)\) and \(\sigma_{y'y'} = (e/8\pi)(1 - \alpha/\beta)\). [44]

Let us suppose that \(\alpha > 0\) and \(\beta > 0\), and in this case, we have \(\Gamma'(0) < \Gamma'(\pi/2)\). The Rashba–Dresselhaus system has a smaller band-splitting of 2m(α − β)/ℏ^2 along the [110] direction on the Fermi surface. On the other hand, the system has a larger band-splitting (2m(α + β)/ℏ^2) along the [110] direction. When the electric field is applied along the k′_y direction ([110]), the spin-Hall response along the k′_z direction indeed has a value larger than e/8π, i.e., |\(\sigma_{x'y'}\)| > e/8π, as shown above. Interestingly, when \(\alpha\) is very close to \(\beta\) in magnitude, equation (B.3) is very close to unity. The ISHC in the Rashba–Dresselhaus system would transit from \(\sigma_{x'y'} \sim +e/4\pi\) to \(\sigma_{x'y'} \sim -e/4\pi\) upon tuning the Rashba coupling via the gate voltage [45].

The Rashba coupling and the Dresselhaus coupling are usually of the same order of magnitude in a GaAs quantum well [46]. In a II–VI semiconductor, the Rashba coupling is larger than the Dresselhaus coupling, while in a III–V semiconductor, the Dresselhaus coupling is larger than the Rashba coupling [46]. In narrow-gap compounds, Rashba coupling dominates [47].

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