

Geometric Origin of Intrinsic Spin Hall Effect in an Inhomogeneous Electric Field

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Geometric Origin of Intrinsic Spin Hall Effect in an Inhomogeneous Electric Field

In recent years, the spin Hall effect has been received great attention because of its potential application in spintronics and quantum information processing and storage. However, this effect is usually studied under the external homogeneous electric field. Understanding how the inhomogeneous electric field affects the spin Hall effect is still lacking. Here, we give the general expression for the intrinsic spin Hall conductivity in the presence of the inhomogeneous electric field, which is shown to be expressed through gauge-invariant geometric quantities. On the other hand, when people get physical intuition on transport phenomena from the wave packet, one issue appears. It is shown that the conductivity obtained from the conventional wave packet approach cannot be fully consistent with the one predicted by the Kubo-Greenwood formula. Here, we attempt to solve this problem.

Introduction The spin Hall effect (SHE) is a spin-accumulation phenomenon on the boundaries of a 2D system caused by the spin-dependent transverse deflection of the charge current [1–4]. This phenomenon has been received significant attention because it can be applied to spintronics by offering a core mechanism for the generation and detection of spin current [5, 6]. Depending on the origin of the SHE, it is categorized into the intrinsic and extrinsic SHE. While the relativistic spin-orbit coupling (SOC) plays the crucial role in both cases, the intrinsic SHE arises from the intrinsic band structure, whereas the extrinsic one is due to the impurities with large SOC [7–10]. The intrinsic SHE has been of great interest because its underlying mechanism is irrelevant to the random impurities unlike the extrinsic case and the giant spin Hall conductivity (SHC) of several materials such as Pt is presumed to be originating from this effect [6, 11–26].

While the previous works are mostly performed in spatially uniform fields, it has been noted that the application of nonuniform fields could lead to a variety of new phenomena, and even offer us access to various geometric quantities of Bloch wave functions. In an inhomogeneous electric field, the Hall conductivity is related to the Hall viscosity for Galilean invariant systems [27–29], the semiclassical equations of motion gain corrections depending on quantum metric [30], and the intrinsic anomalous Hall conductivity (AHC) is expressed through quantum metric, Berry curvature, and fully symmetric rank-3 tensor [31]. Moreover, the nonreciprocal directional dichroism, i.e., the difference of the refractive index between counterpropagating light fields, is connected with quantum metric dipole [32].

In this paper, we investigate the intrinsic SHC in the inhomogeneous field. We consider a two-dimensional two-band system respecting time-reversal symmetry to suppress the anomalous Hall effect. Using the Kubo-Greenwood formula, we obtain the leading correction to the conventional intrinsic SHC in the uniform electric field. We show that such a leading term, which is the square term of the electric field wave vector, depends on band velocity as well as gauge-invariant geometric quantities: quantum metric and interband Berry connection. For Rashba and Dresselhaus systems, we show that the

SHC under a nonuniform field is no longer a universal value. Instead, it can be adjusted by tuning the Fermi energy of the system which allows us to manipulate the spin current.

In this work, we also address an issue about the incompatibility between Kubo-Greenwood formula and semiclassical wave packet approach revealed in the anomalous Hall effect [31]. To this end, we expand the perturbed Hamiltonian in terms of vector potential rather than the scalar potential, and construct the wave packet by the superposition of wave functions in the upper and lower bands rather than the single lower band. We show that thus obtained wave packet yields the SHC and AHC consistent with the Kubo-Greenwood formula.

Generic two-band model We consider a general form of the two-dimensional two-band Hamiltonian

$$H_0(\mathbf{k}) = \frac{\hbar^2 k^2}{2m} + \sum_{i=1}^2 d_i(\mathbf{k})\sigma_i, \quad (1)$$

where $k = |\mathbf{k}| = \sqrt{k_x^2 + k_y^2}$ is the modulus of the electron momentum, σ_i is the Pauli matrix, and $d_i(\mathbf{k})$ is an arbitrary real function. The two eigenenergies of this Hamiltonian are given by $\varepsilon_{\pm, \mathbf{k}} = \hbar^2 k^2 / 2m \pm d(\mathbf{k})$, where $d(\mathbf{k}) = \sqrt{d_1^2(\mathbf{k}) + d_2^2(\mathbf{k})}$. The corresponding Bloch wave functions are obtained as $e^{i\mathbf{k}\cdot\mathbf{r}} (\pm(d_1(\mathbf{k}) - id_2(\mathbf{k}))/d, 1)^T / \sqrt{2}$. We impose the restriction $d_i(\mathbf{k}) = -d_i(-\mathbf{k})$ to reflect time reversal symmetry of our system. The Rashba and Dresselhaus Hamiltonians, representative time-reversal symmetric models, satisfy this relationship. Under such a restriction, the eigenvalues of the system are even functions of the momentum \mathbf{k} .

Spin Hall conductivity In this paper, we consider in-plane electric field polarized along the x -direction and propagating along the y -direction as illustrated in Fig. 1(a), i.e., $\mathbf{E} = E_x \hat{x} e^{iqy - i\omega t} + \text{c.c.}$ [33]. Then the induced transverse spin Hall conductivity in the static limit $\omega \rightarrow 0$ is given by the Kubo-Greenwood formula

$$\sigma_{\text{SH}}(\mathbf{q}) = \frac{-2e\hbar}{S} \sum_{\mathbf{k}} \frac{\text{Im}[\langle \hat{j}_y^z \rangle_{\mathbf{k}, \mathbf{q}} \langle \hat{v}_x \rangle_{\mathbf{k}, \mathbf{q}}^*]}{\Delta \varepsilon_{\mathbf{k}, \mathbf{q}}}, \quad (2)$$

where $-e$ is the charge of the electron, S is the area of the system. We define $\langle \hat{O} \rangle_{\mathbf{k}, \mathbf{q}} \equiv \langle u_{-, \mathbf{k}-\mathbf{q}/2} | \hat{O} | u_{+, \mathbf{k}+\mathbf{q}/2} \rangle$ and

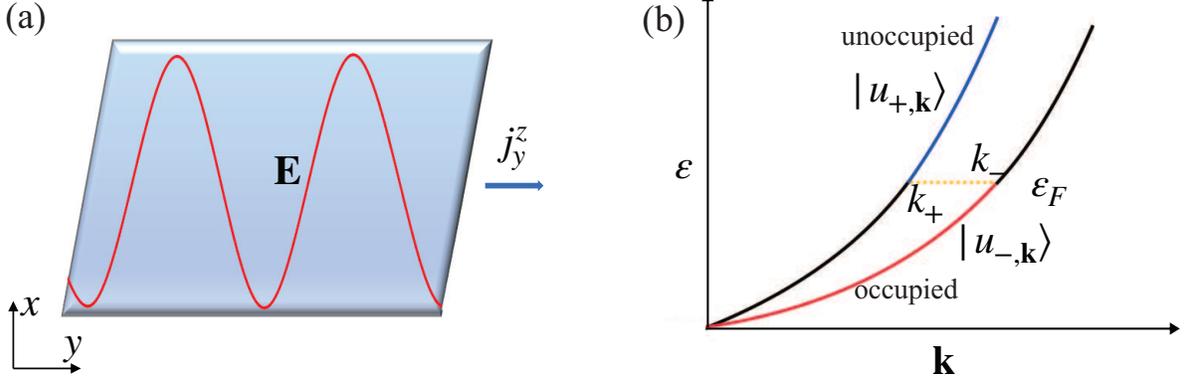


FIG. 1. (a) A two-dimensional system under consideration, where the inhomogeneous in-plane electric field is applied. Spin Hall current flows perpendicular to the polarization direction of the applied field. (b) Schematic energy bands with the Fermi energy ϵ_F higher than the nodal energy.

$\Delta\epsilon_{\mathbf{k}, \mathbf{q}} \equiv \epsilon_{-, \mathbf{k}-\mathbf{q}/2} - \epsilon_{+, \mathbf{k}+\mathbf{q}/2}$, where $|u_{\pm, \mathbf{k}}\rangle$ is the periodic part of Bloch wave functions for the upper unoccupied band (+) and the lower occupied band (-) respectively, as shown in Fig. 1(b). Here $\mathbf{q} = \hat{q}\hat{y}$ represents the momentum transfer due to the modulation of the electric field, \hat{v}_x is the velocity operator along x -direction, and $\hat{j}_y^z = \hbar\{\sigma_3, \hat{v}_y\}/4 = (\hbar^2 k_y/2m)\sigma_3$ is the spin current operator polarized perpendicular to the xy -plane and flowing along the y -direction.

In the uniform field limit ($q \rightarrow 0$), we have the conventional intrinsic SHC

$$\sigma_{\text{SH}}^{(0)} = \frac{-e\hbar^2}{mS} \sum_{\mathbf{k}} \frac{k_y}{\Delta\epsilon_{\mathbf{k}}} A_{+-}^x, \quad (3)$$

where $A_{+-}^x = i\langle u_{+, \mathbf{k}} | \partial_{k_x} | u_{-, \mathbf{k}} \rangle$ is the interband or cross-gap Berry connection [34, 35] along x -axis and $\Delta\epsilon_{\mathbf{k}} \equiv$

$\Delta\epsilon_{\mathbf{k}, 0} = \epsilon_{-, \mathbf{k}} - \epsilon_{+, \mathbf{k}}$ denotes the energy difference between two bands at a given momentum. Here the relation $\langle u_{-, \mathbf{k}} | \sigma_3 | u_{+, \mathbf{k}} \rangle = -1$ is used. While the conventional intrinsic SHC was usually described by the spin Berry curvature [17, 26], we show that it can be characterized by the interband Berry connection in the two-band model.

For nonuniform external electric field with long wavelength excitation, the SHC can be expanded as $\sigma_{\text{SH}}(q) = \sigma_{\text{SH}}^{(0)} + q\sigma_{\text{SH}}^{(1)} + q^2\sigma_{\text{SH}}^{(2)} + O(q^3)$. Due to the time-reversal symmetry of our system, the band velocity and interband Berry connection are odd functions of \mathbf{k} . As a result, the q -linear term vanishes after integration over \mathbf{k} . Then the q^2 term becomes the leading term for the deviation of the SHC from its value under uniform electric field, which is given by [36]

$$\sigma_{\text{SH}}^{(2)} = \frac{e\hbar^2}{4mS} \sum_{\mathbf{k}} k_y \left[\frac{2g_{yy}}{\Delta\epsilon_{\mathbf{k}}} A_{+-}^x + \frac{\partial_{k_y}(v_{-, y} - v_{+, y})}{\Delta\epsilon_{\mathbf{k}}^2} A_{+-}^x + \frac{v_{-, x} - v_{+, x}}{2\Delta\epsilon_{\mathbf{k}}^2} \partial_{k_y} A_{+-}^y + \frac{8\hbar^4 k_x k_y}{m^2 \Delta\epsilon_{\mathbf{k}}^3} A_{+-}^y - \frac{12\hbar^4 k_y^2}{m^2 \Delta\epsilon_{\mathbf{k}}^3} A_{+-}^x \right], \quad (4)$$

where $v_{\pm, i} = \partial_{k_i} \epsilon_{\pm, \mathbf{k}}$ is the group velocity along i -axis ($i = x, y$), $A_{+-}^y = i\langle u_{+, \mathbf{k}} | \partial_{k_y} | u_{-, \mathbf{k}} \rangle$ is the interband Berry connection with respect to k_y , and g_{yy} is the Fubini-Study quantum metric [37] for the filled band given by

$$g_{yy} = \text{Re}[\langle \partial_{k_y} u_{-, \mathbf{k}} | u_{+, \mathbf{k}} \rangle \langle u_{+, \mathbf{k}} | \partial_{k_y} u_{-, \mathbf{k}} \rangle]. \quad (5)$$

Here we have used the relation $\langle u_{\pm, \mathbf{k}} | \sigma_3 | u_{\pm, \mathbf{k}} \rangle = 0$, which means that spin-up and -down are equally distributed in the eigenstate.

Under the gauge transformation $|u_{\pm, \mathbf{k}}\rangle \rightarrow e^{i\phi_{\mathbf{k}}} |u_{\pm, \mathbf{k}}\rangle$, both the interband Berry connection and quantum metric are invariant. Therefore, the correction in (4) is also gauge-invariant. If we impose a further restriction for our system: $d_j(\mathbf{k})$ is a linear function of the momentum,

i.e., $\partial_{k_i}^2 d_j(\mathbf{k}) = 0$, our result (4) can be further simplified because $\partial_{k_i}(v_{-, i} - v_{+, i}) = 4\Delta\epsilon_{\mathbf{k}} g_{ii}$ in such a case [38].

Rashba and Dresselhaus models Let us consider the Rashba model given by $H_0^{\text{R}}(\mathbf{k}) = \hbar^2 k^2/2m + \alpha k_y \sigma_x - \alpha k_x \sigma_y$, where α is the strength of the Rashba SOC. For this system, we have interband Berry connection $A_{+-}^x = k_y/2k^2$, $A_{+-}^y = -k_x/2k^2$, and quantum metric $g_{yy} = k_x^2/4k^4$. Using (3) and (4), the SHC up to q^2 -term is evaluated as

$$\sigma_{\text{SH}}^{\text{R}}(q) = \frac{e}{8\pi} \left[1 + \frac{\hbar^4 q^2}{16m^2 \alpha^2} \left(11 - \frac{5m\alpha^2}{4\hbar^2 \epsilon_F} \right) \right], \quad (6)$$

where ϵ_F is the Fermi energy. As shown in Fig. 2(a), one can adjust the intrinsic SHC by tuning the Fermi energy,

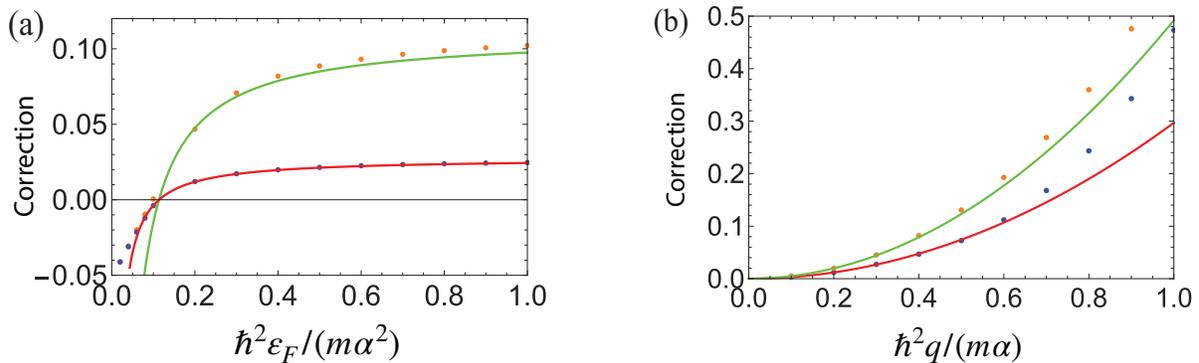


FIG. 2. The correction in unit of $e/(8\pi)$ to the spin Hall conductivity of the Rashba system as a function of (a) the Fermi energy ϵ_F and (b) the wave vector q , respectively. In (a), the green and red lines are the correction $q^2\sigma_{yx}^{(2)}$ with $\hbar^2 q/(m\alpha) = 0.4$ and $\hbar^2 q/(m\alpha) = 0.2$, respectively. In (b), the green and red lines are the correction $q^2\sigma_{yx}^{(2)}$ with $\hbar^2 \epsilon_F/(m\alpha^2) = 0.4$ and $\hbar^2 \epsilon_F/(m\alpha^2) = 0.2$, respectively. The dotted lines refer to the total correction with corresponding parameters.

unlike the uniform electric field case. This may provide us with a new way to manipulate spin current. The spin Hall conductivity (6) obtained from the geometric formula (4) matches well with the exact result from (2) as ϵ_F grows and q decreases as plotted in Fig. 2(a) and (b). Note that the perturbation method is valid for $\hbar^4 q^2/16m^2\alpha^2 \ll 1$.

If we perform the transformation: $d_1(\mathbf{k}) \leftrightarrow d_2(\mathbf{k})$ and $\alpha \rightarrow \beta$, the Rashba system changes to the Dresselhaus model with the Hamiltonian $H_0^D(\mathbf{k}) = \hbar^2 k^2/2m - \beta k_x \sigma_x + \beta k_y \sigma_y$, where β is the Dresselhaus coupling strength. Under such transformation, the band structure and quantum metric remain the same, while the interband Berry connection changes its sign: $A_{+-}^j \rightarrow -A_{+-}^j$. As a result, the SHC of the Dresselhaus system becomes

$$\sigma_{\text{SH}}^D(q) = -\frac{e}{8\pi} \left[1 + \frac{\hbar^4 q^2}{16m^2 \beta^2} \left(11 - \frac{5m\beta^2}{4\hbar^2 \epsilon_F} \right) \right]. \quad (7)$$

There is a sign difference from the result of the Rashba model.

Wave packet approach Conventionally, people get physical intuition for transport phenomena from the semiclassical analysis conducted based on the wave packet dynamics. However, it was mentioned that the AHC calculated from the single-band wave packet method could be inconsistent with the one predicted by the Kubo-Greenwood formula [31]. We show that we should construct the wave packet from two bands for the AHC or SHC to be consistent with the Kubo-Greenwood formula.

Under the presence of the external field, the Hamiltonian of the system is written as $H(\mathbf{k}) = H_0(\mathbf{k}) + H'(\mathbf{k})$. Here $H'(\mathbf{k})$ is the perturbative coupling term with the field given by

$$H'(\mathbf{k}) = e\hat{v}_x A_x, \quad (8)$$

where $A_x = (E_x/i\omega)e^{iqy-i\omega t} + \text{c.c.}$ is the vector potential. It's worth noting that in order to get the transverse

conductivity, we expand the perturbed Hamiltonian in terms of the vector potential rather than scalar potential [39].

A wave packet is usually constructed from the unperturbed Bloch wave function within a single band. However, this conventional way gives inconsistent results with the Kubo-Greenwood formula when calculating AHC [31]. Besides, as can be seen from (3) and (4), the SHC results from the interband coupling. The single-band wave packet method yields a null result for the SHC. Therefore, we use both the upper and lower bands to construct the wave packet as

$$|\psi_-(t)\rangle = \int d\mathbf{k} a(\mathbf{k}, t) e^{i\mathbf{k}\cdot\mathbf{r}} \left(|u_{-, \mathbf{k}-\mathbf{q}/2}\rangle + \frac{H'_{+-}}{\Delta\epsilon_{\mathbf{k}, \mathbf{q}}} |u_{+, \mathbf{k}+\mathbf{q}/2}\rangle \right), \quad (9)$$

where $H'_{+-} = \langle u_{+, \mathbf{k}+\mathbf{q}/2} | H'(\mathbf{k}) | u_{-, \mathbf{k}-\mathbf{q}/2} \rangle$ is the transition matrix element, and the amplitude $a(\mathbf{k}, t)$ satisfies the normalization condition $\int d\mathbf{k} |a(\mathbf{k}, t)|^2 = 1$. One can note that the Bloch wave functions in the upper band are involved in constructing the wave packet in the same manner as the first-order stationary perturbation scheme for the lower band. Similar wave packet structure can be found in Ref. [32, 40] and in the non-Abelian formulation [41].

The spin current flowing along y -direction can be evaluated as

$$j_y^z = \frac{\hbar}{2S} \sum_{\mathbf{k}_c} (\dot{R}_{y\uparrow} - \dot{R}_{y\downarrow}), \quad (10)$$

where \mathbf{k}_c is the momentum of the wave packet, and $R_{y\sigma} = \langle \psi_{-\sigma}(t) | \hat{r}_y | \psi_{-\sigma}(t) \rangle$ is the average position of the spin- σ part of the wave packet given by $|\psi_{-\uparrow}(t)\rangle = (1, 0)|\psi_-(t)\rangle$ and $|\psi_{-\downarrow}(t)\rangle = (0, 1)|\psi_-(t)\rangle$ for spin-up and -down, respectively. Since the expression $\langle \psi_{-\sigma}(t) | \hat{O} | \psi_{-\sigma}(t) \rangle$ is actually $\langle \psi_-(t) | 2\hat{O} + \text{sgn}(\sigma)\{\sigma_3, \hat{O}\} | \psi_-(t) \rangle / 4$, we have

$$\dot{R}_{y\sigma} = \langle \psi_-(t) | \hat{v}_y / 2 + \text{sgn}(\sigma) \hat{j}_y^z / \hbar | \psi_-(t) \rangle, \quad (11)$$

where $\text{sgn}(\sigma) = 1(-1)$ for spin-up(down). It is worth to note that in this paper, we use the classical form of the spin current operator $\hat{j}_y^z = \hbar\{\sigma_3, \hat{v}_y\}/4$ [9, 25] to substitute the effective spin current operator $(\hbar/2)d(\hat{r}_y\sigma_3)/dt$ [42]. Besides, for time-reversal symmetric system, there is no anomalous Hall effect, i.e., $\langle\psi_-(t)|\hat{v}_y|\psi_-(t)\rangle = 0$. Therefore in such a case, the velocities in spin-up and -down basis satisfy the relation: $\dot{R}_{y\uparrow} = -\dot{R}_{y\downarrow} = \langle\psi_-(t)|\hat{j}_y^z|\psi_-(t)\rangle/\hbar$, which indicates that the spin-up and -down part of wave packet have opposite velocity. On the other hand, for time-reversal symmetry breaking system, the charge current along y -direction is

$$j_y = \frac{-e}{S} \sum_{\mathbf{k}_c} \dot{R}_y = \frac{-e}{S} \sum_{\mathbf{k}_c} (\dot{R}_{y\uparrow} + \dot{R}_{y\downarrow}), \quad (12)$$

where $R_y = \langle\psi_-(t)|\hat{r}_y|\psi_-(t)\rangle = R_{y\uparrow} + R_{y\downarrow}$ is the position of the wave packet.

The spin current and charge current can be written in the same form $j = \frac{1}{S} \sum_{\mathbf{k}_c} \langle\psi_-(t)|\hat{j}|\psi_-(t)\rangle$, where \hat{j} is \hat{j}_y^z for spin current or $\hat{j}_y = -e\hat{v}_y$ for charge current. Substituting (9) into it, we have

$$j = \frac{1}{S} \sum_{\mathbf{k}_c} \int d\mathbf{k} a^2(\mathbf{k}, t) \frac{\langle u_{-, \mathbf{k}-\frac{\mathbf{q}}{2}} | \hat{j} | u_{+, \mathbf{k}+\frac{\mathbf{q}}{2}} \rangle H'_{+-}}{\Delta\varepsilon_{\mathbf{k}, \mathbf{q}}} + \text{c.c.} \quad (13)$$

According to Fermi's golden rule, we take ω as $-\Delta\varepsilon_{\mathbf{k}, \mathbf{q}}/\hbar$ for the transition matrix element H'_{+-} and $\Delta\varepsilon_{\mathbf{k}, \mathbf{q}}/\hbar$ for the transition matrix element H'_{-+} . Then from (8) and (13), the conductivity $j/(E_x e^{iqy - i\omega t})$ can be obtained as

$$\sigma(\mathbf{q}) = \frac{-2e\hbar}{S} \sum_{\mathbf{k}_c} \frac{\text{Im}[\langle \hat{j} \rangle_{\mathbf{k}_c, \mathbf{q}} \langle \hat{v}_x \rangle_{\mathbf{k}_c, \mathbf{q}}^*]}{\Delta\varepsilon_{\mathbf{k}_c, \mathbf{q}}}, \quad (14)$$

where $\sigma(\mathbf{q})$ represents the SHC or AHC depending on the choice of \hat{j} . Here we have taken $|a(\mathbf{k}, t)|^2 \approx \delta(\mathbf{k} - \mathbf{k}_c)$, i.e., the wave packet is sharply peaked at the momentum \mathbf{k}_c . One can note that the Kubo-Greenwood formula is reproduced from the wave packet approach, i.e., the two-band wave packet approach is compatible with the Kubo-Greenwood formula.

Discussion and conclusion In this work, we mainly restrict our system to be the time reversal symmetry. If we relax our restrictions, the leading correction to the SHC is generally the first order term of the electric field wave vector q :

$$\sigma_{\text{SH}}^{(1)} = \frac{-e\hbar^2}{2mS} \sum_{\mathbf{k}} \sum_{s=\pm} k_y \left[\frac{v_{s,y}}{\Delta\varepsilon_{\mathbf{k}}^2} A_{+-}^x - \frac{v_{s,x}}{2\Delta\varepsilon_{\mathbf{k}}^2} A_{+-}^y \right], \quad (15)$$

where the interband Berry connection A_{+-} is generally not an odd function of \mathbf{k} . If we break the time-reversal symmetry by adding the mass term $M\sigma_3$ to our Hamiltonian, we have $\sigma_{\text{SH}}^{(1)} = (e\hbar^2/2mS) \sum_{\mathbf{k}, s} k_y \sigma_{-+} [(v_{s,y}/\Delta\varepsilon_{\mathbf{k}}^2) \text{Re}A_{+-}^x -$

$(v_{s,x}/2\Delta\varepsilon_{\mathbf{k}}^2) \text{Re}A_{+-}^y]$, where $\sigma_{-+} = \langle u_{-, \mathbf{k}} | \sigma_3 | u_{+, \mathbf{k}} \rangle = -d(\mathbf{k})/\sqrt{d(\mathbf{k})^2 + M^2}$.

Here, we investigate the system with two-by-two Hamiltonian. One future direction would be to study the intrinsic SHE for the system with four-by-four Dirac Hamiltonian $H(\mathbf{k}) = \varepsilon_0(\mathbf{k}) + \sum_{i=1}^5 d_i(\mathbf{k})\Gamma_i$ [7, 8], where $\varepsilon_0(\mathbf{k})$, $d_i(\mathbf{k})$ are real functions of the momentum \mathbf{k} , and Γ_i are four-by-four Dirac matrices satisfying the anti-commutation relations $\{\Gamma_i, \Gamma_j\} = 2\delta_{ij}$. Another direction would be to investigate how the SHC is modified under the presence of the external inhomogeneous electric field for the Hamiltonian $H(\mathbf{k}) = \sum_{i=1}^5 d_i(\mathbf{k})\Gamma_i + \sum_{i<j=1}^5 d_{ij}(\mathbf{k})\Gamma_{ij}$ [43], where $\Gamma_{ij} = [\Gamma_i, \Gamma_j]/(2i)$.

The SHC formula of the Rashba and Dresselhaus models can be tested in many materials hosting Rashba type SOC such as (i) 2D interfaces of InAlAs/InGaAs [44] and LaAlO₃/SrTiO₃ [45] and (ii) surfaces of heavy materials like Au [46] and BiAg(111) [47, 48]. By using the well-known experimental techniques probing intrinsic spin Hall effect [4, 7, 9, 49, 50], we expect to detect the intriguing Fermi level-dependence of the q^2 -term of the SHC under the spatially modulating electric field by tuning its wavelength.

In summary, we have studied the intrinsic spin Hall conductivity for a two-dimensional time-reversal symmetric system under an inhomogeneous electric field. We have derived a general formula for the leading correction, which is second-order in the electric field wave vector, to the conventional intrinsic spin Hall conductivity under the uniform electric field and showed that it is determined by the gauge-invariant geometric quantities: quantum metric and interband Berry connection. We have showed that for Rashba and Dresselhaus systems, the inhomogeneous intrinsic spin Hall conductivity is adjustable with the Fermi energy and the electric field wave vector. We have demonstrated that the incompatibility between the conventional wave packet description and the Kubo-Greenwood formula can be addressed by the modified wave packet approach.

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