Strong spin-Hall and Nernst effects in a \(p\)-band semimetal

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Abstract

Since spin currents can be generated, detected, and manipulated via the spin Hall effect (SHE), the design of strong SHE materials has become a focus in the field of spintronics. Because of the recent experimental progress also the spin Nernst effect (SNE), the thermoelectrical counterpart of the SHE, has attracted much interest. Empirically strong SHEs and SNEs are associated with \(d\)-band compounds, such as transition metals and their alloys – the largest spin Hall conductivity (SHC) in a \(p\)-band material is \(\sim 450 \, (h/e) \, (\Omega \cdot \text{cm})^{-1}\) for a Bi-Sb alloy, which is only about a fifth of platinum. This raises the question whether either the SHE and SNE are naturally suppressed in \(p\)-bands compounds, or favourable \(p\)-band systems were just not identified yet. Here we consider the \(p\)-band semimetal InBi, and predict it has a record SHC \(\sigma_{xy}^z \approx 1100 \, (h/e) \, (\Omega \cdot \text{cm})^{-1}\) which is due to the presence of nodal-lines in its band structure. Also the spin-Nernst conductivity \(\alpha_{yx}^y \approx 1.2 \, (h/e) \, (A/m \cdot K)\) is very large, but our analysis shows its origin is different as the maximum appears in a different tensor element. This insight gained on InBi provides guiding principles to obtain a strong SHE and SNE in \(p\)-band materials and establishes a more comprehensive understanding of the relationship between the SHE and SNE.

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The joint utilisation of the spin and charge degree of freedom in solids is the main target of spintronics, in which the spin current generation, detection, and manipulation are the three crucial objectives [1–3]. The spin Hall effect (SHE) provides an effective technology to convert the charge current into a pure spin current, where an applied electric field can generate a transverse spin current with the spin polarization perpendicular to both the spin and charge currents [4–7]. Vice versa, the inverse SHE provides an effective method to manipulate the spin current without a magnetic field [5, 8]. Due to this versatility the SHE has attracted extensive interest in recent years, and much effort has been devoted to the theoretical understanding and engineering of strong SHE materials [6, 8–13].

In general the SHE has two distinct origins, an extrinsic contribution from the scattering and an intrinsic one from the band structure. The intrinsic part can be formulated via the spin Berry curvature (SBC) similar to the anomalous Hall effect [7, 14, 15]. Apart from the SHE, a transverse spin current can be generated by a temperature gradient instead of an electric field, which constitutes the spin Nernst effect (SNE) [16–18]. The SNE can also be formulated via the Kubo formula approach based on the electronic band structure [9, 10, 15, 19–24]. Thus the electronic band structure plays a crucial role in searching and designing strong SHE and SNE materials.

Though the precise reason is not clear to date, empirically materials with a strong SHE are primarily dominated by $d$-orbital-related compounds [7, 12, 13, 25, 26] such as $5d$-transition metals and alloys. The largest spin Hall conductivity (SHC) found in $p$-band materials is in a Bi-Sb alloy [27, 28] at only around 450 ($\hbar/e/(\Omega \cdot cm)^{-1}$). Very recently, it was found that the nodal line band structure could generate strong SHCs because of the large local SBC [29, 30]. Employing this guiding principle, we theoretically predict a large intrinsic SHC of about 1100 ($\hbar/e/(\Omega \cdot cm)^{-1}$) in the $p$-band semimetal InBi. Substitution of the electric field by a temperature gradient, reveals a large spin Nernst conductivity (SNC) of about 1.2 ($\hbar/e/(A/m \cdot K)$) at 300 K. This shows that the SNE and SHE can be strongly enhanced by the topological band structure, and that the large SNC and SHC need not be intrinsically weak in cheaper and therefore commercially more attractive $p$-band materials. Though both the intrinsic SHE and SNE can be understood from the SBC, their largest value appears at different tensor elements, implying different origins.

To understand the effect of the nodal line band structure on the SHE and especially the SNE, we first consider two simple systems by effective model Hamiltonians. From the
FIG. 1. **Band structure, SHC, and SNC in the effective BHZ model.** (a) Nodal line energy dispersion of the high symmetry effective BHZ model without the inclusion of SOC. (b) SOC breaks the nodal line with opening a global band gap after SOC is taken into consideration. The distribution of SBC and SNBC at charge neutral point are given above and below the energy dispersion. (c-d) Energy-dependent SHC and SNC, respectively. (e-h) The same as (a-d) but for the symmetry-reduced model. The color bars are in arbitrary units.

high-symmetry Benervig-Hughes-Zhang (BHZ) model for quantum spin Hall insulators [31], where \( s_z \) is maintained as a good quantum number (see the method section), the band structure is presented as a nodal line without considering spin-orbit coupling (SOC). As soon as SOC is taken into consideration, the linear band crossing is gapped and leads to a quantized spin Hall conductance in the band gap [29]. Though the spin Hall conductance reaches the maximum value at the charge neutral point, the spin Nernst conductance is zero there because of the electron and hole symmetry. Comparing the SBC and spin Nernst Berry curvature (SNBC) distribution in reciprocal space, it is found that the SNBC is zero at any \( k \)-point, while the SBC has a strong hot ring from the nodal-line-like band anti-crossing (see Fig. 1(b)). From Eq. (4), one can find that the SNBC is actually a redistribution of the SBC because of the temperature effect, which should be cancelled out by the electron-hole symmetry. To break the electron-hole symmetry, we have reduced the symmetry of the effective model Hamiltonian, making the system non-insulating. Compared to the high-symmetry model, the nodal line in the symmetry-reduced model has a dispersion in energy...
space, and the Fermi velocities are different along the $x$ and $y$ directions. As there is no global gap, the spin Hall conductance is not quantized anymore (Figs. 1(f–g)). Meanwhile, a finite spin Nernst conductance appears at the charge neutral point. In Figs. 1(b,f), we also analysed the SBC and SNBC distribution in the $k_x - k_y$ plane. Because of the dispersion of the nodal ring, the high intensity of the SBC changes from a hot ring to two hotspots, resulting in a non-zero SNBC, as presented in the lower panel of Fig. 1(f). By integrating the SNBC, one can obtain a non-zero spin Nernst conductance at the charge neutral point. Therefore, the non-zero SNC must break the balance of the SHC distribution in energy space.

**FIG. 2.** **Lattice and electronic band structure for InBi.** (a) Tetragonal lattice structure in InBi with space group $P4/nmm$. The lattice parameters are $a = b = 4.9846$ Å and $c = 4.8116$ Å. (b) Nodal line distribution in BZ. Here only the nodal lines without the inclusion of SOC are shown, and they are gapped out by SOC. (c-d) Energy dispersion without and with the inclusion of SOC. The nodal ring linear band crossings in $k_z = 0$, $k_{x,y} = 0$, and $k_x \pm k_y = 0$ planes, are labeled by orange, cyan, and green circles, respectively, in (c). The band anticrossing opened by SOC on the $\Gamma$-$M$ is also labeled by an orange circle. The nodal line on $\Gamma$-$Z$ is highlighted by magenta. The transition point of band occupation are labeled by black dots in (d).

The specific material InBi has been reported to exhibit nonsymmorphic symmetry-protected nodal lines at the edge of the Brillouin zone (BZ) [32]. However, these kinds of nodal lines are just band degeneracies from band folding between different BZs. According
to previous studies, this kind of nodal line normally does not exhibit any topological charge or SBC and, therefore, cannot generate the SHE and SNE [30]. In the current work, we find another type of nodal line inside the BZ protected by mirror symmetry and rotation symmetry, which generates a strong SHE and SNE. As shown in Fig. 2 (b), there are four classes of nodal lines, located in the high-symmetry planes of $k_{x,y}=0$, $k_{z}=0$, and $k_{x} \pm k_{y}=0$, and high-symmetry line of $\Gamma - Z$, respectively. Without including the SOC, the inverted bands have opposite mirror eigenvalues of 1 and -1, respectively, in the planes of $k_{x,y}=0$, $k_{z}=0$, and $k_{x} \pm k_{y}=0$, leading to the double degeneracy (not considering the spin degree of freedom) of nodal line linear band crossings. Along the high-symmetry line of $\Gamma - Z$, the double band degeneracy (highlighted by magenta in Fig. 2(c)) is due to the $c_{4}$ rotation symmetry with respect to the $z$-axis. As long as SOC is taken into consideration, the spin rotation symmetry is broken and the linear band crossings are also gapped out, as indicated in Figs. 2(c-d). This kind of band anti-crossing from the SOC is often accompanied by strong band entanglements and yields a large SBC.

FIG. 3. **SHC and SNC in InBi.** (a, b) Energy dependent SHC and SNC for the three independent tensor elements. (c,d) The evolution of SHC and SNC as the function of temperature. The solid curves and empty circles in (d) are from equation (4) and Mott relation, respectively.

The SHC($\sigma_{i,j}^{k}$) and SNC($\alpha_{i,j}^{k}$; $i, j, k = x, y, z$) are $3 \times 3 \times 3$ tensors, representing the spin
current $\vec{J}^k_{si}$ generated by the electric field $\vec{E}$ via $\vec{J}^k_{si} = \sum_j \sigma^k_{ij} \vec{E}_j$ and temperature gradient $\vec{\nabla}T$ by $\vec{J}^k_{si} = \sum_j \alpha^k_{ij} \vec{\nabla}T_j$, where $\vec{J}^k_{si}$ flows along the $i$-direction with the spin-polarization along the $k$-direction, and $\vec{E}_j$ and $\vec{\nabla}T_j$ are the $j$-component of the electric field $\vec{E}$ and temperature gradient $\vec{\nabla}T$, respectively. Based on linear response theory, for the specific space group $P4/nmm$, there are only three independent tensor elements for both the SHC and SNC tensor \[33–35\]:

$$X^x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & X^x_{yz} \\ 0 & -X^y_{xz} & 0 \end{pmatrix}, \quad X^y = \begin{pmatrix} 0 & 0 & -X^x_{yz} \\ 0 & 0 & 0 \end{pmatrix}, \quad X^z = \begin{pmatrix} 0 & X^z_{xy} & 0 \\ -X^z_{xy} & 0 & 0 \end{pmatrix}$$

(1)

where $X=\sigma$ and $\alpha$ represent the SHC and SNC, respectively. Therefore, there are only three independent non-zero elements, following the relation of $X^z_{xy} = -X^z_{yx}$, $X^y_{zx} = -X^x_{zy}$, and $X^x_{yz} = X^y_{xz}$.

Our calculations are fully consistent with the symmetry analysis. From the energy-dependent SHC (Fig. 3(a)), one can see that the largest tensor element appears at $\sigma^z_{xy}$, which can reach up to about 1100 ($((\hbar/e)(\Omega \cdot cm)^{-1}$). Thus far, this is the only SHC above 1000 ($((\hbar/e)(\Omega \cdot cm)^{-1}$) in the reported $p$-orbital compounds. This large value is robust in a large energy window from $E_0-0.5$ eV to the charge neutral points in the hole-doped range. Therefore, hole doping is preferred from the SHE point of view. Furthermore, we find that the SHC is robust with respect to temperature. The SHC only varies less than 5% from 0 K to room temperature, which is very similar to that in platinum [16].

From the above model analysis, we already know that a large SHC does not imply a large SNC. To obtain a large SNC, the balance of the SHC distribution in energy space must be broken. Based on this understanding, the robustness of the SHC in energy space is not beneficial for the SNE, and a large SNC should not appear at $\alpha^z_{xy}$. Indeed, the tensor element of $\alpha^z_{xy}$ is very small, at about 0.2 ($((\hbar/e)(A/m \cdot K)$) at 300 K. However, a quite large SNC is achieved at $\alpha^z_{xy}$, which can reach up to about 1.2 ($((\hbar/e)(A/m \cdot K)$) at 300 K. Because the SNE is very sensitive to temperature, we also analysed the evolution of the SNC as a function of temperature. As presented in Fig. 3(c), $\alpha^z_{xy}$ is near-zero at low temperatures below 100 K, and the $\alpha^y_{zx}$ and $\alpha^z_{xy}$ are also small ($\sim 0.5 ((\hbar/e)(A/m \cdot K))$. All three components increase steadily with temperature, but $\alpha^y_{zx}$ and $\alpha^z_{xy}$ increase much faster.
TABLE I. SHC, SHA, SNC, and SNA for InBi and Pt. The chemical potential is at charge neutral point, and the temperature is 300 K. The unit for SHC and SNC are \((h/e)(\Omega \cdot cm)^{-1}\) and \(((h/e)(A/m \cdot K))\), respectively.

|        | SHC | SHA | SNC | SNA  |
|--------|-----|-----|-----|------|
| InBi   | X_{xy}^z | 1100 | 0.3 | 0.2  | 0.04 |
| Pt     | X_{xy}^z | 2200 | 0.11| 3.0  | 0.20 |

than \(\alpha_{xy}^z\). This is the reason why \(\alpha_{xy}^z\) is so small even above 300 K.

For the conversion efficiency of the charge and heat current to the spin current not only the absolute values of the SHC and SNC are important, but also the spin Hall angle (SHA) and the spin nernst angle (SNA). Due to the lack of experimental values for the electrical conductivity and thermopower of InBi film, we have just used the bulk values to estimate the SHA and SNA. Because of the large SHC \((\sigma_{xy}^z)\) and small charge conductivity \[36\], the SHA \((\theta_{SH,xy}^z)\) can reach up to 0.3 (see Table I). Hence, the SHA in InBi is close to or even larger than that in the 5d transition metals of Pt, W, and Ta. Similarly, in combination with a large SNC and low thermalpower, the SNA can reach up to 0.21 and 0.28 for \(\theta_{SN,yz}^y\) and \(\theta_{SN,xz}^y\), respectively. It should be noted that the thermalpower in bulk is normally much larger than that in film form, so the SNA should also be much larger.

At low temperature, the SNC can be understood from the Mott relation as the derivative of the SHC with respect to energy \[37\] [38]:

\[
\alpha_{ij}^k = -\frac{\pi^2 k_B^2 T}{3e} \frac{\partial \sigma_{ij}^k(E)}{\partial E}
\]

At a temperature of about 10 K, the SNC from both the Mott relation and SNBC formalism converge to about zero. From Fig. 3 (c), one can easily see that the ANC from the two different formalisms of formula (2) and (3) agree very well with each other at low temperatures from 10 to 100 K. As the slopes of the energy-dependent SHC for \(\sigma_{xz}^y\) and \(\sigma_{yz}^x\) are significantly sharper than that in \(\alpha_{xy}^z\), \(\alpha_{xz}^y\) and \(\alpha_{yz}^x\) are much larger than \(\alpha_{xy}^z\) at temperatures far away from 0 K.

From Eqs. (3) and (4), one can see that the intrinsic SHC and SNC can be understood as the integral of the SBC and SNBC in the whole BZ. As the maximum elements are different
FIG. 4. **Local Berry curvature** $\Omega_{xy}^{S,z}(\vec{k})$ and $\Omega_{xy}^{SN,z}(\vec{k})$ **distribution on high symmetry planes** (a-c) and (d-f) are SBC and SNBC distribution on the three planes of $k_z=0$, $k_y=0$, and $k_x+k_y=0$ planes, respectively. The nodal lines are also shown by orange, cyan, green circles, and magenta curves, respectively. The color bars are in arbitrary units.

For the SHC and SNC, we choose the SBC and SNBC from two different components of $\sigma(\alpha)_{xy}^z$ and $\sigma(\alpha)_{xx}^y$ to observe their distribution and temperature effect for the evolution from the SBC to SNBC. From the above band structure analysis, we know that the special band structures mainly focus on the high-symmetry planes of $k_{x,y}=0$, $k_z=0$, and $k_x \pm k_y=0$, and high-symmetry line of $\Gamma - Z$. Therefore, we have analysed the SBC and SNBC distribution in all the three planes of $k_{x,y}=0$, $k_z=0$, and $k_x+k_y=0$.

First, we analysed the component of $\Omega_{xy}^{S,z}$, which contributes to the large tensor element for the SHC. Fixing the energy at the charge neutral point, as shown in Fig. 4(a), the large SBC in the $k_z=0$ plane is mainly dominated by the $\Gamma$-centred nodal ring. In addition, there exist other hotspots on the $\Gamma-M$ line near the $M$ point, which is not exactly located...
on the nodal ring. This is because the SBC is indeed determined by the band structure with the SOC. The gapless linear band crossing transforms to a band anti-crossing by the SOC. Comparing the linear crossing point $K1$ (highlighted by orange circle) in Fig. 2(b) and the corresponding band anti-crossing point $K1'$ in Fig. 2(c), we can find that the $K1'$ is much closer to the $M$ point than $K1$. Therefore, the hotspots along $\Gamma$-$M$ do not exactly lie on the corner of the gapless nodal ring. In addition, the Fermi level does not lie in the band gap of the band anti-crossing but slightly cuts the conduction band, which also implies the strong entanglement between the conduction and valence band around the band anti-crossing points.

Meanwhile, in the $k_y=0$ plane, there are two types of hotspots, one from the nodal ring in the $k_y=0$ plane and the other on the line $Z$-$\Gamma$-$Z$. The $\Omega_{x'y}^{S,z}$ from the nodal line on $Z$-$\Gamma$-$Z$ is much larger, which is related to the magenta bands in Figs. 2(c–d). There are also two types of hotspots in the $k_x + k_y=0$ plane, one from $Z$-$\Gamma$-$Z$ as that in the $k_y=0$ plane and the other from the $Z$-point-centred nodal ring. From Figs. 4(b–c), one can find some empty parts with a zero SBC and shape edge transition, such as the $\Gamma$- and $Z$-centred areas. This is due to the shape evolution of the band occupation, such as the band around the $\Gamma$ point, as shown in Fig. 2(d). For the $k$ point from $R$ to $\Gamma$, the valence band changes from an occupied band to a non-occupied band after a transition $k$ point (highlighted by the black dot). Similar behaviour is also exhibited for the other areas with an empty SBC.

After taking the temperature effect into consideration, the SNBC ($\Omega_{x'y}^{SN,z}$) also mainly originates from the four classes of nodal lines as that for the SBC. The main difference is that the shape edge transitions in the empty SBC areas are replaced by the hotspot of the SNBC (see Figs. 4(d–f)). This is because the temperature effect smoothens considerably the transition of the band occupation, and the shape transition of the SBC around the edge of the empty area yields a large SNBC.

Similar to $\Omega_{x'y}^{S,z}$, the component of $\Omega_{x'x}^{S,y}$ is dominated by the four classes of nodal lines, but the volume of the negative part is larger than that of $\Omega_{x'y}^{S,z}$ (see Figs. 5(a–c)), leading to a relatively smaller absolute value for the SHC tensor element $\sigma_{yx}^y$. As the negative SNBC($\Omega_{x'x}^{NS,y}$) primarily originates from the sharp transition of the SBC around the edge of the zone with an empty SBC, the small magnitude of $\Omega_{x'y}^{S,y}$ generates a relatively small SNBC for the same tensor component. Comparing Figs. 4 and 5, the $\Gamma$-centred negative hot rings for $\Omega_{x'y}^{SN,z}$ in Figs. 4(d) and (f) are almost invisible in Figs. 5(d) and (f) for $\Omega_{x'x}^{SN,y}$. 

FIG. 5. Local Berry curvature distribution on high symmetry planes for the component of $\Omega_{S,y}^{z}(\vec{k})$ and $\Omega_{SN,y}^{z}(\vec{k})$ (a-c) and (d-f) are SBC and SNBC distribution on the three planes of $k_z=0$, $k_y=0$, and $k_x+k_y=0$ planes, respectively. The nodal lines are also shown by orange, cyan, green circles, and magenta curves, respectively. The color bars are in arbitrary units.

Moreover, the $\Gamma$-centred negative hot ring for $\Omega_{SN,y}^{z}$ in Fig. 5(e) is also considerably weaker than $\Omega_{xy}^{SN,z}$ in Fig. 5(d). Because both components of $\alpha_{xy}^z$ and $\alpha_{yz}^x$ are positive values, the smaller negative $\Omega_{SN,y}^{z}$ directly leads to a larger $\alpha_{xy}^z$ in comparison to $\alpha_{yz}^x$.

In summary, from our calculations we predict a large SHC and SNC in the $p$-band semimetal InBi. Due to the contribution of the nodal lines in the band structure of InBi, the $\sigma_{zy}^x$ component of the SHC can reach up to about 1100 ($\hbar/e (\Omega \cdot cm)^{-1}$), the only SHC above 1000 ($\hbar/e (\Omega \cdot cm)^{-1}$) in the reported $p$-band systems. In contrast to the intuition that a large SHC is always accompanied by a large SNC, we find that the largest value for the SHC and SNC appear in a different third-order tensor element. The size of the SNC is mainly dependent on the breaking of the balance of the SHC distribution in energy space.
and gives the largest SNC of about 1.2 \((\hbar/e)(A/m\cdot K)\) at the tensor element \(\alpha_{zx}^y\), which is close to that in the 5d transition metal platinum. These results on InBi provide more general guiding principles to obtain a strong SHE and SNE in commercially more attractive \(p\)-band compounds and establishes a more comprehensive understanding of the relationship between the SHE and SNE in these materials.

**Method** First-principles calculations were performed using the localized atomic orbital basis and the full potential, as implemented in the Full Potential Local Orbital code (FPLO) \(^{39}\). Exchange and correlations are considered in the generalized gradient approximation, following the Perdew–Burke–Ernzerhof parametrization scheme \(^{40}\). We employed the experimental lattice constants in all our calculations \(^{32}\). We constructed a high-symmetry tight binding Hamiltonian by projecting the Bloch states onto atomic orbital-like Wannier functions and computed the SHC by the linear-response Kubo formula approach \(^{7,15}\):

\[
\sigma_{ij}^k = e \int_{BZ} \frac{d\vec{k}}{(2\pi)^3} \sum_n f_{nk}\Omega_{n,ij}^S(k),
\]

\[
\Omega_{n,ij}^S(k) = -2Im \sum_{n \neq n'} \frac{\langle n\vec{k}|J_i|n'\vec{k}\rangle \langle n'\vec{k}|v_j|n\vec{k}\rangle}{(E_{nk} - E_{n'k})^2},
\]

where \(f_{nk}\) is the Fermi–Dirac distribution for the \(n\)-th band. \(J_i^k = \frac{1}{2}\{v_i, s_k\}\) is the spin current operator with spin operator \(s\), velocity operator \(v_i\), and \(i,j,k = x,y,z\). \(|n\vec{k}\) is the eigenvector for the Hamiltonian \(H\) at eigenvalue \(E_{nk}\). \(\Omega_{n,ij}^S(k)\) is referred to as the SBC for the \(n\)-th band at point \(\vec{k}\) in analogy to the ordinary Berry curvature. The SNC is calculated via

\[
\alpha_{ij}^k = \frac{1}{T} \int_{BZ} \frac{d^3k}{(2\pi)^3} \sum_n \Omega_{n,ij}^S(k)[(E_n - E_F)f_{nk} + k_BT\ln(1 + \exp \frac{E_n - E_F}{k_BT})],
\]

A 500 \(\times\) 500 \(\times\) 500 \(k\)-grid in the BZ was used for the integral of the SHC and SNC. For convenience, we call \(\Omega_{n,ij}^{SN,k} = \Omega_{n,ij}^S(k)[(E_n - E_F)f_{nk} + k_BT\ln(1 + \exp \frac{E_n - E_F}{k_BT})]\) the SNBC.

The BHZ model \(^{31}\) around the \(\Gamma\) point is written in the form of

\[
H_{\text{eff}}(\vec{k}) = \begin{pmatrix} H(\vec{k}) & H^*(-\vec{k}) \\ H^*(\vec{k}) & H(\vec{k}) \end{pmatrix}
\]

\[
H(\vec{k}) = \varepsilon(\vec{k}) + d_i(\vec{k})\sigma_i
\]

where \(\sigma_i\) are the Pauli matrices, \(d_1 + id_2 = A(k_x + ik_y)\), and \(d_3 = M - B(k_x^2 + k_y^2)\). In our calculations, for Figs. 1(a–c), we have set the parameters of \(A = -0.1\ \text{eV}\ \hbar, B = -0.5\ \text{eV}\).
\[ A^2, \text{ and } M = 0.1 \text{ eV}. \]

In order to obtain a non-zero SNC, we break the balance of the SHC by reducing the symmetry:

\[
H_{\text{eff}}(\vec{k}) = \begin{pmatrix}
H'(\vec{k}) & 0 \\
0 & H'^*(-\vec{k})
\end{pmatrix}
\]

where

\[
H'(\vec{k}) = d'_1\sigma_1 + d'_2\sigma_2 + \begin{pmatrix}
M_1 - (B_1k_x^2 + B_2k_y^2) & 0 \\
0 & -[M_2 - (B_2k_x^2 + B_1k_y^2)]
\end{pmatrix}
\]

(6)

where \(d'_1 + id'_2 = A_1k_x + iA_2k_y\). The parameters are \(A_1=0.05\) eV Å, \(A_2=0.1\) eV Å, \(B_1=-1\) eV Å\(^2\), \(B_2=-0.5\) eV Å\(^2\), \(M_1=-0.3\) eV, and \(M_1=-0.5\) eV.

To perform the integral in the whole BZ, we projected the continuous \(\vec{k} \cdot \vec{p}\) model to the lattice by the replacement of \(k_i = (1/a)\sin(ak_i)\) and \(k_i^2 = (2/a^2)(1 - \cos(ak_i))\) with lattice constant \(a=1\) Å.

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[1] S. A. Wolf, D. D. Awschalom, R. A. Buhrman, J. M. Daughton, S. v. Molnr, M. L. Roukes, A. Y. Chtchelkanova, and D. M. Treger, “pintronics: A spin-based electronics vision for the future,” Science, vol. 294, p. 1488, 2001.

[2] I. Zutic, J. Fabian, and S. Sarma, “Spintronics: Fundamentals and applications,” Reviews of Modern Physics, vol. 76, p. 323, 2004.

[3] S. Bader and S. Parkin, “Spintronics,” Annual Review of Condensed Matter Physics, vol. 1, p. 71, 2010.

[4] M. I. Dyakonov and V. I. Perel, “Possibility of orienting electron spins with current,” Journal of Experimental and Theoretical Physics Letters, vol. 13, p. 467, 1971.

[5] J. E. Hirsch, “Spin hall effect,” Physical Review Letters, vol. 83, p. 1834, 1999.
[6] Y. K. Kato, R. C. Myers, A. C. Gossard, and D. D. Awschalom, “Observation of the spin hall effect in semiconductors,” *Science*, vol. 306, p. 1910, 2004.

[7] J. Sinova, S. O. Valenzuela, J. Wunderlich, C. Back, and T. Jungwirth, “Spin hall effects,” *Rev. Mod. Phys.*, vol. 87, p. 1213, 2015.

[8] S. O. Valenzuela and M. Tinkham, “Direct electronic measurement of the spin hall effect,” *Nature*, vol. 442, p. 176, 2006.

[9] S. Murakami, N. Nagaosa, and S.-C. Zhang, “Dissipationless quantum spin current at room temperature,” *Science*, vol. 301, p. 1348, 2003.

[10] J. Sinova, D. Culcer, Q. Niu, N. A. Sinitsyn, T. Jungwirth, and A. H. MacDonald, “Universal intrinsic spin hall effect,” *Physical Review Letters*, vol. 92, p. 126603, 2004.

[11] G. Y. G. Yao, Y. Yao, and Q. Niu, “Ab initio calculation of the intrinsic spin hall effect in semiconductors,” *Physical Review Letters*, vol. 94, p. 226601, 2005.

[12] T. Tanaka, H. Kontani, M. Naito, T. Naito, D. S. Hirashima, K. Yamada, and J. Inoue, “Intrinsic spin Hall effect and orbital Hall effect in 4d and 5d transition metals,” *Phys. Rev. B*, vol. 77, p. 165117, Apr. 2008.

[13] A. Hoffmann, “Advances in magnetics: Spin hall effects in metals,” *IEEE Transactions on Magnetics*, vol. 49, p. 5172, 2013.

[14] N. Nagaosa, J. Sinova, S. Onoda, A. H. MacDonald, and N. P. Ong, “Anomalous hall effect,” *Reviews of Modern Physics*, vol. 82, p. 1539, 2010.

[15] D. Xiao, M.-C. Chang, and Q. Niu, “Berry phase effects on electronic properties,” *Rev. Mod. Phys.*, vol. 82, pp. 1959–2007, July 2010.

[16] S. Meyer, Y.-T. Chen, S. Wimmer, M. Althammer, T. Wimmer, R. Schlitz, S. Geprags, H. Huebl, D. Kdderitzsch, H. Ebert, G. E. W. Bauer, R. Gross, and S. T. B. Goennenwein, “Observation of the spin nernst effect,” *Nature Materials*, vol. 16, p. 977, 2017.

[17] P. Sheng, Y. Sakuraba, Y.-C. Lau, S. Takahashi, S. Mitani, and M. Hayashi, “The spin nernst effect in tungsten,” *Science advances*, vol. 3, no. 11, p. e1701503, 2017.

[18] D.-J. Kim, C.-Y. Jeon, J.-G. Choi, J. W. Lee, S. Surabhi, J.-R. Jeong, K.-J. Lee, and B.-G. Park, “Observation of transverse spin nernst magnetoresistance induced by thermal spin current in ferromagnet/non-magnet bilayers,” *Nature Communications*, vol. 8, no. 1, p. 1400, 2017.

[19] B. A. Bernevig and S.-C. Zhang, “Intrinsic spin hall effect in the two-dimensional hole gas,”
[20] S.-g. Cheng, Y. Xing, Q.-f. Sun, and X. Xie, “Spin nernst effect and nernst effect in two-dimensional electron systems,” Physical Review B, vol. 78, no. 4, p. 045302, 2008.

[21] G. E. W. Bauer, E. Saitoh, and B. J. v. Wees, “Spin caloritronics,” Nature Materials, vol. 11, p. 391, 2012.

[22] K. Tauber, M. Gradhand, D. V. Fedorov, and I. Mertig, “Extrinsic spin nernst effect from first principles,” Physical review letters, vol. 109, no. 2, p. 026601, 2012.

[23] K. Tauber, D. V. Fedorov, M. Gradhand, and I. Mertig, “Spin hall and spin nernst effect in dilute ternary alloys,” Physical Review B, vol. 87, no. 16, p. 161114, 2013.

[24] S. Wimmer, D. Ködderitzsch, K. Chadova, and H. Ebert, “First-principles linear response description of the spin nernst effect,” Physical Review B, vol. 88, no. 20, p. 201108, 2013.

[25] T. Kimura, Y. Otani, T. Sato, S. Takahashi, and S. Maekawa, “Room-temperature reversible spin hall effect,” Physical Review Letters, vol. 98, p. 156601, 2007.

[26] E. Saitoh, M. Ueda, H. Miyajima, and G. Tatara, “Conversion of spin current into charge current at room temperature: Inverse spin-hall effect,” Applied physics letters, vol. 88, no. 18, p. 182509, 2006.

[27] C. Sahin and M. E. Flatte, “Tunable giant spin hall conductivities in a strong spin-orbit semimetal: Bi1-xSbX,” Physical Review Letters, vol. 114, p. 107201, 2015.

[28] J. Fan and J. Eom, “Direct electrical observation of spin hall effect in bi film,” Applied Physics Letters, vol. 92, p. 142101, 2008.

[29] Y. Sun, Y. Zhang, C. Felser, and B. Yan, “Strong intrinsic spin Hall effect in the TaAs family of Weyl semimetals,” Phys. Rev. Lett., vol. 117, p. 146403, Apr. 2016.

[30] Y. Sun, Y. Zhang, C.-X. Liu, C. Felser, and B. Yan, “Dirac nodal lines and induced spin hall effect in metallic rutile oxides,” Physical Review B, vol. 95, no. 23, p. 235104, 2017.

[31] B. A. Bernevig, T. L. Hughes, and S.-C. Z. Zhang, “Quantum Spin Hall Effect and Topological Phase Transition in HgTe Quantum Wells,” Science, vol. 314, p. 1757, 2006.

[32] S. A. Ekahana, S.-C. Wu, J. Jiang, K. Okawa, D. Prabhakaran, C.-C. Huang, S.-K. Mo, T. Sasagawa, C. Felser, B. Yan, Z. Liu, and Y. Chen, “Observation of nodal line in non-symmorphic topological semimetal inbi,” New J. Phys., vol. 19, p. 065007, 2017.

[33] W. H. Kleiner, “Space-time symmetry of transport coeffients,” Physical Review, vol. 142, p. 318, 1966.
[34] M. Seemann, D. Koedderitzsch, S. Wimmer, and H. Ebert, “Symmetry-imposed shape of linear response tensors,” *Phys. Rev. B*, vol. 92, p. 155138, 2015.

[35] Y. Zhang, Y. Sun, H. Yang, J. Železný, S. P. Parkin, C. Felser, and B. Yan, “Strong anisotropic anomalous hall effect and spin hall effect in the chiral antiferromagnetic compounds mn 3 x (x= ge, sn, ga, ir, rh, and pt),” *Physical Review B*, vol. 95, no. 7, p. 075128, 2017.

[36] G. Cooper, G. Saunders, and A. Lawson, “The electrical resistivity and thermoelectric power of inbi and in2bi,” *Journal of Physics and Chemistry of Solids*, vol. 25, no. 11, pp. 1277–1278, 1964.

[37] W.-L. Lee, S. Watauchi, V. L. Miller, R. J. Cava, and N. P. Ong, “Anomalous hall heat current and nemst effect in the cucr2se4-xbrx ferromagnet,” *Physical Review Letters*, vol. 93, p. 226601, 2004.

[38] D. Xiao, Y. Yao, Z. Fang, and Q. Niu, “Berry-phase effect in anomalous thermoelectric transport,” *Physical Review Letters*, vol. 97, p. 026603, 2006.

[39] K. Koepernik and H. Eschrig, “Full-potential nonorthogonal local-orbital minimum-basis band-structure scheme,” *Phys. Rev. B*, vol. 59, p. 1743, 1999.

[40] J. P. Perdew, K. Burke, and M. Ernzerhof, “Generalized gradient approximation made simple,” *Phys. Rev. Lett.*, vol. 77, p. 3865, 1996.