1. Introduction

Weyl semimetals (WSMs) are a novel topological quantum state in condensed matter [1–7], which are characterized by the existence of a set of linear-dispersive band-touching points, known as the Weyl nodes. The Weyl nodes always appear in pairs, of which the quasiparticles carry opposite chirality. In the momentum space the Weyl node acts like a source or drain of the Berry curvature, resulting in the Fermi arc surface states which take a form of a finite segment terminated at the Weyl nodes [8–11]. Besides, WSMs also manifest lots of exotic properties in quantum transport, such as chiral...
anomaly induced negative magnetoresistance [12–18], chiral magnetic effect [19, 20], weak anti-localization [21], double Andreev reflections [22], etc. Due to their unique gapless bulk states, the Fermi arc surface states and special transport properties, WSMs have attracted significant attention [23–31]. For example, Lundgren and Chen et al investigate the electronic contribution to the thermal conductivity and the thermopower of Weyl and Dirac semimetals using the Boltzmann equation [23, 24]. Igarashi et al theoretically study electronic transport in the WSM nanowires under magnetic fields [25], and demonstrate that the interplay between the Fermi-arc surface states and the bulk Landau levels plays a crucial role in the magnetotransport.

The spin Nernst effect refers to a transverse spin current caused by the longitudinal temperature gradient in a system with spin–orbit coupling [32]. Recently, this effect has been observed for the first time in a six-terminal Hall-bar Platinum thin film system [33], which makes it one of the most exciting subjects in spintronics. To date, more and more research groups are studying the spin Nernst effect in various systems of different materials. For example, Sheng et al [34] observed the spin Nernst effect in W/CoFeB/MgO heterostructures, and Bose et al [35] observed the heat current to spin current conversion in a non-magnetic Platinum by the spin Nernst effect at room temperature. Similar to the Nernst coefficient [36, 37], the spin Nernst coefficient is also more sensitive to the details of the spin density of states of the system than the spin Hall conductance. The spin Nernst effect also offers a possibility of controlling the electron spin current in spintronics applications [33–35]. Furthermore, the non-dissipative pure spin current not only deepens the understanding of the phenomenon of non-dissipative quantum transport, but also contributes to the development of novel low power-consumption nanoscale spintronic devices [38, 39].

Due to its potential application in spintronics, the spin Nernst phenomenon has long been the focus of theoretical research and has attracted wide attention of researchers [32, 40–44]. Early in 2008, Cheng and Sun [32] first theoretically studied the spin Nernst effect in a two-dimensional electron gas system with spin–orbit coupling under a perpendicular magnetic field. It was found that the spin–orbit coupling can lead to splitting of the Nernst peak, and the spin Nernst coefficient increases with the spin–orbit coupling strength, but weakens with the increase of the magnetic field. Thereafter, a lot of theoretical works have studied the spin Nernst effect in various systems in depth [40–42]. Tauber et al calculated the influence of impurities on the Nernst effect [40], and found that the direction and magnitude of spin current can be modulated by changing the type of impurity. Rothe et al investigated the spin-dependent thermoelectric transport in quantum spin Hall insulators based on HgTe/CdTe quantum wells in the absence of magnetic fields [41]. It was found that the oscillatory character of the spin Nernst coefficients in the bulk gap were caused by the finite overlap of the edge states from opposite sample boundaries. Wimmer et al presented the first-principles description of the spin Nernst effect based on the Kubo–Streda formalism [42], and used this method to study the spin Nernst effect of diluted and concentrated alloys.

In WSMs, spin-momentum locking correlates the spin direction with the orbital motion of electrons. The spin direction is parallel or anti-parallel with the momentum direction due to the well conserved chirality of each Weyl node, making WSMs a good platform for investigating the spin transport. However, up to now, no investigations of the spin Nernst effect in WSMs have been reported, although the Nernst effect in WSMs were investigated by some recent works [45–52].

In addition, we also note that the spin current is a tensor [53–55], which has $3 \times 3 = 9$ elements, describing the direction of the electron motion and the direction of the spin, respectively. While in a lead, electrons have to move along the lead, but its spin direction may still be in the $x$, $y$, and $z$ directions. In this case, the spin current has three non-zero elements, $I_{ix}$, $I_{iy}$, and $I_{iz}$. Here $I_{ii}$ ($i = x, y$ and $z$) represents an electron moving along the lead with its spin in the $i$ direction. However, all previous studies investigated only the element $I_{iz}$ in the spin Nernst effect, but the spin currents $I_{ix}$ and $I_{iy}$ have never been studied.

In this paper, we carry out a theoretical study of the spin Nernst effect of WSMs under the perpendicular magnetic fields by using the Landauer–Büttiker formula combining with the nonequilibrium Green’s function method. We consider a time-reversal symmetry breaking WSMs in a mesoscopic four-terminal cross-bar device. The three elements of the spin Nernst coefficients are calculated at different temperatures in three connection modes ($x$-$z$, $z$-$x$ and $x$-$y$ modes). We find that the spin Nernst effect in the WSMs has the essential difference with the traditional spin Nernst effect. So we call it the anomalous spin Nernst effect. The anomalous behavior is that (1) the $z$ direction element of the spin Nernst coefficients is zero at the zero magnetic field, and it appears at the presence of the magnetic field, in contrary to the traditional one induced by the spin–orbit coupling, and (2) the $x$ and $y$ direction elements of the spin currents in the two transverse leads flows out or flows in together, which is essentially different with the traditional one, where the spin current flows out from one lead and flows in on the other. In addition, the spin Nernst coefficients show the strongly anisotropic characteristics in space. For the $x$-$z$ and $z$-$x$ connection modes the spin Nernst coefficients show a series of peaks, and the peak positions are independent of the magnetic field, but they strongly oscillate and are very sensitive to the magnetic field for the $x$-$y$ mode. Moreover, through the analysis with both the continuous Hamiltonian and discrete Hamiltonian, the inversion-type symmetry, the mirror-reversal-type symmetry and the electron–hole-type symmetry are found, which lead to the spin Nernst coefficients being odd function or even function of the Fermi energy, the magnetic field and the transverse terminals.

The rest of the paper is organized as follows. In section 2, the effective tight-binding Hamiltonian is introduced, and the formalisms for calculating the spin Nernst coefficients $N_{ix}$, $N_{iy}$ and $N_{iz}$ are derived. In sections 3–5, we study the spin Nernst
As mentioned above, WSMs are anisotropic and the spin Nernst effect strongly depends on both the direction of thermal gradient and direction of transverse lead connection. There are totally six different connection modes, x-z, x-y, y-x, y-z, z-x and z-y, for the connection of the four leads. Here i-j mode \((i,j) = (x,y,z)\) represents that thermal gradient is applied in the i direction and the spin current is measured in the j direction, i.e. the lead-1 and lead-2 connect the rectangular center WSM region at the i direction and lead-3 and lead-4 are at the j direction. However, \(k_i\) and \(k_j\) in equation (1) are equivalent and only \(k_i\) is special. This means that the x and y directions are equivalent, which results in an equal spin Nernst coefficient in the two modes x-z and y-z (x-y and y-x, z-x and z-y). So there are only three non-equivalent cases of the six modes. Thereafter, we consider three non-equivalent x-z, x-y and x-x modes (see figures 1(c)–(e)). For example, for the x-z mode, the longitudinal thermal gradient \(\Delta T\) is added in the x direction, and the spin current is measured in the z direction. The width in the y direction is assumed to be wide where the periodic boundary condition can be used, so the momentum \(k_y\) is a good quantum number. We also consider a magnetic field applied in the y direction, that is, perpendicular to the transport plane. For the z-x (x-y) mode, the width in the y (z) direction is set to be wide and the momentum \(k_x\) (\(k_z\)) is a good quantum number. The magnetic field is applied in the y (z) direction, which is perpendicular to the transport plane still.

Based on the Hamiltonian of equation (1), we here propose the two-band tight-binding discrete model on a simple cubic lattice. For x-z and z-x modes, the momentum \(k_x\) is a good quantum number, and the tight-binding lattice models can be written as

\[
H(k_y) = \sum_i [c_i^\dagger T_0 c_i + c_j^\dagger T_x c_j + \delta t c_j^\dagger T_y c_j + \text{H.c.}],
\]

\[
T_0 = 4t\sigma_z + 2t\sigma_y \sin k_x a - 2t\sigma_x \cos k_x a,
\]

\[
T_x = [-i\sigma_z - it\sigma_y] e^{-i(\phi_{j+1})},
\]

\[
T_y = i\sigma_z e^{-i(\phi_{i+1})}.
\]

For x-y mode, the momentum \(k_y\) is a good quantum number, and the tight-binding lattice model is written as

\[
H(k_y) = \sum_i [c_i^\dagger R_0 c_i + c_j^\dagger R_x c_j + \delta t c_j^\dagger R_y c_j + \text{H.c.}],
\]

\[
R_0 = 4t\sigma_z + 2t\sigma_y \cos k_x a,
\]

\[
R_x = [-i\sigma_z - it\sigma_y] e^{-i(\phi_{j+1})},
\]

\[
R_y = -t\sigma_z - it\sigma_y,
\]

where \(a\) is the lattice constant, and \(c_j = (c_{j+1}, c_{j-1})\) is the annihilation operator at site \(j\) with spin \(\uparrow, \downarrow\); \(\phi_{i+1}\) in equation (2) but \(\phi_{j+1}\) in equation (3). The effect of perpendicular magnetic field is included by adding a phase term \(\phi_{mn} = -\int_{-\infty}^{\infty} \mathbf{A}(r) \cdot \mathbf{d} / \phi_0\), with the vector potential \(\mathbf{A} = (B_z - B_y, 0, B_y)\) and the flux quanta \(\phi_0 = h / e\). In the numerical calculations, we set the lattice constant \(a = 1.0\) nm.
and the Fermi velocity \( v = 3.09 \times 10^5 \text{ m s}^{-1} \) [57]. The magnetic field is expressed in terms of the lattice magnetic flux \( \phi \) with \( \phi = B a^2/2 \pi q \). Here \( \phi \) is 0.005, the magnetic field \( B \) is about 20.7 T. The size of center region is \( W \times L = 40a \times 8a \) (see the grey region in figure 1(b)). For the samples of other sizes, the conclusions are similar.

Considering a small temperature gradient \( \Delta T \) and a zero bias applied on the longitudinal lead-1 and lead-2, we can set the temperatures \( T_1 = T + \Delta T/2 \), \( T_2 = T - \Delta T/2 \), and \( T_3 = T = T \), and the biases \( V_q = 0 \) (\( q = 1, 2, 3, 4 \)), as shown in figure 1(b). Under the drive of the temperature gradient, the spin current is induced in the transverse lead-3 and lead-4. In usual, the spin current is a tensor and it has \( 3 \times 3 = 9 \) elements that respectively describe the direction of the electron motion and the direction of the spin [53–55]. While in the lead, the flow direction has to be along the lead direction, but the spin direction may still be in the \( x, y, z \) directions. So the spin current in the transverse lead may have three non-zero elements, \( I_{qxx}, I_{qyx} \) and \( I_{qzx} \). Here \( I_{qyi} = (i = x, y, z) \) represents an electron moving along the lead-\( q \) with its spin in the \( i \) direction. Below we first derive the expression of the particle current \( J_{q\sigma} \) (\( \sigma = \uparrow, \downarrow \) or \( \sigma = +, - \)), which describes the particle current with the spin pointing the \( \sigma \) direction in the lead-\( q \). From the Landauer–Büttiker formula, the particle current \( J_{q\sigma} \) can be expressed as [32, 44],

\[
J_{q\sigma} = \frac{1}{4} \sum_{k} \sum_{\mu} \int T_{q\sigma,p}(E, k) [f_\mu(E) - f_\mu(E)] \, dE, \tag{4}
\]

where \( T_{q\sigma,p}(E, k) \) is the transmission coefficient for the incident carrier from the lead-\( p \) with momentum \( k \) to the \( \sigma \) mode at the lead-\( q \). The expression of the particle current \( J_{q\sigma} \) in equation (4) is obtained from the Hamiltonian in equation (2). For the Hamiltonian in equation (3), the sum over \( k \) and \( T_{q\sigma,p}(E, k) \) should be replaced by the sum over \( k \) and \( T_{q\sigma,p}(E, k) \). Hereafter, we assume that the transverse lead-3 and lead-4 are normal conductance without spin–orbit coupling. So the spin in the transverse leads is a good quantum number and the \( \sigma \) mode represents the transport mode with its spin pointing to \( \sigma \) direction. On the other hand, we set that the lead-1 and lead-2 are the semi-infinite WSM leads which are the same as the rectangular center region. That is to say, the lead-1/center WSM region/lead-2 forms a perfect WSM nanowire. In equation (4),

\[
f_\mu(E, \mu_q, T_q) = \frac{1}{\exp(E - \mu_q)/k_B T_q + 1}, \tag{5}
\]

is the electronic Fermi distribution function of the lead-\( q \), where the chemical potential \( \mu_q = E_F + eV_q \) with the Fermi energy \( E_F \) [37], and \( k_B \) is the Boltzmann constant.

By using the nonequilibrium Green’s function method, the transmission coefficient \( T_{q\sigma,p}(E, k) \) can be obtained as:

\[
T_{q\sigma,p}(E, k) = \text{Tr}[\Gamma_{q\sigma,p} G^p T_p G^\sigma], \tag{6}
\]

in which \( \Gamma_{q\sigma,p}(E) = i[\Sigma_{q\sigma,p}^\prime(E) - \Sigma_{q\sigma,p}^\prime\prime(E)] \) and \( \Gamma_{p}(E) = i[\Sigma_{p}^\prime(E) - \Sigma_{p}^\prime\prime(E)] \) are the linewith functions. \( \Sigma_{q\sigma,p}^\prime \) and \( \Sigma_{p}^\prime \) are the retarded self-energy due to the coupling between the lead and the center WSM region. In equation (6), the Green’s function \( G^\sigma(E) = [G^\sigma]^\dagger = [E - \mathbf{H}_0 - \Sigma_{q\sigma}^\prime(E) - \Sigma_{q\sigma}^\prime\prime(E)]^{-1} \), with \( \mathbf{H}_0 \) being the Hamiltonian of center scattering region [36, 58].

For the normal transverse lead-3 and lead-4, the self-energy functions are \( \Sigma_{q\sigma}^\prime = -\frac{i}{2} \text{Im} \, \mathbf{u} \cdot \mathbf{m} \cdot \mathbf{u} \), where \( \mathbf{I} \) describes the coupling strength between lead-\( q \) and the central region. In the numerical calculation, we consider the coupling strength with \( \Gamma = 5.0 \). \( \mathbf{m}_1 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \) for \( \sigma = \uparrow \) and \( \mathbf{m}_2 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \) for \( \sigma = \downarrow \). \( \mathbf{u} \) is the unitary matrix which rotates the spin \( z \) axis into \( i \) direction. Specifically, the unitary matrix \( \mathbf{u} \) \((i = x, y, z)\) is

\[
\mathbf{u}_x = \frac{\sqrt{2}}{2} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}, \tag{7}
\]

\[
\mathbf{u}_y = \frac{\sqrt{2}}{2} \begin{pmatrix} i & 1 \\ -i & 1 \end{pmatrix}, \tag{8}
\]

\[
\mathbf{u}_z = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{9}
\]

For the lead-3 and lead-4, the self-energy functions \( \Sigma_{q}^\prime = \Sigma_{q\uparrow}^\prime + \Sigma_{q\downarrow}^\prime = \Sigma_{q\uparrow}^\prime + \Sigma_{q\downarrow}^\prime = \Sigma_{q\uparrow}^\prime + \Sigma_{q\downarrow}^\prime \). For the semi-infinite WSM lead-1 and lead-2, the self-energy functions \( \Sigma_{p}^\prime \) can be calculated numerically [36, 59].

After obtaining the particle current \( J_{q\sigma} \), the charge current in lead-\( q \) can be obtained as \( I_{q\mu} = e[I_{q\uparrow} + I_{q\downarrow}] = e[I_{q\uparrow} + I_{q\downarrow}] = e[I_{q\uparrow} + I_{q\downarrow}] \) and the spin current is \( I_{q\mu} = e[I_{q\uparrow} + I_{q\downarrow}] \), straightforwardly. Note here the charge current has an element \( I_{q\mu} \) only, but the spin current has three non-zero elements, \( I_{qxx}, I_{qyx} \) and \( I_{qzx} \), because that the charge current is vector but the spin current is a tensor [53–55]. The spin Nernst coefficients in the lead-3 and lead-4 are defined as \( N_{q\sigma} = I_{q\sigma} / \Delta T \). Here, \( N_{q\sigma} \) with \( q = 3, 4 \) and \( i = x, y, z \) denote the spin current induced in the transverse lead-3 and lead-4 with the spin direction in the \( i \)-direction by the longitudinal thermal gradient. At the small thermal gradient limits, the spin Nernst coefficients \( N_{q\sigma} \) can be reduced to [32, 44]

\[
N_{q\sigma} = \frac{1}{2} \sum_{k} \left( \Delta T_{q\sigma} \right) \frac{E - E_F}{k_B T_q} f_0(1 - f_0) \, dE, \tag{10}
\]

where \( \Delta T_{q\sigma} = T_{q\uparrow,\sigma} - T_{q\downarrow,\sigma} \), and \( f_0 \) is the Fermi distribution function at the zero thermal gradient and zero bias.

### 3. The thermospin transport in the x-z mode

First, we study the spin Nernst coefficients \( N_{3z}, N_{3x}, N_{3y} \), in the case of x-z transport mode. In this x-z mode, the thermal gradient is applied in the \( x \) direction, the spin current is measured at the \( z \) direction, and the magnetic field is in the \( y \) direction which is perpendicular to the transport \( x-z \) plane. Figures 2(a) and 3(a) show \( N_{3z} \) and \( N_{3x} \) as functions
of Fermi energy $E_F$ for different temperatures at the zero magnetic field. When the magnetic field $B = 0$, the spin Nernst coefficient $N_{3z}$ is exactly zero regardless of the temperature, but $N_{3x} \neq 0$ and $N_{3y} \neq 0$. $N_{3y}$ is not shown here, and it is non-zero but is much smaller than the $N_{3x}$. $N_{3x}$ and $N_{3y}$ exhibit a series of peaks at the low temperatures. With the increase of temperature $T$, $N_{3x}$ and $N_{3y}$ increase as a whole, then some oscillation peaks merge. The oscillation peaks of $N_{3x}$ and $N_{3y}$ become sparser at the higher temperature, and the peak spacings of $N_{3x}$ and $N_{3y}$ become larger (see figure 3(a)).

In order to explain the origin of the non-zero spin Nernst coefficient $N_{3x}$, we plot the transmission coefficient $T_{3x,p}$ at the momentum $k_y = 0$ and the momentum resolved spin Nernst coefficient $N_{3x}$ at several specific momentum $k_y, a = 0$ and $\pm 0.1$ in figures 4(a) and (b). While the energy $E$ just crosses discrete transverse channels, the transmission coefficients suddenly jump and show a series
with the opposite chirality and these red arrows represent the spin polarization direction. \( k_x \) from the Weyl cones. (b) A sketch of the Fermi surface in the lead-3. When the incident carriers are from the lead-1 with \( k_y = 0 \) and consider that the carriers are scattered from the lead-1 to lead-3. The two Fermi surfaces of the two Weyl cones with the opposite chirality and these red arrows represent the spin polarization direction.

\[
\begin{align*}
T_{3x\sigma,1} & = T_{3x\sigma,2} \\
T_{3x\pi,1} & = T_{3x\pi,2}
\end{align*}
\]

\[
\begin{align*}
E(k) & = E_F \\
k_x & = 0
\end{align*}
\]

\[
\begin{align*}
N_{3x} & = 0 \\
k_y & = 0
\end{align*}
\]

\[
\begin{align*}
T = 10K
\end{align*}
\]

\[
\begin{align*}
k_x & = 0 \\
k_y & = 0
\end{align*}
\]

\[
\begin{align*}
E_F & = 0 \\
E_P & = 60
\end{align*}
\]

\[
\begin{align*}
\text{Figure 4.} & \quad (a) \text{ shows the curves of the transmission coefficient } T_{3x\sigma,\phi} \text{ versus the incident energy } E \text{ with perpendicular magnetic field } \phi = 0 \text{ and momentum } k_y = 0. (b) \text{ is the momentum resolved spin Nernst coefficient } N_{3x} \text{ versus the Fermi energy } E_F \text{ for } k_y, a = 0, -0.1 \text{ and } 0.1 \text{ with } \phi = 0 \text{ and temperatures } T = 10K.
\end{align*}
\]

\[
\begin{align*}
\text{Figure 5.} & \quad (a) \text{ Schematic illustrations for two opposite-chirality Weyl cones. For a given Fermi energy, a round Fermi surface can be gotten from the Weyl cones. (b) A sketch of the Fermi surface in the } k_x, k_y \text{ momentum space at } k_y = 0. \text{ Here the two circles are the Fermi surfaces of the two Weyl cones with the opposite chirality and these red arrows represent the spin polarization direction.}
\end{align*}
\]
From the relations of equations (12) and (13), one can obtain that the transmission coefficients have the following relations:

\[ N_{3k/x}(E_F, \phi) = N_{4k/x}(E_F, \phi). \]  

(15)

That is, under the longitudinal thermal gradient drive, the z direction element of the spin current flows from the lead-3 through the center WSM region to the lead-4, which is the same as the conventional spin Nernst effect. However, the x (y) direction element of the spin current in the lead-3 and lead-4 flows out or flows in together, in contrary to the traditional one. So the x and y direction elements of the spin Nernst coefficient is also anomalous. In figure 6, we show the flowing direction and the spin polarization direction for the spin currents \( I_{sz} \) and \( I_{sx} \) in the lead-3 and lead-4. Here \( I_{sz} \) in the lead-3 and lead-4 flows out or flows in together, which are very different with the traditional spin Hall effect and spin Nernst effect.

These relations of the spin Nernst coefficients in equations (11) and (15) can also be obtained by analyzing the symmetry of the WSM Hamiltonian. From the continuous Hamiltonian in equation (1) and the discrete Hamiltonian in equation (2), we find that the WSM has three symmetries: the inversion-type symmetry, the mirror-reversal-type symmetry and the electron–hole–type symmetry.

3.1. The inversion-type symmetry

In the continuous Hamiltonian in equation (1), we take the transformation \( (k_x, k_y, k_z) \rightarrow (-k_x, -k_y, -k_z) \) and rotate the spin by 180° around spin z axis (i.e. \( \sigma_z \rightarrow \sigma_z, \sigma_x \rightarrow -\sigma_x \) and \( \sigma_y \rightarrow -\sigma_y \)). Or in the discrete Hamiltonian in equation (2), we take the transformation \( c_{j\uparrow} \rightarrow ic_{j\downarrow}, c_{j\downarrow} \rightarrow -ic_{j\uparrow} \) and \( k_z \rightarrow -k_z \). Under this transformation the Hamiltonian \( H \) is invariant, but the lead-1 (lead-3) and lead-2 (lead-4) exchange with each other. So from this inversion symmetry, we can obtain the transmission coefficients have the following relations:

\[ T_{3\sigma,1}(E_F, \phi, k_y) = T_{4\sigma,2}(E_F, \phi, -k_y), \]  

(16)

\[ T_{3\sigma,2}(E_F, \phi, k_y) = T_{4\sigma,1}(E_F, \phi, -k_y), \]  

(17)

\[ T_{3\sigma/\sigma,1}(E_F, \phi, k_y) = T_{4\sigma/\sigma,2}(E_F, \phi, -k_y), \]  

(18)

\[ T_{3\sigma/\sigma,2}(E_F, \phi, k_y) = T_{4\sigma/\sigma,1}(E_F, \phi, k_y), \]  

(19)

where \( \sigma = \downarrow \) for \( \sigma = \uparrow \) and \( \sigma = \uparrow \) for \( \sigma = \downarrow \). Then, by combining equations (16)–(19) and (10), and summing over \( k_y \), we can get the relations in equations (14) and (15) of the spin Nernst coefficients in lead-3 and lead-4, straightforwardly.

3.2. The mirror-reversal-type symmetry

If in the continuous Hamiltonian in equation (1), we take \( k_z \rightarrow -k_z \) and the magnetic flux \( \phi \rightarrow -\phi \), or if in the discrete Hamiltonian in equation (2), we take \( c_{j\uparrow,\sigma} \rightarrow c_{j\downarrow,\sigma} \) and \( \phi \rightarrow -\phi \), the Hamiltonian \( H \) remains the same. Under this transformation, the lead-3 and lead-4 exchange with each other. So from this mirror-reversal-type symmetry, we have:
\[ T_{3\sigma,p}(E_F, \phi, k_y) = T_{4\bar{\sigma},p}(E_F, -\phi, k_y), \]

where \( p = 1, 2 \). Then to substitute these relations of the transmission coefficients into the expressions of \( N_{s\sigma} \) in equation (10), one can get the relation between the spin Nernst coefficients \( N_{s3i} \) and \( N_{s4i} \) of the lead-3 and lead-4,

\[ N_{s3i}(E_F, \phi) = N_{s4i}(E_F, -\phi), \quad i = x, y, z. \]  

By combining with equations (21) and (14), (15), we draw the relations in equations (12) and (13), that is, the spin Nernst coefficient \( N_{s3z} \) is an odd function of the magnetic flux \( \phi \) but \( N_{s3x} \) and \( N_{s3y} \) are even functions of \( \phi \).

### 3.3. The electron–hole-type symmetry

In the discrete Hamiltonian in equation (2), if we take the transformation: \( c_{j\uparrow} \rightarrow \tilde{c}_{j\downarrow}, c_{j\downarrow} \rightarrow \tilde{c}_{j\uparrow}, k_y \rightarrow -k_y \) and \( \phi \rightarrow -\phi \), the Hamiltonian \( H \) is invariant. In this transformation, the electron annihilation operator is changed into the hole annihilation operator, and so it is an electron–hole-type transformation and the energy \( E \) will change into \(-E\). Due to the electron–hole-type symmetry, we can get the relations of the transmission coefficients:

\[ T_{3\sigma,p}(E, \phi, k_y) = T_{3\bar{\sigma},p}(-E, -\phi, k_y), \]
\[ T_{3\sigma \rho}(E, \phi, k_y) = T_{3\sigma \rho}(-E, -\phi, -k_y), \]
\[ T_{3\sigma \rho}(E, \phi, k_y) = T_{3\sigma \rho}(-E, -\phi, k_y). \]

To substitute these relations of \( T_{3\sigma \rho}(E, \phi, k_y) \) into the expressions of \( N_{\text{ef}} \) in equation (10), one can obtain the relations of the spin Nernst coefficients between positive and negative Fermi energy:
\[ N_{3\sigma}(E_F, \phi) = N_{3\sigma}(-E_F, -\phi), \]
\[ N_{3\sigma}/(E_F, \phi) = -N_{3\sigma}/(E_F, -\phi). \]

Then by combining with equations (12) and (13), we have \( N_{3\sigma}(E_F, \phi) = -N_{3\sigma}(-E_F, -\phi) \) (i = x, y, z) straightforwardly. This means that the spin Nernst coefficients \( N_{3\sigma x}, N_{3\sigma y} \) and \( N_{3\sigma z} \) are all odd functions of the Fermi energy \( E_F \) regardless of other parameters (e.g. temperature, magnetic flux, etc), which are completely consistent with the numerical results (see figures 2 and 3).

4. The thermospin transport in the z-x mode

In this section, we study the thermospin transport behaviors in the z-x transport mode. In this z-x connection mode, the longitudinal thermal gradient is applied in the z direction, the transverse spin current is measured at the x direction, and the magnetic field is still in the y direction which is perpendicular to the transport z-x plane. The spin Nernst coefficients \( N_{3\sigma x} \) and \( N_{3\sigma y} \) versus the Fermi energy \( E_F \) for the different magnetic field \( \phi \) and different temperatures are shown in figures 7 and 8, respectively. When the magnetic field is absent with \( \phi = 0 \), the spin Nernst coefficients \( N_{3\sigma x}, N_{3\sigma y} \) and \( N_{3\sigma z} \) are all zero. In particular, \( N_{3\sigma z} = N_{3\sigma x} = N_{3\sigma y} = 0 \) can remain regardless of the temperature, the size of the center WSM region, and Fermi energy. This indicates that there is no spin Nernst effect in the z-x transport mode at the zero magnetic field, although there exists the spin–orbit coupling in the WSM.

The absence of spin Nernst effect at the zero magnetic field can be explained with aids of the momentum-spin locking bands as shown in figure 5(b). As mentioned in section 3, for a given momentum \( \mathbf{k} = (k_x, k_y) \), the spin expectation value of the state \( \Psi_{k \pm} = (\cos \theta, 0, -\sin \theta) \) at one Weyl cone and \( \Psi_{k -} = (\sin \theta, 0, \cos \theta) \) at the other Weyl cone, with \( \theta \) being the angle between \( \mathbf{k} \) and \( k_y \) (see figure 5(b)). In the z-x mode, the lead-1 and lead-2 are along the z direction. Let us consider the incident carriers from the lead-1 which is along +z direction. So the state with positive momentum \( k_y \) contributes the transmission coefficients and the spin Nernst coefficients. From figure 5(b), one can see the \( x \) direction elements of the spin polarization for the \(+k_y \) and \(-k_y \) states \( (\Psi_{(+k_y,k_x)} \) and \( \Psi_{(-k_y,k_x)} \) are just opposite, so the \( x \) direction element of spin Nernst coefficients, \( N_{3\sigma y} \), contributed by the \(+k_y \) and \(-k_y \) states cancel each other, leading to \( N_{3\sigma x} = 0 \) regardless of the parameters of the system. On the other hand, the \( z \) direction elements of the spin polarization of states \( \Psi_{k \pm} \) at the two Weyl cones with opposite-chirality are exactly opposite, so the \( z \) direction element of spin Nernst coefficients contributed by the two Weyl cones cancel each other also, so that \( N_{3\sigma z} = 0 \).

When the perpendicular magnetic field \( \phi \) along the y direction is applied, the spin Nernst coefficients \( N_{3\sigma x}, N_{3\sigma y} \) and \( N_{3\sigma z} \) appear with the finite values (see figures 7(b)–(d) and 8(b)–(d)). With the increase of \( \phi \), the spin Nernst coefficients increase rapidly at the beginning, then slowly, but generally keeps increasing. These results seem to indicate that the spin Nernst effect is caused by magnetic field, not by the spin–orbit coupling. So it is an anomalous spin Nernst effect and is essentially different with the traditional spin Nernst effect which can appear at the zero magnetic field. This anomalous spin Nernst effect originates from the combination of the magnetic field and the peculiar band structure of the WSMs. Here the spin Nernst coefficients \( N_{3\sigma x} \) and \( N_{3\sigma y} \) show some peaks (see figures 7 and 8). \( N_{3\sigma x} \) has the positive peaks while \( E_F > 0 \) and the negative peaks at \( E_F < 0 \). All peaks of \( N_{3\sigma y} \) are negative regardless of the value of Fermi energy \( E_F \). While \( E_F \) is near the Weyl nodes, \( N_{3\sigma y} \) has the highest peak but \( N_{3\sigma x} \) is very small. When the temperature \( T \) rises, the height and position of the peaks of \( N_{3\sigma x} \) and \( N_{3\sigma y} \) slightly increase, but the peak positions remain almost unchanged. In particular, the details of the curves of \( N_{3\sigma y}/E_F \) for the different \( \phi \) are very similar (see figures 8(b)–(d)). Here \( N_{3\sigma x} \) is not shown. \( N_{3\sigma x} \) and \( N_{3\sigma y} \) have similar characteristics and they are about the same value.

In order to explain the origination of the peaks in the curves of the spin Nernst coefficients versus Fermi energy, we show the momentum resolved spin Nernst coefficient \( N_{3\sigma y} \) for the different magnetic fields in figure 9. Here each curve of \( N_{3\sigma y} \) shows a high peak. The peak position is about at \( E_F = 2ak_y \), \( h v k_y \). For example, while \( k_y = \pi/30a \) and \( v = 3.09 \times 10^5 \text{ m s}^{-1} \), \( h v k_y \approx 21.3 \text{ meV} \), which is just the peak position of \( N_{3\sigma y} \) at \( k_y = \pi/30a \). In fact, for a given momentum \( k_y \), the WSMs in Hamiltonians (1) and (2) reduce into the two-dimensional system, and the Landau levels form under the strong magnetic field \( B \). The Landau levels are at \( \pm \sqrt{(hv k_y)^2 + 2(hv)^2 eBn} \) with the level index \( n = 0, \pm 1, \pm 2, \ldots \). That is, the peak position of the momentum resolved \( N_{3\sigma y} \) is just at the zeroth Landau level. Because that the zeroth Landau level is not almost affected by the magnetic field \( B \), the peak position as well the details of the curves \( N_{3\sigma y}/E_F \) and \( N_{3\sigma y}/E_F \) in figures 7–9 are almost independent of \( B \) also. In addition, in the numerical calculations, we consider that the thickness of the WSMs in y direction is 61a. If we consider a thicker WSM, the values of momentum \( k_y \) would become denser, and the peak numbers at the curves of \( N_{3\sigma y}/E_F \) in figure 8 increase. For a very thick WSM, these peaks merge and cause large a spin Nernst coefficient \( N_{3\sigma y} \) over a wide \( E_F \) range.

In addition, from figures 7 and 8, we can see that the \( z \) direction element of spin Nernst coefficient, \( N_{3\sigma z} \), is an odd function of the Fermi energy \( E_F \), but the \( x \) and \( y \) direction elements, \( N_{3\sigma x} \) and \( N_{3\sigma y} \), are even functions of \( E_F \). That is, the spin Nernst coefficients have the following relations:
The relations of spin Nernst coefficients \( N_{3z}(E_F, \phi) = -N_{3z}(-E_F, \phi) \), \( N_{3x/\gamma}(E_F, \phi) = N_{3x/\gamma}(-E_F, \phi) \) are derived from the three symmetries mentioned equations (27)–(28).

These relations are different with the \( x-z \) mode, in which all elements of the spin Nernst coefficients are odd functions of \( E_F \) (see equation (11)).

Moreover, the calculation results show all elements of the spin Nernst coefficients are the odd functions of the magnetic field \( \phi, i.e.

\[ N_{3i}(E_F, \phi) = -N_{3i}(E_F, -\phi), \quad i = x, y, z. \]

From the relations of the odd functions of \( \phi \), we can obtain \( N_{3i}(E_F) = 0 \) at the \( \phi = 0 \) straightforwardly.

Let us study the relation of the spin Nernst coefficients at the transverse lead-3 and lead-4. From calculation results, we obtain that \( N_{3x} \) and \( N_{4x} \) have the relations as:

\[ N_{3x}(E_F, \phi) = -N_{4x}(E_F, -\phi), \quad (30) \]

\[ N_{3x/\gamma}(E_F, \phi) = N_{4x/\gamma}(E_F, -\phi). \quad (31) \]

These relations are the same as that in the \( x-z \) mode (see equations (14) and (15)). That is, under longitudinal thermal gradient drive, the \( z \) direction element of the spin current, \( I_{3z} \), flows from a transverse lead through the center WSM region to the other transverse lead, but the \( x \) and \( y \) direction elements, \( I_{3x} \) and \( I_{3y} \), in two transverse leads flow out or flow in together, as shown in figure 6.

In fact, these relations of the spin Nernst coefficients in equations (27)–(31) obtained from the numerical results can analytically be derived from the three symmetries mentioned above also. First, from the inversion-type symmetry, one can get that the transmission coefficients in the \( z-x \) transport mode have the relations as shown in equations (16)–(19) still. So the relations of spin Nernst coefficients \( N_{3i} \) and \( N_{4i} \) in the transverse lead-3 and lead-4 in equations (30) and (31) can be obtained straightforwardly.

Second, in the mirror-reversal-type symmetry, the momentum \( k_i \to -k_i \), and the magnetic flux \( \phi \to -\phi \). That is, the longitudinal lead-1 and lead-2 exchange with each other. Therefore from the mirror-reversal-type symmetry, we get the relations of the transmission coefficients:

\[ T_{3x/\gamma}(E, \phi, k_i) = T_{3x/\gamma}(E, -\phi, k_i). \]

To substitute these relations of \( T_{3x/\gamma} \) into the expression of the spin Nernst coefficients in equation (10), one has:

\[ \tilde{N}_{3x/\gamma}(E_F, \phi, k_i) = -\tilde{N}_{3x/\gamma}(E_F, -\phi, k_i). \]

Then by summing over the momentum \( k_i \), the relations in equation (29), the spin Nernst coefficients being the odd functions of the magnetic field \( \phi \), can be obtained straightforwardly.

Third, from the electron–hole-type symmetry, we can get the relations of the transmission coefficients:

\[ T_{3\sigma,\pi}(E, \phi, k_i) = T_{3\sigma,\pi}(E, -\phi, -k_i). \]

\[ T_{3\sigma,\pi}(E, \phi, k_i) = T_{3\sigma,\pi}(E, -\phi, -k_i). \]

which are the same as the relations in equations (22)–(24) in the \( x-z \) mode case. Then to substitute these relations of \( T_{3\sigma,\pi} \) into equation (10), we obtain

\[ \tilde{N}_{3x}(E_F, \phi, k_i) = \tilde{N}_{3x}(-E_F, -\phi, -k_i), \]

\[ \tilde{N}_{3x/\gamma}(E_F, \phi, k_i) = -\tilde{N}_{3x/\gamma}(-E_F, -\phi, -k_i). \]

To combine the above equations with the equation (33), we have:

\[ \tilde{N}_{3x}(E_F, \phi, k_i) = -\tilde{N}_{3x}(-E_F, \phi, -k_i), \]

\[ \tilde{N}_{3x/\gamma}(E_F, \phi, k_i) = -\tilde{N}_{3x/\gamma}(-E_F, \phi, -k_i). \]

The analytical results in equation (39) obtained from systemic symmetry completely agree with the numerical calculations in figure 9. At last, by summing over the momentum \( k_i \) in figure 9. The momentum resolved spin Nernst coefficient \( \tilde{N}_{3z} \) versus the Fermi energy \( E_F \) for \( k_i = 0, \pm \pi/30 \) and \( \pm \pi/15 \) with temperatures \( T = 10K \) and the magnetic field \( \phi = 0 \) (a), \( \phi = 0.005 \) (b), \( \phi = 0.01 \) (c) and \( \phi = 0.05 \) (d).
equations (38) and (39), one get the relations in equations (27) and (28), i.e. the $z$ direction element of spin Nernst coefficient being an odd function of the Fermi energy but the $x$ and $y$ direction elements being even functions. In short, all the relations (in equations (27) and (31)) of the spin Nernst coefficients over the Fermi energy, the magnetic field and the transverse terminals obtained from the numerical calculations can also be derived by the systemic symmetry analysis.

5. The thermospin transport in the $x$-$y$ mode

In this section, we study the thermospin transport behaviors in the $x$-$y$ connection mode. In this $x$-$y$ mode, the longitudinal thermal gradient is added in the $x$ direction, the transverse spin current is measured at the $y$ direction, and the magnetic field is in the $z$ direction as shown in figures 2(b) and (e). Figures 10(a) and 11(a) show the spin Nernst coefficients $N_{3x}$ versus Fermi energy $E_F$ for different temperatures at the zero magnetic field ($\phi = 0$). Here three elements $N_{3z}$, $N_{3x}$ and $N_{3y}$ are all non-zero even if at $\phi = 0$, which are essentially different from that of the $x$-$z$ and $z$-$x$ modes. $N_{3z}$ is an even function of the Fermi energy with $N_{3z}(E_F) = N_{3z}(-E_F)$, while $N_{3x}$ and $N_{3y}$ are odd functions with $N_{3x/y}(E_F) = -N_{3x/y}(-E_F)$. $N_{3z}$ shows some negative peaks but the value of $N_{3z}$ is very small. On the other hand, $N_{3x}$ strongly oscillates between the positive and negative values. The oscillation amplitude of $N_{3x}$ is quite large and it can be over $0.05k_B$. With the increase of temperature $T$, the peak height of $N_{3z}$ almost remains and the oscillation amplitude of $N_{3x}$ slightly reduces. $N_{3y}$ has the similar characteristics as $N_{3z}$, but the value of $N_{3y}$ is much smaller than $N_{3x}$.
Let us explain why $N_{3z}$ has a large value and all three elements of spin Nernst coefficients are non-zero in the $x$-$y$ connection mode. In the case of the $x$-$y$ mode, the spin Nernst coefficients are mainly contributed by these carriers with $k_z$ near 0. The Weyl Hamiltonian with $k_z = 0$ can be approximated as $\mathbf{H}_\parallel = i\hbar v(k_z \sigma_z + k_x \sigma_x)$. Here the Hamiltonian $\mathbf{H}_\perp$ of two Weyl cones near $\mathbf{K}_\perp$ are the same. So the spin Nernst coefficients from two Weyl cones can not cancel always, which is essentially different with the $x$-$z$ and $z$-$x$ modes as shown in figure 5. In addition, if we consider the incident carriers from the lead-1, the states with the positive momentum $k_z$ contribute the spin Nernst coefficients. Note for all positive $k_z$ states, the $x$ direction elements of their spin polarization have the same sign, leading to a large value of $N_{3z}$.

Next, we study the effect of the magnetic field on the spin Nernst effect. Figures 10(b)–(d) show the spin Nernst coefficients $N_{3z}$, and $N_{3x}$ for the magnetic field $\phi = 0.005$, $\phi = 0.01$ and $\phi = 0.05$, respectively. With the increase of the magnetic field $\phi$, the $x$ direction element of the spin Nernst coefficient $N_{3x}$ increases as a whole. But it does not increase monotonously, e.g. $N_{3z}$ at $\phi = 0.01$ is smaller than the value at $\phi = 0.005$ (see figures 10(b) and (c)). The $x$ direction element, $N_{3x}$, still keeps the large value and the strong irregular oscillation in the presence of the magnetic field. In addition, when $\phi \neq 0$, the spin Nernst coefficient $N_{3x}$ is both non-odd and non-even function of the Fermi energy $E_F$ and magnetic field $\phi$. However, when the Fermi energy $E_F$ and the magnetic field $\phi$ change the sign at the same time, the spin Nernst coefficients have the relations:

$$N_{3z}(E_F, \phi) = N_{3z}(-E_F, -\phi),$$

(40)

$$N_{3x/y}(E_F, \phi) = -N_{3x/y}(-E_F, -\phi).$$

(41)

Furthermore, from the numerical results, we also get the relations of the spin Nernst coefficients at the transverse lead-3 and lead-4:

$$N_{3z}(E_F, \phi) = N_{3z}(-E_F, -\phi),$$

(42)

$$N_{3x/y}(E_F, \phi) = -N_{3x/y}(-E_F, -\phi).$$

(43)

That is, the $z$ direction element of the spin current, $I_{3z}$, flows from a transverse lead through the center WSM region to the other transverse lead which is the same with the conventional spin Nernst effect. But the $x$ and $y$ direction elements, $I_{3x}$ and $I_{3y}$, in two transverse leads flow out or flow in together, as shown in figure 6, which is abnormal. These relations in equations (42) and (43) are the same as that in the $x$-$z$ and $z$-$x$ modes.

Let us analytically derive the relations in equations (40)–(43) from the system’s symmetry. First, the mirror-reversal-type symmetry in the $x$-$y$ mode is slightly different with that in the $x$-$z$ and $z$-$x$ modes, because of the difference of the direction of the magnetic field. In the present $x$-$y$ mode, we take the transformation of the momentum $k_z \rightarrow -k_z$ and the magnetic flux $\phi \rightarrow \phi$ (i.e. the magnetic field does not need an inverse sign), the Hamiltonian $\mathbf{H}$ is invariant. From this mirror-reversal symmetry, although we can obtain $T_{3z/1}(E_F, \phi, k_z) = T_{3z/1}(E_F, \phi, -k_z)$ and $T_{3x/2}(E_F, \phi, k_z) = T_{3x/2}(E_F, \phi, -k_z)$ with $i = x, y, z$, from these relations of the transmission coefficients one only gets $N_{3z}(E_F, \phi) = N_{3z}(E_F, \phi)$. Second, from the inversion symmetry, we have

$$T_{3z/\sigma,1}(E_F, \phi, k_z) = T_{3z/\sigma,1}(E_F, \phi, -k_z),$$

(44)

$$T_{3z/\sigma,2}(E_F, \phi, k_z) = T_{3z/\sigma,2}(E_F, \phi, -k_z),$$

(45)

$$T_{3z/\gamma,1}(E_F, \phi, k_z) = T_{3z/\gamma,1}(E_F, \phi, -k_z),$$

(46)

$$T_{3z/\gamma,2}(E_F, \phi, k_z) = T_{3z/\gamma,2}(E_F, \phi, -k_z).$$

(47)

These relations of the transmission coefficients are similar with that in equations (16)–(19) for the $z$-$x$ and $x$-$z$ modes. To combine these relations and equation (10), the relations of spin Nernst coefficients $N_{3i}$ and $N_{3i}$ in the two transverse lead-3 and lead-4 in equations (42) and (43) can be derived analytically. From the above results, we find that the inversion symmetry makes that the spin current $I_3$ flows from a transverse lead to the other transverse lead and the spin currents $I_{3x}$ and $I_{3y}$ in two transverse leads flow out or flow in together in all three ($x$-$z$, $z$-$x$ and $x$-$y$) connection modes.

Finally, from the electron–hole-type symmetry, we can get the relations of the transmission coefficients:

$$T_{3x/\sigma, p}(E, \phi, k_z) = T_{3x/\sigma, p}(-E, -\phi, -k_z),$$

(48)

$$T_{3x/\sigma, p}(E, \phi, k_z) = T_{3x/\sigma, p}(-E, -\phi, -k_z),$$

(49)

$$T_{3y/\sigma, p}(E, \phi, k_z) = T_{3y/\sigma, p}(-E, -\phi, -k_z).$$

(50)

To substitute these relations of transmission coefficients into the expressions of spin Nernst coefficients in equation (10), one can analytically obtain the relations of the spin Nernst coefficients in equations (40) and (41), straightforwardly.

6. Conclusions

In summary, we study the spin Nernst effect for the Weyl semimetals under the perpendicular magnetic fields. By using nonequilibrium Green function method combining with the tight-binding Hamiltonian, three elements of the spin currents and spin Nernst coefficients at the transverse leads are derived. Due to the anisotropy of the Weyl semimetals, the spin Nernst coefficients are strongly dependent on both the direction of thermal gradient and the direction of the transverse lead connection. There are three non-equivalent modes ($x$-$z$, $z$-$x$ and $x$-$y$ modes), which are studied in detail. For the $i$-$j$ mode ($i, j = x, y, z$), the thermal gradient is applied in the $i$ direction and the spin current is measured in the $j$ direction. We find that the spin Nernst effect in the Weyl semimetals is essentially different with the traditional spin Nernst effect. So we call it the anomalous spin Nernst effect. Its anomalous behavior is manifested in the following two aspects. (1) The spin Nernst coefficients are zero at the zero magnetic field, and they appear in the presence of the magnetic field. This seems that the spin Nernst effect is caused by the magnetic field, in contrary to the traditional one induced by the spin–orbit coupling. (2) The $x$ and $y$ direction elements of the
spin currents in the two transverse leads flows out or flows in together. This is very different with the traditional one, where the spin current flows out from one transverse lead and flows in on the other transverse lead.

In addition, we show that the Weyl semimetals have the inversion-type symmetry, the mirror-reversal-type symmetry and the electron–hole-type symmetry. From the three symmetry, the spin Nernst coefficients are odd functions or even functions of the Fermi energy, the magnetic field and the transverse terminals. In particular, these odd or even relations of the spin Nernst coefficients analytically obtained from symmetries are completely consistent with the numerical calculation results. Furthermore, the spin Nernst coefficients show the strong anisotropic characteristics. At the zero magnetic field, the x direction elements of the spin Nernst coefficients are zero for the x-z and z-x modes, but it has non-zero value for the x-y mode. In the presence of the magnetic field, for the x-z and z-x modes the spin Nernst coefficients show a series of peaks and the peak positions are independent of the magnetic field and temperatures. But for the x-y mode, the spin Nernst coefficients strongly oscillate between the positive and negative values and are very sensitive to the magnetic field. These strongly anisotropic behaviors of the spin Weyl semimetals with broken time reversal symmetry. It is also hoped that these anomalous behaviors of the spin Nernst effect will be helpful to control the spin current.

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