Electronic non-coplanar refraction and deflected diffraction of Weyl-node-mismatch junctions

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Abstract
We studied the transport properties of the Weyl-node-mismatch junction, beside which the Weyl nodes are mismatch so that their projections on the interface plane cannot overlap. When electrons of one valley are injected onto the junction, the refraction is not coplanar with the injection-reflection plane. The non-coplanar deviation angle is valley dependent, and so if the injection consists of both valley components, the birefringence will take place. When electrons coming from a narrow rod transit across the junction into the bulk region on the other side, the electrons will be diffracted in the unconfined region. The diffraction is dispersed near the rod-bulk interface and is laterally deflected to the direction along the line connecting the Weyl node projections of incident and transmitted sides.

1. Introduction

The wave-particle duality of electrons allows one to understand the electronic transport as a combination of reflection and refraction. Because of the variety and complexity of electron energy bands in solid media, the electron optics has some interesting features that cannot be observed in usual photon optics. In 2007, Cheianov et al in their milestone paper [1] reported that, when an electron transits through a p–n junction in graphene, the electron experiences a negative refraction, and junction interface plays the role of so-called Veselago lens. The negative refraction of graphene p–n junctions was recently identified in experiment [2], which stimulated the researches on the electron optics in graphene. Such unusually refraction, with the spin and valley degree of freedom being taken into account, results in a variety of spin-dependent and valley-dependent refraction and focusing effects [3–7]. When the p-side or n-side of the junction is strained, the negative refraction is partially boiled and the focusing becomes asymmetric [8]. If an electron ray is injected onto the junction, the hit spot on the interface of reflected ray has a Goos–Hänchen shift [9–11]. When an electron wave passes through a narrow-wide junction, the diffraction wave will be split or collimated in the wide end, depending on the injection valley index [12].

The Weyl semimetal, of which the conduction and valence bands touch linearly with each other at points called Weyl nodes, as a new member of Dirac material family, has drawn much attention in recent years [13]. Weyl nodes exist in pairs, and the partners of one pair have opposite chirality and can be viewed as opposite monopoles of Berry curvature. Weyl materials have chiral anomaly [14, 15], which causes a lot of interesting transport effects such as positive longitudinal magnetoconductivity [16], planar Hall effect [17], and optical gyrotropy [18]. Since the Weyl semimetal is the 3D counterpart of graphene, the fantasy electron optical effects found in graphene are also expected in Weyl semimetals. The 3D version of Klein tunneling in Weyl materials was studied [19], the negative refraction and the Veselago focusing in Weyl semimetals were discussed [19–22], and the Imbert–Fedorov shift and Goos–Hänchen shift, for the reflection as well as the transmission in Weyl materials, were reported [23–26].

In this paper, we investigated the transmission problem and electron optics of a Weyl junction. The two sides of the junction are made up with the same Weyl semimetal, while the material for one side is rotated slightly relative to that of the other side, so that the projections of Weyl nodes of two sides cannot overlap with each other.

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on the interface. The right panel of figure 1 shows two possible realizations for the junction system. Electrons injected onto the interface will experience a non-coplanar refraction, as demonstrated in the left panel of figure 1. The non-coplanar deviation angle depends on incident orientation, Weyl node configuration, and valley index. If the injection consists of both valley components, the transmission will show birefraction feature. The transmission probability has maximum when the injection takes a special incident orientation. The conduction of the junction versus incident energy has a gap at low energy end, and when the energy is greater than a critical value, the conductance increases from then on. If the junction is constructed with a narrow rod and a large bulk, the electrons will be diffracted in the unconfined region when electrons are injected from the rod. The diffraction is dispersed near the rod export, that is a common diffraction feature, and the diffraction wave is laterally deflected to opposite sides for different valleys, that will cause the valley Hall effect. The deflected diffraction is quite remarkable when the incident wavevector is comparable to the node-mismatch distance and fades out in large wavevector limit. These interesting transport effects result from Lorenz force at the interface, which is caused by the Weyl-node-mismatch and exerted on electrons transiting through the interface. The conclusions also suit for the Dirac semimetals from band inversion.

2. Model and calculations

The minimal Hamiltonian of Weyl semimetal of positive chirality reads

\[ H = \mathbf{q} \cdot \boldsymbol{\sigma}, \]

where \( \mathbf{q} = \mathbf{k} - \mathbf{k}_0 \) is the wavevector relative to the Weyl node, with \( \mathbf{k} \) and \( \mathbf{k}_0 \) being the wavevector and the Weyl node measured from \( \Gamma \) point (the other Weyl node of negative chirality locates at \( -\mathbf{k}_0 \)). In the equation, the Fermi velocity \( v_F \) and the reduced Planck constant \( \hbar \) are set to be unity. The eigen energies and eigen states of the Hamiltonian in equation (1) can be straight obtained as

\[ E_{\pm} = \pm \sqrt{\mathbf{q}^2 + \Delta}, \quad |\psi_{\pm}\rangle = \begin{pmatrix} \cos(\theta/2) \\ \pm e^{i\varphi} \sin(\theta/2) \end{pmatrix}, \]

where \( \theta \) and \( \varphi \) are respectively the polar angle and azimuthal angle of \( \mathbf{q} \). At this stage, we only calculate the electronic transport of conduction band (\( E > 0 \)) near the positive chiral node, the conclusions will be extended to the other node and to cases of \( E < 0 \) at the end of this section.

The junction interface is set to be the \( x-y \) plane and thus the \( z \)-axis is normal to it. We consider that an electron is injected with state \( |i\rangle \) from region \( z < 0 \), reflected into state \( |r\rangle \), and transmitted into state \( |t\rangle \) in region \( z > 0 \). The states of reflection and transmission can be generally written as
In the limit \( d \to 0 \), the triangle in figure 2(b) reduces into a line, \( q_{1||} \) overlaps with \( q_{2||} \), \( \Delta \varphi \) vanishes, and the refraction is reduced into the normal one.

The line of \( d \) divides the projection plane into two half planes. If point \( A \) falls on the upper-half plane, the electron experiences a right-handed screw when it enters the refraction region, and if the point lands on the lower-half plane, a left-handed screw happens. If point \( A \) falls exactly on the boundary line, \( \Delta \varphi \) will be \( \pi \) or 0, depending on point \( A \) between or beyond the end points of \( d \).
Like the optical refraction, the polar angle torque, that is described by $\Delta \theta = \theta_2 - \theta_1$, occurs when electrons enter the refraction region, and it can be calculated by

$$\sin \Delta \theta = \frac{1}{q^2} (q_{1z} q_{2||} - q_{2z} q_{1||}).$$

(8)

In the limit $d \to 0$, we have $\Delta \theta = 0$, and the refraction effect disappears.

The midperpendicular of $d$ splits the projection plane into left and right parts (see figure 2(b)). If point $A$ falls on the left part, we have $q_{1||} < q_{2||}$ and $q_{1z} > q_{2z}$. For this case, $\Delta \theta$ is positive, that means the electron experiences a backward screw when it goes across the interface. Otherwise, the forward crew refraction happens.

The transmission probability $T$ is defined by $|\psi_2|^2 / |\psi_1|$, where $\psi_2 = q_2 / q$ (It is calculated by $\partial E / \partial q_z$) is the velocity normal to the interface plane. After some tedious calculations, we obtain a compact expression of $T$, that is

$$T = \frac{4 q_{1z} q_{2z}}{(q_{1z} + q_{2z})^2 + d^2}. \tag{9}$$

Figure 3 shows the transmission probability at different energies. For transmission, the in-plane wavevector $k_z$ corresponds to a point on $k_x-k_y$ plane. (Point $A$ in figure 2.) To ensure $q_{1||} < q$, the point must lie in the circle that is centered at point $O_1$ and has the radius $q = E$. Because the refraction does not change the energy, the point has to fall within another circle centered at $O_2$, having the same radius. The two conditions must be met simultaneously and so the transmission is only non-zero in the intersection area of the two circles. If point $A$ is outside the intersection region, the electron will be totally reflected. We fix the incident polar angle and let its azimuthal angle $\varphi_1$ change a turn. When $\varphi_1$ sweeps over the intersection region, the transmission sharply arises and changes flatly in the intersection area.

The maximum transmission can be found when point $A$ settles at the center of the intersection region, and it can be calculated by setting $q_{1z} = q_{2z}$ in equation (9), saying

$$T_m = \frac{q_{2z}^2}{q^2} = \cos^2 \theta_1, \tag{10}$$

in which the relation $q^2 = q_{1z}^2 + d^2 / 4$ is used. When the transmission takes its maximum, the injection direction is not normal to the interface, but has the incident angle $\theta_1 = \arcsin(d/2q)$. For this case, we have $\theta_1 = \theta_2$ and $\Delta \varphi = \pi$, that means the refraction and reflection directions orient opposite exactly.

The conductance (in units of conductance quanta $e^2/h$, where $e$ and $h$ are electron charge and Planck constant) across the junction per unite interface area can be calculated as

$$G(E) = \frac{1}{(2\pi)^2} \int_{q_{1||} \leq E} dq_{1||} T(E, q_{1||}). \tag{11}$$

Figure 4(a) shows the conductance as function of incident energy. There is a conductance gap on the curve in the interval $[0, d/2]$. This is because that in the interval, the two circles in figure 3 do not intersect, and then the conductance is zero. When the energy becomes higher, the two circles intersect and the area of intersection gets larger, and the conductance increases from zero on. The gap can be seen more clearly on the curve of $G/G_0$ in
where $G_0 = q^2 / 4\pi$ is the conductance of the Weyl material without the junction. When $E \gg d$, the ratio $G/G_0$ tends to be unity and the junction has no effect for the transport.

Now we consider the junction is made up of a rod and a semi-infinite bulk. When an electron beam of a given energy comes from the rod and enters the bulk region, it is refracted, simultaneously diffracted, and a local density of states (LDOS) caused by the injection is distributed in the whole diffraction region. How the LDOS looks like can be understood by means of the semiclassical method proposed in [12]. Here we describe the problem as following.

Though the rod radius is finite, we assume that the cross section is large enough to ensure that the spinor plane wave $|\psi\rangle$ can be viewed as the eigen state in the rod. The LDOS in the rod contributed by the incident state is

$$ f(x, y, z) = \begin{cases} 1/(\pi R^2), & x^2 + y^2 \leq R, \\ 0, & x^2 + y^2 > R, \end{cases} \quad (12) $$

where $R$ is the radius of the rod. The incident state $|\psi\rangle$ is refracted into $|\psi_t\rangle$ and correspondingly, the LDOS is transformed to $|\psi_t\rangle^2 f$ at the interface. Thereafter, the state propagates freely and a LDOS distribution in the infinite region is formed. Such a LDOS likes a non-divergent searchlight beam. The beam has the same cross section as it accommodated in the rod, while its orientation is different from that of the rod (see figure 5). The orientation of the searchlight beam is the same as that of velocity in the bulk region, which is parallel to the vector $q_2$. One incident state labeled by $q_1$ corresponds to one transmitted state labeled by $q_2$. The LDOS of the searchlight beam is described as

$$ D_{q_1} = |\psi(q_1)|^2 f(x - x', y - y', z), \quad (13) $$
where

\[ x' = z \tan \theta_z \cos \varphi_2, \]
\[ y' = z \tan \theta_z \sin \varphi_2, \]

are the coordinates of the cross section center.

An injected electron beam of energy \( E \) consists of all incident states having the same vector length \( \mathbf{q}_1 = E \). These states are all refracted and propagate in the diffraction region. Every state has its own LDOS in the transmission region, and the total LDOS contributed by all injection states of energy \( E \) is

\[ D(E) = \frac{1}{(2\pi)^2} \int_{|\mathbf{q}_1| \leq E} d\mathbf{q}_1 \langle \mathbf{D}(\mathbf{q}_1) \rangle_{\mathbf{q}_1 = E}. \]  

Figure 6 shows the total LDOS distribution induced by injection with certain energies. One can see the injected beam is dispersed and deflected, and the deflection is apparent when \( E \lesssim d \) and is negligible for \( E \gg d \). Because the total LDOS in equation (15) is a combination of beams in all directions, it is natural that the transmitted wave is dispersed in the non-confined region. The deflection of transmission can be qualitatively understood by semiclassical mechanism [27]. The mismatch of the Weyl nodes results in an in-plane wavevector \( \mathbf{q}_{21} \) (See the arrows originated from \( O_2 \) in figure 3), which is also the in-plane orientation of the searchlight beam in equation (13). The configuration of these \( \mathbf{q}_{21} \) determines the manner of diffraction disperse and deflection. For the case of \( E < d \), all \( \mathbf{q}_{21} \) are oriented leftwards, as indicated in the upper-left panel of figure 3, and so the beam of energy \( E \) is deflected severely. When \( E > d \) but \( E \) does not dominate over, there is a larger portion of \( \mathbf{q}_{21} \) in the intersection is leftwards and a smaller portion pointing rightwards, as shown in the lower-left panel of figure 3. For this case, the deflection is still leftwards but more dispersed and less deflected. For the large energy limit \( E/d \to \infty \), the deflection effect tends to be negligible.

All the above calculations and discussions are based on that the electron is injected from the conduction band and from the valley of positive chirality. The transport properties for the valence band electrons and for the other valley can be obtained respectively by reversing the sign of incident energy (the velocity is opposite to wavevector \( \mathbf{q} \) for this case) and exchanging the projection points of the Weyl nodes \( O_1 \) and \( O_2 \) in figure 2). Under either operation, the leftward (rightward) screw of the non-coplanar refraction and leftward (rightward) deflection of diffraction will be both reversed to rightward (leftward), and the transmission as well as the conductance remains unchanged. If the injected wavefunction is superposed with both valleys, the components of the two valleys are respectively refracted differently. In other words, the birefraction occurs.

Most Weyl semimetals experimentally verified are of the inversion-broken type and have many Weyl node-pairs [28, 29]. The Weyl node-pairs often lie at different energies. Every node plays its own role in transport.
according to above analysis, and each Weyl node-pair can be treated individually with its own incident energy. The calculations can also be applied for the Dirac semimetal from band inversion [30–32], which has even number of two-fold Dirac points away from $\Gamma$ point and can be regarded as two Weyl materials overlap in real space.

3. Summary

We studied the transmission properties of Weyl-node-mismatch junctions. When electrons transit through the interface, the refraction of the junction is non-coplanar and valley dependent, thus the birefringence happens if the injection consists of both valley components. The non-coplanar angle depends on the relative orientation between the direction of injection and that of Weyl-node-mismatch mapping on the junction interface. When the injection energy is greater than a critical value, which is determined by the Weyl-node-mismatch distance on the interface, the conductance arises and increases, otherwise, it is totally suppressed due to that the injection and transmission circles cannot intersect. If electrons are injected from a narrow rod, transit the junction and go into a bulk, they will be diffracted and dispersed in the bulk region. The diffraction is deflected oppositely for different valleys. Our conclusions are not limited to Weyl semimetals, but also valid for Dirac semimetals from band inversion.

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