Vortex of beam shift induced by mono-chiral interface states

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Abstract

If an electron beam hits onto the interface of a Weyl-node-mismatch junction, a shift of the beam center on the interface happens when the beam is reflected or transmitted, where the junction consists of two materials of the same Weyl semimetal and one of them is rotated with respect to the other by an angle. We calculate the longitudinal and transverse shift components (the Goos–Hänchen and Imbert–Fedorov shifts). The reflection shift for total reflection cases is much more remarkable than the shift for transmitted cases. There exists a semi-vortex structure of the reflection shift on the in-plane k-space. The vortex is induced by the touch between bulk bands and interface bands. The formation of such interface bands is explained by the pulley-group model, in which the Weyl cones serve as wheels and the surface and interface bands act as ropes. A surface rope connects wheels of opposite chiralities, and an interface rope links the wheels for the two side materials of the same chirality.

1. Introduction

The similarity between electron in graphene and photon in medias spurs extensive studies on electron optics in graphene under different configurations, and a lot of interesting features, that cannot be observed in usual photon optics, were discovered. A graphene p–n junction is a negative refraction interface for electrons [1], which was recently verified in transport experiment [2]. The unusually refraction, with considering the factors such as spin, valley, strain, and band warping, results in a variety of refraction and focusing effects [4, 3, 5–8]. In a strained graphene channel, the Fabry–Pérot states can carry a pure valley current [9]. If an electron beam is injected onto the junction interface, the spot of reflected beam has a shift relative to that of incident beam on the interface [10–12]. When an electron wave comes from a narrow ribbon into a bulk region, it is diffracted in split [13].

The Weyl semimetal, that accommodates pairs of Dirac points named by Weyl nodes, can be regarded as the 3D counterpart of graphene, has drawn much attention in recent years [14–16]. The Weyl nodes of one pair possess opposite chiralities and are the source and sink of Berry curvature. The chiral anomaly [17, 18], that happens when electric field in direction of magnetic field and can pump electrons between Weyl nodes, leads to interesting transport effects such as negative longitudinal magnetoresistance [19–22], planar Hall effect [23] and optical gyrotropy [24]. When electrons transit through a Weyl junction, the refraction is non-coplanar with the injection-reflection plane [25]. The novel electron optics effects ever found in graphene are expected in Weyl semimetals. The 3D version of Klein tunneling, negative refraction and Veselago focusing were discussed in Weyl semimetals [26–29]. The electron beam shift on p–n junction interfaces has not only longitudinal but also transverse components, respectively called Goos–Hänchen (GH) and Imbert–Fedorov (IF) shifts, the latter of which does not exist in graphene [30–32], and the beam shift for transmission that was not noticed in solid media previously, was pointed out recently [30]. When an electron beam is injected from a Weyl semimetal to an insulator and reflected, the shift is extremely sensitive to the existence of surface bands, and a semi-vortex structure in the in-plane k-space was found locating where the surface band touches and bulk band [33].
In this paper, we investigated the electron beam shift, both the GH and IF components, on the interface as a function of in-plane wavevector of a Weyl-node-mismatch junction. The junction, that is demonstrated in the left panel of figure 1, is constructed with two identical Weyl semimetals with one side material is rotated with respect to the other side. The Weyl nodes of the same chirality of two sides are mismatch, and Weyl-node-mismatch line, that connects the two node projections on the interface, plays important role for the beam shift. The injection beam has non-zero transmission when real wavevector is allowed on the transmitted side, and it is totally reflected when real wavevector is forbidden there. For both reflection and transmission beams, the GH shift is anti-symmetric, and the IF shift is symmetric relative to the Weyl-node-mismatch line in the transmitted region. The reflection shift in the total reflection region has no symmetry and is quite larger than that in the transmitted region. We found a semi-vortex in reflection shift for the total reflection case. The vortex is a signal of new surface energy bands appearing at the junction interface. The interface bands are formed by the interaction between the surface bands of materials of two sides at the interface. The interface bands are topological objects, they are tangent with the same chirality Weyl cones of different sides, and the tangency induces the vortex of reflection shift. We used a pulley-group model to explain the interface bands under various situations.

2. Theory of beam shift

We begin with the minimal Hamiltonian of Weyl semimetal of positive chirality

\[
H = \mathbf{q} \cdot \mathbf{\sigma} = \begin{pmatrix} q_x & q_z - i q_y \\ q_z + i q_y & -q_x \end{pmatrix},
\]

where \( \mathbf{\sigma} = (\sigma_x, \sigma_y, \sigma_z) \) is the vector of Pauli matrices in spin (pseudo-spin) space, \( \mathbf{q} = \mathbf{k} - \mathbf{k}_0 \) is the reduced wavevector with respect to the Weyl node \( \mathbf{k}_0 \) (The 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 omitted for simplifying the notation. The eigen energies and eigen states of the Hamiltonian is straight solved as

\[
E_{\pm} = \pm q_z, \quad |\psi_{\pm}\rangle = \frac{1}{\sqrt{|2E|}} \begin{pmatrix} e^{-i \varphi/2} \sqrt{E + q_z} \\ \pm e^{i \varphi/2} \sqrt{E - q_z} \end{pmatrix},
\]

where \( \varphi \) is the azimuthal angle. In the equation \( q_z \) can be either real or imaginary, of which the former and latter correspond to the propagating and evanescent modes respectively. In this section, we will only consider the electronic transport near the positive chiral node for the conduction band, and later the conclusions will be extended to the other situations with some modifications.

The Weyl-node-mismatch junction is illustrated in figure 1, which is made up of two identical Weyl materials with one of them is torqued by an angle. The junction interface is set to be the \( x-y \) plane. We consider the physical process that an eigen state of conduction band (\( E > 0 \)) 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 injection and transmission are propagating ones and can be written as
where $\mathbf{r}$ is the position vector, $\theta = \arctan |q_n|^2$ is the polar angle of $q$, and the relation
\[
\cos^2 \theta/2 = (E + q_n)/2E
\]
for propagating states is used. In the equation and from here on, the quantities with subscripts 1 and 2 mean respectively those of the incident and transmitted sides, and the parallel symbol is used to imply the component projected on the interface. For the transmission, $q_n$ could be either real or imaginary, corresponding to non-zero transmission or total reflection case. The transmitted state covering either case is
\[
|t\rangle = \frac{1}{\sqrt{2E}} \begin{pmatrix} e^{i\varphi_1/2} \sqrt{E + q_{2z}} e^{i\theta_2} r e^{i\theta_2} \\ e^{i\varphi_1/2} \sqrt{E - q_{2z}} e^{i\theta_2} r e^{i\theta_2} \end{pmatrix}.
\]
(4)

The energy conservation results in $q_1 = q_2 = q$. The wavefunction continuity requires the plane waves of two sides coincide, saying, $k_{1||} = k_{2||} = k_{||}$ and simultaneously demands the spinor parts of two sides equivalent to each other at the interface, saying
\[
\begin{pmatrix} e^{-i\varphi_1/2} \sin \frac{\theta_1}{2} \\ e^{i\varphi_1/2} \sin \frac{\theta_1}{2} \end{pmatrix} + \mathbf{r} \begin{pmatrix} e^{-i\varphi_2/2} \sin \frac{\theta_2}{2} \\ e^{i\varphi_2/2} \sin \frac{\theta_2}{2} \end{pmatrix} = t \sqrt{2E} \begin{pmatrix} e^{-i\varphi_1/2} \sqrt{E + q_{2z}} \\ e^{i\varphi_2/2} \sqrt{E - q_{2z}} \end{pmatrix},
\]
(5)

where $\mathbf{r}$ and $\mathbf{t}$ are the reflection and transmission coefficients. The equation allows us to work out the two coefficients as
\[
r = -\frac{a}{b} = |r| e^{i\gamma_r}, \quad t = -\frac{\cos \theta_1}{b} = |t| e^{i\gamma_t},
\]
(6)

where $\gamma_r$ and $\gamma_t$ are the complex angles of $r$ and $t$ respectively, and $a$ and $b$ are two dimensionless quantities defined by
\[
a = \frac{e^{i\Delta \varphi/2} \cos \frac{\theta_1}{2} \sqrt{E - q_{2z}} - e^{-i\Delta \varphi/2} \sin \frac{\theta_1}{2} \sqrt{E + q_{2z}}}{\sqrt{2E}},
\]
\[
b = \frac{e^{i\Delta \varphi/2} \sin \frac{\theta_1}{2} \sqrt{E - q_{2z}} - e^{-i\Delta \varphi/2} \cos \frac{\theta_1}{2} \sqrt{E + q_{2z}}}{\sqrt{2E}},
\]
(7)

with $\Delta \varphi = \varphi_2 - \varphi_1$.

An electron beam is superposed by infinite of plane waves, and the incident electron beam can be generally described by
\[
|B_i(E)\rangle = \int f(E, \mathbf{k}_i) |i(\mathbf{k}_i)\rangle d\mathbf{k}_i ||,
\]
where $f$ is a function reflecting the beam profile distribution in $k_x$-$k_y$ plane. A typical choice of the profile is the Gaussian distribution function. On the interface ($z = 0$), the integration results in different beam spot centers in real space for different spin (pseudo-spin) components. For the spin up and down components, the spot centers are calculated to be $\varphi_1/2$ and $-\varphi_1/2$. The calculation details are not shown here but presented in appendix A.

According to equation (3), the spin up and down components for the injection are weighted by the probabilities $\cos^2(\theta_1/2)$ and $\sin^2(\theta_1/2)$ respectively, where the prime symbol means the gradient operation in $k_x$-$k_y$ plane. The incident center can be regarded as the weighted mean average over the two components, and it is worked out to be
\[
R_i = \frac{1}{2} \varphi_1' \cos \theta_1.
\]
(9)

The incident beam is reflected and transmitted away, and the wavefunctions of reflection and transmission beams are
\[ |B_r(E)| = \int f(E, k_1) |r(k_1)| \, dk_1 \]
\[ |B_t(E)| = \int f(E, k_1) |r(k_1)| \, dk_1 \]

For the reflection and transmission, the beam centers of spin up and down components are \( \gamma^r - \varphi^r \) and \( \gamma^t + \varphi^t \), respectively (see appendix A). The two components are weighted by \( \sin^2(\theta_1/2) \) and \( \cos^2(\theta_1/2) \) for the reflection, and are weighted by \( \cos^2(\theta_2/2) \) and \( \sin^2(\theta_2/2) \) for the transmission, according to equations (5) and (4). By averaging over the spin components, the reflection and transmission beam centers are

\[
R_r = -\gamma_r' - \frac{1}{2} \varphi_r' \cos \theta_1
\]
\[
R_t = -\gamma_t' + \frac{1}{2} \varphi_t' \cos \theta_2.
\]

The shifts of reflection and transmission with respect to the incident center are defined by \( S_r = R_r - R \) and \( S_t = R_t - R \), respectively, and they are calculated as

\[
S_r = -\gamma_r' - \varphi_r' \cos \theta_1,
\]
\[
S_t = -\gamma_t' + \frac{1}{2}(\varphi_t' \cos \theta_2 - \varphi_r' \cos \theta_1).
\]

To obtain the explicit results of the shifts, we have to work out \( \gamma' \) and \( \gamma' \) first. The detailed calculation of them can be found in appendix B.

The GF and IF shift components can be obtained by projecting the shifts on the longitudinal and transverse directions, saying

\[
S_{GF} = S \cdot \hat{q}_l \]
\[
S_{IF} = S \cdot \hat{\varphi}_l.
\]

where \( \hat{q}_l \) and \( \hat{\varphi}_l \) are the longitudinal and tangent unit vectors respectively. Equation (13) is applied on both the reflection and the transmission beams.

3. Calculation results

We establish the \( k_x \)-axis normal to the interface, and the \( k_x-k_y \) plane projections of Weyl nodes belong to the incident and transmitted sides are \((0, 0)\) and \((d, 0)\), which are referred as points \( O_1 \) and \( O_2 \) from here on, respectively. The line connecting \( O_1 \) and \( O_2 \) will be called as the line of \( d \), and the length \( d \) reflects the Weyl-node-mismatch. The transmission and reflection shift, as well as their GH and IF components for the incident energy \( E = 1.5d \) are shown in figure 2. Since both the incident and transmitted states must be propagating ones, the constraints \( q_{11} < q \) and \( q_{1||} < q \) have to be satisfied. The former and the latter constraints define two circles with radius \( q \) and centered at \( O_1 \) and \( O_2 \) respectively, and the two circles will be referred as incident circle and transmitted circle in the following. The transmission shift can only be defined in the intersection region of the two circles, and the intersection area will be named by transmission region. In the incident circle excluding the transmission region, the transmission probability is zero and the total reflection occurs, and we will refer this area as total reflection region.

For the transmission, the GF and IF components are odd and even symmetric with respect to the line of \( d \) and take zero on the line. The shift magnitude is both up–down and left–right symmetric. The shift orients approximately (anti)parallel to the line of \( d \) in the most area of the transmission region. The reflection shift in the transmission region has some similar features as those of the transmission shift. The GH and IF components are odd and even symmetric, they are zero on the line of \( d \), and the shift orients almost horizontally. However, the shift magnitude only has up–down symmetry but is not left–right symmetric.

In the total reflection region, no transmission shift is defined and the reflection shift is quite different. The shift is much more remarkable than that in the transmission region and it has not any symmetry at all. Averagely saying, the shift orients from the total reflection region to the transmission region, and the direction of shift is exactly horizontal on the line of \( d \) because the IF component is zero there. The shift discontinues at the boundary between the two regions, and the discontinuity was also reported in other junction systems [30]. Near the boundary, the shift is divergent on the total reflection side while keeps finite on the transmission side.

The most interesting thing is that there is a semi-vortex structure at the edge of the total reflection region. To identify the semi-vortex, we settle a circle of radius 0.01\( d \), which crosses point vortex center point (labeled by \( A \) in the figure) and is tangent to the incident circle. The radius is chosen to ensure that the circle does not intersect with the boundary between two regions (The circle size is exaggerated). We observe the orientation of reflection
shift when a point on the circle moves from point $A$ anti-clockwise. The calculated result is presented in the inset of figure 2. The orientation angle evolves smoothly and changes amount of $\pi$.

Figure 3 shows the vortex structure in reflection shift for different incident energies. When the energy decreases, the radius of incident and transmitted circles becomes smaller, and the total reflection region expands with the position of vortex center unchanged. If the energy $E < d/2$, the two circles do not intersect, the transmission region disappears, the electron cannot transit through the junction and the total reflection occurs in the whole incident circle with the vortex structure preserved. When the incident energy increases, the transmission region expands, the total reflection area shrinks, and the shift is weakened in both regions. If $E \gg d$, the transmission region almost occupies the whole transmitted circle, the total reflection region shrinks into a very slim crescent. However, point $A$ cannot be covered by the transmission region even for high energy cases and the vortex center survives still there.

If one reverses the relative rotation of beside materials so that the injected and transmitted circles exchange their positions, the substitution $d \rightarrow -d$ should be taken in the calculation results. The vortex center appears at the opposite edge of the incident circle while the vortex curl keeps unchanged. When the injected electron is from valence band, its velocity is opposite to $q$. For this case, the replacement $\varphi \rightarrow -\varphi$ is applied in the results, which leads to that both the vortex position is flipped and the vortex curl is reversed. For the other valley
injection, not only $\phi \to -\phi$ but also $d \to -d$ are applied. The combination of the two operations results in that, the vortex position remains intact while the vortex curl is reversed.

4. Interface energy bands

The vortex structure of reflection shift, whose center lies on the edge of the incident circle, is the signal of surface band existence [33]. Since the surface bands of the lower and upper materials meet at the interface, they will merge and reconstruct new interface bands. A reasonable guess is that the vortex is induced by the joint between interface bands and bulk bands.

An interface state, that locates near the interface and extends in the bulk, satisfies equation (2) in the two side materials simultaneously. The interface band can be determined by the wavefunction continuity at junction interface, saying,

$$\begin{align*}
\begin{pmatrix}
    e^{-i\xi_1^2/2} \sqrt{E + q_{1z}} \\
    e^{-i\xi_2^2/2} \sqrt{E - q_{2z}}
\end{pmatrix} & \propto
\begin{pmatrix}
    e^{-i\xi_1^2/2} \sqrt{E + q_{2z}} \\
    e^{-i\xi_2^2/2} \sqrt{E - q_{1z}}
\end{pmatrix}.
\end{align*}$$

(14)

Because the interface states decay away in real space, the wavevector must be imaginary either in the upper or in the lower materials. We denote the imaginary wavevectors as $q_{1z} = -i\kappa_1$ and $q_{2z} = i\kappa_2$ in the lower and upper materials, respectively, where $\kappa_1$ and $\kappa_2$ are the decay rates in the two side materials. By substitute the imaginary wavevectors in the above equation, we have

$$\Delta\phi = \xi_1 + \xi_2,$$

(15)

where $\xi_1$ and $\xi_2$ are the complex angles of $E + i\kappa_1$ and $E + i\kappa_2$ respectively.

The solutions of equation (15) can be obtained with the help of figure 4. One can easily verify that, all the points on the line tangent up to the incident and transmitted circles satisfy the above equation. The touch point between the incident circle and the interface band line is just the vortex center of shift. The energy relation

$$E^2 = q^2 - \kappa^2$$

on both sides results in the interface band dispersion $E = q$. Because of $\kappa_1 + \kappa_2 = d$, if an interface state attenuates on one side rapidly, it decays on the other side slowly. In the figure, the incident and transmitted circles are separated well, while the above conclusions are not changed when they intersect.

The interface band has its topological origination. The incident and transmitted materials have their own Berry curvatures $\Omega = q/2q^3$. We consider a $k$-space plane that is perpendicular to the line of $d$ (line $O_1O_2$). On the plane, one can define a 2D Chern number $C = (2\pi)^{-1} \int \Omega \cdot dq_\perp dq_\parallel$ with $\Omega_x = q_x/2q^3$ being the Berry curvature component along $k_x$ direction. The Chern number on the plane is calculated to be $C = \text{sgn}(q_x)/2$. When the plane is placed between points $O_1$ and $O_2$, we have $q_{1x} > 0$ and $q_{2x} < 0$, and the Chern numbers for the incident and transmitted materials take $+1/2$ and $-1/2$ respectively. This means the interface is a topological domain wall for the chosen value of $k_x$, and the Chern number difference $C_1 - C_2 = 1$ is number of energy band localized near the interface [34–36]. If the plane cuts the line outside of $O_1$ and $O_2$, the values of $q_x$
for both side materials have the same sign, so Chern number difference is zero. This is the reason why an interface band appears in the interval of $k_x$ between $O_1$ and $O_2$.

The interface band can also be understood by the mixture of surface bands in real space. The lower panels in figure 4 show how the surface bands at the interface merge into new interface bands. Cutting the Weyl cones of a Weyl semimetal at the positive incident energy, we have two circles enclosing the Weyl points and two surface band lines connecting the two circles by tangent way. One line represents the surface states on the bottom surface, and the other means those on the top surface. The Weyl pairs of the two side materials orient non-parallelly, and the two Weyl dipole vectors cross in the same $k$-space. When the two materials are jointed to form the junction, the surface bands of both side materials on the interface are spoiled and new interface bands appear. The interface bands are the tangent lines connecting the incident and transmitted circles of same chirality. The calculations in this paper are based on the positive chirality incidence. For the other chirality injection, the transmitted circle lies left to incident one, and point $A$ locates at the same position with respect to the Weyl point of negative chirality. Unlike the surface bands of semimetals, the interface bands have no counter-flowing partners, and the current carried by them is neutralized by the surface bands. One can see that these circles connected by surface and interface bands looks like a set of wheels winded on by a closed rope.

Because the surface bands and interface bands are all topological objects, the closed rope cannot be broken by adiabatic Hamiltonian deformation and weak perturbation, the pulley-group model is a powerful tool to analysis interface bands for more complicated situations. We consider that not only the in-plane rotation of one side material happens but also the out-of-plane rotation is allowed. The latter rotation results in that the interface projection of its Weyl dipole vector is shortened. We initialize the junction as before (see figure 4), and change the in-plane and out-plane rotations, so as that the transmitted circle moves around the incident one by a half-turn and the incident and transmitted circles exchange their positions. The process is illustrated in the upper panels of figure 5. One can find that point $A$ moves on the incident circle, and finally get to the opposite side, consistence with our former statements.

When there is a potential difference across the interface, the Weyl node pairs of two sides lie at different energies, and the incident and transmitted circles are of different size. The lower panels of figure 5 demonstrate how the system evolves when the energy decrease from above both Weyl node energies. With the energy decreases, the both circles shrink, and one of them is reduced into a point for certain energy, then the circle revivals on the valance band. For this case, the interface band is co-tangent with the two circles in a kink way. Finally, the two circles become both valance band ones, and point $A$ moves to the other side on the incident circle of valence type, in accordance with our previous conclusion.

![Figure 5. Evolution of interface band when (Upper panels) the positions of incident and transmitted circles change and when (Lower panels) the energy is decreased. The incident and transmitted circles of valance band are marked by gray-filling. The blue, red, and purple lines denote respectively the bottom surface band, top surface band, and interface band.](image-url)
5. Summary

We calculated the electron beam shift for reflection and transmission on the interface of a Weyl-node-mismatch junction, and the interface states on the junction interface were analyzed. The GH shift and IF shift are antisymmetric and symmetric with respect to the Weyl-node-mismatch line in the transmitted region. The reflection shift in the total reflection region is dominant in magnitude. A semi-vortex for reflection shift locates at the tangency point between the interface band and the incident circle. The interface band links the incident and transmitted circles of the same chirality. We found the origin of the interface bands can be well explained by a pulley-group model, which reflects the topological nature of the interface states and can be applied for a variety of situations.

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Appendix A. Shifts of gaussian beam center

A typical choice of the cross-section profile of beam in k-space is the Gaussian distribution function
\[ f \propto \exp\left((-k\delta - k)^2/2\Gamma^2\right) \]
with \( k \) being the beam center and \( \Gamma \) being the effective width. The integrations in equations (8) and (10) are always of the form
\[ \int e^{-(k\delta - k)^2/2\Gamma^2} \exp(i\vec{k} \cdot \vec{r}) \, d\vec{k} \]
where \( g \) is a function of \( k \) and takes \( \mp \varphi_1/2, \varphi_1/2 \) and \( \varphi_2/2 \) for spin up/down incident, reflection and transmission beams, respectively. If \( \Gamma \) is small enough to ensure \( g \) can be viewed as a slow varying function, we can expanding \( g \) at \( k \) up to the first order and we have
\[ e^{ig} = \exp[i(g)_{k_1} \cdot (k_1 - \bar{k}_1)]. \]
Substituting the expression into equation (A1), one can find the integration is proportional to
\[ \int e^{-(k\delta - k)^2/2\Gamma^2} \exp[i(k_1 - \bar{k}_1) \cdot (\vec{r} + (g')_{k_1} \cdot \vec{r})] \, d\vec{k}_1 \]
\[ \propto \exp[-2\Gamma^2 (\vec{r} + (g')_{k_1} \cdot \vec{r})]. \]
It describe also a Gaussian beam in real space with the center being \(-(g')_{k_1}\) and the width \( (2\Gamma)^{-1} \). The centers of the spin-up/down components of injection are thus \( \pm \varphi_1'/2 \), here and in the main text, the subscript \( \bar{k}_1 \) is omitted for concision. The spin-up/down beam centers for reflection are \(-\gamma_1' \pm \varphi_1'/2\) and those for transmission are \(-\gamma_1' \pm \varphi_1'/2\).

Appendix B. Calculation of \( \gamma_1' \) and \( \gamma_1'' \)

Denoting the complex phases of \( a \) and \( b \) in equation (6) as \( \phi_a \) and \( \phi_b \) respectively, we have \( \gamma_1' = \phi'_a - \phi'_b \) and \( \gamma_1'' = -\phi'_b \). In the following, we will calculate the shifts for the propagating transmission case \( (|r^2| < 1) \) and the total reflection case \( (|r^2| = 1) \) separately.

For the case of non-zero transmission, we have
\[ \phi'_a = \frac{1}{4|a|^2} \left[ \Delta \varphi'(\cos \theta_1 - \cos \varphi_2) + \frac{d}{\bar{q}} (\theta'_1 \sin \varphi_1 - \theta'_2 \sin \varphi_2) \right], \]
\[ \phi'_b = \frac{1}{4|b|^2} \left[ \Delta \varphi'\cos \theta_1 + \cos \varphi_2 + \frac{d}{\bar{q}} (\theta'_1 \sin \varphi_1 + \theta'_2 \sin \varphi_2) \right]. \]

Generally saying, the shift consists of the linear combination of vectors \( \varphi'_1, \theta'_1, \varphi'_2 \) and \( \theta'_2 \), and these gradients can be calculated as
\[ \varphi' = \frac{\hat{\varphi}}{\bar{q}_1}, \quad \theta' = \frac{\hat{\theta}}{\bar{q}_2}. \]

The equation can be applied for either the injection side or the transmission side, and in the equation \( \hat{\varphi} \) and \( \hat{\theta} \) is the tangent and radial unit vectors with respect to point O1 or O2.
For the case of total reflection, the transmission probability (not the transmission coefficient) is zero, the transmission shift cannot be defined and need not to be considered. Because $\theta_2$, that describes the polar angle of transmission, makes no sense now, the shift for total reflection needs to be re-calculated. The wavevector $q_{2z} = i\kappa_2$ is pure imaginary for the total reflection case. The energy is related with the wavevector components by $E' = q_{2x}^2 + q_{2z}^2$. Recalling that $\xi_2'$ is the complex angle of $E + iq_{2z}$, we have $E + q_{2z} = q_{2z}e^{i\xi_2'}$. Applying it in equation (6) and carrying the calculation on, we obtain

$$\phi' = \frac{1}{2} \left( \frac{\Delta \varphi - \xi_2'}{\sin \theta_1} \cos \theta_1 + \sin(\Delta \varphi - \xi_2') \frac{\theta'}{\sin \theta_1} \right) .$$

(B3)

In the equation, all the gradients except for $\xi_2'$ are given in equation (B2), and $\xi_2'$ is calculated by

$$\xi_2' = \frac{q}{\kappa_2} \cdot \frac{\hat{q}_{2z}}{q_{2z}} .$$

(B4)

Because of $a = b^*$ for the total reflection case, that can be easily verified in equation (6), we have $\phi_b = -\phi_a$ and $\gamma_f' = 2\phi_a$.

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