Hall effect and orbital magnetism of Dirac electrons with spin-orbit interactions

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Abstract. Hall effects and orbital magnetism are investigated for Dirac electrons in solid with spin-orbit interactions. The conductivity, the Hall conductivity, the Hall coefficient and the orbital susceptibility are calculated on the basis of the gauge-invariant Kubo formula in the Luttinger-Kohn representation. The Hall coefficient exhibits peaks at the band-edge and changes its sign at the middle of the band gap. A novel contribution to the Hall conductivity, which is generated by the interband effects of a magnetic field, is found near the band-edge region. The origin of this novel contribution is discussed referring to the orbital susceptibility.

1. Introduction

In resent years, there has been a renewed interest in the problem of Dirac electrons in solids, which has an electron dispersion of Dirac electron $E(k) \propto \sqrt{v^2k^2 + \Delta^2}$ (Fig. 1)[1]. (Here $2\Delta$ is a band gap and $v$ the velocity of electrons.) Graphite[3, 4] and bismuth[5, 6] are the typical Dirac electron systems in solids, which have been known since old days[7]. Adding to these old Dirac electrons, new materials of Dirac electrons, such as the graphene[8, 9], $\alpha$-ET$_2$I$_3$[10] and HgTe quantum well[11], have been discovered. Furthermore, Bi and its alloys have been attracting renewed interest in the context of the spin Hall effect[12, 13], the three dimensional fractional quantum Hall effect[14], and nanoscience[15, 16]. In spite of these fascinating behaviors, there has been no theoretical analysis especially in the weak field limit. In order to understand these

![Figure 1. Band structure of pure bismuth near the $L$-point in the Brillouine zone. The chemical potential is $\mu \sim 27$ meV from the band-edge of the conduction band, and the band gap is $2\Delta \sim 14$ meV[2].](image-url)
phenomena, it is indispensable to understand the motion of electrons and holes of Bi-type Dirac electrons in a magnetic field.

Electrons in a crystal can be described in terms of Bloch electron. In a magnetic field, \( H \), it is often useful to utilize the Peierls substitution, where the effective Hamiltonian is described by \( \mathcal{H}_{\text{eff}} = E_n(k + eA/c) \) except for the Zeeman effect. Here, the \( n \)-th Bloch band is characterized by an energy function \( E_n(k) \) for zero field. In a magnetic field, however, the Bloch wave function is distorted so as to hybridize with another Bloch state. These terms will be referred to as non-diagonal terms, and the effects which are not taken into account by the Peierls substitution will be referred as the interband effects of a magnetic field[17, 18]. Although the interband effect is a fundamental problem even for non-interacting electron systems, it has been studied only in limited cases.

The significance of the interband effects is recognized through the studies of the orbital magnetism[19]. In most cases, the orbital susceptibility, \( \chi \), obtained by the Peierls substitution, the Landau-Peierls (LP) formula[20], is used for the comparison with the experimental results. However, the LP formula fails to explain the anomalous behavior of Bi[21, 22, 23]. Adams pointed out, in the study of the diamagnetism of Bi, that the LP formula gives insufficient results in cases where the energy gaps between some bands are much smaller than the Fermi energy[24]. In such cases, a term corresponding to complicated “roundabout” interband transition of electrons gives large contributions. McClure adopted the Adam’s idea and succeeded to explain the large diamagnetism of graphite[4, 25], which also could not be explained with the LP formula[26, 27]. This work now becomes the basis of the recent study of graphite-type Dirac electrons, such as graphene[28, 29, 30, 31] and \( \alpha \)-ET\(_2\)I\(_3\)[32].

As for Bi, it is more complicated because of the large spin-orbit coupling of the order of 1.5 eV[2]. The spin-orbit interaction couples the bands separated with a band gap, and causes a remarkable effect of interplay of spins and orbital motion of electrons. The effective \( g \)-factor become much larger than that of free electrons owing to the orbital motion (\( g \) can exceed 200 for Bi). The orbital diamagnetism and the spin paramagnetism are mixed together by the strong spin-orbit coupling, so that they can no longer be well separated. The anomalously large diamagnetism of Bi finally explained not only qualitatively but also quantitatively[33], by considering the spin-orbit coupling, the interband effects and the special band structure of Dirac electron, together with the theoretical improvements of the exact formula of the orbital susceptibility[34, 35, 36, 37, 38, 39].

The Dirac electrons of this Bi-type, i.e., that with the spin-orbit interactions has not been examined in detail contrary to the graphite-type one. In the present paper, we shall investigate the orbital susceptibility and the Hall effects of the Bi-type Dirac electrons. A new contribution to the Hall conductivity due to the interband effects is found, and the its origin is discussed referring to the orbital susceptibility. A peak structure of the Hall coefficient at the band edge is also found.

### 2. Theory

We consider a three-dimensional two-band model which consists of a pair of doubly degenerate bands (due to spin) as

\[
\mathcal{H} = \frac{p^2}{2m} + V + \frac{\nabla^2 V}{8 (mc)^2} + \frac{p \cdot s \times \nabla V}{2 (mc)^2},
\]

where \( V \) is the crystal potential, \( s \) is the spin, and the last term is the spin-orbit interaction. The extrema of bands are not at the center of the Brillouin zone. Such a two-band model was introduced by Cohen and Blount for Bi[5]. Wolf express Eq. (1) in an elegant way, which is
essentially identical to the Dirac Hamiltonian as[6, 40]

\[ \mathcal{H} = \Delta \beta + iv \sum_{\mu} k_{\mu} \beta \sigma_{\mu} \]

\[ = \begin{pmatrix} \Delta & 0 & ivk_z & iv(k_x - ik_y) \\ 0 & \Delta & iv(k_x + ik_y) & -ivk_z \\ -ivk_z & iv(-k_x + ik_y) & -\Delta & 0 \\ -iv(k_x + ik_y) & ivk_z & 0 & -\Delta \end{pmatrix}, \]  

where

\[ \alpha = \begin{pmatrix} 0 & \sigma_{\mu} \\ \sigma_{\mu} & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \]

with \( \sigma_i \)'s being the Pauli spin matrices. The origin of the energy is taken at the center of the band gap \( 2\Delta \). Following Wolff, we have discarded the \( p^2/2m \) term since this term is usually small. This “relativistic” Hamiltonian already includes spin-orbit interactions, and then it can be expressed only in terms of \( 4 \times 4 \) matrices. This is essentially different from the Dirac electrons without spin-orbit interactions, which can be written in terms of \( 2 \times 2 \) matrices[28, 29, 30, 31, 32, 45].

It must be noted that this Hamiltonian is not in the Bloch representation but in the Luttinger-Kohn (LK) representation[46]. The wave function, \( \psi_{nk} \), is expressed in the form

\[ \psi_{nk} = u_{nk_0}(r)e^{ik_0r}, \]

where \( u_{nk_0} \) being the periodic part of the Bloch function at a wave number \( k_0 \). Only in this representation, the wave function in a magnetic field is correctly represented[47]. Furthermore, we can obtain straightforwardly the gauge-invariant results for various response functions[47, 48]. Note that the LK representation is exact and related to the international Symposium on Molecular Conductors (ISMC 2008) IOP Publishing Journal of Physics: Conference Series 132 (2008) 012004 doi:10.1088/1742-6596/132/1/012004

2.1. Conductivity

We calculate the conductivity, \( \sigma_{xx} \), and the Hall conductivity, \( \sigma_{xy} \), on the basis of the Kubo formula in the LK representation[47]. The diagonal conductivity \( \sigma_{xx} \) is given by

\[ \sigma_{xx}(\omega) = \frac{e^2}{i\omega} \{ \Phi_{xx}(\omega + i0) - \Phi_{xx}(0 + i0) \}, \]  

\[ \Phi_{xx}(i\omega_m) = -T \sum_n \sum_k \text{Tr} \mathcal{G}_x \mathcal{G}_- \gamma_x \]

\[ = -4e^2\nu^2 T \sum_n \sum_k \frac{i\varepsilon_n (i\varepsilon_n - i\omega_m) - \frac{1}{3} v^2k^2 - \Delta^2}{(i\varepsilon_n)^2 - v^2k^2 - \Delta^2} \{ (i\varepsilon_n - i\omega_m)^2 - v^2k^2 - \Delta^2 \}, \]

where the velocity matrix is \( \gamma_{\mu} = \partial \mathcal{H}/\partial k_{\mu} = iv\beta \sigma_{\mu} \), and the Green function is given by

\[ \mathcal{G} = (i\varepsilon_n - \mathcal{H})^{-1} (\mathcal{G}_- = (i\varepsilon_n - i\omega_m - \mathcal{H})^{-1}) \]  

with \( \varepsilon_n = i\varepsilon_n + i\Gamma \text{sgn}(\varepsilon_n) \) (\( \varepsilon_n = (2n + 1)\pi T \)). Here we have introduced a finite damping, \( \Gamma \), for electrons as in Ref. [30] to represent the effects of impurity scattering present in actual materials. We assume for the sake of simplicity and clarity that \( \Gamma \) is independent from energy and momentum, though the impurity scattering may somewhat vary \( \Gamma \) as has been shown by Shon and Ando[45]. Then, we obtain

\[ \sigma_{xx} = -\frac{e^2}{\pi \delta \nu} \int_{-\infty}^{\infty} d\varepsilon f'(\varepsilon - \mu) \int_0^{\infty} dX \left[ \frac{X^2(\varepsilon^2 + \Gamma^2 - \frac{1}{3} X^2 - \Delta^2)}{\{ (\varepsilon + i\Gamma)^2 - X^2 - \Delta^2 \} \{ (\varepsilon - i\Gamma)^2 - X^2 - \Delta^2 \}} - \frac{X^2 \{ (\varepsilon + i\Gamma)^2 - \frac{1}{3} X^2 - \Delta^2 \}}{2 \{ (\varepsilon + i\Gamma)^2 - X^2 - \Delta^2 \}^2} + \text{c.c.} \right]. \]
Finally, we obtain

$$\sigma_{xx} = e^2 \Gamma^2 / \left( 2 \pi^2 v \sqrt{\Gamma^2 + \Delta^2} \right).$$

2.2. Hall Conductivity

The off-diagonal conductivity $\sigma_{xy}$ is given by the following formula within the linear response theory[47]:

$$\sigma_{\mu \nu} = \frac{1}{i \omega} K_{\mu \nu}^{\alpha}(q, \omega) A_{q \alpha}.$$  \hspace{1cm} (7)

The kernel $K_{\mu \nu}^{\alpha}$ have the gauge-invariant form as

$$K_{\mu \nu}^{\alpha} = - \frac{e^3}{2mc} (q_{\mu} \delta_{\nu \alpha} - q_{\nu} \delta_{\mu \alpha}) T \sum_n \sum_k \text{Tr} \left[ G_{- \gamma \mu} G_{\gamma \mu} G - G_{- \gamma \mu} G_{- \gamma \mu} G \right]$$

$$- \frac{e^3}{2c} (q_{\mu} \delta_{\nu \alpha} - q_{\nu} \delta_{\mu \alpha}) T \sum_n \sum_k \text{Tr} \left[ G_{- \gamma \nu} G_{- \gamma \mu} G_{\gamma \mu} G_{- \gamma \nu} G_{- \gamma \mu} G \right]$$

$$+ \gamma \mu G_{\gamma \nu} \gamma \mu G_{- \gamma \mu} G_{- \gamma \nu} G_{\gamma \mu} G_{- \gamma \mu} G_{- \gamma \nu} G_{\gamma \mu} G_{\gamma \mu} G_{\gamma \nu} - G_{- \gamma \mu} G_{\gamma \nu} G_{\gamma \mu} G_{\gamma \nu} G_{\gamma \mu} G_{\gamma \nu} - G_{- \gamma \mu} G_{\gamma \nu} G_{\gamma \mu} G_{\gamma \nu} G_{\gamma \mu} G_{\gamma \nu}].$$  \hspace{1cm} (8)

In the present Hamiltonian, the $k^2/2m$ term is discarded, so that the contribution of the first term vanishes. Here $i(q_{\mu} A_{q \nu} - q_{\nu} A_{q \mu}) = H$ is to be noted. Then $\sigma_{xy}$ is given by

$$\sigma_{xy} = \frac{1}{i \omega} \frac{8e^3 v^4}{2c} (-iH) T \sum_n \sum_k \frac{i \omega_m (2i \xi_n - i \omega_m) \{i \xi_n (i \xi_n - i \omega_m) + v^2 (k_x^2 - k_y^2 - k_z^2) - \Delta^2 \}}{(i \xi_n^2 - v^2 k^2 - \Delta^2)^2 (i \xi_n - i \omega_m)^2 - v^2 k^2 - \Delta^2)^2}.$$  \hspace{1cm} (9)

Finally, we obtain

$$\sigma_{xy} = \frac{e^3 v H}{12 \pi^2 c} \int_{-\infty}^{\infty} \frac{d \varepsilon}{\varepsilon} \left[ \frac{\varepsilon + i \Gamma}{\{ (\varepsilon + i \Gamma)^2 - \Delta^2 \}^{3/2} + \text{c.c.}} \right] f(\varepsilon - \mu)$$

$$+ \left( \frac{-2 \Gamma^2 - \Gamma^2 \Delta^2 + (\Delta^2 - \varepsilon^2)^2 + 2 \Gamma^2 \varepsilon - i \Gamma \mu (\Delta^2 - \varepsilon^2)}{2 \Gamma^2 \varepsilon^2 \sqrt{\varepsilon^2 - \Gamma^2 - \Delta^2} + 2 i \Gamma \varepsilon} + \text{c.c.} \right) f'(\varepsilon - \mu) \text{sgn}(\varepsilon).$$  \hspace{1cm} (10)

2.3. Orbital Susceptibility

The orbital susceptibility, $\chi$, in the limit of weak magnetic field is obtained by the following formula[48]

$$\chi = \frac{e^2}{c^2} T \sum_n \sum_k \text{Tr} G_{\gamma \mu} G_{\gamma \mu} G_{\gamma \mu} G_{\gamma \mu} G_{\gamma \mu}.$$  \hspace{1cm} (11)

which is exact even for any Bloch electrons. With the present Hamiltonian, this formula gives

$$\chi = -\frac{4e^2 v^4}{c^2} T \sum_n \left[ \frac{1}{\{ (i \xi_n)^2 - v^2 k^2 - \Delta^2 \}^2} - \frac{8 v^4 k_x^2 k_y^2}{\{ (i \xi_n)^2 - v^2 k^2 - \Delta^2 \}^2} \right].$$  \hspace{1cm} (12)

And then we obtain at $T = 0$ in the form

$$\chi = \frac{e^2 v}{c^2 \pi^2} \frac{4}{15} \int_{-\infty}^{\infty} d \varepsilon f(\varepsilon) \left[ \frac{1}{\sqrt{\varepsilon + i \Gamma}^2 - \Delta^2} + \text{c.c.} \right] \text{sgn}(\varepsilon).$$  \hspace{1cm} (13)
3. Results & Discussions

3.1. Conductivities

The chemical potential dependence of $\sigma_{xx}$ and $\sigma_{xy}$ at $T = 0$ are shown in Fig. 2 (a) and (b), respectively. They are normalized by a factor $\sigma_{xx0} = e^2/\pi^2v$ and $\sigma_{xy0} = e^3v/12\pi^2c$. Away from the band-edge, $|\mu| \ll \Delta$, $\sigma_{xx} \propto \mu^2$ and $\sigma_{xy} \propto -\mu$, which are consistent with the results obtained by the Bloch band picture (or the intraband contributions). Note that for the two-dimensional systems, present calculation gives $\sigma_{xx} \propto |\mu|$ and $\sigma_{xy} \propto \text{const.}$, which are consistent with the previous works[30, 31, 32]. In the insulating region, $|\mu| < \Delta$, both conductivities have small
values due to $\Gamma$. These non-zero values produce an anomalous property of the Hall coefficient.

3.2. Hall Coefficient

For a two band system, it is puzzling how $R_H$ behaves in the band gap region $|\mu| < \Delta$. In the free electron system, $R_H$ is proportional to $1/n_e e c$, $n_e$ being the carrier density of electrons. Thus it should diverge for $|\mu| \leq \Delta$, since $n_e = 0$. More precisely, if we start from the general expression, $R_H = \sigma_{xy}/H \sigma_{xx} \sigma_{yy}$, valid even in the multi-band cases, we obtain $R_H \to 0/0$ for $|\mu| < \Delta$. Namely, it is not trivial whether $R_H$ converges or diverges and then the property of $R_H$ in the band gap region is quite puzzling.

The Hall conductivity defined by $R_H = \sigma_{xy}/\sigma_{xx}^2 H$ as a function of $\mu$ is shown in Fig. 2 (c) with $R_{H0} = \sigma_{xy0}/\sigma_{xx0}^2 H$. Away from the band-edge, $R_H \propto -{\mu}^3$, which is also consistent with the Bloch band picture since the carrier density is proportional to $|\mu|^3$ in three dimension. The remarkable features are seen for the band-edge and insulating regions. A sharp peak appears at the band-edges, $\mu = \pm \Delta$, and a rapid sign-change occurs through $\mu = 0$. Note that there is no carriers at $T = 0$ of $|\mu| < \Delta$ in clean systems. Nevertheless, it is surprising that $R_H$ does not diverge but has small values. The sign change of $R_H$ through $\mu = 0$ has been seen also in the case of the Dirac electrons of graphite type ($2 \times 2$) with $\Delta = 0[30, 32]$. In the gapless case, however, the peak structure appears simultaneously with the sign change at $\mu = 0$. By contrast, our results for $\Delta > 0$ show that the peak appears at the band-edges apart from the sign change at $\mu = 0$.

3.3. Orbital Susceptibility

The orbital susceptibility is shown in Fig. 2 (d) as a function of $\mu$. The result shows that the diamagnetism is largest when $\mu$ is located in the band gap, where the density of states vanishes. At the band-edge, $\chi$ shows a kink and then decreases as $\chi \propto \log(\mu/\Delta)$. The result is consistent with the previous work of $\chi$ calculated by use of the Wigner representation$[33]$. The theoretical results explain well the experimental results$[22, 23]$ (a clear kink structure at the band-edge is actually seen in the experimental results by Wehrl). Both experimental and theoretical results imply that the electric current flows even in the insulating region when a magnetic field is applied. This current is non-dissipative, i.e., thermodynamic as in the case of the persistent currents in superconductivity. It is similar to the atomic diamagnetism, but the present orbital current must be extended in space than the atomic size.

3.4. Interband Effect of a Magnetic Field

Here we study the interband effects of a magnetic field on $\sigma_{xy}$. The interband contribution, $\sigma_{xy}^{\text{inter}}$, can be extracted from $\sigma_{xy}$ by subtracting the intraband contribution, $\sigma_{xy}^{\text{intra}}$, as

$$\sigma_{xy}^{\text{inter}} = \sigma_{xy} - \sigma_{xy}^{\text{intra}}. \tag{14}$$

The intraband contribution is the Hall conductivity calculated within the intraband approximation, i.e., the Bloch band picture: the Green function is given by $G = [i\varepsilon_n - E_n(k)]^{-1}$. Then $\sigma_{xy}^{\text{intra}}$ is calculated as

$$\sigma_{xy}^{\text{intra}} = -\frac{e^3 v_H}{6\pi^3 c} \sum_{n=\pm} \int_{-\infty}^{\infty} d\varepsilon f'(\varepsilon - \mu) \int_0^{\infty} dX \frac{n X^4}{[E_n(X)]^3} \frac{4\Gamma^3}{3[(\varepsilon - E_n(X))^2 + \Gamma^2]^3}, \tag{15}$$

where $E_\pm(X) = \pm \sqrt{X^2 + \Delta^2}$. The apparent expression of Eq. (15) is quite different from that of Eq. (10). Despite that, they agree with each other except for the band-edge region, showing the validity of the Bloch band approximation away from the band gap. Near the band-edge
region, on the other hand, $\sigma_{\text{intra}}$ does not agree with $\sigma_{xy}$, namely, the interband contribution $\sigma_{\text{inter}}$ becomes large.

The obtained $\sigma_{\text{inter}}$ is shown in Fig. 2 (d). Remarkable properties are discovered as follows. The interband contribution $\sigma_{xy}^{\text{inter}}$ takes the largest value at the band-edge, while it damps away from the band-edge as $\sigma_{xy}^{\text{inter}} \propto -1/\mu$. Furthermore, $\sigma_{xy}^{\text{inter}}$ does not depend on $\Gamma$ so much. These properties are completely different from that of $\sigma_{\text{intra}}^{\text{xy}}$, which increases as $|\sigma_{\text{intra}}^{\text{xy}}| \propto \mu$ away from the band-edge, and largely depends on $\Gamma$ as $\sigma_{\text{intra}}^{\text{xy}} \sim \Gamma^{-2}$. (Note that the vertical axis of Fig. 2 (b) includes a factor $\Gamma^2$.) These fundamental differences indicate that the nature of $\sigma_{xy}^{\text{inter}}$ is different from that of $\sigma_{xy}^{\text{intra}}$.

The ratio of $\sigma_{xy}^{\text{inter}}$ to $\sigma_{xy}$ is small for $\Gamma < \Delta$, but become large for $\Gamma > \Delta$. Figure 2 (f) shows $\sigma_{xy}$, $\sigma_{\text{intra}}^{\text{xy}}$ and $\sigma_{xy}^{\text{inter}}$ for $\Delta/\Gamma = 0.1$ as a function of $\mu/\Gamma$. For $|\mu| < \Gamma$, $\sigma_{xy}^{\text{inter}}$ exceeds $\sigma_{\text{intra}}^{\text{xy}}$, so that the shoulder structure appears at around $|\mu| \sim \Gamma$. If this structure is detected, it will be a direct observation of the interband contribution. Note that this structure is the same nature of the small peak just above/below $\mu = 0$ for the gapless Dirac electrons ($2 \times 2$) in two-dimension[30].

Now, let us discuss the physical origin of the interband contribution. The nature of $\sigma_{xy}^{\text{inter}}$ is closely related to that of the orbital susceptibility. In the insulating region, electric current flows circularly in a magnetic field, generating the diamagnetism (Fig. 3 (a)). This current is non-dissipative, and there are no electrons going through the crystal, so that it does not contribute to the Hall conductivity. In the band-edge region, on the other hand, there exist the conduction electrons, which can go through the crystal. The electrons which belong to a local diamagnetic orbital then start to transfer to the neighboring orbitals by hybridizing with the conduction electrons (Fig. 3 (b)). Consequently, electrons can go through the crystal by this transfer between local diamagnetic orbital and generate contributions to the Hall conductivity, namely, $\sigma_{xy}^{\text{inter}}$. The local diamagnetic current, which is non-dissipative, has largest values for $|\mu| \leq \Delta$ and decreases away from the band-edge. Correspondingly, $|\sigma_{xy}^{\text{inter}}|$ actually decreases away from the band-edge. This supports the present picture.

4. Conclusion

We have studied the Hall effects and the orbital susceptibility of the Dirac electron with spin-orbit interactions on the basis of the gauge-invariant Kubo formula in the Luttinger-Kohn representation. The Hall coefficient exhibits remarkable peaks at the band-edge, $\mu = \pm \Delta$, and changes its sign through $\mu = 0$. A novel contribution to the Hall conductivity, which is generated due to the interband effect of a magnetic field, is found. This contribution, $\sigma_{xy}^{\text{inter}}$, has the largest value at the band-edge and decreases away from the band-edge. This property is quite different from the conventional Hall conductivity obtained by the Bloch band picture,
\[ \sigma_{\text{intra}}^{xy}, \] but is similar to that of the orbital susceptibility. So \( \sigma_{\text{inter}}^{xy} \) is tightly related with the diamagnetic current which is non-dissipative.

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The general Dirac Hamiltonian and the reciprocal effective mass tensor are given as

\[ \mathcal{H} = \Delta \beta + \frac{k^2}{2m} + ik \cdot \left[ \sum_{\mu=1}^{3} W(\mu) \beta \alpha_\mu \right] = \begin{pmatrix}
\frac{k^2}{2m} + \Delta & 0 & k \cdot \langle 1|v|3 \rangle & k \cdot \langle 1|v|4 \rangle \\
0 & \frac{k^2}{2m} + \Delta & k \cdot \langle 2|v|3 \rangle & k \cdot \langle 2|v|4 \rangle \\
k \cdot \langle 3|v|1 \rangle & k \cdot \langle 3|v|2 \rangle & \frac{k^2}{2m} - \Delta & 0 \\
k \cdot \langle 4|v|1 \rangle & k \cdot \langle 4|v|2 \rangle & 0 & \frac{k^2}{2m} - \Delta
\end{pmatrix}, \quad (16) \]

\[ \vec{\alpha} = \Delta^{-1} \sum_{\mu} W(\mu), \] by Wolff, respectively [6]. Here, \( W \) corresponds to the matrix elements of the velocity operator. For the electron ellipsoids at \( L \)-point of Bi, only \( \alpha_{xx}, \alpha_{yy}, \alpha_{zz} \) are finite [5]. If we take the principal axis along the electron ellipsoids at \( L \)-point of Bi, we can reduce to diagonal three parameters. In the model used here, we assumed these three parameters are set to be equal, namely, \( \vec{\alpha} \) to be proportional to a unit matrix.

The band gap is mainly due to the lattice distortion [42, 43], which is considered to be the first example of the Peierls distortion [44, 17]. The real crystal of bismuth has a rhombohedral lattice with two atoms per unit cell. This structure is generated by stretching of a face centered cubic lattice along one of the body diagonals, followed by a relative displacement of neighbouring atoms along this diagonal.

[40] The general Dirac Hamiltonian and the reciprocal effective mass tensor are given as

\[ \mathcal{H} = \Delta \beta + \frac{k^2}{2m} + ik \cdot \left[ \sum_{\mu=1}^{3} W(\mu) \beta \alpha_\mu \right] = \begin{pmatrix}
\frac{k^2}{2m} + \Delta & 0 & k \cdot \langle 1|v|3 \rangle & k \cdot \langle 1|v|4 \rangle \\
0 & \frac{k^2}{2m} + \Delta & k \cdot \langle 2|v|3 \rangle & k \cdot \langle 2|v|4 \rangle \\
k \cdot \langle 3|v|1 \rangle & k \cdot \langle 3|v|2 \rangle & \frac{k^2}{2m} - \Delta & 0 \\
k \cdot \langle 4|v|1 \rangle & k \cdot \langle 4|v|2 \rangle & 0 & \frac{k^2}{2m} - \Delta
\end{pmatrix}, \quad (16) \]

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