Anomalous conductivity of two-dimensional Dirac electrons in organic conductor under pressures

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Dirac electrons in organic conductor \(\alpha\)-(BEDT-TTF)\(_2\)I\(_3\) under pressures, which exhibit anomalous conductivity being nearly constant at high temperatures, have been examined using a two-dimensional tight-binding model (TB) model with both the impurity and electron-phonon (e-p) scatterings. A crucial role of scattering by acoustic phonon is shown based on the previous study for a model with simple Dirac cone [Phys. Rev. B 98, 161205 (2018)]. In addition to diagonal conductivity \(\sigma_{xx} = \sigma_{yy}\) and \(\sigma_{xy}\), off-diagonal conductivity \(\sigma_{xy}\) exists due to a tilted Dirac cone, where \(y(x)\) corresponds to a direction parallel (perpendicular) to a stacking axis of molecules. This \(\sigma_{xy}\) results in a rotation of axis of the principal value \(\sigma_{\pm}\). Since the conductivity at high temperatures is suppressed by the e-p scattering on the Dirac cone, the increase of temperature results in a broad maximum for \(\sigma_y\) and a nearly constant \(\sigma_x\) for a moderate choice of the e-p coupling constant. Further a correlation effect is examined employing a mean-field for the on-site and nearest-neighbor-site interactions. Anisotropic behavior of \(\sigma_x\), \((\nu = x \text{ and } y)\) is discussed by comparing with experiments of organic conductors, which present nearly constant resistivity at high temperatures.

1. Introduction

Since the discovery of two-dimensional massless Dirac fermions,\(^1\) the extensive studies have been explored in various materials. Among them, noticeable phenomena of Dirac electrons in molecular crystals,\(^2\) have been studied in organic conductor \(\alpha\)-(BEDT-TTF)\(_2\)I\(_3\) (BEDT-TTF=bis(ethylenedithio)tetrathiafulvalene). After noting that the density of states (DOS) vanishes linearly at the Fermi energy,\(^3\) the two-dimensional Dirac cone with a zero-gap state (ZGS)\(^5\) was found using a tight-binding (TB) model, where transfer energies are estimated from the extended H\"{u}ckel method.\(^6\) The existence of such Dirac cone was verified by first-principles DFT calculation,\(^7\) which has been used for studying further \(\alpha\)-(BEDT-TTF)\(_2\)I\(_3\) under hydrostatic pressures.\(^8\)

There are common features among organic conductors with isostructure salts,\(^9,10\) \(\alpha\)-D\(_2\)I\(_3\) (D = ET, STF, and BETS), where ET = BEDT-TTF, STF = bis(ethylenedithio)tetrathiafulvalene, and BETS = bis(ethylenedithio)tetraselenafalvalene. These salts display an energy band with a Dirac cone\(^5,11-13\) and the resistivity at high temperatures shows nearly constant behavior,\(^9,10,14-18\) while the conventional metal shows the linearly increasing one. Such unconventional behavior was also observed in Dirac electrons with nodal line semimetals of single-component molecular conductors\(^19-23\) Thus, it has been believed that the nearly constant behavior in resistivity at high temperatures is attributable to the intrinsic property of the Dirac electrons.

The Dirac electrons of these organic conductors at a zero doping display ZGS, where DOS around the chemical potential increases from zero linearly. A two-band model with such ZGS shows that the static conductivity at absolute zero temperature remains finite with a universal value, i.e., independent of the magnitude of impurity scattering owing to a quantum effect. The effect of impurity has been examined in detail by applying a self-consistent Born approximation.\(^24\) It is further shown that the conductivity increases with increasing the doping. The tilting of the Dirac cone, which also increases the conductivity, provides the anisotropic conductivity and the deviation of the current from the applied electric field.\(^25\) The conductivity at finite temperatures depends on the magnitude of the impurity scattering, \(\Gamma\) which is proportional to the inverse of the life time by the disorder. With increasing temperature \((T)\), the conductivity remains unchanged for \(T \ll \Gamma\), while it increases for \(\Gamma \ll T.\(^26\)\) Noting that \(\Gamma \sim 0.0003 \text{ eV for organic conductors,}\(^2\) a monotonous increase of the conductivity at finite temperature \(T > 0.0005 \text{ eV is expected. However the measurement of the conductivity (or resistivity) on the above organic conductor shows the almost constant behavior at high temperatures. To comprehend such an exotic phenomena, the acoustic phonon scatterings has been proposed as a possible mechanism, where a simple model of Dirac cone without tilting displays a reasonable suppression of the conductivity at high temperatures.\(^27\) Then, it is needed to verify that such a model with both Dirac cone and the e-p interaction quantitatively accounts for the behavior of the organic conductor.

The purpose of the present paper is to demonstrate the role of the acoustic phonon in \(\alpha\)-(BEDT-TTF)\(_2\)I\(_3\), which gives rise to anomalous conductivity being nearly constant at high temperatures. We clarify characteristics of Dirac electrons with large tilting\(^28-30\) where transfer energies between molecules are estimated from the X-ray diffraction experiment and DFT. A TB model with transfer energies of \(\alpha\)-(BEDT-TTF)\(_2\)I\(_3\) under pressures is

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examined, which are well known compared with those of other isostructural salts, BETS and STF. Since the tilted Dirac cone is also obtained for BETS \cite{12} and STF, \cite{13} it is expected that the present TB model provides a common feature for these salts, i.e., the nearly constant conductivity at high temperatures.

The paper is organized as follows. In Sect. 2, model and formulation are given for both the uniaxial and hydrostatic pressure, where the latter case is examined by adding site potential due to interaction. In Sect. 3, after examining the chemical potential and density of states (DOS), the conductivity is calculated for \( \alpha \)-\( (\text{BEDT-TTF})_2I_3 \) under both uniaxial and hydrostatic pressures. Sect. 4 is devoted to summary and discussion.

2. Model and Formulation

We consider a two-dimensional system per spin, which is given by,

\[
H_{\text{total}} = H_0 + H_1 + H_p + H_{e-p} + H_{\text{imp}}.
\]

(1)

\( H_0 \) describes a TB model of organic conductor \( \alpha \)-\( (\text{BEDT-TTF})_2I_3 \) consisting of four molecules per unit cell (Fig. 1). \( H_1 \) describes a site potential, which is obtained from a mean field of short range repulsive interactions. \( H_p \) and \( H_{e-p} \) denote an acoustic phonon and an electron-phonon (e-p) interaction. \( H_{\text{imp}} \) is the impurity potential. The terms \( H_0 + H_p + H_{e-p} \) are the Fröhlich Hamiltonian \cite{31} applied to the present Dirac electron system. The unit of the energy is taken as eV.

2.1 Energy band

First, we derive the energy band for \( H = H_0 + H_1 \) and the associated quantities. A TB model, \( H_0 \), is expressed as

\[
H_0 = \sum_{i,j=1}^{N} t_{i,j;\alpha,\beta} a_{i,\alpha}^\dagger a_{j,\beta} = \sum_{k}^{N} t_{\alpha,\beta}(k)a_{\alpha}^\dagger(k)a_{\beta}(k),
\]

(2)

where \( a_{i,\alpha}^\dagger \) denotes a creation operator of an electron of molecule \( \alpha \) \( [\text{A}(1), \text{A}'(2), \text{B}(3), \text{C}(4)] \) at the \( i \)-th lattice site. \( N \) is a total number of the square lattice sites and \( t_{i,j;\alpha,\beta} \) are the transfer energies for the nearest and next-nearest neighbor sites, which are shown in Fig. 1. A Fourier transform for the operator \( a_{j,\alpha} \) is given by \( a_{j,\alpha} = 1/N^{1/2} \sum_{k} a_{\alpha}(k) \exp[i(k \cdot r_j)] \), where \( k = (k_x, k_y) \) and the lattice constant is taken as unity. The quantity \( H_1 \) corresponds to a site potential, \( V_\alpha \), acting on the \( \alpha \) site, where \( V_\alpha = V_{\Lambda} \) due to an inversion symmetry around the cross in Fig. 1. The Hamiltonian \( H_1 \) is obtained as

\[
H_1 = \sum_{\alpha} \left( V_\alpha - V_{\Lambda} \right) \tilde{n}_\alpha = \tilde{V}_B \tilde{n}_B + \tilde{V}_C \tilde{n}_C,
\]

(3)

where \( \tilde{V}_\alpha \) denotes a potential measured from that of the \( \text{A} \) site and \( \tilde{n}_\alpha = a_{\alpha}^\dagger(k)a_{\alpha}(k). \) From Eqs. (2) and (3), \( H \) is written as

\[
H = \sum_{k} \sum_{\alpha,\beta} a_{\alpha}^\dagger(k)h_{\alpha,\beta}a_{\beta}(k),
\]

(4)

where matrix elements, \( h_{\alpha,\beta} \), are given as follows.

\[
\begin{align*}
  h_{12}(k) &= a_3 + a_2 Y, & (5a) \\
  h_{13}(k) &= b_3 + b_2 X, & (5b) \\
  h_{14}(k) &= b_4 Y + b_1 XY, & (5c) \\
  h_{23}(k) &= b_2 + b_3 X, & (5d) \\
  h_{24}(k) &= b_1 + b_4 X, & (5e) \\
  h_{34}(k) &= 2a_1 , & (5f) \\
  h_{11}(k) &= a_{1d}(Y + Y^*) , & (5g) \\
  h_{33}(k) &= a_{3d}(Y + Y^*) + \tilde{V}_B , & (5h) \\
  h_{44}(k) &= a_{4d}(Y + Y^*) + \tilde{V}_C , & (5i) \\
\end{align*}
\]

and \( h_{ij}(k) = h_{ji}(k) \), where \( X = \exp[ik_0x] = \tilde{X}^* \) and \( Y = \exp[ik_0y] = \tilde{Y}^* \). The matrix elements of \( H_1 \) are \( \tilde{V}_B \) for \( \alpha = \beta = 3 \), \( \tilde{V}_C \) for \( \alpha = \beta = 4 \) and zero otherwise. Equation (4) is diagonalized as

\[
H = \sum_{k} \sum_{\gamma} c_\gamma^\dagger(k)E_\gamma(k)c_\gamma(k),
\]

(6a)

where \( E_1(k) > E_2(k) > E_3(k) > E_4(k) \) and

\[
c_\gamma(k) = \sum_{\alpha} c_{\alpha}(k)a_{\alpha}(k).
\]

(6b)

The Dirac point \( (k_D) \) is obtained from

\[
E_1(k_D) = E_2(k_D) = \epsilon_D.
\]

(7)
The ZGS is obtained when $\epsilon_D$ becomes equal to the chemical potential at $T=0$.

In the present paper, the site potentials $\bar{V}_B$ and $\bar{V}_C$ in $H_1$ are given by the mean-field of short-range repulsive interactions,

$$
\bar{V}_B = (n_B - n_A)U/2 + 2V_0(n_C - n_A) + 2V_b(2n_A - n_B - n_C),
$$

(8a)

$$
\bar{V}_C = (n_C - n_A)U/2 + 2V_0(n_B - n_A) + 2V_b(2n_A - n_B - n_C),
$$

(8b)

where $U$ is the on-site repulsive interaction and $V_a$ ($V_b$) denotes the nearest neighbour interaction along the $y$ ($x$) axis. $n_{\alpha}$ denotes a local density corresponding to an electron number per unit cell at the $\alpha$ site. From $E_\gamma$, $n_{\alpha}$ including both spin $\uparrow$ and $\downarrow$ is calculated as

$$
n_{\alpha} = \frac{2}{N} \sum_k \langle \hat{n}_{\alpha}(k) \rangle_H = \frac{2}{N} \sum_k \sum_\gamma d^{*}_{\gamma\alpha}(k)d_{\gamma\alpha}(k)f(E_\gamma(k) - \mu),
$$

(9)

which is determined self-consistently. $n_A = n_{A'}$ due to transfer energies being symmetric with respect to the inversion center between $A$ and $A'$ in Fig. 1. In Eq. (9), $\langle \hat{n}_{\alpha}(k) \rangle = 1/\exp(\exp(\epsilon/T) + 1)$ with $T$ being temperature in the unit of eV and $k_B = 1$. The chemical potential $\mu$ is determined from the three-quarter-filled condition, which is given by

$$
1/N \sum_k \sum_\gamma f(E_\gamma(k) - \mu) = \int_{-\infty}^{\infty} \text{d}\omega D(\omega)f(\omega) = 3,
$$

(10)

where

$$
D(\omega) = \frac{1}{N} \sum_k \sum_\gamma \delta(\omega - E_\gamma(k)).
$$

(11)

$D(\omega)$ denotes DOS per spin and per unit cell, which satisfies $\int \text{d}\omega D(\omega) = 4$. Note that $n_A + n_{A'} + n_B + n_C = 6$ from Eq. (10). We use $\mu(T)$ at finite $T$ and $\mu(0)$ at $T=0$.

### 2.2 Scattering by phonon and impurity

In Eq. (1), the third term denotes the harmonic phonon given by $H_p = \sum_q \omega_q b_q^\dagger b_q$ with $\omega_q = v_s|q|$ and $h = 1$, while the forth term is the e-p interaction expressed as

$$
H_{e-p} = \sum_{k\gamma} \sum_q \alpha_{q} c^\dagger_{\gamma}(k + q)c_{\gamma}(k)\phi_q,
$$

(12)

with $\phi_q = b_q + b_{q}^\dagger$. We introduce a coupling constant $\lambda = |\alpha_q|^2/\omega_q$ which becomes independent of $|q|$ for small $|q|$. The e-p scattering is considered within the same band (i.e., intraband) due to the energy conservation with $v \gg v_s$, where $v \sim 0.05$ denotes the averaged velocity of Dirac cone. The last term of Eq. (1), $H_{\text{imp}}$, denotes a normal impurity scattering, which is introduced to obtain the finite conductivity and to avoid the infinite conductivity in the presence of only the e-p interaction.

Noting that the band is three-quarter filled owing to 2:1 salt, we calculate an energy difference defined by

$$
\Delta(k) = E_1(k) - E_2(k),
$$

(13)

where the Dirac point $k_D$ is obtained from $\Delta(k_D) = 0$ as shown in the next section. Since $E_\gamma(k_D) = \mu$ ($\gamma = 1, 2$) for the present ZGS, the low temperature property is determined from $|E_\gamma(k) - \mu| \ll T$.

The damping of the electron of the $\gamma$ band, which is defined by $\Gamma_\gamma$, is obtained from the electron Green function expression as

$$
G_\gamma(k, i\omega_n) = \frac{i\omega_n - E_{\gamma,k} + i\Gamma_\gamma}{\omega_n^2 + \Gamma_\gamma^2},
$$

(14a)

$$
\Gamma_\gamma = \Gamma + \gamma_{\text{ph}},
$$

(14b)

where $\gamma_{\text{ph}} = -\text{Im}\Sigma_\gamma(k, E_{\gamma,k} - \mu)$ with $\Sigma_\gamma(k, E_{\gamma,k} - \mu)$ being a self-energy by the e-p interaction. The real part of the self-energy can be neglected for small doping. The quantity $\Gamma$ comes from another self-energy by the impurity scattering. Note that $\gamma_{\text{ph}}$ does not depend on $\Gamma$, and that the ratio $\gamma_{\text{ph}}/T$ is crucial to determine the $T$ dependence of the conductivity. The quantity $\Sigma_\gamma(k, \omega)$ is $\Sigma_\gamma(k, i\omega_n)$ with $\omega_n \rightarrow -\omega + 0$ is estimated as

$$
\Sigma_\gamma(k, i\omega_n) = T \sum_m \sum_q |\alpha_q|^2 \times

\frac{1}{i\omega_n + \xi_\gamma,k + q + 2\omega_q/\omega_m + \omega_q},
$$

(15)

which is a product of electron and phonon Green functions. $\omega_n = (2n + 1)\pi T$, $\omega_m = 2\pi m T$ with $m$ and $n$ being integers. $\xi_\gamma,k = E_{\gamma,k} - \mu$. Applying the previous result, we obtain

$$
\Gamma_{\gamma_{\text{ph}}} = C_0 R \times T|\xi_{\gamma,k}|,
$$

(16a)

$$
R = \frac{\lambda}{\lambda_0},
$$

(16b)

where $C_0 = 6.25\lambda_0/(2\pi v_s^2)$. For $v \simeq 0.05$ and $\lambda_0/2\pi v_s = 0.1$, we obtain $C_0 \simeq 12.5$ (eV)$^{-1}$. $R$ denotes a normalized e-p coupling constant.

Using the component of the wave function $d_{\alpha\gamma}$ in Eq. (6b), the response function per spin and per site is calculated as

$$
\sigma_{\alpha\beta}(T) = \frac{e^2}{\pi \hbar N} \sum_k \sum_{\gamma,\gamma'} v_{\alpha\gamma}(k)^* v_{\gamma'\beta}(k)

\int_{-\infty}^{\infty} \text{d}\epsilon \left( -\frac{\partial f(\epsilon)}{\partial \epsilon} \right)

\times \frac{\Gamma_{\gamma'}}{(\epsilon - \xi_{\gamma,k})^2 + \Gamma_{\gamma'}^2} \times \frac{\Gamma_{\gamma'}^2}{(\epsilon - \xi_{\gamma',k})^2 + \Gamma_{\gamma'}^2},
$$

(17)

$$
v_{\alpha\gamma}(k) = \sum_{\alpha'\beta} d_{\alpha\gamma}(k) \frac{\partial H_{\alpha'\beta}}{\partial k_{\nu}} d_{\beta\gamma}(k),
$$

(18)

where $\nu = x$ and $y$. $h = 2\pi \hbar$ and $e$ denote a Plank’s constant and electric charge, respectively.

In terms of $\sigma_{xx} = \sigma_\alpha = A$, $\sigma_{yy} = \sigma_\gamma = B$, and $\sigma_{xy} = C$, the current $(J_x, J_y)$ obtained from a response to an
The relations between \((\sigma_1, \sigma_2, \phi)\) and \((A, B, C)\) are
\[
\tan 2\phi = \frac{2C}{A - B},
\]
\[
\sigma_1 = \sigma_- = \frac{1}{2} [A + B - \sqrt{(A - B)^2 + 4C^2}],
\]
\[
\sigma_2 = \frac{1}{2} [A + B + \sqrt{(A - B)^2 + 4C^2}].
\]

Note that \(\phi < 0\) for \(C > 0\) and \(\phi > 0\) for \(C < 0\), where \(0 < |\phi| < \pi/4\) for \(B > A\) and \(\pi/4 < |\phi| < \pi/2\) for \(A > B\).

It is noted that Eq. (17) can be understood using DOS when \(k\) dependence of \(\psi_{\sigma n}^0\), close to the Dirac point is small. In fact, as shown in the next section, with increasing temperature the conductivity in the absence of the e-p interaction increases monotonously due to the increase of DOS since the chemical potential moves away from that of the Dirac point.\(^{25}\)

\section*{3. Conductivity of Dirac Electrons}

We calculate the conductivity for the TB model with transfer energies shown in Fig. 1. The direction of molecular stacking is given by the \(y\) axis, while that perpendicular to the stacking is given by the \(x\) axis. The nearest neighbour (NN) transfer energies are examined for both uniaxial pressure and hydrostatic pressure, while those of next nearest neighbor (NNN) sites are added only for hydrostatic pressure.\(^7\) In the following calculations, the conductivity is normalized by \(e^2/\hbar\) and the energy is scaled by eV. First we examine the case of uniaxial pressure \((P = 6)\) without site potential, and study next a case of hydrostatic pressure with site potential to comprehend the similarity and dissimilarity.

\subsection*{3.1 \(\alpha-(\text{BEDT-TTF})_2\text{I}_3\) under uniaxial pressures}

The TB model under uniaxial pressure \(P\) is calculated using nearest neighbor transfer energies at \(P\) kbar, which are given by \(a_1 = -0.028(1 + 0.089P)\), \(a_2 = -0.048(1 + 0.167P)\), \(a_3 = 0.02(1 - 0.025P)\), \(b_1 = 0.123\), \(b_2 = 0.140(1 + 0.011P)\), \(b_3 = 0.062(10.032P)\), and \(b_4 = 0.025.\(^5\)}

There are following characteristics in the band structure. Figure 2(a) shows the ZGS at \(P = 6\) kbar, where \(E_1(k)\) and \(E_2(k)\) touch at the Dirac points \(k_D = (0, 0.57, 0.30)\)π with an energy \(E_D = \mu = 0.178\) due to three-quarter-filled band. In fact, energies of the conduction and valence bands \(E_1(k)\) and \(E_2(k)\) exist for \(0 < E_1(k) - \mu < 0.19\) and \(-0.11 < E_2(k) - \mu < 0\), respectively. Such ZGS shows a relation \(E_2(Y) < E_D < E_1(X) < E_1(M)\), where \(Y, X\) and \(M\) are TRIMs given by \(\Gamma = (0, 0)\pi, X = (1, 0)\pi, Y = (0, 1)\pi,\) and \(M = (1, 1)\pi\). Note that, for \(P = 4\) and 8, \(\mu = 0.172,\) and 0.185 and \(k_D = (0.6, 0.35)\pi\) and \((0.55, 0.25)\pi\), respectively. Figure 2(b) shows contour plots of \(E_1(k) - E_2(k)\), as the function of \(\delta k = k - k_D\) in a small region around \(k_D\). The line surrounding the orange region given by \(E_1(k) - E_2(k) < 0.03\), is almost a circle suggesting that the velocity of the Dirac cone is isotropic. Figure 2(c) shows \(E_0(k) - \epsilon_D\). The Dirac point is located at the darkest region, where the ellipse for the fixed \(E_0(k) - \epsilon_D\) suggests a tilted Dirac cone. Note that the axis of the cone shows slight rotation clockwise from the \(x_k\) axis, which plays a crucial role for the transport property as shown later. Figure 2(d) shows \(E_2(k) - \epsilon_D\). The Dirac point is located at the brightest region, where the ellipse for the fixed \(E_2(k) - \epsilon_D\) also suggests a tilted Dirac cone. We define a phase \(\phi_0(<0)\) (\(\phi_2\)) as a tilting angle of \(E_1(k) - E_2(k)\) measured from the \(k_x\) axis. Since \(E_1(k)\) and \(E_2(k)\) form a pair of Dirac cone, \(\phi_2 - \phi_1 = \pi\) for \(k\) in the limit of the f Dirac point. The deviation from the limiting value increases with increasing \(\delta k_D\). The tilting parameter is given by \(\eta \sim 0.8\).

Figure 3 shows the temperature \((T)\) dependence of the chemical potential \((\mu(T))\) at \(P = 6\) (solid line) and a hydrostatic pressure \(P_{\text{hydro}}\) (dashed line), where the corresponding DOS as a function of \(\omega - \mu\) is shown in the inset. With increasing \(T\), \(\mu\) varies slowly suggesting that the \(T\) dependence of \(\mu\) on \(\sigma_1\) is negligibly small. In fact, the \(T\) dependence of \(\mu\) in Eq. (16a) may be ignored for \(\sigma_1(T)\) at low temperatures. We verified that \(\mu(T)\) can be replaced by \(\mu(0)\) in \(\xi_{\sigma, k}\) for \(0 < T < 0.015\) \((0 < T < 0.013)\) which is the range of temperature of the following numerical calculation of \(\sigma_1\) under the pressure of \(P = 6\) kbar \(P_{\text{hydro}}\). The DOS close to the chemical potential shows a linear dependence with respect to \(\omega - \mu\), where \(\mu\) is the chemical potential at \(T = 0\). The slight decrease of the chemical potential at low temperatures comes from the peak above the chemical potential corresponding to the van hove singularity at \(E_1(X)\) in DOS. The increase of \(\mu\) above the minimum occurs since the van hove singularity at \(E_2(Y)\) below the chemical potential has a large peak compared with that of \(E_1(X)\). Similar behavior is found for \(P_{\text{hydro}}\), which shows the increase of the band width.

Figure 4 shows the temperature dependence of conductivity of \(\sigma_1\) \((\nu = x, y, xy, +, -)\) without the e-p interaction, where \(P = 6\) and and \(\Gamma = 0.0005\). For another choice of \(\Gamma = 0.001\), \(\sigma_x\) and \(\sigma_y\) becomes smaller, while \(\sigma_z\) is smaller for \(T > 0.011\) and \(\sigma_z\) is larger for...
The conductivity in the zero limit of $T$ is given by $\sigma_x(0) \simeq 0.06$ and $\sigma_y(0) \simeq 0.09$, respectively which are compared with that of the universal value of $1/2\pi^2 = 0.051$. The slightly larger value in the present case comes from the tilting of the Dirac cone.\textsuperscript{25} At low temperatures, we obtain an equality $\sigma_y > \sigma_x$, which can be understood as follows. Figure 2(b) shows a nearly isotropic velocity of the Dirac cone, while Figs. 2(c) and 2(d) present a large tilting of the Dirac cone along the $k_y$ direction. Our previous calculation of a tilted Dirac cone shows that the conductivity becomes maximum for the direction perpendicular to a tilting axis.\textsuperscript{25} Thus we obtain $\sigma_y > \sigma_x$ at low temperature in the present case. Compared with such inequality at low temperatures, an opposite relation of $\sigma_x > \sigma_y$ is found for $T > 0.012$. The transport at high temperatures is determined by electrons with higher energy, where the transfer energy along the $x$ direction is larger than that of $y$ direction. Such crossover occurs at lower $T$ for larger $\Gamma$. This is compatible with a fact that the reduction of $\sigma_y$ by $\Gamma$ is larger than that of $\sigma_x$. We also note that such crossover occurs at higher $T$ for $P=8$ (not shown here).

The dashed line in Fig. 4 shows the $T$ dependence of the principal value $\sigma_\perp$. In the limit of $T=0$, we obtain $\sigma_\perp(0) \simeq 0.092$ and $\sigma_\parallel(0) \simeq 0.067$, which give $\sigma_\perp(0)/\sigma_\parallel \simeq 1.8$ and $\sigma_\parallel(0)/\sigma_\perp \simeq 1.32$ with $\sigma_\parallel = 1/(2\pi^2)$. These results are compatible with the analytical results of tilted Dirac cone where $\sigma_\perp/\sigma_\parallel = 1.84$ and $\sigma_\parallel/\sigma_\perp = 1.19$ for $\eta = 0.84$.\textsuperscript{25} The behavior of $\sigma_\parallel$ being linear in $T$ resembles that of DOS around $\omega = \mu$ in the inset of Fig. 3, which is found for $|\omega - \mu| < 0.015$. The inset displays $T$ dependence of $\phi$, where $\phi < 0$ due to $\sigma_{xy} > 0$ and $\sigma_y > \sigma_x$ at low temperatures as seen from Fig. Eq. (21a). With increasing $T$, $\phi$ decreases and becomes smaller than $-\pi/4$ at a temperature corresponding to $\sigma_x = \sigma_y$, where the axis close to $\sigma_\perp$ changes from $k_y$ axis to the $k_x$ axis. Thus the principal axes rotate clockwise with an angle $\phi(\leq 0)$ (see Eq. (20c)).

As shown in Fig. 4 (P=6), $\sigma_\nu$ increases monotonously as the function of $T$, which is different from the experiment showing nearly constant behavior at high temper-
Such exotic T dependence of $\sigma_{\nu}$ is examined next by taking account of the e-p interaction, which is expected to reduce $\sigma_{\nu}$. Using Eq. (14b) and (16a), $\sigma_{\nu}$ of Eq. (17) is calculated, where $\Gamma$ in the absence of the e-p interaction is replaced by $\Gamma_{\nu}(=\Gamma + \Gamma_{\nu}^{ph})$. Owing to the T dependence of $\Gamma_{\nu}^{ph}$, $\Gamma$ is dominant at low T while $\Gamma_{\nu}^{ph}$ is dominant at high T. Note that such crossover with increasing T depends on $R$.

Figure 5 shows the T dependence of $\sigma_{\nu} (\nu = x, y, xy)$ in the presence of the e-p interaction with some choices of $R$. Compared with $\sigma_{\nu}$ with $R = 0$ (Fig. 4), $\sigma_{\nu}$ with $R \neq 0$ is reduced noticeably. At temperatures around $T \sim 0.015$, $\sigma_{x}$ is nearly constant, while $\sigma_{y}$ takes a broad maximum at lower temperatures. Noting that the difference in $\sigma_{x}$ and $\sigma_{y}$ at low temperatures is noticeably reduced at high temperatures, it is found that the tilting effect of the Dirac cone in the presence of moderate strength of $R$ varies with increasing temperatures. The $R$ dependence on $\sigma_{xy}$ is small. The crossover temperature corresponding to $\sigma_{xy} = \sigma_{x}$ decreases with increasing $R$, since the reduction of $\sigma_{y}$ is larger than that of $\sigma_{x}$. The nearly constant behavior of $\sigma_{x}$ is understood as follows. In the absence of the e-p interaction, $\sigma_{x}$ as a function of $T$ increases linearly, which comes from DOS determined by the Dirac cone. However for $R \neq 0$, the noticeable effect of the acoustic phonon emerges at finite temperatures. As shown in Eq. (14b), the electron is scattered by both normal impurity (I) and the e-p interaction ($\Gamma_{\nu}^{ph}$), where the increase of the latter at finite temperature is seen from Eq. (16a). However, compared with the conventional metal with a Fermi surface, where the increase of temperature gives rise to a large enhancement of the e-p scattering to suppress the conductivity, the effect of the e-p scattering in the case of the Dirac cone close to the three-quarter-filled band is strongly reduced due to a constraint by the energy-momentum conservation. Thus, we obtain nearly constant behavior or a broad maximum in $\sigma_{\nu}$, due to a competition between the enhancement by DOS of the Dirac cone and the suppression by the e-p interaction.

Figure 6 shows the T dependence of the principal values $\sigma_{\pm}$ corresponding to Fig. 5. Since $\sigma_{+}$ and $\sigma_{-}$ give the upper and lower bound of the conductivity, these quantities are convenient to comprehend experiments even when the exact correspondence between the crystal axis and the direction of the applied electric field is not known. In the inset, the rotation angle is shown, where $\phi < 0$ for $\sigma_{xy} > 0$ and $\sigma_{y} > \sigma_{x}$. The angle $|\phi|$ increases and exceeds $\pi/4$ at a certain temperature ($\sigma_{+} = \sigma_{-}$), implying that the axis of $\sigma_{x}$ becomes closer to $k_{xy}$-axis at high temperatures. Since $\sigma_{+}$ and $\sigma_{-}$ have a common feature of a broad maximum with increasing $T$, we examine the origin of such maximum of $\sigma_{\nu}$ by using a numerical fitting of $\sigma_{\pm}$. We apply a fitting formula given by

$$\sigma_{\nu} = \sigma_{0,\nu} + \frac{a_{\nu} T^{2}}{1 + b_{\nu} T^{2}/(1 + c_{\nu} T^{2})},$$

(22a)

which is shown by symbols for $R=2$ in Fig. 6. Fitting parameters $a_{\nu}$, $b_{\nu}$, and $c_{\nu}$ in Eq. (22a) are obtained as follows. First, $\sigma_{x}$ in the absence of the e-p interaction is fitted by $\sigma_{0,x}$ and $a_{x}$. Next, the T dependence around a maximum is fitted by $b_{x}$ and $c_{x}$. These coefficients are estimated as $\sigma_{0,x} = 0.08$, $a_{x} = 0.1$, $b_{x} = 0.046 c_{x} = 0.1$ and $\sigma_{0,y} = 0.06$, $a_{y} = 0.053$, $b_{y} = 0.028 c_{y} = 0.031$ for $R=2$. Such a formula can be derived based on a simplified model, where $\sigma_{+} \sim \sigma_{-} \sim \sigma_{0}$. Note that $\Gamma_{\nu}^{ph}$ is obtained in Eq. (16a) and $\sigma \simeq a_{\nu} T^{2}/\Gamma$ with $a_{\nu} = o(0.1)$ without e-p interaction. Taking $\Gamma$ replaced by $\Gamma + \Gamma_{\nu}^{ph}$ and employing an idea $|<\xi,|>\sim T$ with $<|$ being an average value in the summation of Eq. (15),
we obtain
\[ \sigma \simeq a'_p 10^{3T} \left( 1 + C_0 RT^2 / \Gamma \right), \]  
(22b)
with \( C_0 = 12.5 \) and \( \Gamma = 0.0005 \). Both equations Eqs. (22a) and (22b) are compatible due to \( C_0 RT^2 / \Gamma \simeq b_1 \cdot 10^{3T^2} \) with \( R = 2 \). From Eq. (22b), it is found that a maximum of \( \sigma \) as a function of \( T \) is obtained by a competition between the increase of DOS (the numerator) and the suppression the denominator by the e-p interaction of competition. Equation (22b) suggests that \( \sigma \) decreases with increasing \( R \).

### 3.2 \( \alpha-(BEDT-TTF)_2I_3 \) under hydrostatic pressures

We examine Dirac electrons under hydrostatic pressure using the TB model with NN \((a_1, \ldots, b_4)\) and NNN \((a_{1d}, \ldots, a_{4d})\) transfer energies, which are given by\(^7\)
\[ a_1 = -0.0267, \quad a_2 = -0.0511, \quad a_3 = 0.0323, \quad b_1 = 0.1241, \quad b_2 = 0.1296, \quad b_3 = 0.0513, \quad b_4 = 0.0152, \quad a_{1d} = 0.0119, \quad a_{3d} = 0.0046, \quad \text{and} \quad a_{4d} = 0.0060. \]
We use the site potentials given by Eqs. (8a) and (8b).\(^8\) They are estimated as \( V_B = 0.0511, \quad V_C = 0.0032 \) for \( U = 0.4, \quad V_0 = 0.17, \quad \text{and} \quad V_0 = 0.05, \) where \( n_A = n_A' = 1.46, \quad n_B = 1.37, \) and \( n_C = 1.71, \) with \( \nu = 0.172 \) at \( T = 0 \).

Band energies \( E_j(k) \) under hydrostatic pressure, which have Dirac cones similar to Fig. 2, show the following difference. Figure 7(a) shows the conduction and valence bands \((0 < E_1(k) - \mu < 0.15)\) and \((-0.09 < E_2(k) - \mu < 0)\) in the first Brillouin zone, which touch at the Dirac points \( k_D = (0.69, 0.44)\pi \). Compared with Fig. 2(a), the band width of both \( E_1(k) \) and \( E_2(k) \) is slightly large and the Dirac points move away from the \( \Gamma \) point. In Fig. 7(b), the energy difference between \( E_1 \) and \( E_2 \) is shown, where the orange region with \( E_1 - E_2 < 0.03 \) suggests the enhanced anisotropy of the velocity of Dirac cone, e.g., an ellipse with the ratio of major and minor axes being \( \simeq 1.2 \). Figure 7(c) shows that the tilting angle \( \phi > 0 \) of \( E_1(k) - \mu \) measured from \( k_{x_0} \) axis has the sign opposite to that of Fig. 2(c). As shown later, such difference in the sign results in the difference of the current direction, i.e., the rotation with respect to the applied electric field. Figure 7(d) shows \( E_2(k) - \mu \) forming a pair of Dirac cone with that of Fig. 7(c), where the deviation of the tilting axis from \( k_{x_0} \) axis is opposite to that of Fig. 2(d).

Now we examine the electric conductivity. Figure 8 shows conductivity \( \sigma_{\nu_x} \), the solid line, (dashed line) denotes \( \sigma_{x}, \sigma_{y}, \) and \( \sigma_{xy} (\sigma_{\pm}) \). Note that \( \sigma_{xy} < 0 \) and has the sign opposite to that of the uni-axial pressure (Fig. 4). The conductivity \( \sigma_{\nu_x} \) at low temperatures of Fig. 8 is compared with that of Fig. 4. A difference between \( \sigma_{\nu_x} \) and \( \sigma_{\nu_y} \) in the former case is reduced due to hydrostatic pressure, which suppresses an increase of \( \sigma_{xy}(> \sigma_x) \) caused by a uniaxial pressure applied along the \( y \) direction. Figure 8 also shows the principal value \( \sigma_{\pm} \) of the conductivity, where \( \phi > 0 \) in the inset denotes an angle between the \( \sigma_- \) axis and the \( k_x \) axis. With increasing \( T \), the difference between \( \sigma_{\nu_x} \) and \( \sigma_{\nu_y} \) increases but is small compared with that of Fig. 4. This comes from a difference at low temperature, where \( \sigma_{xy} - \sigma_x \) for the uniaxial pressure is larger than that for the hydrostatic pressure. The sign, \( \phi > 0 \), which is in contrast to that of Fig. 4, is understood from Eq. (21a), since \( \sigma_{xy} < 0 \) and \( \phi/\pi(>0) \) (the inset) from Eq. (21a).

Now, we examine the effect of the e-p scattering on the \( T \) dependence of conductivity with some choices of \( R \), Eq. (16b), where the effect of the site potential is included in the energy band. Figure 9 shows \( \sigma_{\nu_x} \) with the fixed \( R = 1, 2, \) and 3, in which visible suppression of \( \sigma \) by \( R \) is seen compared with that of Fig. 8 \( (R = 0) \).
The crossover temperature, where $\sigma_y > \sigma_x$ at low temperatures and $\sigma_x > \sigma_y$ at high temperatures, decreases with increasing $R$. The slow increase toward the nearly constant behavior at high $T$ is seen for $\sigma_x$ while a broad maximum is found for $\sigma_y$. $\sigma_{xy}$ as a function of $T$ takes a minimum and followed by the change of the sign for large $R$.

Here, to understand the effect of site potentials under hydrostatic pressures, we show the $T$ dependence of $\sigma_\nu$ ($\nu = x, y$, and $xy$) without site potentials in Fig. 10 and compare with that in Fig. 9. The effect of the variation of $\mu(T)$ on $\sigma_\nu$ is negligibly small, where $\mu(0) = 0.168$.

In Fig. 10, the nearly constant behavior is obtained for $\sigma_x$ with $R = 2$ and 3. The sign of $\sigma_{xy}(> 0)$ is opposite to that of Fig. 9 at low $T$. Noting that Fig. 10 resembles Fig. 5, the sign of $\sigma_{xy}$ with + (-) at low temperatures corresponds to the absence (presence) of interactions. From Figs. 10 and 9, it turns out that the site potentials enhance $\sigma_x$ but suppress $\sigma_y$. The suppression of $\sigma_y$ is reasonable, since there is alternation of site potentials of $V_B$ and $V_C$ along the $y$ direction on the B-C chain. However, the origin of the enhancement of $\sigma_x$ is not clear, since the transfer energies $b_j$ in Fig. 1 are complicated for the electron transfer along the $x$ direction.

4. Summary and Discussion

We calculated the $T$ dependence of conductivity $\sigma_\nu$ of Dirac electrons in organic conductor ET under both uniaxial and hydrostatic pressures to examine the nearly constant behaviors at high temperatures. Extending the previous case, where the role of the e-p interaction was examined using the simple two bands of the Dirac cone, we examined the case of ET salts, where the transfer energy of the tight-binding model was obtained from the extended Hückel method and DFT. Such a model provides anomalous $T$ dependence of conductivity due to the tilted Dirac cone. With a moderate choice of the e-p interaction, our result suggests the almost constant conductivity at high temperature. The presence of the off-diagonal component ($\sigma_{xy}$), which is associated with the deviation of the tilting axis of the Dirac cone from the $k_x$ or $k_y$ axis, results in the principal axis with clockwise or anticlockwise rotation depending on the sign of $\sigma_{xy}$. Within the mean-field theory, we examined the effect of interactions on the conductivity with the tilted Dirac cone. Compared with $\sigma_x$ without interactions, $\sigma_x$ is enhanced but $\sigma_y$ is suppressed.

Here, we note on the role of the e-p interaction$^{27}$ in the nodal line semimetal $[\text{Pd}(\text{dddt})_2]$, which also exhibits similar resistivity at high $T$.$^{19}$ Although the system differs due to a line of Dirac points in 3D momentum space, electrons close to the nodal line show rather robust 2D DOS. Taking a moderate magnitude of the e-p coupling constant, the almost $T$ independent conductivity in the 2D plane has been obtained.$^{15}$

Finally, we compare our result with that of experiment. Temperature dependence of resistance (corresponding to the inverse of the conductivity) under hydrostatic pressures shows nearly constant behavior at high temperatures and a minimum at low temperatures, while the minimum is invisible for uniaxial pressure.$^{2}$ Our results show the broad maximum for $\sigma_y$ and mototonous variation for $\sigma_x$. Although we obtain the qualitative coincidence, the detail correspondence between them e.g., the direction of measurement is needed for the quantitative comparison. It also remains a future problem to clarify if the conductivity under pressure suggests the presence of interaction. The validity of our present calculation may be examined by the measurement of the deviation angle of the principal axis, i.e., the clockwise (anticlockwise) for the case without interaction (with interaction).

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