Tilted Dirac Cone Effect on Interlayer Magnetoresistance in $\alpha$-(BEDT-TTF)$_2$I$_3$

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We report the effect of Dirac cone tilting on interlayer magnetoresistance in $\alpha$-(BEDT-TTF)$_2$I$_3$, which is a Dirac semimetal under pressure. Fitting of the experimental data by the theoretical formula suggests that the system is close to a type-II Dirac semimetal.

The discovery of an unconventional half-integer quantum Hall effect in graphene[10] has stimulated intensive research on massless Dirac fermion systems. When a conduction band and a valence band touch at a single point in energy–momentum space with linear energy dispersion, the system is called a massless Dirac fermion system. The touching points appear as points known as Dirac points. Despite the Fermi velocity of those Dirac fermions being much smaller than the speed of light, they are described by the relativistic Dirac equation. The half-integer quantum Hall effect is a consequence of their unusual electronic structure[9] if the Dirac points are at the Fermi energy, the system is called a Dirac semimetal. A number of Dirac fermion systems have been discovered, including surface states of topological insulators[9]. There is also intensive research on Weyl fermions[11] which are a two-component analog of Dirac fermions. In general, the energy dispersion of Dirac fermions, which has a cone-like shape called a Dirac cone, is tilted from the energy axis in energy–momentum space. In Dirac or Weyl semimetals, both electron and hole pockets appear if the tilt is large enough. Such a system is called a type-II Dirac or Weyl semimetal[12] where Lorentz invariance is broken, and physical properties are very different from the usual Dirac or Weyl fermions, which are called type I.

In this paper, we report the effect of the Dirac cone tilt on the interlayer magnetoresistance in $\alpha$-(BEDT-TTF)$_2$I$_3$, which is a Dirac semimetal under pressure[13]. We found that the tilt of the Dirac cone is very large and the system is close to a type-II Dirac semimetal.

To investigate the tilt of the Dirac cone, we may consider a single Dirac point, though there are two Dirac points in $\alpha$-(BEDT-TTF)$_2$I$_3$ because the tilt of the other Dirac cone is the same. The Hamiltonian is described by the following $2 \times 2$ matrix[14]

$$\mathcal{H} (k_x, k_y) = \begin{pmatrix} v_0 k_x + v_y k_y & v_x k_x - i v_y k_y \\ v_x k_x + i v_y k_y & v_0 k_y + v_y k_x \end{pmatrix}, \quad (1)$$

where we set $\hbar = 1$ and $(k_x, k_y)$ is the wave vector in the two-dimensional Brillouin zone. The anisotropy in the Fermi velocity is parameterized by $\alpha = \sqrt{v_y/v_x}$. The vector $(v_0, v_y)$ is associated with the tilt of the Dirac cone. The angle between the $k_x$ axis and the tilt direction is defined by

$$\gamma = \tan^{-1}\left(\frac{v_y}{v_0} \frac{v_x}{v_0} \right). \quad (2)$$

The tilt of the Dirac cone is described by the following parameter:

$$\eta = \sqrt{\left(\frac{v_y}{v_0} \frac{v_x}{v_0}\right)^2 + \left(\frac{v_y}{v_0} \frac{v_x}{v_0}\right)^2}. \quad (3)$$

If $\eta < 1$, the system is a type-I Dirac semimetal. If $\eta > 1$, the system is a type-II Dirac semimetal.

Under a magnetic field $B = B (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$, the interlayer magnetotransport is governed by the zero-energy Landau level because the Fermi energy is at the Dirac point[13][14]. At zero temperature, the interlayer resistivity is given by[15]

$$\rho_{zz} = \frac{A}{B_0 \sin \theta \exp \left(-B \frac{1}{2}(\alpha/\ell_z)^2 I(\phi) \cot \theta \right)} \cdot (4)$$

where $A$ is a parameter inversely proportional to the density of states and the square of the interlayer hopping[13] and $B_0$ is a parameter associated with impurity scattering. The value of this latter parameter is estimated as $B_0 = 0.7$ T from the magnetic field dependence of the interlayer magnetoresistance[13]. $\rho_{zz}$ depends on the azimuthal angle $\phi$ through the following function[15]

$$I(\phi) = \left(\frac{\alpha \sin \phi \cos \gamma - \frac{1}{\alpha} \cos \phi \sin \gamma}{\lambda \sin \phi \sin \gamma + \frac{1}{\alpha} \cos \phi \cos \gamma} \right)^2 \cdot (5)$$

$$+ \frac{1}{\lambda} \left(\frac{\alpha \sin \phi \cos \gamma - \frac{1}{\alpha} \cos \phi \sin \gamma}{\lambda \sin \phi \sin \gamma + \frac{1}{\alpha} \cos \phi \cos \gamma} \right)^2 \cdot (6)$$

where $\lambda = \sqrt{1 - \eta^2}$. $\alpha_c$ is the lattice constant for the $c$ axis, and $\ell_z = 1/\sqrt{eB\sin \theta}$ is the magnetic length with $e$ being the electron charge. From the analysis of the tight-binding model for $\alpha$-(BEDT-TTF)$_2$I$_3$[13] we find $\gamma = 89.0^\circ$, $\alpha = 1.2$, and $\lambda = 0.40$. (For the other Dirac cone, we find $\gamma = 269.0^\circ$.) When $\alpha \neq 1$, there is a contribution from the Fermi surface anisotropy to the $\phi$ dependence of $\rho_{zz}$. However, $\alpha$ is close to 1, and so we set $\alpha = 1.2$ in the following analysis. As a result, the fitting parameters are $A$, $\lambda$, and $\gamma$.

Experiments were conducted as follows: A sample on which four electrical leads (gold wire with a diameter of 15 μm) are attached by carbon paste was placed into a Teflon capsule filled with the pressure medium (Ishimatsu DN-oil 7373). The capsule was then set into a clamp-type pressure cell made of hard alloy MP35N, and hydrostatic pressure of up to 1.7
The pressure was examined by recording the change in the resistance of Manganin wire at room temperature. The resistance of the crystal was measured by using a conventional dc method with an electrical current of 0.1 µA along the $c$ crystal axis, which is normal to the two-dimensional plane. In the investigation, the interlayer magnetoresistance $\rho_{zz}$ was measured as a function of the azimuthal angle $\phi$ in a magnetic field of 7 T at 4.2 K.

The experimental result was fitted by formula (4), as shown in Fig. 1. The parameter values obtained by the fitting are listed in Table I. From this analysis, we find that $\eta$ is less than one but very close to one. Therefore, the Dirac cone in $\alpha$-(BEDT-TTF)$_2$I$_3$ is almost at the boundary between types I and II. We also find that the direction of the tilt is approximately along the $k_x$ axis, or the $b$ axis, because $\rho_{zz}$ is maximum when the magnetic field is in the direction of the tilt. This is consistent with the tight-binding calculation and the first-principles calculation. Note that the value of $\lambda$ increases as $\theta$ decreases. This behavior is understood as follows: As $\theta$ decreases, mixing between the Landau levels increases. This suppresses the anisotropy associated with the interlayer hopping of the zero-energy Landau level wave function. Meanwhile, $I(\phi) \sim \cos^2\phi/\lambda$, for $\lambda \ll 1$. Therefore, to describe the suppression of the anisotropy using formula (4), we need a large $\lambda$ value. By contrast, the parameter $\gamma$ does not depend on $\theta$ because the Landau level mixing does not affect the anisotropy. In addition, the value is not much different from the $\gamma = 1.0^\circ$ value evaluated from the tight-binding model. The parameter $A$ increases as $\theta$ increases. This is understood from the reduction of the density of states at the Fermi energy owing to lifting of spin degeneracy by the Zeeman energy.

To conclude, we have measured the anisotropy of the interlayer resistivity and fitted the experimental data by using a theoretical formula. From the analysis, we have found that the Dirac cone of $\alpha$-(BEDT-TTF)$_2$I$_3$ is almost at the boundary between types I and II. The signature of massive carriers in the in-plane magnetotransport might be related to this fact. Because the electronic structure of $\alpha$-(BEDT-TTF)$_2$I$_3$ is controlled by pressure, we may expect that a type-II Dirac semimetal is realized in $\alpha$-(BEDT-TTF)$_2$I$_3$ under high pressure, a subject that is left for future research.

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![FIG. 1. (Color online) Azimuthal angle $\phi$ dependence of the interlayer resistivity $\rho_{zz}$ for different values of $\theta$. The experimental data are fitted by using the theoretical formula [3], which are shown by lines. The inset shows the layers of Dirac fermions and the crystal axes $a$, $b$, and $c$. The $b$ (a) axis corresponds to the $x$ ($y$) axis.](image)

| $\theta$ (degrees) | $A$ (arbitrary units) | $\lambda$ | $\gamma$ (degrees) | $I - \eta$ |
|------------------|----------------------|-----------|-------------------|------------|
| 40               | 55.9                 | 0.0275    | 3.86              | 3.78 x 10^{-4} |
| 30               | 47.1                 | 0.0345    | 4.56              | 5.95 x 10^{-4} |
| 20               | 43.1                 | 0.0547    | 3.50              | 1.50 x 10^{-3} |

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