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Theory of in-plane magnetoresistance in two-dimensional massless Dirac fermion system

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We present the theory of the in-plane magnetoresistance in two-dimensional massless Dirac fermion systems including the Zeeman splitting and the electron-electron interaction effect on the Landau level broadening within a random phase approximation. With the decrease in temperature, we find a characteristic temperature dependence of the in-plane magnetoresistance showing a minimum followed by an enhancement with a plateau. The theory is in good agreement with the experiment of the layered organic conductor α-(BEDT-TTF)$_2$I$_3$ under pressure. In-plane magnetoresistance of graphene is also discussed based on this theory.

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I. INTRODUCTION

Since the discovery of unconventional integer quantum-Hall effect in graphene,[1,2] which is a single atomic sheet of graphite, massless Dirac fermions realized in condensed-matter systems have attracted much attention. Under magnetic field, a remarkable difference between conventional two-dimensional electron systems and two-dimensional Dirac fermion systems appears in the Landau-level structure. In conventional electrons, the Landau-level energies are equally spaced. Meanwhile the Landau-level energies in Dirac fermions with the Fermi velocity v are given by

$$E_n = \mathrm{sgn}(n)\frac{\hbar v}{\ell_B}\sqrt{2|n|}, \tag{1}$$

where $n=0,\pm 1,\pm 2,\ldots$ and $\ell_B=\sqrt{\hbar/eB}$ is the magnetic length.[3] For the case of Dirac fermions, the Landau levels are unevenly spaced. What makes a crucial difference compared to the case of conventional electrons is the existence of the zero-energy Landau level that plays a central role for the unconventional integer quantum-Hall effect.[4]

Massless Dirac fermion systems are not restricted to a purely two-dimensional system. The layered organic conductor α-(BEDT-TTF)$_2$I$_3$ under pressure shows remarkable physical properties associated with a Dirac fermion spectrum.[5] Theoretically it has been predicted that this system is a massless Dirac fermion system,[6,7] where the Fermi energy is at the Dirac point and the Dirac cone is tilted.[8–10] This massless Dirac fermion spectrum is supported by first-principles calculations.[11,12] Experimentally the observation of the negative interlayer magnetoresistance[13] supports the massless Dirac fermion spectrum. Application of the magnetic field decreases the interlayer resistivity. This negative interlayer magnetoresistance is consistent with the existence of the zero-energy Landau level.[14] The interlayer resistance decreases in proportion to the inverse of the applied magnetic field. This magnetic field dependence arises from the zero-energy Landau-level degeneracy.

In this organic Dirac fermion system, an intriguing in-plane magnetoresistance was observed.[5] Under magnetic field, the in-plane resistivity decreases gradually as the temperature T is decreased for $T>100$ K. After reaching a broad minimum around 100 K, the resistivity increases and then shows a narrow plateau region around several Kelvin. After that the resistivity increases again as the temperature is decreased further.

In this paper, we present the theory of the in-plane magnetoresistance in massless Dirac fermion systems including the Landau-level broadening effect due to the Coulomb interaction between Dirac fermions and the Zeeman energy splitting. We compute the in-plane longitudinal conductivity by the Kubo formula using the Landau-level wave functions for massless Dirac fermions. The Coulomb interaction effect on the Landau-level broadening is computed by the random-phase approximation. The result is consistent with the in-plane magnetoresistance observed in α-(BEDT-TTF)$_2$I$_3$.[5] The theory is also applied to graphene.

II. MODEL

For the description of two-dimensional Dirac fermions in the x-y plane, we introduce two component spinor field operator $\psi_\sigma(x,y)$, where $\sigma=\pm$ denotes the spin. In graphene and α-(BEDT-TTF)$_2$I$_3$, there are two Dirac points in the Brillouin zone. We assume that Dirac fermions are degenerate with respect to these valley degrees of freedom. We do not consider intervalley interaction and focus on the single-valley properties. The Hamiltonian is given by $\mathcal{H}=\mathcal{H}_0+\mathcal{V}_C$, where

$$\mathcal{H}_0=\sum_\sigma\int dx\int dy\,\psi_\sigma^\dagger(x,y)\hbar v(\hat{k}_x\sigma_x+\hat{k}_y\sigma_y)\psi_\sigma(x,y) \tag{2}$$

with $\hat{k}_{x,y}=-i\partial_{x,y}$ and $\sigma_{x,y}$ the Pauli matrices. The term $\mathcal{V}_C$ describes the Coulomb interaction between Dirac fermions, $\mathcal{V}_C=(1/2)\Sigma_{\mathbf{q}}V_{\mathbf{q}}\rho_{\mathbf{q}}\rho_{-\mathbf{q}}$, where $V_q=2\pi e^2/(4\pi\epsilon_0\epsilon|\mathbf{q}|)$ with ϵ the dielectric constant. Throughout this paper, we assume that the Fermi energy is at the Dirac point. We do not include the effect of the Dirac cone tilt in α-(BEDT-TTF)$_2$I$_3$ (Ref. 8) because it turns out that tilt is unimportant for understanding the main features of the in-plane magnetoresistance of α-(BEDT-TTF)$_2$I$_3$ as we shall see below.

In a magnetic field, the kinetic energy of Dirac fermions is quantized into Landau levels, Eq. (1). Taking the Landau gauge $\mathbf{A}=(0,Bx)$, the Landau-level wave functions are represented by $\Phi_{n,k}(x,y)=\exp(iky)\phi_{n,k}(x)/\sqrt{L_y}$, where L_y is the system size in the y direction and

$$\phi_{n,k}(x) = \frac{C_n}{\sqrt{\ell_B}}\left[\begin{pmatrix} -i \,\mathrm{sgn}\, n \\ 0 \end{pmatrix} h_{|n|-1}\left(\frac{x}{\ell_B}+k\ell_B\right) + \begin{pmatrix} 0 \\ 1 \end{pmatrix} h_{|n|}\left(\frac{x}{\ell_B}+k\ell_B\right)\right] \quad (3)$$

with $C_0=1$ and $C_n=1/\sqrt{2}$ for $n\neq 0$, and $\mathrm{sgn}\, n=1(-1)$ for $n>0(n<0)$ and $\mathrm{sgn}\, n=0$ for $n=0$.

Here $h_n(\xi)$ are the eigenstates of the harmonic oscillator Hamiltonian $-\partial_\xi^2/2+\xi^2/2$, $h_n(\xi)=H_n(\xi)\exp(-\xi^2/2)/(2^{n/2}\pi^{1/4}\sqrt{n!})$, with $H_n(\xi)$ the Hermite polynomial.

In terms of the Landau-level wave functions, the field operator $\psi_\sigma(x,y)$ is represented by $\psi_\sigma(x,y)=\Sigma_{n,k}\Phi_{n,k}(x,y)c_{n,k,\sigma}$. Using this form, we find that the Fourier transform of the density operator $\rho(x,y)=\Sigma_\sigma\psi_\sigma^\dagger(x,y)\psi_\sigma(x,y)$ is

$$\rho_{\mathbf{q}} = e^{-q^2\ell_B^2/4}e^{i/2q_xq_y\ell_B^2}\sum_{n_1,n_2,k,\sigma} e^{iq_xk\ell_B^2}F_{n_1,n_2}(\mathbf{q})c^\dagger_{n_1,k,\sigma}c_{n_2,k+q_y,\sigma}, \quad (4)$$

where the function $F_{n_1,n_2}(\mathbf{q})$ is defined by[15]

$$F_{n_1,n_2}(\mathbf{q}) = C_{n_1}C_{n_2}[J_{|n_1|,|n_2|}(\mathbf{q}) + \mathrm{sgn}(n_1n_2)J_{|n_1|-1,|n_2|-1}(\mathbf{q})]. \quad (5)$$

For $n_1>n_2$, the function $J_{n_1,n_2}(\mathbf{q})$ has the following form:

$$J_{n_1,n_2}(\mathbf{q}) = \sqrt{\frac{n_1!}{n_2!}}\left(\frac{-iq_x-q_y}{\sqrt{2}}\ell_B\right)^{n_1-n_2}L_{n_2}^{n_1-n_2}\left(\frac{q^2\ell_B^2}{2}\right) \quad (6)$$

and $J_{n_2,n_1}(\mathbf{q})=[J_{n_1,n_2}(\mathbf{q})]^*$. Here $L_n^m(x)$ are the associated Laguerre polynomials.

III. COULOMB INTERACTION EFFECT ON THE LANDAU-LEVEL BROADENING

Now we compute the Coulomb interaction effect on the scattering rate of Dirac fermions that leads to the Landau-level broadening. As we shall show below the temperature dependence of the Landau-level broadening gives rise to a broad minimum in the in-plane resistivity that appears around $T=T_{\min}$. (For the case of α-(BEDT-TTF)$_2$I$_3$, it has been reported[5] that $T_{\min}\sim 100$ K.) Although it is easy to include the Zeeman splitting in the calculation of the Landau-level broadening, we present the calculation for the spinless case because the interaction effect plays an important role at high temperatures where many Dirac fermions are excited from the zero-energy Landau level while the Zeeman spin-splitting effect is negligible.

The single-particle Matsubara Green's function for the Landau level with the index n is $G_n(i\omega_\nu)=1/[i\omega_\nu-E_n-\Sigma_n(i\omega_\nu)]$, where $\omega_\nu=(2\nu+1)\pi k_BT$ is the fermion Matsubara frequency. Within the random phase approximation, the self-energy $\Sigma_n(i\omega_\nu)$ is described by

$$\Sigma_n(i\omega_\nu) = -\frac{k_BT}{2\pi\ell_B^2}\sum_{\mathbf{q},n',i\Omega_{\nu'}}\frac{V_{\mathbf{q}}}{1-V_{\mathbf{q}}D_{\mathbf{q}}(i\Omega_{\nu'})} \times F_{n,n'}(\mathbf{q})F_{n',n}(-\mathbf{q})G_{n'}(i\omega_\nu+i\Omega_{\nu'}), \quad (7)$$

where

$$D_{\mathbf{q}}(i\Omega_\nu) = -\frac{e^{-q^2\ell_B^2/2}}{2\pi\ell_B^2}\sum_{n_1,n_2}F_{n_1,n_2}(\mathbf{q})F_{n_2,n_1}(-\mathbf{q}) \times \frac{f(E_{n_1})-f(E_{n_2})}{i\Omega_\nu-E_{n_1}+E_{n_2}}. \quad (8)$$

The summation over the boson Matsubara frequency $\Omega_{\nu'}$ in Eq. (7) is carried out by using the spectral representation of $V_{\mathbf{q}}(i\Omega_\nu)\equiv V_{\mathbf{q}}/[1-V_{\mathbf{q}}D_{\mathbf{q}}(i\Omega_\nu)]$. Performing the analytic continuation $i\omega_\nu\to\omega+i\delta$ with δ an infinitesimal number and after some algebra, we obtain

$$\Sigma_n(\omega+i\delta) = -\frac{1}{4\pi^3\ell_B^2}\int_{-\infty}^{\infty}d\varepsilon\int_0^\infty dqq\,\mathrm{Im}[V_{\mathbf{q}}(\varepsilon+i\delta)] \times\sum_{n'}F_{n,n'}(\mathbf{q})F_{n',n}(-\mathbf{q})\frac{n(\varepsilon)+f(E_{n'})}{\omega+i\delta-E_{n'}+\varepsilon}. \quad (9)$$

The imaginary part of the self-energy, $-\mathrm{Im}\,\Sigma_n(\omega+i\delta)$, leads to the Landau level broadening. Instead, we use an approximate form, $\Gamma_n^C\equiv-\mathrm{Im}\,\Sigma_n(E_n+i\delta)$. We do not attempt to compute this quantity in a self-consistent manner. The Coulomb interaction plays an important role if there are large numbers of excited Dirac fermions. However, the number of the excited Dirac fermions is suppressed at temperatures less than the Landau-level energy gap. In such a regime, we may treat the Coulomb interaction perturbatively.

Figure 1(a) shows Γ_n^C for different Landau levels where we set[16] $\sqrt{2/B}\hbar v/\ell_B=10$ K/T$^{-1/2}$ and $\epsilon=300$ that were estimated[17] from the analysis of the interlayer magnetoresistance in α-(BEDT-TTF)$_2$I$_3$. (Note that at ambient pressure a large dielectric constant that is the same order of magnitude as our value has been reported.[18])

In the numerical calculation, we used the recursion formula for the function $\sqrt{n!/(n+k)!}x^{k/2}\exp(-x/2)L_n^k(x)$ instead of the recursion formula for the associated Laguerre polynomials because $L_n^k(x)$ and the factorials can be huge for Landau levels with $|n|\gg 1$. The summation with respect to the Landau levels is taken from $n=-50$ to 50. At temperatures below ~ 10 K, Γ_n^C remain constant. This behavior is understood from the energy gaps created by the Landau-level structure: the Coulomb interaction plays an important role when there are excited Dirac fermions to higher Landau levels. In order to excite Dirac fermions to higher Landau levels, the temperature should be larger than the energy gap created by the Landau levels. Thus, the characteristic temperatures are determined from the energy gaps between the Landau levels. As shown in Fig. 1(a), Γ_0^C behaves remarkably differently while the other $\Gamma_n^C(n\neq 0)$ behaves similarly. At low temperature below 30 K the effect of the electron-electron interaction is rapidly suppressed because of the large

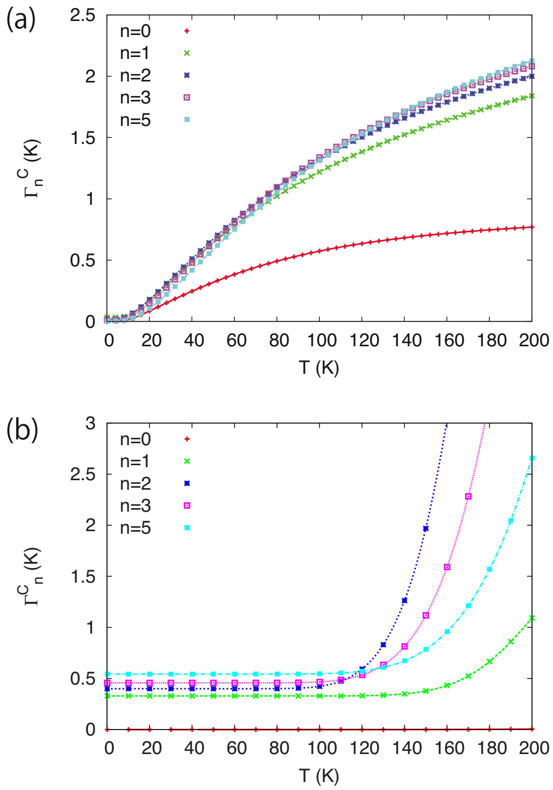

FIG. 1. (Color online) (a) Temperature dependence of Γ_n^C at $B=10$ T for different Landau levels with $\delta=0.1$ for α-(BEDT-TTF)$_2$I$_3$. (b) Temperature dependence of Γ_n^C at $B=10$ T for graphene.

energy gap between the zero-energy Landau level and the $|n|=1$ Landau level. Reflecting this fact, Γ_n^C decreases as we increase the magnetic field because the Landau-level energy gaps increase.

Figure 1(b) shows Γ_n^C for graphene where we take $\epsilon=2.5$ for the dielectric constant[19] and $\sqrt{2/B}\hbar v/\ell_B=400$ K/T$^{-1/2}$ for the Landau-level structure parameter.[4] Although the temperature dependence of Γ_n^C is different from Fig. 1(a) because of the parameter differences, it is common that the $n=0$ Landau-level component behaves differently as compared with the $n=0$ Landau level. Since the Landau-level energy gaps between the $n=0$ Landau level and the $n=1$ Landau level for graphene is about 1000 K, the value of Γ_0^C is negligible in the temperature range shown in Fig. 1(b). This result is consistent with the experiment[20] suggesting that the zero-energy Landau level is quite sharp in shape compared with the other Landau levels. Compared to α-(BEDT-TTF)$_2$I$_3$, the almost temperature independent region extended until $\sim$120 K. This is because the Landau-level energy spacing in graphene is larger than that in α-(BEDT-TTF)$_2$I$_3$. As shown in Fig. 1(b) the interaction effect on Γ_n^C is negligible for $T<100$ K due to the large separation between the Landau levels.

IV. IN-PLANE MAGNETORESISTANCE

Now we compute the in-plane longitudinal conductivity σ_{xx} using the Kubo formula[21]

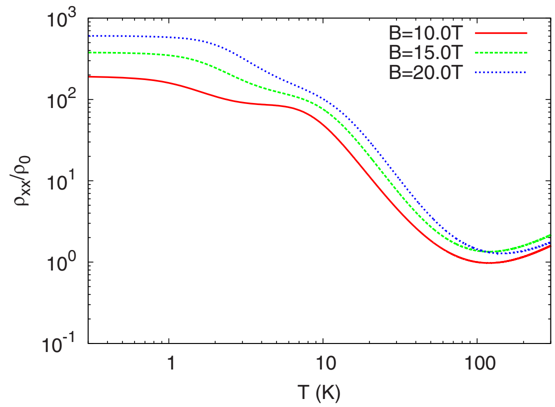

FIG. 2. (Color online) The in-plane resistivity for different magnetic fields with $\Gamma_0=2$ K. The normalization parameter ρ_0 is taken as $\rho_0=\rho_{xx}(100\text{ K})$ at $B=10$ T to compare with the experiment in Ref. 5.

$$\sigma_{xx}=\frac{e^2}{\hbar}\left(\frac{\hbar v}{\ell_B}\right)^2\sum_{n,\sigma}C_n\int_{-\infty}^{\infty}dE\left(-\frac{\partial f}{\partial E}\right)\times\frac{\Gamma_n/\pi}{(E-E_{n,\sigma})^2+\Gamma_n^2}\left[\frac{\Gamma_{|n|+1}/\pi}{(E-E_{|n|+1,\sigma})^2+\Gamma_{|n|+1}^2}+\frac{\Gamma_{-|n|-1}/\pi}{(E-E_{-|n|-1,\sigma})^2+\Gamma_{-|n|-1}^2}\right], \tag{10}$$

where f is the Fermi distribution function and the Zeeman energy splitting is included as $E_{n,\sigma}=E_n+g\mu_B\sigma B/2$. Here μ_B is the Bohr magnetron and we set $g=2$. The scattering rate is assumed to be $\Gamma_n=\Gamma_0+\Gamma_n^C$, where Γ_0 is associated with impurity scattering. In the following calculation we take $\Gamma_0=2$ K that was estimated from analysis of the interlayer magnetoresistance data[13] at low temperatures.[16] To reduce the numerical computation time we use Páde approximants for the temperature dependence of Γ_n^C. For Landau levels with $n\neq0$ we used the same Páde approximant for Γ_1^C because Γ_n^C with $n\neq0$ behave similarly as shown in Fig. 1(a).

Figure 2 shows the in-plane resistivity, $\rho_{xx}=1/\sigma_{xx}$ for different magnetic fields. Note that $\sigma_{xy}=0$ because the Fermi energy is at the Dirac point. Here we assume particle-hole symmetry so that the Fermi energy is fixed to the Dirac point even at finite temperatures. The minima appear around $T_{\min}\simeq100$ K. These minima appear because of the onset of the Landau-level splitting effect: The Landau levels with $|n|<10$ are well separated each other. But those separations are unimportant for $T\sim100$ K because of the temperature broadening effect due to the derivative of the Fermi distribution function in Eq. (10). For $T>100$ K, Landau levels with $|n|\leq10$ are almost continuously distributed because $|E_{n+1}-E_n|<\Gamma_{n+1}+\Gamma_n$. For $T<100$ K, we find that $|E_{10\pm1}-E_{10}|>\Gamma_{10\pm1}+\Gamma_{10}$ from the temperature dependence of Γ_n^C. So the Landau level splitting effect appears for $T<100$ K. We computed σ_{xx} without including Γ_n^C, and confirmed that the temperature dependence of ρ_{xx} for $T>100$ K mainly arises from the temperature dependence of Γ_n^C.

The appearance of a minimum at a characteristic temperature $T_{\min}$ in the in-plane magnetoresistance suggests that $T_{\min}$ is a crossover temperature from the interaction dominant regime to the almost noninteracting regime: for $T>T_{\min}$, the Landau-level broadening smears out the Landau-level energy spectrum. In this regime, the Landau-level spacing is unimportant, and the electron-electron interaction, which requires the excitations from one Landau level to higher Landau levels, plays an important role. By contrast for $T<T_{\min}$, the Landau-level broadening is less than the Landau-level spacing. Thus, the excitations from one Landau level to higher Landau levels are suppressed. The characteristic temperature $T_{\min}$ depends on ϵ, v, and B. Although there is no simple analytical formula for $T_{\min}$, one can determine $T_{\min}$ from the in-plane magnetoresistance measurement. The same analysis can be applied to the surface states of three dimensional topological insulators.[22,23]

With decreasing the temperature from ~ 100 K the resistivity increases because the number of Landau levels contributing to σ_{xx} decreases. Below 10 K a narrow plateau region appears. If we compute ρ_{xx} omitting the Zeeman energy splitting, we have a peak instead of the plateau and ρ_{xx} approaches a universal curve that is independent of the magnetic field. The peak position is scaled by $\sqrt{B}$. So the presence of the plateau is associated with the Landau-level splitting between $n=0$ and $n=\pm 1$. Namely, including the Zeeman energy splitting transforms the peak to the plateau. For $T<2\Gamma_0$, ρ_{xx} turns to increase again, and then ρ_{xx} approaches a temperature-independent value. We note that for a conventional parabolic dispersion case ρ_{xx} monotonically increases with decreasing the temperature because the Landau levels are equally spaced.

All features stated above are consistent with the experiment[5] except for $T<2\Gamma_0$. In the experiment, ρ_{xx} does not approach a temperature-independent value for $T<1$ K but increases further with decreasing temperature changing the slope at a characteristic temperature $T_{\exp}$. This behavior suggests that there is an another Landau level splitting probably associated with valley splitting. In Ref. 24, a Kosterlitz-Thouless transition scenario was proposed. We will investigate this point further in a future publication.

Now we comment on the tilt of the Dirac cone. In α-(BEDT-TTF)$_2$I$_3$, theoretical calculations suggest that the Dirac cone is tilted.[8] In the presence of the tilt of the Dirac cone, the Landau-level wave functions are deformed[10] that leads to anisotropy of the resistivity. However, the features of the in-plane magnetoresistance are unaffected by the tilt. The temperature dependence of the in-plane magnetoresistance is determined by the Landau-level structure. Since the tilt of the Dirac cone just leads to a modification of the overall factor of the Landau-level energies and does not affect the Landau-level structure qualitatively,[10] the tilt is unimportant for the temperature dependence of the in-plane magnetoresistance.

Using the theory, we are able to understand some results about σ_{xx} in graphene. Figure 3 shows σ_{xx} for different Γ_0 at

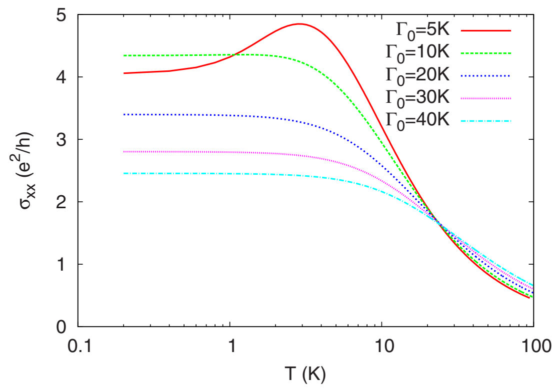

FIG. 3. (Color online) The temperature dependence of σ_{xx} for graphene for different Γ_0 at $B=10$ T.

$B=10$ T. We computed σ_{xx} for $B>10$ T as well (not shown) and found similar behaviors. The results with $\Gamma_0>10$ K are in good agreement with the experiment[25] for $B<8$ T. Experimentally Γ_0 is estimated[19] as $\Gamma_0\sim 30$ K. For clean samples with Γ_0, we should observe a peak associated with the Zeeman splitting around $T=2\Gamma_0-\mu_B B$. For $\Gamma_0=5$ K, the peak appears around $2\Gamma_0-\mu_B B\sim 3$ K as shown in Fig. 3. In the experiment reported in Ref. 25, σ_{xx} decreases at low temperatures for $B>10$ T. To understand this behavior, we need to assume that a valley splitting occurs as discussed in the literature.[26]

V. CONCLUSION

In conclusion, we have investigated the in-plane resistivity of Dirac fermions under magnetic field. We have included the Landau-level structure, the Zeeman energy splitting, and the Coulomb interaction effect between Dirac fermions. The Coulomb interaction plays an important role at high temperatures, where Dirac fermions are excited from the zero-energy Landau level. We found that the $n=0$ Landau level behaves differently compared to the other Landau levels. The features observed in α-(BEDT-TTF)$_2$I$_3$ are consistent with our result except for $T<1$ K where a valley splitting may play an important role. This theory has also been applied to graphene. We have found a consistent behavior with an existing experimental data and have predicted the presence of a peak structure of conductivity in clean samples.

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