Corrigendum: Semiclassical Boltzmann transport theory of few-layer black phosphorus in various phases (2019 2D Mater. 6 025016)

Sanghyun Park, Seungchan Woo and Hongki Min

Department of Physics and Astronomy, Seoul National University, Seoul 08826, Republic of Korea
E-mail: hmin@snu.ac.kr

In our paper, figures 3–10 and 14 have factor errors, and we present the fixed figures below. The factor errors do not affect the conclusions of the original paper.

**Figure 3.** Calculated dc conductivities (a)–(c) \(\sigma_{xx}/\sigma_0\) and (d)–(f) \(\sigma_{yy}/\sigma_0\) as a function of Fermi energy at the semi-Dirac transition point \(\Delta = 0\) for (a) and (d) short-range impurities, (b) and (d) charged impurities with \(\alpha_0 = 1000\), and (c) and (f) charged impurities with \(\alpha_0 = 1\). Here, \(\sigma_0 = e^2 k^2_0 c^2 / 16\pi\hbar n_{imp}\).
Figure 4. Calculated dc conductivities (a)–(c) $\sigma_{xx}$ and (d)–(f) $\sigma_{yy}$ as a function of Fermi energy in the insulator phase with $\Delta = 1$ for (a) and (d) short-range impurities, (b) and (d) charged impurities with $\alpha_0 = 1000$, and (c), (f) charged impurities with $\alpha_0 = 1$.

Figure 5. Calculated dc conductivities (a)–(c) $\sigma_{xx}$ and (d)–(f) $\sigma_{yy}$ as a function of Fermi energy in the Dirac semimetal phase with $\Delta = -1$ for (a) and (d) short-range impurities, (b) and (d) charged impurities with $\alpha_0 = 1000$, and (c), (f) charged impurities with $\alpha_0 = 1$. 
Figure 6. (a)–(c) $d \log \sigma_{xx}/d \log \varepsilon_F$ and (d)–(f) $d \log \sigma_{yy}/d \log \varepsilon_F$ as a function of $\alpha_0$ for charged impurities in each phase. The red dashed lines represent the Fermi energy exponents obtained in the strong screening limit. Here, $\varepsilon_F = \varepsilon_0$ for the semi-Dirac transition point, $\varepsilon_F = 1.01 \varepsilon_0$ for the gapped insulator phase, and $\varepsilon_F = 0.01 \varepsilon_0$ for the Dirac phase are used for the calculation.

Figure 7. Calculated dc conductivities (a)–(c) $\sigma_{xx}$ and (d)–(f) $\sigma_{yy}$ as a function of the temperature at the semi-Dirac transition point ($\Delta = 0$) for (a) and (d) short-range impurities, (b) and (d) charged impurities with $\alpha_0 = 1000$, and (c), (f) charged impurities with $\alpha_0 = 1$. Here, if the temperature is normalized by $T_F = \varepsilon_F/k_B$, the result is independent of $\varepsilon_F$ at the semi-Dirac transition point. The blue dashed-dotted lines and red dashed lines represent fitting by the corresponding asymptotic form in the low- and high-temperature limits, respectively.
Figure 8. Calculated dc conductivities (a)–(c) $\sigma_{xx}$ and (d)–(f) $\sigma_{yy}$ in the low-density limit as a function of the temperature in the insulator phase with $\Delta = 1$ for (a) and (d) short-range impurities, (b) and (d) charged impurities with $\alpha_0 = 1000$, and (c), (f) charged impurities with $\alpha_0 = 1$. Here, $\varepsilon_F = 1.1 \varepsilon_0$ is used for the calculation. The blue dashed-dotted lines represent the result for the gapped 2DEG system, and the red dashed lines represent power-law fitting by the asymptotic form of the semi-Dirac transition point in the high-temperature limit.

Figure 9. Calculated dc conductivities (a)–(c) $\sigma_{xx}$ and (d)–(f) $\sigma_{yy}$ in the low-density limit as a function of the temperature in the Dirac semimetal phase with $\Delta = -1$ for (a) and (d) short-range impurities, (b) and (d) charged impurities with $\alpha_0 = 1000$, and (c), (f) charged impurities with $\alpha_0 = 1$. Here, $\varepsilon_F = 0.01 \varepsilon_0$ is used for the calculation. The blue dashed-dotted lines and red dashed lines represent fitting by the corresponding asymptotic form in the low- and high-temperature limits, respectively.
Figure 10. Calculated dc conductivities (a)–(c) $\sigma_{xx}$ and (d)–(f) $\sigma_{yy}$ immediately below the van Hove singularity point as a function of the temperature in the Dirac semimetal phase with $\Delta = 1$ for (a) and (d) short-range impurities, (b) and (d) charged impurities with $\alpha_0 = 1000$, and (c), (f) charged impurities with $\alpha_0 = 1$. Here, $\varepsilon_F = 0.9\varepsilon_0$ is used for the calculation.

Figure 14. Calculated dc conductivities as a function of the temperature for the gapped 2DEG system in the low-density limit with $\Delta = 1$ for (a) short-range impurities, (b) charged impurities with $\alpha_0 = 1000$, and (c) charged impurities with $\alpha_0 = 1$. Here, $\varepsilon_F = 1.1\varepsilon_0$ is used for the calculation. The red dashed lines and blue dashed-dotted lines represent the conductivity of the insulator phase (with the same Fermi energy) $\sigma_{xx}^{\text{ins}}$ and $\sigma_{yy}^{\text{ins}}$, respectively.

ORCID iDs

Sanghyun Park ♦ https://orcid.org/0000-0001-6347-1289
Seungchan Woo ♦ https://orcid.org/0000-0003-1103-6773
Hongki Min ♦ https://orcid.org/0000-0001-5043-2432
1. Introduction

Since the discovery of graphene [1, 2], which is a carbon allotrope of two-dimensional (2D) honeycomb lattice, 2D materials have been one of the most active research areas in condensed matter physics. Black phosphorus (BP) is a 2D material with van der Waals layered structure composed of phosphorus atoms, and it has recently attracted considerable attention [3, 4]. As a layered semiconductor in its natural form, BP has a tunable band gap, and manipulation of its band gap through various methods has been validated by multiple theoretical and experimental reports [5]. Notable examples of the band gap tuning include thickness change [6, 7], strain control [8], pressure [9], electronic gating [10–12], and chemical doping [13]. Some of the band gap manipulation methods [9, 13] demonstrated that the band gap can be tuned to zero, showing the semi-Dirac state with a combination of linear and quadratic dispersions [14], which is also predicted in TiO$_2$/VO$_2$ heterostructures [15, 16]. Moreover, the band gap can be inverted, leading to the Dirac semimetal phase [17–19].

Due to its anisotropic electronic band structure, BP shows many peculiar transport properties such as large in-plane anisotropic transport [20, 21]. The effects of temperature [10, 22, 23], the number of layers [10], and substrate [22] on the anisotropic transport properties of BP have been studied experimentally. Furthermore, the transport properties of BP have been studied theoretically [24–29], demonstrating its anisotropic nature in energy- and temperature-dependent transport. However, there has been no systematic study on the anisotropic transport of BP in each phase, fully considering the anisotropy of the system and the interband scattering. In this study, we theoretically investigate the transport properties of BP in the gapped insulator phase, gapless Dirac semimetal phase, or gapless semi-Dirac transition point between the two phases. Using the fully anisotropic multiband Boltzmann transport theory, we systematically study the dc conductivity of few-layer BP as a function of the carrier density and temperature by varying the band gap tuning parameter, and determine the characteristic density and temperature dependence corresponding to each phase.
Figure 1. (a)–(c) Energy dispersions and (d)–(f) the corresponding Fermi surfaces of few-layer BP for the ((a) and (c)) insulator phase, ((b) and (e)) semi-Dirac transition point, and ((c) and (f)) Dirac semimetal phase.

Figure 2. (a)–(c) Calculated DOS and (d) and (e) the carrier density as a function of Fermi energy for the ((a) and (c)) insulator phase, ((b) and (e)) semi-Dirac transition point, and ((c) and (f)) Dirac semimetal phase. Here, $\Delta \equiv \frac{\varepsilon_g}{\varepsilon_0}$ is the band gap tuning parameter, and $g = 2$ and $c = 1$ are used for calculation.
2. Methods

2.1. Model

By expanding the tight-binding lattice model of few-layer BP [4, 30, 31], the corresponding low-energy effective Hamiltonian can be obtained as [32–36]

\[ H = \left( \frac{\hbar^2 k_x^2}{2m^*} + \frac{\varepsilon_g}{2} \right) \sigma_x + \hbar v_0 k_y \sigma_y, \]  

(1)

where \( m^* \) is the effective mass along the zigzag \((x)\) direction, \( v_0 \) is the band velocity along the armchair \((y)\) direction, \( \varepsilon_g \) is the size of the band gap (which will be used as a tuning parameter), and \( \sigma_x \) and \( \sigma_y \) are the Pauli matrices. The eigenenergies of the Hamiltonian are given by \( \varepsilon_{\pm} = \pm \sqrt{\left( \frac{\hbar^2 k_x^2}{2m^*} + \frac{\varepsilon_g}{2} \right)^2 + \hbar^2 v_0^2 k_y^2}; \) thus, the Hamiltonian \( H \) has a direct band gap for \( \varepsilon_g > 0 \), a semi-Dirac band touching point at \((k_x, k_y) = (0, 0)\) for \( \varepsilon_g = 0 \), or two Dirac points at \((k_x, k_y) = (\pm \sqrt{\frac{\varepsilon_g}{\hbar^2 v_0^2}}, 0)\) for \( \varepsilon_g < 0 \). The characteristic energy scales along the zigzag and armchair directions are given by \( \varepsilon_0 = \frac{\hbar^2 k_x^2}{2m^*} \) and \( \hbar v_0 k_y \), respectively, where \( k_0 = a^{-1} \) and \( a \) is the lattice constant. We introduce the dimensionless parameters \( \Delta = \frac{\varepsilon_g}{\varepsilon_0} \) and \( c = \frac{\hbar v_0 k_y}{\varepsilon_0} \), which represent a gap tuning parameter and the ratio of the characteristic energy scales along the zigzag and armchair directions, respectively. Throughout the paper, we use \( c = 1 \) and the spin degeneracy \( g = 2 \) for the calculation. We will discuss the effect of higher-order terms omitted in equation (1) in section 5.

Figure 1 shows the energy dispersion and the corresponding Fermi surface of few-layer BP in each phase. Initially, few-layer BP without band gap tuning is in the gapped insulator phase, as shown in figure 1(a). As the band gap \( \varepsilon_g \) decreases (for example, upon applying a perpendicular electric field), eventually it vanishes and the system is described by the semi-Dirac Hamiltonian in equation (1) with \( \varepsilon_g = 0 \), as shown in figure 1(b). If the band gap decreases even further and becomes negative (\( \varepsilon_g < 0 \)), band inversion occurs, which has been achieved experimentally using surface doping [17, 18] and external pressure [19].

In the gapped insulator phase, the inherent anisotropy of the system is less evident and the system at low densities resembles typical semiconductors with a different effective mass in each direction. At the semi-Dirac transition point, the energy dispersion becomes linear (quadratic) along the armchair (zigzag) direction, as shown in figure 1(e). At the Dirac semimetal phase, the anisotropy in the energy dispersion becomes more pronounced and the Fermi sur-
face vastly changes its shape depending on the value of the Fermi energy $\varepsilon_F$. For $\varepsilon_F < \varepsilon_g/2$, the Fermi surface becomes two distinct lines, as shown in figure 1(f), whereas for $\varepsilon_F > \varepsilon_g/2$, the two Fermi surfaces become joined completely, forming a closed line. At $\varepsilon_F = \varepsilon_g/2$, a van Hove singularity occurs in the density of states (DOS), as explained below.

Figure 2 shows the DOS and the carrier density as a function of Fermi energy for each phase. At the semi-Dirac transition point, the DOS is simply given by $D(\varepsilon) \sim \varepsilon^{1/2}$ (figure 2(a)), and the carrier density (which is an energy integral of the DOS up to $\varepsilon_F$) is given by $n \sim \varepsilon_F^{3/2}$ (figure 2(d)). (See appendix A for the detailed derivations of the DOS and the carrier density.) In the gapped insulator phase, both DOS at $\varepsilon_F$ and carrier density vanish for $\varepsilon_F < \varepsilon_g/2$, whereas for $\varepsilon_F > \varepsilon_g/2$, they follow those of the semi-Dirac transition point as $\varepsilon_F$ increases (figures 2(b) and (e)). In the Dirac semimetal phase, when $\varepsilon_F$ is very small, the system resembles a typical 2D Dirac semimetal such as graphene; thus, $D(\varepsilon) \sim \varepsilon^2$. As $\varepsilon_F$ increases and approaches $\varepsilon_g/2$ near the top of the inverted band, the band dispersion effectively becomes hyperbolic paraboloid with a different sign in each direction in momentum space. Subsequently, a van Hove singularity occurs in the DOS, diverging logarithmically with $D(\varepsilon) \sim -\log(|\varepsilon| - \varepsilon)^{-1}$ [37]. If $\varepsilon_F$ increases further, the DOS and the carrier density follow those of the semi-Dirac transition point with a discontinuous energy derivative in the DOS at the van Hove singularity (figures 2(c) and (f)).

Notably, as the energy dispersion and the Fermi surface are anisotropic, and the Fermi energy can cross multiple bands, we cannot naively use the conventional Boltzmann transport theory assuming an isotropic single-band system. Thus, the anisotropic multiband Boltzmann transport theory is necessary to calculate the dc conductivity of such systems, as explained in section 2.2.

2.2. Boltzmann transport theory in anisotropic multiband systems

We use semiclassical Boltzmann transport theory to calculate the density and temperature dependence of the dc conductivity of few-layer BP in each phase in the presence of impurities, assuming elastic scattering (see section 5 for the limitation of the current approach). In the Boltzmann transport theory, electron states are described by the non-equilibrium distribution function $f = f(\mathbf{r}, \mathbf{k}, t)$. Its time rate of change is balanced out by the collision term, which represents the total scattering probability per unit time, i.e. $rac{df}{dt} = \left(\frac{df}{dt}\right)_{\text{coll}}$.

We assume a spatially homogeneous system without explicit time dependence in the distribution function, i.e. $f = f_k$. Thus, the time derivative of the
distribution function is given by \( \frac{df}{dt} = \hat{k} \cdot \frac{\partial f}{\partial k} \), whereas the collision term is given by

\[
\left( \frac{df}{dt} \right)_{\text{coll}} = - \int \frac{d^4k}{(2\pi)^4} W_{kk'} (f_k - f_{k'}),
\]

where \( W_{kk'} = \frac{2}{\pi} n_{\text{imp}} |V_{kk'}|^2 \delta (\varepsilon_k - \varepsilon_{k'}) \) is the transition rate from \( k \) to \( k' \) for an elastic scattering with the impurity potential \( V_{kk'} \) and the impurity density \( n_{\text{imp}} \). In the presence of a uniform electric field \( E \), \( \hbar k = (-e)E \), and to the leading order in \( E \),

\[
\frac{df_k}{dt} \approx (-e)E \cdot \frac{\partial f^{(0)}_k}{\hbar \partial k} = (-e)E \cdot v_k \frac{\partial f^{(0)}_k}{\partial \varepsilon_k},
\]

where \( v_k = \frac{1}{\hbar} \frac{\partial \varepsilon_k}{\partial k} \) and \( f^{(0)}_k = f^{(0)}(\varepsilon_k) = \left[ \rho (\varepsilon - \mu) + 1 \right]^{-1} \) is the Fermi–Dirac distribution function at equilibrium with \( \beta = \frac{1}{k_B T} \) and the chemical potential \( \mu \). Assume that, to the leading order in \( E \), the non-equilibrium distribution function \( f_k \) is given by \( f_k \equiv f^{(0)}(\varepsilon_k) + \delta f_k \) at energy \( \varepsilon = \varepsilon_k \). Thus, from \( \frac{df}{dt} = \left( \frac{df}{dt} \right)_{\text{coll}} \), we obtain

\[
(-e)E \cdot v_k S^{(0)}(\varepsilon) = \int \frac{d^4k'}{(2\pi)^4} W_{kk'} (\delta f_k - \delta f_{k'}),
\]

where \( S^{(0)}(\varepsilon) = - \frac{\partial f^{(0)}(\varepsilon)}{\partial \varepsilon} \). If the Fermi energy crosses multiple energy bands, equation (4) is generalized to [38, 39]

\[
(-e)E \cdot v_k S^{(0)}(\varepsilon) = \sum_{\alpha'} \int \frac{d^4k'}{(2\pi)^4} W_{kk'}^{\alpha\alpha'} (\delta f_k^{\alpha} - \delta f_{k'}^{\alpha'}),
\]

where \( \alpha \) and \( \alpha' \) are band indices.

We parameterize \( \delta f_k^{\alpha} \) in the following form [40–42]:

\[
\delta f_k^{\alpha} = (-e) \left( \sum_{i=1}^{d} E^{(i)} v^{(i)}_k \tau^{(i)}_k \right) S^{(0)}(\varepsilon),
\]

where \( E^{(i)}, v^{(i)}_k \), and \( \tau^{(i)}_k \) are the electric field, velocity, and relaxation time, respectively, along the \( i \)th direction for each band. After matching each coefficient in \( E^{(i)} \), we obtain the following integral equation for the relaxation time:

\[
1 = \sum_{\alpha'} \int \frac{d^4k'}{(2\pi)^4} W_{kk'}^{\alpha\alpha'} \left( \frac{}{v^{(i)}_k} \right) \left( \frac{}{v^{(i)}_k} \right) \left( \frac{}{v^{(i)}_k} \right). \]

This is a coupled integral equation relating the relaxation times at different angles in different bands, which correctly considers the anisotropy and multiple

**Figure 5.** Calculated dc conductivities (a)–(c) \( \sigma_x \) and (d)–(f) \( \sigma_y \) as a function of Fermi energy in the Dirac semimetal phase with \( \Delta = -1 \) for (a) and (d) short-range impurities, (b) and (d) charged impurities with \( \alpha_0 = 1000 \), and (c) and (f) charged impurities with \( \alpha_0 = 1 \).
bands of the system. Note that, for an isotropic single-band system \( \tau^{(i)}_{\kappa \alpha} = \tau(\varepsilon) \) for a given energy \( \varepsilon = \varepsilon_{\kappa \alpha} \), equation (7) is reduced to the well-known expression for the relaxation time given by [43]

\[
\frac{1}{\tau_k} = \int \frac{d^2 k'}{(2\pi)^2} W_{kk'} (1 - \cos \theta_{kk'}). \tag{8}
\]

The current density \( J \) induced by an electric field \( E \) is thus given by

\[
j^{(i)} = g \sum_\alpha \int \frac{d^2 k}{(2\pi)^2} (-e) \tau_{\kappa \alpha} \delta_{k \alpha} \equiv \sum_j \sigma_{ij} E^{(i)}, \tag{9}
\]

where \( \sigma_{ij} \) is the conductivity tensor given by

\[
\sigma_{ij} = e g^2 \sum_\alpha \int \frac{d^2 k}{(2\pi)^2} S^{(0)}(\varepsilon) \tau^{(i)}_{\kappa \alpha} \tau^{(j)}_{\kappa' \alpha} \tau_{\kappa \alpha}. \tag{10}
\]

We find that the Hall conductivity \( (i \neq j) \) vanishes, thus we consider only the diagonal part of the dc conductivity \( (i = j) \).

3. Density dependence of dc conductivity

Using the anisotropic multiband Boltzmann transport theory developed in section 2.2, we calculate the dc conductivity of few-layer BP as a function of the carrier density or Fermi energy at zero temperature for each phase: the semi-Dirac transition point \((\Delta = 0)\), gapped insulator phase \((\Delta > 0)\), and Dirac semimetal phase \((\Delta < 0)\), all of which can be expressed by equation (1).

As for the impurity potential, we consider two types of impurity scattering: short-range impurities and long-range Coulomb impurities (or charged impurities). Short-range impurities originate from lattice defects, vacancies, dislocations, etc, and their potential form is given by a constant in momentum space, \( V_{kk'} = V_{\text{short}} \), as they are approximately represented by the delta function in real space. For charged impurities distributed randomly in the background, the impurity potential is given by \( V_{kk'} = \frac{2e^2}{q|q|} \) in 2D, where \( \epsilon(q) \) is the dielectric function for \( q = k - k' \).

Within the Thomas–Fermi approximation, \( \epsilon(q) \) can be approximated as \( \epsilon(q) \approx \kappa (1 + q_{TF} / |q|) \), where \( \kappa \) is the background dielectric constant, \( q_{TF} = \frac{2\pi e^2}{\kappa} D(\varepsilon_F) \) is the Thomas–Fermi wave vector, and \( D(\varepsilon_F) \) is the total DOS at the Fermi energy \( \varepsilon_F \) (including all the contributions from the bands crossing \( \varepsilon_F \) and the spin degeneracy). The interaction strength for charged impurities can be characterized by an effective fine structure constant \( \alpha_0 = \frac{e^2}{\pi\varepsilon_0} \). Note that \( q_{TF} \propto g\alpha_0 \). Thus, the screening strength for Coulomb impurities is also characterized by \( \alpha_0 \).

Figure 6. (a)–(c) \( d \log \sigma_{xx}/d \log \varepsilon_F \) and (d)–(f) \( d \log \sigma_{xx}/d \log \varepsilon_F \) as a function of \( \alpha_0 \) for charged impurities in each phase. The red dashed lines represent the Fermi energy exponents obtained in the strong screening limit. Here, \( \varepsilon_F = \varepsilon_0 \) for the semi-Dirac transition point, \( \varepsilon_F = 1.01\varepsilon_0 \) for the gapped insulator phase, and \( \varepsilon_F = 0.01\varepsilon_0 \) for the Dirac phase are used for the calculation.
3.1. Semi-Dirac transition point
First, let us consider the semi-Dirac transition point ($\Delta = 0$). Figure 3 shows the Fermi energy dependence of the dc conductivity at the semi-Dirac transition point. The characteristic density or Fermi energy dependence of the dc conductivity can be understood as follows. From equation (10) with $\tau_i^{(F)} \sim \frac{D_F^{1/2}}{v_i^{(F)}}$, we expect $\sigma_{ii} \sim \frac{D_F^{1/2}}{v_i^{(F)}}$ at the Fermi energy along the $i$th direction, and $V_F^2$ is the angle-averaged squared impurity potential at the Fermi energy. At the semi-Dirac transition point, $D_F^{1/2}$ and the Fermi velocity in each direction is given by $v_F^{(x)} \sim \frac{\epsilon_{F}}{T_F}$ and $v_F^{(y)} \sim \frac{\epsilon_{F}}{T_F}$, from which we can deduce the power-law behavior of the dc conductivity. (See appendix A for the detailed derivations of the power-law dependences.)

For short-range impurities, $V_F$ is a constant independent of density; in this case, we obtain

$$\sigma_{xx} \sim \frac{\epsilon_{F}^{1/2}}{n},$$

(11a)

$$\sigma_{yy} \sim \frac{\epsilon_{F}^{1/2}}{n^{0}}.$$  

(11b)

For charged impurities, in the strong screening limit ($g\alpha_0 \gg 1$), $V_F \sim q_F^{-1} \sim D_F^{-1} \sim \frac{\epsilon_{F}^{1/2}}{T_F}$; thus, we obtain

$$\sigma_{xx} \sim \epsilon_{F}^{1/2} \sim n^{1},$$

(12a)

$$\sigma_{yy} \sim \epsilon_{F}^{1/2} \sim n^{0}.$$  

(12b)

At general screening strength, the power-law behavior is determined by the competition between the screening wave vector and the momentum transfer. We present the numerically calculated power-law behavior for the semi-Dirac transition point and for the other phases in figure 6.

3.2. Insulator phase
Figure 4 shows the Fermi energy dependence of the dc conductivity in the insulator phase ($\Delta > 0$). In the insulator phase, the power-law dependence of the dc conductivity at low densities becomes similar to that of 2D electron gas (2DEG) with a different effective mass in each direction. (See appendix C1 for detailed derivations.)

For short-range impurities, the power-law dependence of the dc conductivity at low densities is given by...
σ_{xx} \sim \varepsilon_F, \quad (13a)
\sigma_{yy} \sim \varepsilon_F. \quad (13b)

For charged impurities, in the strong screening limit, at low densities, we obtain

σ_{xx} \sim \varepsilon_0^2 F, \quad (14a)
σ_{yy} \sim \varepsilon_0^2 F. \quad (14b)

Note that, as the Fermi energy or the carrier density increases, the power-law dependence becomes similar to that of the semi-Dirac transition point.

### 3.3. Dirac semimetal phase

Figure 5 shows the Fermi energy dependence of the dc conductivity in the Dirac semimetal phase (Δ < 0). In the Dirac semimetal phase, the power-law dependence of the dc conductivity at low densities becomes similar to that of graphene but with a different Fermi velocity in each direction. (See appendix C2 for detailed derivations.)

For short-range impurities, the power-law dependence of the dc conductivity at low densities is given by

σ_{xx} \sim \varepsilon_0 F, \quad (15a)
σ_{yy} \sim \varepsilon_0 F. \quad (15b)

For charged impurities, in the strong screening limit, at low densities, we obtain

σ_{xx} \sim \varepsilon_F^2, \quad (16a)
σ_{yy} \sim \varepsilon_F^2. \quad (16b)

Near the van Hove singularity, ε_F \approx ±\varepsilon_g / 2, the DOS diverges logarithmically and it dominates the overall power-law behavior of conductivity. Therefore, for short-range impurities, the conductivity becomes

σ_{xx} \sim \left(-\log (|\Delta| - \varepsilon_F)\right)^{-1}, \quad (17a)
σ_{yy} \sim \left(-\log (|\Delta| - \varepsilon_F)\right)^{-1}. \quad (17b)

For charged impurities, due to the dominant contribution from the diverging Thomas–Fermi wave vector qTF \propto D(ε_F), the conductivity is largely given by the square of the DOS as follows:

σ_{xx} \sim \log (|\Delta| - \varepsilon_F)^2, \quad (18a)
σ_{yy} \sim \log (|\Delta| - \varepsilon_F)^2. \quad (18b)

As the Fermi energy or the carrier density increases further, the power-law dependence of the dc...
conductivity becomes similar to that of the semi-Dirac transition point, as in the insulator phase.

Figure 6 shows the evolution of the Fermi-energy power law of the dc conductivity as a function of the screening strength $\alpha_0$ for each phase in the low carrier density limit. For the insulator phase and the semi-Dirac transition point, the Fermi-energy exponent decreases, whereas for the Dirac semimetal phase, it shows a non-monotonic behavior with a dip structure, which originates from the interband-like scattering between two distinct Fermi surfaces shown in figure 1(f). As the screening strength increases, all the Fermi-energy exponents approach the corresponding power law estimated in the strong screening limit.

4. Temperature dependence of dc conductivity

We can apply the anisotropic multiband Boltzmann transport theory developed in section 2.2 to the dc conductivity at finite temperature. In equation (10), the finite temperature affects the conductivity through the Fermi distribution and the temperature-dependent screening for the charged impurity potential. At finite temperatures, the chemical potential of the system also deviates from the Fermi energy $\varepsilon_F$ due to the broadening of the Fermi distribution function. From the invariance of carrier density $n$ with respect to temperature $T$, we obtain the temperature dependence of the chemical potential $\mu(T)$. For charged impurities, the finite temperature Thomas–Fermi screening wave vector is given by $q_{TF}(T) = \frac{2\pi}{\varepsilon_0} \frac{\alpha_0}{e} \frac{\partial n}{\partial \mu}$ for 2D systems. (See appendix D for the detailed derivation of the temperature dependence of the chemical potential and Thomas–Fermi wave vector). In this section, we calculate the dc conductivity of few-layer BP as a function of the temperature for each phase. The detailed derivation of the temperature-dependent conductivity is presented in appendices E and F.

4.1. Semi-Dirac transition point

From the power-law dependence of the DOS, $D(\varepsilon) \sim \varepsilon^{1/2}$ at the semi-Dirac transition point (figure 2(a)), we can obtain the asymptotic behaviors of $\mu(T)$ and $q_{TF}(T)$ in a relatively straightforward manner. In the low- and high-temperature limits, the chemical potential at the semi-Dirac transition point is given by

$$\mu = \begin{cases} 1 - \frac{\varepsilon_F^2}{2T} \left( \frac{T}{\varepsilon_F} \right)^2 & (T \ll T_F), \\ \frac{1}{2 \sqrt{\pi(\frac{\varepsilon_F}{T})^{3/2}}} & (T \gg T_F), \end{cases} \quad (19)$$
whereas the Thomas–Fermi wave vector is given by

\[ q_{\text{TF}}(T) = \begin{cases} \frac{1}{\pi^2} \left( \frac{T}{T_F} \right)^2 & (T \ll T_F), \\ 2\eta \left( \frac{1}{2} \right) \Gamma \left( \frac{1}{2} \right) \left( \frac{T}{T_F} \right)^2 & (T \gg T_F), \end{cases} \]

where \( \Gamma \) is the Gamma function and \( \eta \) is the Dirichlet eta function [44]. In a single-band system, \( q_{\text{TF}}(T) \) typically decreases with the temperature at high temperatures, whereas at the semi-Dirac transition point, \( q_{\text{TF}}(T) \) increases with the temperature due to the thermal excitation of carriers participating in the screening.

Figure 7 shows the temperature dependence of the dc conductivity at the semi-Dirac transition point, normalized by the zero-temperature conductivity value in each direction. For short-range impurities, we determine that the asymptotic behavior is given by

\[ \frac{\sigma_{xx}(T)}{\sigma_{xx}(0)} = \begin{cases} 1 - \frac{x^2}{\pi^2} \left( \frac{T}{T_F} \right)^2 & (T \ll T_F), \\ \log 2 \left( \frac{T}{T_F} \right)^2 & (T \gg T_F), \end{cases} \]

\[ \frac{\sigma_{yy}(T)}{\sigma_{yy}(0)} = \begin{cases} 1 - e^{-T_{\text{ff}}/T} & (T \ll T_F), \\ \frac{1}{2} + \frac{1}{8n(1)^{1/2}} \left( \frac{T}{T_F} \right)^{-1} & (T \gg T_F). \end{cases} \]

For charged impurities, the asymptotic behavior is given by

\[ \frac{\sigma_{xx}(T)}{\sigma_{xx}(0)} = \begin{cases} 1 + C_{xx} \left( \frac{T}{T_F} \right)^2 & (T \ll T_F), \\ D_{xx} \left( \frac{T}{T_F} \right)^2 & (T \gg T_F), \end{cases} \]

\[ \frac{\sigma_{yy}(T)}{\sigma_{yy}(0)} = \begin{cases} 1 + C_{yy} \left( \frac{T}{T_F} \right)^2 & (T \ll T_F), \\ D_{yy} \left( \frac{T}{T_F} \right)^2 & (T \gg T_F), \end{cases} \]

where \( C_{ii} \) (\( D_{ii} \)) indicates the low- (high-) temperature coefficients. In the strong screening limit, the coefficients become \( C_{xx} = 0 \), \( D_{xx} = \frac{x^2}{\pi^2} \), \( C_{yy} = -\frac{x^2}{4} \), and \( D_{yy} = \log 2 \). As the screening strength decreases, the high-temperature coefficients \( D_{ii} \) remain positive, whereas the low-temperature coefficients \( C_{ii} \) decrease and we expect that the initially negative or vanishing \( C_{ii} \) would eventually become positive in the weak screening limit. (See appendix E for the detailed derivations of the coefficients \( C_{ii} \) and \( D_{ii} \).)

The temperature dependence in the high-temperature limit can be easily understood by replacing \( \varepsilon \) with \( T \) in the Fermi energy dependence of dc conductivity (equations (11) and (12)). At high temperatures, \( \sigma_{yy}(T) \) for short-range impurities decreases with the temperature, showing a metallic behavior. Other-

---

**Figure 10.** Calculated dc conductivities (a)–(c) \( \sigma_{xx} \) and (d)–(f) \( \sigma_{yy} \) immediately below the van Hove singularity point as a function of the temperature in the Dirac semimetal phase with \( \Delta = 1 \) for ((a) and (d)) short-range impurities, ((b) and (d)) charged impurities with \( \alpha_0 = 1000 \), and ((c) and (f)) charged impurities with \( \alpha_0 = 1 \). Here, \( \varepsilon_f = 0.9\varepsilon_0 \) is used for the calculation.
wise, the conductivities increase with the temperature, showing an insulating behavior. Note that the high-temperature asymptotic form for charged impurities is obtained by considering the effect of the energy averaging and that of the temperature-dependent screening separately. It correctly predicts the temperature power-law dependence but not the coefficients in the asymptotic form, showing a discrepancy with the numerical result, as the effect of temperature cannot be simply separated into the energy averaging and the temperature-dependent screening at high temperatures.

4.2. Insulator phase

Figure 8 shows the temperature dependence of the dc conductivity in the insulator phase with the fixed Fermi energy of $\varepsilon_F = 1.1\varepsilon_0$, which corresponds to the low-density limit. At zero temperature, the insulator phase in the low-density limit can be effectively considered as a gapped 2DEG (with anisotropic effective masses). Similarly, at finite temperatures, the temperature-dependent conductivity of the insulator phase in the low-density limit resembles that of the gapped 2DEG system (blue dash-dotted lines in figure 8), especially in the low-temperature limit. In the high-temperature limit, the power-law behavior of the temperature-dependent conductivity for the insulator phase becomes similar to that of the semi-Dirac transition point (equations (21) and (22)), because thermally excited carriers above the gap contribute to the conductivity. (See appendix F for the temperature dependence of the chemical potential, Thomas–Fermi screening wave vector, and conductivity of the gapped 2DEG system.)

In the high-density limit, the temperature dependence of dc conductivity in the insulator phase resembles that of the semi-Dirac transition point.

4.3. Dirac semimetal phase

Figure 9 shows the calculated temperature-dependent conductivity in the Dirac semimetal phase, with the fixed Fermi energy of $\varepsilon_F = 0.01\varepsilon_0$, which corresponds to the low-density limit. At low densities, the Dirac semimetal phase can be effectively considered as graphene (with anisotropic velocities); thus, we can understand its temperature-dependent conductivity behavior using the result of graphene. (See appendix F for the temperature dependence of the chemical potential, Thomas–Fermi screening wave vector, and conductivity of graphene.) For graphene with short-range impurities, the asymptotic form of the temperature-dependent conductivity becomes

$$\frac{\sigma_{g\beta}(T)}{\sigma_{g\beta}(0)} = \begin{cases} 1 - \frac{\varepsilon_F}{T} \left( \frac{T}{T_F} \right)^2 & (T \ll T_F), \\ \frac{1}{16\log^2 \left( \frac{T}{T_F} \right)} & (T \gg T_F), \end{cases}$$

(23)

whereas for charged impurities in the strong screening limit, the asymptotic form of the temperature-dependent conductivity becomes

$$\sigma_{g\beta}(T) = \begin{cases} 1 - \frac{\varepsilon_F}{T} \left( \frac{T}{T_F} \right)^2 & (T \ll T_F), \\ \frac{1}{16\log^2 \left( \frac{T}{T_F} \right)} & (T \gg T_F), \end{cases}$$

(24)

Similarly to the result of the semi-Dirac transition point, the high-temperature asymptotic form for charged impurities correctly captures the temperature power-law dependence (but not the exact coefficient value, as discussed in section 4.1).

Figure 10 shows the temperature dependence of the dc conductivity in the Dirac semimetal phase immediately below the van Hove singularity point, exhibiting a nonmonotonic behavior with temperature. As explained earlier, the temperature dependence of the dc conductivity is determined by the energy averaging with $S^{01}(\varepsilon)$ broadened by temperature, and by the temperature-dependent screening for charged impurities. Thus, if the Fermi energy is near the van Hove singularity, the distance between the Fermi energy and the van Hove singularity sets an important energy scale for the temperature dependence, $k_BT_1 \equiv |\varepsilon_F - \varepsilon_0|$. For charged impurities, the conductivity first increases, showing a peak at $T_1$, and thereafter decreases, showing a dip at $T_{2d} \sim 0.5T_F$ corresponding to the minimum of $q_{TF}(T)$ (figure D3(e) in the appendix). For short-range impurities, the conductivity first decreases, showing a dip at $T_1$, and thereafter increases, showing a peak at $T_{2d} \sim 0.25T_F$. These dips and peaks are from the temperature-dependent evolution of the chemical potential $\mu(T)$ (figure D3(b) in the appendix), shifting the central point of the energy averaging.

In the high-density limit, the temperature dependence of dc conductivity in the Dirac semimetal phase resembles that of the semi-Dirac transition point.

5. Discussion and conclusion

When we consider both short-range and charged impurities, assuming that each scattering mechanism is independent, the total scattering rate is obtained by adding their scattering rates in accordance with Matthiessen’s rule. Note that the scattering mechanism with a higher scattering rate (or equivalently a lower conductivity) dominates the resulting conductivity. From the obtained Fermi-energy power-law dependence of dc conductivity, we can determine the dominant scattering mechanism. At the semi-Dirac transition point, we can observe from equation (11) and figures 6(a) and (d) that, for both $\sigma_{xx}$ and $\sigma_{yy}$, the Fermi-energy power law for short-range impurities is always smaller than that of charged impurities. This indicates that, at low densities, charged impurities are dominant over short-range impurities, whereas at high densities, short-range impurities are dominant over charged impurities. In the insulator phase, at low densities, the system can be approximated as a 2DEG and the Fermi-energy power laws for short-range and charged impurities are almost comparable (except in

11
the no-screening limit) as shown in equation (13) and figures 6(b) and (e). At high densities, the power-law dependence follows that of the semi-Dirac transition point; thus, short-range impurities dominate over charged impurities. In the Dirac semimetal phase, at low densities, the Fermi-energy power law for short-range impurities is always smaller than that of charged impurities as shown in equation (15) and figures 6(c) and (f); thus, charged impurities are dominant over short-range impurities as in the case of graphene. At high densities, short-range impurities become dominant over charged impurities, following the trend of the semi-Dirac transition point. Note that, near the van Hove singularities, charged impurities are highly screened due to the enhanced DOS, and thus, short-range impurities are dominant over charged impurities [39].

Our analysis is based on the semiclassical Boltzmann transport theory, which is known to be valid in the high-density limit. At low densities, the effect of potential fluctuations induced by spatially inhomogeneous impurities becomes important, which is not captured by our approach assuming a spatially homogeneous system. At the semi-Dirac transition point or in the Dirac semimetal phase, the potential fluctuation is expected to result in a minimum conductivity [45–47]. In the insulator phase, if the band gap is sufficiently large, the effect of the potential fluctuation might be limited. The interplay of the impurity potential fluctuation, temperature, and band gap would be an interesting future research direction.

Finally, we wish to mention the additional parabolic term $\frac{\hbar^2 k_y^2}{2m^*}\sigma_x$ omitted in equation (1) along the armchair (y) direction beyond the lowest order [48]. This term could affect the dc conductivity, especially at high densities above the crossover Fermi energy $\varepsilon_F^\prime = \frac{2m^*\gamma}{\hbar^2}$, where the effective Hamiltonian in equation (1) is no longer valid. For example, at the semi-Dirac transition point with $\varepsilon_F \gg \varepsilon_F^\prime$, the parabolic term becomes dominant over the linear term along the armchair direction; thus, $\sigma_{xx}$ and $\sigma_{yy}$ will follow those of (anisotropic) 2DEG.

In summary, we calculate the dc conductivity of few-layer BP as a function of the density and temperature using the anisotropic multiband Boltzmann transport theory, which is essential when the effect of anisotropic energy dispersion or interband scattering becomes important. We find that the dc conductivities in the Boltzmann limit show characteristic density and temperature dependence in each phase, which could be used as a signature of the tunable electronic structure of BP in transport measurements.

Acknowledgments

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No. 2018R1A2B6007837) and Creative-Pioneering Researchers Program through Seoul National University (SNU).

Appendix A. Eigenstates and density of states

In this section, we provide a detailed explanation on the model Hamiltonian of few-layer BP, and its various properties including DOS. In the model Hamiltonian given by equation (1) in the main text, the exact values of $m^*$ and $\nu_0$ depend on the number of layers and the gap tuning parameter. We introduce the normalization constants $k_0 \equiv a^{-1}$ and $\varepsilon_0 \equiv \frac{\hbar^2 k_0^2}{2m^*}$; thus, the Hamiltonian becomes

$$H = \varepsilon_0 \begin{pmatrix} 0 & \tilde{k}_x - ic\tilde{k}_y + \Delta \\ \tilde{k}_x + ic\tilde{k}_y + \Delta & 0 \end{pmatrix}, \quad (A.1)$$

where $\tilde{k} = k/k_0$, $c = \hbar\nu_0 k_0/\varepsilon_0$, and $\Delta \equiv \frac{\varepsilon_0}{2k_0}$. To avoid difficulties associated with anisotropic dispersion, we consider the following coordinate transformation with

$$k_x \to \alpha k_0 (r \cos \phi - \Delta)^2, \quad \alpha = \pm 1$$

where $\phi \in [-\phi_{\text{max}}(r), \phi_{\text{max}}(r)]$. This coordinate transformation changes the Hamiltonian into the following form:

$$H = \varepsilon_0 r \begin{pmatrix} 0 & e^{-i\phi} \\ e^{i\phi} & 0 \end{pmatrix}. \quad (A.4)$$

In the transformed coordinates, the energy dispersion is given by $\varepsilon_{\pm}(r) = \pm \varepsilon_0 r$ and the corresponding eigenstates are given by

$$|+\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ e^{i\phi} \end{pmatrix}, \quad (A.5a)$$

$$|-\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -e^{i\phi} \end{pmatrix}. \quad (A.5b)$$

The Jacobian $\mathcal{J}$ corresponding to this transformation is given by

$$\mathcal{J} = \begin{vmatrix} \frac{\partial k_x}{\partial r} & \frac{\partial k_x}{\partial \phi} \\ \frac{\partial k_y}{\partial r} & \frac{\partial k_y}{\partial \phi} \end{vmatrix} = \frac{k_0^2 r}{2c\sqrt{r} \cos \phi - \Delta} \equiv \mathcal{J}(r, \phi). \quad (A.6)$$
Note that, for the $+$ band, the band velocity $v_k^{(i)} = \frac{1}{\hbar} \frac{\partial E_k^{(i)}}{\partial k}$ can be expressed as
\[ v_k^{(i)} = 2\alpha v_0 \cos \phi \sqrt{r \cos \phi - \Delta}, \tag{A.7a} \]
\[ v_k^{(i)} = v_0 \sin \phi, \tag{A.7b} \]
where $v_0 = \frac{\hbar}{\sqrt{2m_0}}$.

The DOS at the semi-Dirac transition point ($\Delta = 0$) at the energy $\varepsilon > 0$ can be obtained analytically as
\[ D(\varepsilon) = g \int \frac{d^2 k}{(2\pi)^2} \delta (\varepsilon - E_+ k) \]
\[ = 2 g \int_0^\infty dr \int_0^{\pi} d\phi \sqrt{r^2 \cos^2 \phi - \Delta^2} (\varepsilon - \varepsilon_0 r) \]
\[ = \frac{2 g k_0^2 \sqrt{2} K(1/2)}{2\pi e_0} \left( \frac{\varepsilon}{\varepsilon_0} \right)^{1/2}, \tag{A.8} \]
where $g$ is the spin degeneracy, and the factor 2 originates from the duplicate parts of the Fermi surfaces parameterized by $\alpha = \pm 1$. Here, $K(k) = \sum_{n=0}^{\infty} [2(n+1)!/(2n)!] k^2n$ is the complete elliptic integral of the first kind with $K(1/2) \approx 1.854$ [44]. Note that the Thomas–Fermi wave vector is determined by the DOS at the Fermi energy $\varepsilon_F$ given by
\[ q_{TF} = \frac{2\pi e^2}{\hbar} D(\varepsilon_F) = \frac{4g \alpha_0 k_0^2 \sqrt{2} K(1/2)}{\pi e} \left( \frac{\varepsilon_F}{\varepsilon_0} \right)^{1/2}, \tag{A.9} \]
where $\alpha_0 = \frac{e^2}{\hbar n_0}$ is the effective fine structure constant. The carrier density is thus given by
\[ n = \int_0^{\varepsilon_F} d\varepsilon D(\varepsilon) = n_0 \frac{4 g \sqrt{2} K(1/2)}{3\pi e} \left( \frac{\varepsilon_F}{\varepsilon_0} \right)^{1/2}, \tag{A.10} \]
where $n_0 = k_0^2$. Note that $\varepsilon_F \sim n^2$ and $D(\varepsilon_F) \sim n^2$.

Figure 2 in the main text shows the calculated DOS and the carrier density for each phase.

**Appendix B. Density dependence of dc conductivity in BP**

In this section, we derive the dc conductivity at zero temperature for 2D multiband systems with anisotropic energy dispersion. To consider the anisotropy of the energy dispersion, we express the multiband anisotropic Boltzmann equation in equation (7) using the transformed coordinates in equation (A.6) as follows:

\[ 1 = \sum_{\alpha} \int_0^{\varepsilon_F} dr' \int_{-\phi_{\text{max}}(r')}^{\phi_{\text{max}}(r')} d\phi' \frac{J(r', \phi'}{(2\pi)^2} W_{\alpha'}^{\alpha}(r') \left( \frac{\varepsilon}{\varepsilon_0} \right) \]
\[ 1 = P_{n-1}^{(j)} \mathcal{D}_{n-1}^{(j)} - \sum_{n'} P_{n-1}^{(j)} \mathcal{D}_{n-1}^{(j)} + P_{n-1}^{(j)} \mathcal{D}_{n-1}^{(j)} - \sum_{n'} P_{n-1}^{(j)} \mathcal{D}_{n-1}^{(j)}, \]  

(B.6b)

where \( P_{n}^{(j)} = \mathcal{D}_{n}^{(j)}(\phi_n) \) is an N-vector and \( P_{n'}^{(j)} = \mathcal{D}_{n'}^{(j)}(\phi_n, \phi_{n'}) \Delta \phi \) is an \( N \times N \) matrix, which correlates the different \( \phi \)-dependent relaxation times for a given \((\alpha, \alpha')\) combination. Note that equation \[(B.6a)\] shares the basic structure with the multiband scattering formula \([38, 39]\) (which accounts for the scattering between each half of the Fermi surface) and the anisotropic scattering formula \([42]\) (which accounts for the scattering between different \( \phi \) and \( \phi' \) points). Furthermore, equation \[(B.6a)\] is a \( 2N \times 2N \) matrix equation with two independent indices \((\alpha, \phi_n)\), i.e. index \( \alpha \) for each half of the Fermi surfaces and the \( \phi \)-discretization index \( \nu \).

Thus, the dc conductivity at zero temperature is given by

\[ \sigma_{ij} = g e^2 \sum_{\alpha} \int \left( \dfrac{d^2 k}{2\pi^2} \right)^2 \delta(\varepsilon_k - \varepsilon_F)(\varepsilon_k)^{n_{\alpha}^{(j)}}(\varepsilon_k)^{n_{\alpha}^{(j)}} \]

\[ = g e^2 \sum_{\alpha} \int_0^{\infty} d\phi \int_0^{\pi} d\phi' \phi \delta(\varepsilon_k - \varepsilon_F)(\varepsilon_k)^{n_{\alpha}^{(j)}}(\varepsilon_k)^{n_{\alpha}^{(j)}} \]

\[ = \sigma_0 \sum_{\alpha} \int_0^{\infty} d\phi \int_0^{\pi} d\phi' \phi \delta(\varepsilon_k - \varepsilon_F)(\varepsilon_k)^{n_{\alpha}^{(j)}}(\varepsilon_k)^{n_{\alpha}^{(j)}} \]

(B.7)

where \( \sigma_0 = g e^2 \rho_v v_0 \tau_0 \), \( \tau_0 = \tau_0^{(i)} / \tau_0 \), and \( \tau_0^{(i)} = \tau_0^{(i)} / \tau_0 \).

Thus, from equation \((A.7a)\), we have

\[ \sigma_{xx} = 2 \sum_{\alpha} \int_0^{\infty} d\phi \int_0^{\infty} d\phi' \phi \cos^2 \phi \sqrt{\bar{T}_F} \cos \phi - \Delta V_{\alpha}^{(x)}(\phi), \]

(B.8a)

\[ \sigma_{yy} = 2 \sum_{\alpha} \int_0^{\infty} d\phi \int_0^{\infty} d\phi' \phi \sin^2 \phi \sqrt{\bar{T}_F} \cos \phi - \Delta V_{\alpha}^{(y)}(\phi). \]

(B.8b)

Note that \( \tau_0, \nu_0, \nu_0 \), and \( \tau_0 \) are the density-independent normalization constants in units of time, velocity, DOS, and conductivity, respectively.

**Appendix C. Low-density approximate models for the insulator phase and Dirac semimetal phase**

In this section, we derive the dc conductivity of low-density approximate models for the insulator phase and Dirac semimetal phase. Note that the only anisotropy considered in these models is the anisotropy in the effective mass or velocity with the same power-law dependence in momentum.

**C.1. Insulator phase at low densities**

For the insulator phase, as well as the Dirac semimetal phase discussed later, the DOS and carrier density do not follow the simple power-law behavior. Therefore, we utilize approximate models to understand the asymptotic behavior of dc conductivity at low densities. When \(|\varepsilon_F| > |\varepsilon_F^0|\) but the carrier density is sufficiently small, the system can be approximated as a two-dimensional electron gas (2DEG). From the series expansion at the minimum point of the conduction band, we have

\[ \varepsilon(k) = \varepsilon_0 \left( \dfrac{k_x}{k_F} \right)^2 + \varepsilon_F^0 \left( \dfrac{k_y}{k_F} \right)^2 \]

\[ = \dfrac{\hbar^2 k_x^2}{2m_x} + \dfrac{\hbar^2 k_y^2}{2m_y}, \]

(C.1)

where \( m_x = \frac{\hbar^2 c^2}{2\varepsilon_F} \) and \( m_y = \frac{\Delta \hbar^2 c^2}{\varepsilon_F} \).

For comparison, we first consider a 2DEG with an isotropic energy dispersion given by

\[ \varepsilon(k) = \dfrac{\hbar^2 k^2}{2m}. \]

(C.2)

As the system is isotropic, we can readily calculate the conductivity of each case using the Einstein relation

\[ \sigma_{\text{iso}} = e^2 D(\varepsilon_F) D, \]

(C.3)

where \( D = \frac{\varepsilon_F}{\tau_F} \) is the diffusion constant and \( D(\varepsilon) = \frac{\varepsilon_F}{\tau_F} \) is the DOS for the isotropic 2DEG. The relaxation time at the Fermi energy \( \tau_F \) is given by

\[ \frac{1}{\tau_F} = \frac{2\pi n_{\text{imp}}}{\hbar} \int \dfrac{d^2 k}{(2\pi)^2} |V_{kk'}|^2 (\varepsilon - \varepsilon_F)(1 - \cos \phi') \]

\[ = \frac{2\pi n_{\text{imp}}}{\hbar} \frac{m}{2\pi \hbar^2} \int_0^{\pi} d\phi' \left( \frac{2\pi}{\hbar^2} \right) |V_{\phi'}|^2 (1 - \cos \phi') \]

\[ = \frac{2\pi n_{\text{imp}}}{\hbar} \frac{m}{2\pi \hbar^2} V_{\text{DEG}}^2, \]

(C.4)

where \( V_{\phi'} \) is the angle-dependent potential on the Fermisurface and \( V_{\text{DEG}}^2 = \frac{1}{2 \pi} \frac{d^2 k}{(2\pi)^2} |V_{\phi'}|^2 (1 - \cos \phi') \) is the angle-averaged square of the impurity potential.

Therefore, the dc conductivity of the isotropic 2DEG is given by

\[ \sigma_{\text{iso}} = e^2 \left( \frac{2m}{\hbar^2} \right) \left( \frac{V_{\phi'}^2}{2\pi} \right) \left( \frac{\hbar}{2\pi n_{\text{imp}} m V_{\text{DEG}}^2} \right) \]

\[ = \frac{g e^2 h}{2\pi n_{\text{imp}} m V_{\text{DEG}}^2}, \]

(C.5)

where \( V_{\text{DEG}} = \frac{\varepsilon_F^0}{\tau_F} \) and \( \varepsilon_F = \frac{\delta \varepsilon_F^0}{\tau_F} \).

Now, let us consider the Fermi energy dependence of the dc conductivity using the Einstein relation in equation \((C.3)\). For short-range impurities, \( V_{\text{DEG}}^2 \) is a constant independent of \( \varepsilon_F \); thus, we have

\[ \sigma \sim \varepsilon_F. \]

(C.6)

Here, we used \( V_{\phi'}^2 \sim k_F^2 \sim \varepsilon_F \). For charged impurities in the strong screening limit, \( V_{\text{DEG}}^2 \sim q_{TF}^2 \sim D^{-2}(\varepsilon_F) \) is also a constant; thus,

\[ \sigma \sim \varepsilon_F. \]

(C.7)

For the anisotropic 2DEG with different effective masses in each direction, we introduce the following coordinate transformation \([k_x, k_y] \rightarrow (k, \phi)\):
\[
\begin{align*}
  k_x & \rightarrow \sqrt{\frac{m_x}{m}} k \cos \phi, \\
  k_y & \rightarrow \sqrt{\frac{m_y}{m}} k \sin \phi, \\
\end{align*}
\]
which gives the Jacobian \( dk_x dk_y = \sqrt{\frac{m_y}{m}} \frac{dk}{dk} dk \). The band velocity \( v^{(i)}_k \) can be expressed as
\[
  v_k^{(i)} = \frac{\hbar k}{\sqrt{m_{m_x}}} \cos \phi, \\
  v_k^{(i)} = \frac{\hbar k}{\sqrt{m_{m_y}}} \sin \phi.
\]

Subsequently, the energy dispersion becomes isotropic in the transformed coordinates; thus, the DOS is given by
\[
D(\varepsilon) = \frac{g \sqrt{m_x m_y}}{2\pi \hbar^2}. \quad (C.8)
\]

The relaxation time of the anisotropic 2DEG for \( k \) at the Fermi energy can be obtained by solving the coupled integral equation (equation (7) in the main text). For short-range impurities or charged impurities in the strong screening limit, the scattering potential \( V_{kk'} = V_0 \) is independent of the angle, thus it can be shown that \( \tau^{(i)}_s = \tau^{(i)}_s \equiv \tau^{(i)}_s \). Then the coupled equation can be simplified as
\[
\begin{align*}
\frac{1}{\tau^{(j)}} &= \frac{2\pi n_{imp} \hbar}{\sqrt{m_x m_y}} \int_{0}^{2\pi} d\phi \int_{0}^{2\pi} d\phi' \frac{1}{\tau^{(i)}_{\text{imp}} \sqrt{m_x m_y}} \phi^{(i)}_k \left( 1 - \frac{v^{(i)}_k}{v^{(i)}_k} \right) \\
&= \frac{2\pi n_{imp} \hbar}{\sqrt{m_x m_y}} \sqrt{V^2_{2\text{DEG}}}, \quad (C.11)
\end{align*}
\]
where \( V^2_{2\text{DEG}} \equiv \int_{0}^{2\pi} d\phi \int_{0}^{2\pi} d\phi' |V_{kk'}|^2 (1 - \frac{v^{(i)}_k}{v^{(i)}_k}) = |V_0|^2 \) is the angle-averaged square of the impurity potential for the anisotropic 2DEG. Note that \( \tau^{(i)}_s \) is independent of the direction \( i \).

Therefore, the conductivity of the anisotropic 2DEG is given by
\[
\begin{align*}
  \sigma_{ij} &= g e^2 \int \frac{d^2 k}{(2\pi)^2} \delta(\varepsilon - \varepsilon(k))\psi^{(i)}(k) \psi^{(j)}(k) \\
&= \frac{g e^2 \sqrt{m_x m_y}}{2\pi \hbar^2} \frac{h}{\tau_F} \int_{0}^{2\pi} d\phi v^{(i)}_k v^{(j)}_k, \quad (C.12)
\end{align*}
\]
where \( \tau_F \) is the relaxation time at the Fermi energy. When the electric field and the current density are along the \( y \)-direction, the conductivity \( \sigma_{xx} \) becomes
\[
\begin{align*}
  \sigma_{xx} &= \frac{g e^2 \sqrt{m_x m_y}}{2\pi \hbar^2} \frac{h}{\tau_F} \int_{0}^{2\pi} d\phi \frac{1}{2\pi} \left[ v^{(i)}_x \right]^2 \\
&= \frac{g e^2 \hbar e \pi}{2\pi n_{imp} \sqrt{m_x m_y} V^2_{2\text{DEG}}} \frac{m}{m_x}. \quad (C.13)
\end{align*}
\]

Similarly, when the electric field and the current density are along the \( y \)-direction, the conductivity \( \sigma_{yy} \) becomes
\[
\begin{align*}
  \sigma_{yy} &= \frac{g e^2 \sqrt{m_x m_y}}{2\pi \hbar^2} \frac{h}{\tau_F} \int_{0}^{2\pi} d\phi \frac{1}{2\pi} \left[ v^{(i)}_y \right]^2 \\
&= \frac{g e^2 \hbar e \pi}{2\pi n_{imp} \sqrt{m_x m_y} V^2_{2\text{DEG}}} \frac{m}{m_y}. \quad (C.14)
\end{align*}
\]

Therefore, the dc conductivities for the anisotropic case are modified as
\[
\begin{align*}
  \sigma_{xx} &= \sigma_{\text{iso}} \frac{m}{m_x}, \quad (C.15a) \\
  \sigma_{yy} &= \sigma_{\text{iso}} \frac{m}{m_y}. \quad (C.15b)
\end{align*}
\]
Thus, for short-range impurities or charged impurities in the strong screening limit, the Fermi energy dependence of the dc conductivities for the anisotropic 2DEG follows that of the isotropic 2DEG given by equations (C.6) and (C.7).

Note that, as the Fermi energy or the carrier density increases, the insulator phase can no longer be approximated by a 2DEG model, and the energy dispersion follows that of the semi-Dirac transition point. Therefore, the power-law dependence eventually follows that of the semi-Dirac transition point.

### C.2. Dirac semimetal phase at low densities

For the Dirac semimetal phase (\( \Delta < 0 \)), the series expansion at one of the band touching points gives
\[
H(k) = \frac{\hbar}{k_0} \left( 2\sqrt{-\Delta} k_x \sigma_x + c_k \sigma_y \right) \\
\equiv \hbar (v_x k_x \sigma_x + v_y k_y \sigma_y), \quad (C.16)
\]
where \( v_x = \frac{2 \sqrt{-\Delta}}{\hbar k_0} \) and \( v_y = \frac{\sqrt{2}}{\hbar k_0} \).

For comparison, we first consider an isotropic 2D Dirac semimetal with the Hamiltonian given by
\[
H(k) = \hbar v (k_x \sigma_x + k_y \sigma_y). \quad (C.17)
\]
The DOS is thus given by
\[
D(\varepsilon) = \frac{g k}{2\pi \hbar v} = \frac{g e}{2\pi \hbar^2 v^2}. \quad (C.18)
\]
The relaxation time at the Fermi energy \( \tau_F \) is given by
\[
\begin{align*}
\frac{1}{\tau_F} &= \frac{2\pi n_{imp} \hbar}{\sqrt{m_x m_y}} \int_{0}^{2\pi} d\phi \left| V_{kk'} \right|^2 |F_{kk'}^x| \delta(\varepsilon - \varepsilon) (1 - \cos \phi') \\
&= \frac{2\pi n_{imp} \hbar k_0}{2\pi \hbar v} \int_{0}^{2\pi} d\phi' \frac{1}{2\pi} |V_{0x}^i|^2 F(\phi')(1 - \cos \phi') \\
&= \frac{2\pi n_{imp} \hbar k_0}{2\pi \hbar v} V_{0x}^2, \quad (C.19)
\end{align*}
\]
where \( F(\phi') = \frac{1}{2} (1 + \cos \phi') \) is the square of the wave function overlap and \( V_{0x}^i \equiv \int_{0}^{2\pi} d\phi' \left| V_{0x}^i \right|^2 F(\phi')(1 - \cos \phi') \) is the angle-averaged square of the impurity potential. Therefore, the dc conductivity of the isotropic Dirac semimetal is given by
Now, let us consider the Fermi energy dependence of the dc conductivity using the Einstein relation in equation (C.3). For short-range impurities, $V_{\text{imp}}^2$ is a constant independent of $\varepsilon_F$; thus, we have

$$\sigma \sim \varepsilon_F^0,$$  \hspace{1cm} (C.21)

whereas for charged impurities in the strong screening limit, $V_{\text{imp}}^2 \sim k_F^2 \sim \varepsilon_F^2$, and in general, $\sigma \sim \varepsilon_F^2$ for charged impurities.

For the anisotropic Dirac semimetals with different velocities in each direction, we introduce the following coordinate transformation $[(k_x, k_y) \rightarrow (k, \phi)]$:

$$k_x \rightarrow \frac{v}{\epsilon} k \cos \phi,$$
$$k_y \rightarrow \frac{v}{\epsilon} k \sin \phi,$$  \hspace{1cm} (C.23)

which gives the Jacobian $dk_xdk_y = \frac{v}{\epsilon} dv_x dv_y$. The band velocity $v_k^{(i)} = 1/\hbar \partial_{\theta_k}$ can be expressed as $v_k^{(x)} = v_x \cos \phi$, $v_k^{(y)} = v_y \sin \phi$.  \hspace{1cm} (C.24)

Subsequently, the energy dispersion becomes isotropic in the transformed coordinates; thus, the DOS is given by

$$D(\varepsilon) = \frac{g v k}{2\pi \hbar v_x v_y} = \frac{g \varepsilon}{2\pi \hbar^2 v_x v_y}.$$  \hspace{1cm} (C.25)

Similarly, using the same assumptions which were used in equation (C.11), for short-range impurities or charged impurities in the strong screening limit, we can calculate the relaxation time of the anisotropic Dirac semimetals given by

$$\begin{align*}
\tau^{(i)} &= \frac{2\pi \hbar v_x v_y}{g v k} \int \frac{d^2 k}{(2\pi)^2} |V_{kk'}|^2 \delta(\varepsilon_k - \varepsilon_{k'}) \left(1 - \frac{v_{k'}^{(i)}}{v_k^{(i)}}\right) \\
&= \frac{2\pi \hbar v_x v_y}{g v k} \int \frac{d^2 k}{(2\pi)^2} \frac{g v k}{2\pi \hbar v_x v_y} V_{\text{imp}}^2,
\end{align*}$$  \hspace{1cm} (C.26)

where $V_{\text{imp}}^2 \equiv \int \frac{d^2 k}{(2\pi)^2} V_0^2 F(\phi') \left(1 - \frac{v_{k'}^{(i)}}{v_k^{(i)}}\right) = \frac{|V_0|^2}{4}$ is the angle-averaged square of the impurity potential for the anisotropic graphene. Note that $v_{k'}^{(i)}$ for the anisotropic Dirac semimetal is also independent of the direction $i$.

Therefore, the conductivity of the anisotropic Dirac semimetal is given by

$$\begin{align*}
\sigma_{ij} &= \frac{g \varepsilon g v k}{(2\pi)^2} \delta(\varepsilon - \varepsilon(\mathbf{k})) v_{k'}^{(i)} v_k^{(j)} \\
&= \frac{g \varepsilon g v k}{2\pi \hbar v_x v_y} \frac{\tau}{2\pi} \int_0^{2\pi} d\phi \left[\frac{v_k^{(i)}}{v_k^{(j)}}\right]^2.
\end{align*}$$  \hspace{1cm} (C.27)

When the electric field and the current density are along the $x$-direction, the conductivity $\sigma_{xx}$ becomes

$$\begin{align*}
\sigma_{xx} &= \frac{g \varepsilon g v k}{2\pi \hbar v_x v_y} \frac{\tau}{2\pi} \int_0^{2\pi} d\phi \\ &\times \left[\frac{v_k^{(x)}}{v_k^{(y)}}\right]^2, \hspace{1cm} \sigma_{yy} = \frac{g \varepsilon g v k}{2\pi \hbar v_x v_y} \frac{\tau}{2\pi} \int_0^{2\pi} d\phi \cos^2 \phi.
\end{align*}$$  \hspace{1cm} (C.28)

Similarly, when the electric field and the current density are along the $y$-direction, the conductivity $\sigma_{yy}$ becomes

$$\begin{align*}
\sigma_{yy} &= \frac{g \varepsilon g v k}{2\pi \hbar v_x v_y} \frac{\tau}{2\pi} \int_0^{2\pi} d\phi \left[\frac{v_k^{(y)}}{v_k^{(x)}}\right]^2, \hspace{1cm} \sigma_{xx} = \frac{g \varepsilon g v k}{2\pi \hbar v_x v_y} \frac{\tau}{2\pi} \int_0^{2\pi} d\phi \frac{v_k^{(x)}}{v_k^{(y)}}.
\end{align*}$$  \hspace{1cm} (C.29)

Thus, for short-range impurities or charged-impurities in the strong screening limit, the Fermi energy dependence of the dc conductivities for the anisotropic graphene follows that of the isotropic graphene given by equations (C.21) and (C.22).

Near the van Hove singularities, where the energy dispersion can be expanded as $\varepsilon(\mathbf{k})/\varepsilon_0 \approx |\Delta| - k_F^2 + \frac{\tilde{E}_0^2}{\Delta}$, the DOS diverges logarithmically $[37]$, dominating the overall power-law behavior of the conductivity. For short-range impurities, the conductivity becomes

$$\sigma_{xx} \sim -\log(|\Delta| - \varepsilon_F)^{-1},$$  \hspace{1cm} (C.31a)
$$\sigma_{yy} \sim -\log(|\Delta| - \varepsilon_F)^{-1}.$$.  \hspace{1cm} (C.31b)

For the charged impurities near the van Hove singularities, the conductivity becomes

$$\sigma_{xx} \sim |\Delta| - \varepsilon_F|^2,$$  \hspace{1cm} (C.32a)
$$\sigma_{yy} \sim |\Delta| - \varepsilon_F|^2.$$  \hspace{1cm} (C.32b)
Note that, as the Fermi energy or the carrier density increases, the power-law dependence of the dc conductivity follows that of the semi-Dirac transition point, as in the gapped insulator case.

Appendix D. Temperature dependence of chemical potential and Thomas–Fermi wave vector in BP

In this section, we derive the temperature-dependent chemical potential and Thomas–Fermi wave vector of few-layer BP. When the temperature is finite, the chemical potential \( \mu \) deviates from the Fermi energy \( \varepsilon_F \) due to the broadening of the Fermi distribution function \( f^{(0)}(\varepsilon, \mu) = \left[ e^{\beta(\varepsilon - \mu)} + 1 \right]^{-1} \) where \( \beta = \frac{1}{k_B T} \). As the charge carrier density \( n \) does not vary under the temperature change, we have

\[
\begin{align*}
n = \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi} D(\varepsilon) f^{(0)}(\varepsilon, \mu) \\
= \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi} D(\varepsilon) \left[ f^{(0)}(\varepsilon, \mu) + f^{(0)}(-\varepsilon, \mu) \right] \\
\equiv \int_{-\varepsilon^F}^{\varepsilon^F} \frac{d\varepsilon}{2\pi} D(\varepsilon),
\end{align*}
\]

Thus, the carrier density measured from the charge neutral point, \( \Delta n \equiv n|_{\mu=0} - n|_{\mu=0} \), is given by

\[
\Delta n = \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi} D(\varepsilon) \left[ f^{(0)}(\varepsilon, \mu) - f^{(0)}(-\varepsilon, \mu) \right] \\
\equiv \int_{-\varepsilon^F}^{\varepsilon^F} \frac{d\varepsilon}{2\pi} D(\varepsilon),
\]

where the first and second lines represent the carrier density evaluated at the finite and zero temperatures, respectively. Here, we used \( f(-\varepsilon, \mu) = 1 - f(\varepsilon, -\mu) \).

By solving this equality in terms of \( \mu \), we can calculate the chemical potential of the system for a given temperature \( T \). See the Supplemental Material in [42] for the simplified cases.

Subsequently, consider the temperature-dependent Thomas–Fermi wave vector \( q_{TF}(T) \). Note that in 3D, \( q_{TF}(0) = \frac{4\pi}{\kappa} \frac{\partial}{\partial \mu} D(\varepsilon_F) \) and at finite \( T \), \( q_{TF}(T) = \frac{4\pi}{\kappa} \frac{\partial}{\partial \mu} D(\varepsilon_F) \). Thus, we have

\[
\begin{align*}
q_{TF}(T) &= \frac{\beta}{2D(\varepsilon_F)} \int_{0}^{\infty} \frac{d\varepsilon}{2\pi} D(\varepsilon) \\
&\times \left[ \frac{1}{1 + \cosh \beta(\varepsilon - \mu)} + \frac{1}{1 + \cosh \beta(\varepsilon + \mu)} \right].
\end{align*}
\]

For a given \( T \), the chemical potential is calculated using the density invariance in equation (D.2), and subsequently, \( q_{TF}(T) \) is obtained from the above relation.

When the DOS is given by a simple power law with respect to energy, we can analytically obtain the temperature dependence of the chemical potential and Thomas–Fermi wave vector, and their asymptotic behaviors at low and high temperatures.

Consider a gapless electron–hole system with a DOS given by \( D(\varepsilon) = C_\alpha |\varepsilon|^{\alpha-1} \Theta(\varepsilon) \), where \( C_\alpha \) is a constant and \( \Theta(\varepsilon) \) is a step function. Using the results from the Supplemental Materials in [42], we can obtain

\[
\mu = \frac{\varepsilon^F}{\varepsilon^F} = \left( 1 - \frac{\pi^2}{12} \left( \frac{T}{T_F} \right)^2 \right)\left( 1 + \frac{1}{\pi \eta} \right)^{-\frac{\alpha-1}{\alpha}} \left( T \ll T_F \right),
\]

\[
\mu = \frac{\varepsilon^F}{\varepsilon^F} = \left( 1 - \frac{\pi^2}{12} \left( \frac{T}{T_F} \right)^2 \right)\left( 1 + \frac{1}{\pi \eta} \right)^{-\frac{\alpha-1}{\alpha}} \left( T \gg T_F \right),
\]

where \( T_F = \frac{\varepsilon^F}{k_B} \) is the Fermi temperature, \( \eta \) is the Dirichlet eta function, and \( \Gamma \) is the gamma function [44]. For the temperature-dependent Thomas–Fermi wave vector \( q_{TF}(T) \), we obtain

\[
\frac{q_{TF}(T)}{q_{TF}(0)} = \left\{ \begin{array}{ll}
1 - \frac{\pi^2}{12} \left( \frac{T}{T_F} \right)^2 & \left( T \ll T_F \right), \\
\frac{1}{2\eta(\alpha-1)\Gamma(\alpha)} \left( \frac{T}{T_F} \right)^{\frac{\alpha-1}{\alpha}} & \left( T \gg T_F \right),
\end{array} \right.
\]

For few-layer BP at the semi-Dirac transition point, the DOS is given by \( D(\varepsilon) \propto \varepsilon^\frac{3}{2} \); thus, \( \alpha = \frac{3}{2} \). Thus, we have

\[
\frac{q_{TF}(T)}{q_{TF}(0)} = \left\{ \begin{array}{ll}
1 - \frac{\pi^2}{12} \left( \frac{T}{T_F} \right)^2 & \left( T \ll T_F \right), \\
\frac{1}{2\eta(\frac{3}{2})\Gamma(\frac{3}{2})} \left( \frac{T}{T_F} \right)^{\frac{1}{2}} & \left( T \gg T_F \right),
\end{array} \right.
\]

where \( q_{TF}(0) = q_{TF}^G \) is given by equation (A.9).

Figures D1, D2, and D3 show the calculated temperature dependence of the chemical potential \( \mu(T) \) and Thomas–Fermi wave vector \( q_{TF}(T) \) in various phases of BP using equations (D.2) and (D.3), respectively.

Appendix E. Temperature dependence of dc conductivity at the semi-Dirac transition point

Using equation (10) in the main text, we can generalize the conductivity tensor at zero temperature to that at finite temperature. For \( f^{(0)}(\varepsilon) = \left[ z^{-1} e^{\beta \varepsilon} + 1 \right]^{-1} \), where \( z = e^\mu \) is the fugacity, \( S^{(0)}(\varepsilon) = -\frac{\partial f^{(0)}(\varepsilon)}{\partial \mu} = \beta f^{(0)}(\varepsilon) \left[ 1 - f^{(0)}(\varepsilon) \right] = \frac{\beta e^{-\beta \varepsilon}}{e^{-\beta \varepsilon} + 1} \).

Thus, the conductivity at finite temperature is given by
Figure D1. Calculated temperature dependence of (a) chemical potential and (b) Thomas–Fermi wave vector for the semi-Dirac transition point ($\Delta = 0$). Here, the black solid lines represent the numerical result, and the red/blue dashed lines represent the high-/low-temperature asymptotic forms in equations (D.6) and (D.7). If the chemical potential and temperature are normalized by $\varepsilon_F$ and $T_F$, respectively, the result is independent of $\varepsilon_F$ at the semi-Dirac transition point.

Figure D2. Calculated temperature dependence of (a)–(c) chemical potential and (d)–(f) Thomas–Fermi wave vector for the gapped insulator phase with $\Delta = 1$ at (a) and (d) $\varepsilon_F = 1.01\varepsilon_0$, (b) and (e) $\varepsilon_F = 1.1\varepsilon_0$, and (c) and (f) $\varepsilon_F = 1.5\varepsilon_0$. 

2D Mater. 6 (2019) 025016
Thus, from equation (A.7a), we have

\[
\sigma_0(T) = ge^2 \sum_{\alpha} \int_0^\infty \frac{d^2 k}{(2\pi)^2} \left( -\frac{\partial f^{(0)}(\varepsilon_k)}{\partial \varepsilon} \right) \nu^{(i)}_{\alpha \sigma^{(i)}}(\varepsilon_k, \varepsilon_{\alpha \sigma^{(i)}}(\varepsilon_k) \right)
\]

\[
= ge^2 \sum_{\alpha} \int_0^\infty dr \int_0^{\pi} d\phi \frac{k^2_1 \beta \varepsilon^{1-\varepsilon^{(i)}_{\alpha \sigma^{(i)}}(\varepsilon_k)}}{2 \varepsilon \sqrt{r \cos \phi - \Delta}} \varepsilon^{(i)}_{\alpha \sigma^{(i)}}(\varepsilon_k) \varepsilon^{(i)}_{\alpha \sigma^{(i)}}(\varepsilon_k)
\]

\[
= \sigma_0 \sum_{\alpha} \int_0^\infty dr \int_0^{\pi} d\phi \frac{r \beta \varepsilon^{1-\varepsilon^{(i)}_{\alpha \sigma^{(i)}}(\varepsilon_k)}}{2 \varepsilon \sqrt{r \cos \phi - \Delta}} \varepsilon^{(i)}_{\alpha \sigma^{(i)}}(\varepsilon_k) \varepsilon^{(i)}_{\alpha \sigma^{(i)}}(\varepsilon_k).
\]

(E.1)

To derive the asymptotic behaviors of \(\sigma_0(T)\) at low and high temperatures, assume that the relaxation time can be decomposed into energy- and temperature-dependent parts as \(\tau^{(i)}(\varepsilon, T) = \tau^{(i)}(\varepsilon) g^{(i)}(\frac{T}{T_F})\)

where \(g^{(i)}(\frac{T}{T_F})\) is the energy-independent correction term from the temperature-dependent screening effect with \(\frac{T}{T_F}g^{(i)}(0) = 1\). For short-range impurities, \(g^{(i)}(\frac{T}{T_F}) = 1\). For charged Coulomb impurities, we expect \(g^{(i)}(\frac{T}{T_F}) = 1\). At low temperatures, whereas at high temperatures, the energy averaging typically dominates over the screening contribution and we can assume \(g^{(i)}(\frac{T}{T_F}) = 1\). Suppose the following power-law dependence: \(D(\varepsilon) \sim \varepsilon^{1-\gamma}, \varepsilon^{(i)}(\varepsilon) \sim \varepsilon^\gamma, \text{and } \frac{\tau^{(i)}(\varepsilon) \sim \varepsilon^\gamma}.\) Subsequently, byrewrit-
ing equation (E.1) as an energy-integral form, we obtain the asymptotic power-law behavior of the temperature-dependent conductivity at low and high temperatures as

$$\frac{\sigma_{xx}(T)}{\sigma_{xx}(0)} = \begin{cases} 1 + \frac{\pi}{\Gamma} (\delta - \alpha)T - A^{(i)} \left( \frac{T}{T_F} \right)^2 & (T \ll T_F), \\ \Gamma \delta \eta(\delta) \left( \frac{T}{T_F} \right)^\delta & (T \gg T_F), \end{cases}$$

(E.3)

where $\delta = \alpha - 1 + 2\nu + \gamma$. (See the supplemental material of [42] for the detailed derivation of the power-law analysis of the temperature-dependent dc conductivity.) For the semi-Dirac transition point ($\Delta = 0$), $\alpha = \frac{1}{2}$.

For short-range impurities, $\delta \left( \frac{T}{T_F} \right) = 1$ and from the energy dependence of the relaxation time, $\gamma = -\frac{1}{2}$. Thus, from equation (E.2a), the asymptotic behavior is given by

$$\frac{\sigma_{xx}(T)}{\sigma_{xx}(0)} = \begin{cases} 1 - \frac{\pi^2}{12} \left( \frac{T}{T_F} \right)^2 & (T \ll T_F), \\ \log^2 \left( \frac{T}{T_F} \right) & (T \gg T_F), \end{cases}$$

(E.4a)

$$\frac{\sigma_{yy}(T)}{\sigma_{yy}(0)} = \begin{cases} 1 - e^{-T_T/T} & (T \ll T_F), \\ \frac{1}{2} + \frac{1}{8n(1)\Gamma(1)} \left( \frac{T}{T_F} \right)^{-\frac{1}{2}} & (T \gg T_F). \end{cases}$$

(E.4b)

Here, the extra terms in $\sigma_{xy}(T)/\sigma_{yy}(0)$ were obtained through the next-order expansion of the temperature corrections.

For charged impurities in the strong screening limit, $A^{(i)} = \frac{\pi^2}{6}$, which is two times the low-temperature coefficient $\frac{\pi^2}{12}$ in equation (D.7), and $\gamma = \frac{1}{2}$. Thus, we obtain

$$\frac{\sigma_{xy}(T)}{\sigma_{xy}(0)} = \begin{cases} 1 - \frac{\pi^2}{12} \left( \frac{T}{T_F} \right)^2 & (T \ll T_F), \\ \log^2 \left( \frac{T}{T_F} \right) & (T \gg T_F), \end{cases}$$

(E.5a)

$$\frac{\sigma_{yy}(T)}{\sigma_{yy}(0)} = \begin{cases} 1 - \frac{\pi^2}{6} \left( \frac{T}{T_F} \right)^2 & (T \ll T_F), \\ \frac{1}{2} + \frac{1}{16n(1)\Gamma(1)} \left( \frac{T}{T_F} \right)^{-\frac{1}{2}} & (T \gg T_F). \end{cases}$$

(E.5b)

As the screening strength decreases, the low-temperature coefficient in equation (E.3) increases, because the screening coefficient $A^{(i)}$ decreases whereas the other part remains positive.

**Appendix F. Temperature dependence of dc conductivity in the low-density approximate models for the insulator phase and Dirac semimetal phase**

In this section, we present the temperature dependence of the chemical potential, Thomas–Fermi wave vector, and conductivity of the low-density approximate models for the insulator phase and Dirac semimetal phase, which are the gapped 2DEG and graphene, respectively.

**F.1. Insulator phase**

We introduce the gapped 2DEG model system with the energy dispersion given by $\varepsilon(k) = \pm \varepsilon_0 [\Delta + (k/k_0)^2]$ with $\Delta > 0$, to account for the thermal excitation behavior involving the band gap between the valence and conduction bands, similar to the insulator phase. Note that the effects of the difference between the effective mass of each direction are canceled out by zero-temperature normalization.

Figure F1 shows the calculated dc conductivities as a function of the temperature for the gapped 2DEG system in the low-density limit with $\varepsilon_F = 1.1\varepsilon_0$ along with the result of the insulator phase with the same Fermi energy (see also figure 8 in the main text). At low temperatures, the calculated results of temperature-dependent conductivity in the insulator phase show a similar behavior as that of the low-density approximate model. However, as the temperature increases, the discrepancy between the two results increases, and in the high-temperature limit, the conductivity becomes similar to that of the semi-Dirac transition point.

**F.2. Dirac semimetal Phase**

For graphene (which is an approximate model for the Dirac semimetal phase in the low-density limit) from equations (D.4) and (D.5) with $\alpha = 2$, the low- and high-temperature asymptotic behaviors for chemical potential are given by

$$\frac{\mu}{\varepsilon_F} = \begin{cases} 1 - \frac{\pi^2}{6} \left( \frac{T}{T_F} \right)^2 & (T \ll T_F), \\ \frac{1}{16} \log^2 \left( \frac{T}{T_F} \right)^{-\frac{1}{2}} & (T \gg T_F), \end{cases}$$

(E.1)

whereas those for the Thomas–Fermi wave vector are given by

$$\frac{q_{TF}(T)}{q_{TF}(0)} = \begin{cases} 1 - \frac{\pi^2}{6} \left( \frac{T}{T_F} \right)^2 & (T \ll T_F), \\ \frac{1}{2} + \frac{1}{16n(1)\Gamma(1)} \left( \frac{T}{T_F} \right)^{-\frac{1}{2}} & (T \gg T_F). \end{cases}$$

(E.2)

As shown in figures D3(a) and (d), the result of the low-density approximate model and the numerically calculated result of the Dirac semimetal phase in the low-density limit are consistent with each other. For short-range impurities, the asymptotic form of the temperature-dependent conductivity becomes (equation (E.4a) with $\gamma = 0$)

$$\frac{\sigma_{xy}(T)}{\sigma_{xy}(0)} = \begin{cases} 1 - e^{-T_T/T} & (T \ll T_F), \\ \frac{1}{2} + \frac{1}{16n(1)\Gamma(1)} \left( \frac{T}{T_F} \right)^{-\frac{1}{2}} & (T \gg T_F). \end{cases}$$

(E.3)

whereas for charged impurities in the strong screening limit, (equation (E.4a) with $\gamma = 2$)
(a) Short range

\( \sigma(T) \) for (a) short-range impurities, (b) charged impurities with \( \alpha_0 = 1000 \), and (c) charged impurities with \( \alpha_0 = 1 \). Here, \( \epsilon_p = 1.1\epsilon_F \) is used for the calculation. The red dashed lines and blue dashed-dotted lines represent the conductivity of the insulator phase (with the same Fermi energy) \( \sigma_{\text{ins}}^{\alpha_0} \) and \( \sigma_{\text{ins}}^{\alpha_0} \), respectively.

\[
\sigma_{\text{ff}}(T)^{-1} = \begin{cases} 
1 - \frac{2\pi}{T} \left( \frac{\epsilon_p}{T} \right)^2 & (T \ll T_F), \\
\frac{\pi^2}{2} \left( \frac{\epsilon_p}{T} \right)^2 & (T \gg T_F).
\end{cases}
\]

**References**

[1] Castro Neto A H, Guinea F, Peres N M R, Novoselov K S and Geim A K 2009 The electronic properties of graphene *Rev. Mod. Phys.* **81** 109–62

[2] Das Sarma S, Adam S, Hwang E H and Rossi E 2011 Electronic transport in two-dimensional graphene *Rev. Mod. Phys.* **83** 407–70

**ORCID iDs**

Sanghyun Park [https://orcid.org/0000-0001-6347-1289](https://orcid.org/0000-0001-6347-1289)

Seungchan Woo [https://orcid.org/0000-0003-1103-6773](https://orcid.org/0000-0003-1103-6773)

Hongki Min [https://orcid.org/0000-0001-5043-2432](https://orcid.org/0000-0001-5043-2432)

[3] Roldán R and Castellanos-Gomez A 2017 A new bandgap rediscovered: From bulk material to monolayers Angew. Chem. Int. Ed. **56** 8052–72

[4] Chaves A, Jiw, Maassen J and Dumitriu I T 2017 Low theoretical overview of black phosphorus 2D Materials: Properties and Devices ed P Auvors (Cambridge: Cambridge University Press) pp 381–412

[5] Roldán R and Castellanos-Gomez A 2017 A new bandgap tuning knob Nat. Photon. **11** 407

[6] Yang J, Xu R, Pei J, Myint Y W, Wang F, Wang Z, Zhang S, Yu Z, and Lu Y 2015 Optical tuning of exciton and trion emissions in monolayer phosphorene *Light Sci. Appl.* **4** e312

[7] Akr D, Sevik C and Peeters F M 2015 Significant effect of stacking on the electronic and optical properties of few-layer black phosphorus *Phys. Rev. B* **92** 165406

[8] Quereda J, San-Jose P, Parente V, Vaquero–Garzon L, Molina-Mendoza A J, Agrait N, Rubio–Bollinger G, Guinea F, Roldán R and Castellanos–Gomez A 2016 Strong modulation of optical properties in black phosphorus through strain-engineered rippling *Nano Lett.* **16** 2931–7

[9] Xiang Z J et al 2015 Pressure-induced electronic transition in black phosphorus *Phys. Rev. Lett.* **115** 186403

[10] Deng B et al 2017 Efficient electrical control of thin-film black phosphorus bandgap *Nat. Commun.* **8** 14474

[11] Liu Y, Qiu Z, Carvalho A, Bao Y, Xu H, Tan S J R, Liu W, Castro Neto A H, Loh K P and Lu J 2017 Gate-tunable giant Stark effect in few-layer black phosphorus *Nano Lett.* **17** 1970–7

[12] Li L L, Paroens B and Peeters F M 2018 Tuning the electronic properties of gated multilayer phosphorene: a self-consistent tight-binding study *Phys. Rev. B* **97** 155424

[13] Kim J, Baik S S, Ryu S H, Sohn Y, Park S, Park B-G, Denlinger J, Yi Y, Choi H J and Kim K S 2015 Observation of tunable band gap and anisotropic Dirac semimetal state in black phosphorus *Science* **349** 723–6

[14] Banerjee S, Singh R R P, Pardo V and Pickett W E 2009 Tight-binding modeling and low-energy behavior of the semi-dirac point *Phys. Rev. Lett.* **103** 016402

[15] Pardo V and Pickett W E 2009 Half-metallic semi-Dirac-point generated by quantum confinement in TiO2/VO2 Nanostructures *Phys. Rev. Lett.* **102** 166803

[16] Pardo V and Pickett W E 2010 Metal-insulator transition through a semi-Dirac point in oxide nanostructures: VO2 (0 0 1) layers confined within TiO2 *Phys. Rev. B* **81** 035315

[17] Kim J, Baik S S, Jung S W, Sohn Y, Ryu S H, Choi H J, Yang B-J and Kim K S 2017 Two-dimensional dirac fermions protected by space–time inversion symmetry in black phosphorus *Phys. Rev. Lett.* **119** 226801

[18] Ehlen N, Samna A, Senkovskiy B V, Petacca L, Fedorov A V, Profeta G and Grüneis A 2018 Direct observation of a surface resonance state and surface band inversion control in black phosphorus *Phys. Rev. Lett.* **119** 226801

[19] Di Pietro P et al 2018 Emergent dirac carriers across a pressure-induced lifshitz transition in black phosphorus *Phys. Rev. B* **98** 165111

[20] Xia F, Wang H and Jia Y 2014 Rediscovering black phosphorus as an anisotropic layered material for optoelectronics and electronics *Nat. Commun.* **5** 4458

[21] Mishchenko A, Cao Y, Yu G L, Woods C R, Gorbachev R V, Novoselov K S, Geim A K and Levitov L S 2015 Nonlocal response and anamorphosis: the case of few-layer black phosphorus *Nano Lett.* **15** 6991–5

[22] Li T, Zhang Z, Li X, Huang M, Li S, Li S and Wu Y 2017 High field transport of high performance black phosphorus *Nano Lett.* **11** 163507
Illarionov Y Y, Wadh M, Zepa G, Kim J-S, Kim S, Dodabalapur A, Akimawde D and Grasser T 2016 Long-term stability and reliability of black phosphorus field-effect transistors ACS Nano 10 9543–9

Qiao J, Kong X, Hu Z-X, Yang F and Ji W 2014 High-mobility transport anisotropy and linear dichroism in few-layer black phosphorus Nat. Commun. 5 4475

Liu Y, Low T and Ruden P P 2016 Mobility anisotropy in monolayer black phosphorus due to scattering by charged impurities Phys. Rev. B 93 165402

Liu Y and Ruden P P 2017 Temperature-dependent anisotropic charge-carrier mobility limited by ionized impurity scattering in thin-layer black phosphorus Phys. Rev. B 95 165446

Han F W, Xu W, Li L L, Zhang C, Dong H M and Peeters F M 2017 Electronic and transport properties of n-type monolayer black phosphorus at low temperatures Phys. Rev. B 95 115436

Zare M, Rameshti B Z, Ghamsari F G and Asgari R 2017 Thermoelectric transport in monolayer phosphorene Phys. Rev. B 95 045422

Adroguer P, Carpentier D, Montambaux G and Orignac E 2016 Diffusion of dirac fermions across a topological merging transition in two dimensions Phys. Rev. B 93 125313

Rudenko A N and Katsnelson M I 2014 Quasiparticle band structure and tight-binding model for single- and bilayer black phosphorus Phys. Rev. B 89 201408

de Sousa D J P, de Castro L V, da Costa D R, Pereira J M and Low T 2017 Multilayered black phosphorus: from a tight-binding to a continuum description Phys. Rev. B 96 155427

Baik S S, Kim K S, Yi Y and Choi H J 2015 Emergence of two-dimensional massless dirac fermions, chiral pseudospins, and berrys phase in potassium doped few-layer black phosphorus Nano Lett. 15 7788–93

Doh H and Choi H J 2017 Dirac-semimetal phase diagram of two-dimensional black phosphorus 2D Mater. 4 025071

Montambaux G, Piéchon F, Fuchs J-N and Goerbig M O 2009 Merging of dirac points in a two-dimensional crystal Phys. Rev. B 80 153412

Montambaux G, Piéchon F, Fuchs J-N and Goerbig M O 2009 A universal hamiltonian for motion and merging of dirac points in a two-dimensional crystal Eur. Phys. J. B 72 509

de Gail R, Fuchs J-N, Goerbig M, Pichon F and Montambaux G 2012 Manipulation of dirac points in graphene-like crystals Physica B 407 1948 (1992 Proc. of the Int. Workshop on Electronic Crystals (ECRS-2011))

Marder M P 2010 Condensed Matter Physics 2nd edn (New York: Wiley)

Siggia E D and Kwock P C 1970 Properties of electrons in semiconductor inversion layers with many occupied electric subbands. I. Screening and impurity scattering Phys. Rev. B 2 1024–36

Woo S, Hwang E H and Min H 2017 Large negative differential transconductance in multilayer graphene: the role of intersubband scattering 2D Mater. 4 025090

Schliemann J and Loss D 2003 Anisotropic transport in a two-dimensional electron gas in the presence of spin–orbit coupling Phys. Rev. B 68 165311

Výborný K, Kovalev A A, Sinova J and Jungwirth T 2009 Semiclassical framework for the calculation of transport anisotropies Phys. Rev. B 79 045427

Park S, Woo S, Mele E J and Min H 2017 Semiclassical Boltzmann transport theory for multi-Weyl semimetals Phys. Rev. B 95 161113

Ashcroft N W and Mermin N D 1976 Solid State Physics (New York: Brooks/Cole)

Arfken G B, Weber H J and Harris F E 2012 Mathematical Methods for Physicists 7th edn (New York: Academic)

Adam S, Hwang E H, Galitski V M and Das Sarma S 2007 A self-consistent theory for graphene transport Proc. Natl Acad. Sci. 104 18392–7

Li Q, Hwang E H and Das Sarma S 2011 Disorder-induced temperature-dependent transport in graphene: puddles, impurities, activation, and diffusion Phys. Rev. B 84 115442

Ramakrishnan N, Milliarti M and Adam S 2015 Transport and magnetotransport in three-dimensional weyl semimetals Phys. Rev. B 92 245120

Jang J, Ahn S and Min H 2018 Optical conductivity of black phosphorus with a tunable electronic structure (arXiv:1811.07529)