Bilayer Graphene with Long-Range Scatterers
Studied in a Self-Consistent Born Approximation

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The density of states and conductivity are calculated for scatterers with nonzero range in bilayer graphene within a self-consistent Born approximation. For scatterers with a Gaussian potential, the minimum conductivity at zero energy remains universal in the clean limit, but increases with disorder and becomes nonuniversal for long-range scatterers. For charged impurities, we use the Thomas-Fermi approximation for the screening effect. The minimum conductivity increases with impurity concentration but the dependence is not so considerable. When the excited conduction band starts to be populated by electrons, the conductivity increases due to the increase in the screening effect.

Keywords: charged scatterers, impurity scattering, bilayer graphene, graphene, graphite, level broadening, Dirac electron

§1. Introduction

Recently, atomically thin graphenes consisting of a few layers of a monolayer graphite sheet were experimentally fabricated using mechanical exfoliation and epitaxial growth. Several reviews have already been published. Transport properties of graphenes were often studied in a self-consistent Born approximation assuming model short-range scatterers because of simplicity. Quite recently, calculations were extended to the case of long-range scatterers in monolayer graphene. The purpose of this paper is to study density of states and conductivity of bilayer graphene in the presence of scatterers with nonzero range.

In graphenes, their electronic structure strongly varies with the change in the number of layers. The band structure of monolayer graphene is characterized by Dirac-like spectrum in which conduction and valence bands with linear dispersion stick at the K and K' points located at a Brillouin-zone corner. Bilayer graphene has a zero-gap structure, but with quadratic dispersion unlike monolayer, leading to nonzero density of states even at zero energy.

Various theoretical studies were reported on transport properties of bilayer graphene including those within a self-consistent Born approximation. In particular, the conductivity was shown to take at zero energy a universal value twice as large as that in monolayer graphene. In this paper, we extend self-consistent Born approximation to the case of scatterers with nonzero range and calculate the density of states and the conductivity in this system. We first consider scatterers with a Gaussian potential to see explicit dependence on the potential range. In the case of charged impurities, we use the Thomas-Fermi approximation for screening.

The paper is organized as follows: In §2, a brief review is given on the electronic states and the Boltzmann conductivity. The method of calculations of Green's function and static conductivity for long-range scatterers in the self-consistent Born approximation is discussed. In §3 some examples of numerical results are presented for scatterers with a Gaussian potential and for charged impurities. Short summary is given in §4.

§2. Formulation

2.1 Effective-mass description

We consider a bilayer graphene which is arranged in the AB (Bernal) stacking as illustrated in Fig. 1. The upper layer is denoted as 1 and the lower layer denoted as 2. In each layer, a unit cell contains two carbon atoms denoted by A1 and B1 in layer 1 and A2 and B2 in layer 2. For the inter-layer interaction, we include only the coupling between vertically neighboring atoms. Then, electronic states are described by the k p equation:

$$\mathcal{H}_0(\hat{k}) F(r) = \varepsilon F(r),$$

with

$$\mathcal{H}_0(\hat{k}) = \begin{pmatrix} A_1 & B_1 & A_2 & B_2 \\ 0 & \gamma \hat{k}_- & 0 & 0 \\ 0 & 0 & \Delta & 0 \\ 0 & \Delta & 0 & \gamma \hat{k}_- \end{pmatrix},$$

and

$$\hat{k}_\pm = \hat{k}_x \pm i \hat{k}_y,$$

where γ is a band parameter, \(\hat{k} = (\hat{k}_x, \hat{k}_y) = -i \nabla\) is a wave-vector operator, and Δ represents the inter-layer coupling between sites B1 and A2.

The parameters γ and Δ are related to tight-binding parameters γ0 and γ1 through γ = (√3/2)\(a\)γ0 and Δ = γ1, where a is the lattice constant given by a = 2.46 Å, \(\gamma_0 \approx 3.16\) eV, and \(\gamma_1 \approx 0.39\) eV. Couplings between vertically neighboring atoms are known to cause trigonal warping and four band touching points at zero energy in the energy scale of a few meV. Such a structure can easily be washed out in actual bilayer graphenes with disorder and will be neglected in the following.

The states are specified by the set of quantum numbers (s, j) and \(\hat{k}\), with \(\hat{k}\) the wave vector, s = ±1 and −1 for the conduction and valence bands, respectively,

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and integer \( j = 1 \) and \( 2 \) specifying two bands within the conduction or valence bands. The wave function is written as
\[
F_{sjk}(r) = \frac{1}{L} \exp(i\mathbf{k}\cdot\mathbf{r}) U[\theta(\mathbf{k})] F_{sjk},
\]  
(2.4)
where \( L^2 \) is the area of the system, \( k = |\mathbf{k}|, k_x = k \cos \theta(\mathbf{k}), k_y = k \sin \theta(\mathbf{k}), \) and
\[
U(\theta) = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & e^{i\phi} & 0 & 0 \\
0 & 0 & e^{i\theta} & 0 \\
0 & 0 & 0 & e^{2i\theta}
\end{pmatrix}.
\]  
(2.5)
Then, \( F_{sjk} \) satisfies
\[
H_0(k) F_{sjk} = \varepsilon_{sj}(k) F_{sjk},
\]  
(2.6)
with
\[
H_0(k) = \begin{pmatrix}
g(k) & 0 & 0 \\
0 & 0 & \Delta \\
0 & \Delta & 0
\end{pmatrix}.
\]  
(2.7)
Let us define
\[
\varepsilon(k) = \sqrt{(\Delta/2)^2 + (\gamma k)^2},
\]
\[
\gamma k = \varepsilon(k) \sin \psi,
\]
\[
\Delta k = \varepsilon(k) \cos \psi,
\]  
where \( \psi = 0 \) for \( k = 0 \) and \( \psi = \pi/2 \) for \( k \to \infty \). Then, the eigen energies are given by
\[
\varepsilon_{s1}(k) = 2s \varepsilon(k) \sin^2(\psi/2)
\]
\[
= s \left[ \sqrt{\gamma k)^2 + \left(\Delta/2\right)^2} - \frac{\Delta}{2} \right],
\]
\[
\varepsilon_{s2}(k) = 2s \varepsilon(k) \cos^2(\psi/2)
\]
\[
= s \left[ \sqrt{\gamma k)^2 + \left(\Delta/2\right)^2} + \frac{\Delta}{2} \right],
\]  
(2.9)
and the corresponding eigenvectors are given by
\[
F_{s1k} = \frac{1}{\sqrt{2}} \begin{pmatrix}
s \cos(\psi/2) \\
s \sin(\psi/2) \\
- s \sin(\psi/2) \\
- s \cos(\psi/2)
\end{pmatrix},
\]  
(2.10)
\[
F_{s2k} = \frac{1}{\sqrt{2}} \begin{pmatrix}
s \sin(\psi/2) \\
s \cos(\psi/2) \\
- s \cos(\psi/2) \\
- s \sin(\psi/2)
\end{pmatrix}.
\]  
(2.11)
Figure 2 shows these energy bands.

The density of states for \( \varepsilon > 0 \) is given by
\[
D(\varepsilon) = \frac{g_s g_v}{2\pi \gamma^2} \left[ \frac{\Delta}{2} + \varepsilon + \theta(\varepsilon - \Delta) \left( \varepsilon - \frac{\Delta}{2} \right) \right],
\]  
(2.12)
where the spin and valley degeneracies are given by \( g_s = 2 \) and \( g_v = 2 \), respectively, and \( \theta(t) \) is the step function defined by
\[
\theta(t) = \begin{cases} 
1 & (t > 0); \\
0 & (t < 0). 
\end{cases}
\]  
(2.13)
The density of states is obviously symmetric around \( \varepsilon = 0 \).

### 2.2 Self-consistent Born approximation

Let us consider Green’s function defined by
\[
\hat{G}(k, \varepsilon) = \left( \frac{1}{\varepsilon - \hat{H}} \right) = [\varepsilon - H_0(k) - \hat{\Sigma}(k, \varepsilon)]^{-1},
\]  
(2.14)
with
\[
\hat{H} = H_0 + \sum_i v(r - r_i),
\]  
(2.15)
where \( \langle \cdots \rangle \) denotes average over impurity configurations, \( \hat{\Sigma}(k, \varepsilon) \) is the self-energy matrix, and \( v(r) \) is the potential of scatterers. We consider scatterers with isotropic potential
\[
v(r) = \int \frac{dq}{(2\pi)^2} v(q) e^{iqr},
\]  
(2.16)
where \( v(q) = v(q) \) with \( q = |q| \).

In the present isotropic system, the Green’s function is written as
\[
\hat{G}(k, \varepsilon) = U[\theta(\mathbf{k})] \hat{G}(k, \varepsilon) U[\theta(\mathbf{k})]^{-1},
\]  
(2.17)
with
\[
\hat{G}(k, \varepsilon) = [\varepsilon - H_0(k) - \hat{\Sigma}(k, \varepsilon)]^{-1},
\]  
(2.18)
which depends only on \( k \). This shows that the angular variation is expressed in terms of \( U[\theta(\mathbf{k})] \).

Within the self-consistent Born approximation, we have
\[
\hat{\Sigma}(k, \varepsilon) = \int \frac{dk'}{(2\pi)^2} n_i v(k-k') \hat{G}(k', \varepsilon) v(k'-k),
\]  
(2.19)
as diagrammatically shown in Fig. 3 (a). We have
\[
\hat{\Sigma}(k, \varepsilon) = U[\theta(\mathbf{k})] \int \frac{dk'}{(2\pi)^2} n_i v(k-k') U[\theta(k') - \theta(\mathbf{k})] \times \hat{G}(k', \varepsilon) U[\theta(k') - \theta(\mathbf{k})]^{-1} v(k'-k) U[\theta(\mathbf{k})]^{-1}.\]

For any function \( g(k) \), we have
\[
\int \frac{dk'}{(2\pi)^2} v(k-k') e^{i\theta(\varepsilon - \theta(k'))} g(k') v(k'-k) = \int_0^{2\pi} dk' \frac{1}{2\pi} V_n(k,k') g(k'),
\]  
(2.20)
with
\[
V_n(k,k') = \int_0^{2\pi} \frac{d\theta}{2\pi} [v(k-k')]^2 \cos n \theta,
\]  
(2.21)
where \( \theta \) is the angle between \( k \) and \( k' \). Then, we have
\[
\hat{\Sigma}(k, \varepsilon) = U[\theta(\mathbf{k})] \hat{\Sigma}(k, \varepsilon) U[\theta(\mathbf{k})]^{-1},
\]  
(2.22)
with
\[
\hat{\Sigma}(k, \varepsilon) = n_i \int_0^{2\pi} \frac{dk'}{2\pi} \left( \begin{array}{c}
V_{11}^2 G_{11} & V_{12}^0 G_{12} & V_{13}^0 G_{13} & V_{14}^0 G_{14} \\
V_{21}^0 G_{21} & V_{22}^0 G_{22} & V_{23}^0 G_{23} & V_{24}^0 G_{24} \\
V_{31}^0 G_{31} & V_{32}^0 G_{32} & V_{33}^0 G_{33} & V_{34}^0 G_{34} \\
V_{41}^0 G_{41} & V_{42}^0 G_{42} & V_{43}^0 G_{43} & V_{44}^0 G_{44}
\end{array} \right),
\]  
(2.23)
where \( V_n^2 \equiv V_n^0 (k,k') \) and \( G_{11} \equiv G_{11}(k',k), \) etc., for
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simplicity. The self-consistency equation becomes
\[
\hat{G}(k, \varepsilon) = [\varepsilon - \mathcal{H}_0(k) - \hat{\Sigma}(k, \varepsilon)]^{-1}.
\] (2.25)
The conductivity is written as
\[
\sigma = \int \frac{dk}{2\pi} \frac{\partial f}{\partial \varepsilon}(\varepsilon)\sigma(\varepsilon),
\] (2.26)
with
\[
\sigma(\varepsilon) = \frac{g_0g_ve^{2\varepsilon^2}}{4\pi\hbar} \sum_{s',s=\pm1} \int \frac{dk}{2\pi} \text{Tr} \hat{v}_x \hat{G}(k, \varepsilon + i\delta 0)
\times \hat{J}(k, \varepsilon + i\delta 0) \hat{G}(k, \varepsilon + i\delta 0),
\] (2.27)
where
\[
\hat{v}_x = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix},
\] (2.28)
and current vertex part \( \hat{J} \) satisfies the Bethe-Salpeter type equation:
\[
\hat{J}(k, \varepsilon, \varepsilon') = \hat{\nu}_x + \int \frac{dk'}{(2\pi)^2} n_{1v}(k-k') \hat{G}(k', \varepsilon) \hat{J}(k', \varepsilon, \varepsilon')
\times \hat{G}(k', \varepsilon') v(k' - k),
\] (2.29)
as illustrated in Fig. 3 (b).

In order to proceed further, we separate the velocity operator as follows:
\[
\hat{v}_x = \hat{v}_+ + \hat{v}_-,
\] (2.30)
with
\[
\hat{v}_+ = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},
\] (2.31)
\[
\hat{v}_- = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}.
\] (2.32)

We have
\[
\hat{v}_x = e^{i\theta(k)} U[\theta(k)] \hat{v}_x U[\theta(k)]^{-1}
+ e^{-i\theta(k)} U[\theta(k)] \hat{v}_- U[\theta(k)]^{-1},
\] (2.33)
and consequently define
\[
\hat{J}(k, \varepsilon, \varepsilon') = e^{i\theta(k)} U[\theta(k)] \hat{J}_+(k, \varepsilon, \varepsilon') U[\theta(k)]^{-1}
+ e^{-i\theta(k)} U[\theta(k)] \hat{J}_-(k, \varepsilon, \varepsilon') U[\theta(k)]^{-1}.
\] (2.34)

Then, the Bethe-Salpeter-type equation becomes
\[
\hat{J}(k, \varepsilon, \varepsilon') = \hat{v}_x
+ e^{i\theta(k)} U[\theta(k)] \int \frac{dk'}{(2\pi)^2} n_{1v}(k-k') U[\theta(k')-\theta(k)]
\times e^{i\theta(k')-\theta(k)} \hat{G}(k', \varepsilon') \hat{J}_+(k', \varepsilon, \varepsilon') \hat{G}(k', \varepsilon')
\times U[\theta(k')-\theta(k)]^{-1} v(k'-k) U[\theta(k)]^{-1}
+ e^{-i\theta(k)} U[\theta(k)] \int \frac{dk'}{(2\pi)^2} n_{1v}(k-k') U[\theta(k')-\theta(k)]
\times e^{-i\theta(k')-\theta(k)} \hat{G}(k', \varepsilon') \hat{J}_-(k', \varepsilon, \varepsilon') \hat{G}(k', \varepsilon')
\times U[\theta(k')-\theta(k)]^{-1} v(k'-k) U[\theta(k)]^{-1}.
\] (2.35)
Therefore, we have two Bethe-Salpeter equations:
\[
\hat{J}_+(k, \varepsilon, \varepsilon') = \hat{v}_x + n_1 \int_0^\infty \frac{dk'}{2\pi} \text{Tr} \hat{v}_x \hat{G}(k, \varepsilon + i\delta 0)
\times \hat{J}_+(k, \varepsilon + i\delta 0) \hat{G}(k, \varepsilon + i\delta 0),
\] (2.36)
\[
\hat{J}_-(k, \varepsilon, \varepsilon') = \hat{v}_x + n_1 \int_0^\infty \frac{dk'}{2\pi} \text{Re Tr} \hat{v}_x \hat{G}(k, \varepsilon + i\delta 0)
\times \hat{J}_-(k, \varepsilon + i\delta 0) \hat{G}(k, \varepsilon + i\delta 0),
\] (2.37)
with \( \hat{\Sigma}_{\pm} \equiv \hat{G} \hat{J}_\pm \hat{G}' \), where \( \hat{G} \equiv \hat{G}(k', \varepsilon) \), \( \hat{G}' \equiv \hat{G}(k', \varepsilon') \), \( J_\pm \equiv J_\pm (k', \varepsilon, \varepsilon') \), and \( \Xi_{11} \) means the (1,1) element of matrix \( \hat{\Sigma} \), etc., for simplicity. The conductivity becomes
\[
\sigma(\varepsilon) = \frac{g_0g_ve^{2\varepsilon^2}}{4\pi\hbar} \int_0^\infty \frac{dk}{2\pi} \text{Re Tr}
\times [\hat{v}_x \hat{G}(k, \varepsilon + i\delta 0) \hat{J}_-(k, \varepsilon + i\delta 0) \hat{G}(k, \varepsilon - i\delta 0)]
+ \hat{v}_+ \hat{G}(k, \varepsilon + i\delta 0) \hat{J}_+(k, \varepsilon + i\delta 0) \hat{G}(k, \varepsilon - i\delta 0)
- \hat{v}_- \hat{G}(k, \varepsilon + i\delta 0) \hat{J}_-(k, \varepsilon + i\delta 0) \hat{G}(k, \varepsilon + i\delta 0)
+ \hat{v}_- \hat{G}(k, \varepsilon + i\delta 0) \hat{J}_+(k, \varepsilon + i\delta 0) \hat{G}(k, \varepsilon + i\delta 0)].
\] (2.38)

Because of the symmetry between layers 1 and 2 and because \( V_{-n}(k, k')^2 = V_n(k, k')^2 \), Green’s function \( \hat{G}(k, \varepsilon) \) and self-energy \( \Sigma(k, \varepsilon) \) are symmetric under replacements 1 ↔ 4 and 2 ↔ 3, i.e., \( \Sigma_{11} = \Sigma_{44}, \Sigma_{12} = \Sigma_{43}, \) etc. For current vertex part \( \hat{J}(k, \varepsilon, \varepsilon') \), the other hand, \( \hat{J}^+(k, \varepsilon, \varepsilon') \) and \( \hat{J}^-(k, \varepsilon, \varepsilon') \) should be exchanged under these replacements, corresponding to \( \hat{v}_+ \) and \( \hat{v}_- \), i.e., \( \hat{J}_{14} = \hat{J}_{44}, \hat{J}_{13} = \hat{J}_{43} \), etc. This symmetry is not present when an external electric field is applied perpendicular to the layer and bilayer graphene becomes asymmetric.

### 2.3 Boltzmann conductivity

Let us define \( g_{sjk} \) as deviation of the distribution function of states \( (s, j, k) \) to the lowest order in applied electric field \( E \). Then, the Boltzmann equation is given by
\[
(-e)E \cdot \mathbf{v}_{sjk} \left( -\frac{\partial f}{\partial \varepsilon_{sjk}} \right) = \sum_{s',j'} \int \frac{dk'}{(2\pi)^2} \frac{2\pi}{\hbar} \langle |V_{s'j'k'k}^a|^2 \rangle
\times \delta(\varepsilon_{sjk} - \varepsilon_{s'j'k'})(g_{sjk} - g_{s'j'k'}),
\] (2.39)
with
\[
\langle |V_{s'j'k'k}^a|^2 \rangle = n_1 |v(k' - k)|^2 |F_{s'j'k}^a|^2 |U(k'k)|^2,
\] (2.40)
where \( \theta_{kk'} \) is the angle between \( k' \) and \( k \). We shall assume
\[
g_{sjk} = (-e)\tau_{sj}(\varepsilon) \mathbf{v}_{sjk} \cdot E \left( -\frac{\partial f}{\partial \varepsilon_{sjk}} \right),
\] (2.41)
with \( \tau_{sjk} \) being relaxation time to be determined and \( \mathbf{v}_{sjk} \) is the group velocity of state \( (s, j, k) \), i.e., \( \mathbf{v}_{sjk} = \ldots \)
We define a dimensionless parameter characterizing the cutoff-energy is of the order of the half of the area. This parameter is the same as that defined with the partial density of states for band $\epsilon_{sj}(k)$,

\[
D_{sj}(\epsilon) = \int \frac{dk}{(2\pi)^2} \delta(\epsilon - \epsilon_{sj}(k)).
\]

Explicitly, we have

\[
D_{s+1}(\epsilon) = \frac{1}{2\pi\gamma}(\epsilon + \frac{\Delta}{2})_{+},
\]

\[
D_{s+2}(\epsilon) = \frac{1}{2\pi\gamma}(\epsilon - \frac{\Delta}{2})_{+}\theta(\epsilon - \Delta).
\]

§3. Numerical Results and Discussion

3.1 Scatterers with Gaussian potential

In order to see the explicit dependence on the potential range, we first assume scatterers with a Gaussian potential

\[
v(r) = \frac{v_0}{\pi d^2} \exp\left(-\frac{r^2}{d^2}\right),
\]

with range $d$. This gives Fourier transform

\[
v(q) = v_0 \exp\left(-\frac{q^2d^2}{4}\right).
\]

We define a dimensionless parameter characterizing the scattering strength

\[
W = \frac{n_i v_0^2}{4\pi\gamma},
\]

where $n_i$ is the concentration of scatterers per unit area. This parameter is the same as that defined previously\cite{13,15,16} for short-range scatterers with $d \to 0$ ($W = A^{-1}$ in refs. 9–11)

We introduce cutoff energy $\epsilon_c$ and wave vector $k_c$ through

\[
\epsilon_c = \gamma k_c.
\]

The cutoff-energy is of the order of the half of the $\pi$-band width, i.e., $\epsilon_c \approx 3\gamma_0$, for which $k_c \approx \pi/a$. For numerical calculations, we discretize wave vector such that

\[
k_j = \frac{1}{2}\Delta k_0 + \sum_{j'=1}^{j} \Delta k_{j'} \quad (j = 1, \ldots, j_{\text{max}}),
\]

with

\[
\sum_{j=1}^{j_{\text{max}}} \Delta k_{j} = k_c.
\]

For explicit numerical calculations in the following, we use $j_{\text{max}} = 1000$ and

\[
\Delta k_j \propto (j + \alpha)^{\beta},
\]

with $\alpha \approx 0$ and $\beta \approx 1$. Further, we choose $\Delta/\epsilon_c = 0.1$ and introduce wave vector $k_0$ characterizing the energy difference between the lowest and excited conduction band such that

\[
\gamma k_0 = \Delta.
\]

The self-consistency equation for the self-energy and the Bethe-Salpeter-type equation for the current vertex are numerically solved by simple iterations, although actual computational time sometimes becomes very long, in particular, for large disorder.

Figure 4 shows calculated (a) density of states and (b) conductivity as a function of energy for $W = 0.1$. In Fig. 4(a) the dotted line represents the density of states in ideal bilayer graphene and the dashed line represents twice of that in monolayer graphene and in (b) the dotted lines represent the Boltzmann conductivity. Only the region of positive energy is shown because both density of states and conductivity are symmetric with respect to zero energy.

The density of states clearly shows that the energy region affected strongly by the presence of scatterers is limited to $|\epsilon| \lesssim \gamma/d$ for small $d$ such that $dk_0 \leq 0.2$. When the range becomes larger such that $dk_0 \geq 2$, the region affected by scatterers is separated into two, those close to zero energy and close to the bottom of the excited conduction band $\Delta$. In fact, the excited conduction band has significant band tail due to disorder.

At zero energy, the Boltzmann conductivity vanishes due to the vanishing velocity. In the self-consistent Born approximation the conductivity becomes close to the universal value obtained previously for short-range scatterers\cite{12}

\[
\sigma_0 = \frac{g_nv_0^2}{\pi^2\hbar},
\]

which is twice as large as that in monolayer graphene,\cite{9} the universality of which remains as a hot topics.\cite{34–41}

It increases rapidly with energy, becoming larger than the Boltzmann conductivity at sufficiently high energy for long-range scatterers $dk_0 > 0.5$.

The conductivity exhibits a kink-like structure when the energy crosses the bottom of the excited conduction band. This behavior also seen in the Boltzmann conductivity arises due to sudden appearance of interband scattering, which is more dominant than the appearance
of extra conductivity due to additional carriers in the excited conduction band. Apart from the difference in the kink position, the overall behavior of the conductivity is very close to that of the Boltzmann result. Interband matrix elements between the state $k=0$ at the bottom of the excited conduction band and those of the lowest conduction band vanish as is clear in Eqs. (2.10) and (2.11) and therefore the conductivity does not exhibit step-like decrease at the band-crossing point.

Figure 5 shows results in the cleaner case $W=0.02$. In this case, the results become essentially the same as the Boltzmann results except the presence of appreciable tail in the density of states of the excited conduction band. This shows that the Boltzmann conductivity is sufficiently accurate in clean bilayer graphene except at zero energy.

Figure 6 shows the minimum conductivity at zero energy. For very short-range case $dk_c < 1$, the conductivity is nearly independent of $W$. With the increase in the range, the conductivity increases with $W$, takes a maximum at a certain value of $W$, and then starts to decrease. The value of $W$ where the minimum conductivity becomes maximum increases with the range. This figure clearly shows that the conductivity at zero energy is not universal but depends on the degree of the disorder for scatterers with long-range potential. This situation is the same as in monolayer graphene.\(^{16}\)

This increase of the minimum conductivity with $W$ for long-range scatterers can be ascribed to level broadening effects. In fact, states at energy $\epsilon = 0$ have higher $k$ components because of large level broadening. These higher $k$ states are weakly scattered in backward direction and therefore tend to have large contribution to the conductivity and enhance the minimum conductivity.

3.2 Charged Scatterers

We consider charged impurities with screening effect included within a Thomas-Fermi approximation. The potential is

$$v(q) = \frac{\epsilon^2}{\kappa(q+q_s)}, \quad \text{a}(3.10)$$

where $\kappa$ is the static dielectric constant, which is chosen to be 2.5 in the following, and $q_s$ is the Thomas-Fermi screening constant given by

$$q_s = \frac{2\pi \epsilon^2}{\kappa} D(\varepsilon_F), \quad \text{b}(3.11)$$

at zero temperature. The scattering strength is a function of the density of states at the Fermi level and therefore should be determined in a self-consistent manner for each Fermi level. To characterize the impurity concentration, we introduce

$$n_c = \frac{\epsilon^2}{4\pi \gamma^2}, \quad \text{c}(3.12)$$

which roughly corresponds to the number of unit cells in a unit area.

Figure 7 shows some examples of calculated (a) density of states and (b) conductivity. The density of states in the low energy region becomes larger with the concentration of scatterers. Further, the excited conduction band has a long tail in the density of states, its amount being roughly proportional to the concentration.

The minimum conductivity at zero energy becomes slightly larger than the universal value given by eq. (3.9) and increases with the impurity concentration. However, it approximately remains universal because the dependence on $n_i$ is weak as shown in the inset of Fig. 7(b). When the energy exceeds the bottom of the excited conduction band, the Boltzmann conductivity exhibits a discrete jump. This jump is also present in the conductivity in the self-consistent Born approximation, although it is considerably smoothed out. This increase when the excited band is occupied comes from the sudden increase in the screening effect.

The importance of the screening effect may suggest the necessity to treat it more carefully by taking into account its dependence on the wave vector. The screening problem in clean graphenes has been studied in monolayer\(^{39,42−46}\) and bilayer,\(^{47,48}\) showing peculiar wave-vector dependence different from conventional two-dimensional systems. The use of full dielectric function requires its calculation in the present approximation scheme. This task remains very difficult and is left for future.

One important feature of bilayer graphene is that the band structure can be strongly modified due to opening-up of a band gap by applied electric field.\(^{25,49−51}\) The present formulation has not explicitly used the symmetry between layers 1 and 2 and therefore is also applicable to bilayer graphene with nonzero band gap. This problem is left for calculations in the near future.

§4. Summary

The density of states and the conductivity have been calculated for scatterers with nonzero range in the self-consistent Born approximation. The self-energy part appearing in Green’s function explicitly depends on the wave vector and becomes a $(4,4)$ matrix. A self-consistent equation for the self-energy and the current vertex function have been numerically solved. The results for scatterers with Gaussian potential with range $d$ show that both density of states and conductivity are sensitive to the potential range and to the effective scattering strength characterized by dimensionless parameter $W$. With the decrease in the scattering strength the results rapidly approach those in the Boltzmann theory except in the vicinity of zero energy. At zero energy, the minimum conductivity remains universal only for short-range scatterers and becomes nonuniversal for long-range scatterers. This situation seems to be quite similar to the case of monolayer graphene.

For charged impurity scattering, the minimum conductivity increases with the concentration but the dependence is not so considerable. When the excited conduction band starts to be populated by electrons, the conductivity increases due to the increase in the screening effect within the Thomas-Fermi approximation. The overall behavior of the conductivity is well described by
the Boltzmann theory except in the case of high impurity concentration.

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References


Figure Captions

Fig. 1 (Color online) The lattice structure of bilayer graphene. Some representative hopping integrals are shown.

Fig. 2 (Color online) The energy dispersion of a bilayer graphene. The dotted lines show that of a monolayer graphene. The parameter $\Delta = \gamma_1$ represents the interlayer coupling $B_1 \leftrightarrow A_2$.

Fig. 3 (a) A diagramatic representation of the matrix self-energy in the self-consistent Born approxima-
tion. (b) A Bethe-Salpeter-type equation of the current vertex part with velocity operator $(\gamma/h)\hat{e}_x$.

**Fig. 4** (Color online) (a) Calculated density of states and (b) conductivity as a function of energy for scatterers with Gaussian potential with range $d$ in units of $k_0 = \Delta/\gamma$ and dimensionless scattering strength $W = n_i u_i^2/4\pi\gamma^2 = 0.1$. The dotted line in (a) represents the density of states of ideal bilayer graphene and the thin dashed line represents that of two independent monolayer graphenes. The dotted line in (b) shows the Boltzmann conductivity.

**Fig. 5** (Color online) (a) Calculated density of states and (b) conductivity as a function of energy for scatterers with Gaussian potential with $W = 0.02$.

**Fig. 6** (Color online) Calculated minimum conductivity at zero energy versus $W$ for scatterers with Gaussian potential.

**Fig. 7** (Color online) Calculated (a) density of states and (b) conductivity versus the Fermi energy for charged scatterers screened in the Thomas-Fermi approximation. The inset in (b) shows the minimum conductivity versus the impurity concentration.
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\[
\hat{\Sigma}(k,E) = \chi \eta \nu (k \cdot k)^2 \hat{G}(k',E)
\]

(a) \(\hat{\Sigma}(k,E)\) = 

(b) \(\hat{J}(k,E,k',E') = \) 

\[
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\]

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