Charged impurity scattering in graphenes: Effects of environmental screening, band gap, and AA stacking

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Abstract. The conductivity is calculated for dominant charged-impurity scattering in graphenes within a self-consistent Born approximation. In monolayer graphene, environmental dielectric screening is shown to change their effective potential from short to long range. In bilayer graphene, effects of band-gap opening due to asymmetry between two layers caused by perpendicular electric field and effects of AA stacking are considered.

1. Introduction
Recently, atomically thin graphenes consisting of a few layers of monolayer graphite sheet were experimentally fabricated using mechanical exfoliation [1, 2] and epitaxial growth [3, 4]. Several reviews have already been published on their intriguing electronic properties [5, 6, 7, 8]. Transport properties of graphenes were often studied in a self-consistent Born approximation assuming model short-range scatterers because of simplicity [9, 10, 11, 12, 13, 14, 15]. Calculations were extended to the case of long-range scatterers in monolayer graphene [16] and in bilayer graphene [17]. The purpose of this paper is to generalize this scheme to study effects of charged-impurity scattering in the presence of environmental dielectric material for monolayer graphene, effects of asymmetry induced band-gap in bilayer graphene, and properties of bilayer graphene with AA stacking.

2. Environmental effect in monolayer graphene
In graphene, a unit cell contains two carbon atoms, which are denoted by A and B. Two bands having approximately linear dispersion cross the Fermi level (chosen at $\varepsilon = 0$) at K and K’ points of the first Brillouin zone. In an effective-mass or $k \cdot p$ scheme, the electron motion near the K point is described by

$$\gamma(\vec{\sigma} \cdot \hat{\mathbf{k}})\mathbf{F}(\mathbf{r}) = \varepsilon\mathbf{F}(\mathbf{r}),$$  \hspace{1cm} (1)

where $\vec{\sigma} = (\sigma_x, \sigma_y)$ are the Pauli spin matrices, $\hat{\mathbf{k}} = -i\vec{\nabla}$, and $\mathbf{F}(\mathbf{r})$ is a two-component wave function consisting of $F_A$ and $F_B$ describing slowly-varying parts of the amplitude at A and B sites, respectively. This is exactly the same as Weyl’s equation for a neutrino, except that the velocity, given by $v = \gamma/h$, is much smaller than light velocity $c (v \approx c/300)$. For the K’ point, we should replace $\vec{\sigma}$ with its complex conjugate $\vec{\sigma}^\ast$. This equation of motion is quite useful for the description of characteristic features of electronic states in graphene.
The energy dispersion is given by $\varepsilon_{\pm}(k) = \pm \gamma |k|$ and the density of states becomes $D(\varepsilon) = g_s g_v \varepsilon^2 / (2\pi \gamma^2)$, where $g_s = 2$ is the spin degeneracy and $g_v = 2$ is the valley degeneracy corresponding to the K and K’ points. The density of states vanishes at $\varepsilon = 0$ and therefore graphene is often called a zero-gap semiconductor. As will later become clear, however, this is quite inappropriate.

We consider graphene on SiO$_2$ covered by dielectric material with dielectric constant $\varepsilon_{\text{out}}$ on the top side as schematically illustrated in Fig. 1. When screening effect is included within a Thomas-Fermi approximation, the potential of charged impurities in the vicinity of graphene is

$$v_i(q) = \frac{2\pi e^2}{\kappa(q+q_s)},$$

where $q_s$ is the Thomas-Fermi screening constant given by $q_s = (2\pi e^2/\kappa)D(\varepsilon_F)$ and $\kappa$ is the effective dielectric constant given by

$$\kappa = \frac{1}{2}(\kappa_{\text{out}} + \kappa_{\text{ox}}),$$

with $\kappa_{\text{ox}} = 3.9$ for SiO$_2$. Then, the calculation of the density of states and the conductivity is performed by a straightforward extension of the previous work for $\kappa_{\text{out}} = 1$ [16].

Figure 2 shows some examples of (a) calculated density of states and (b) conductivity for $1 \leq \kappa_{\text{out}} \leq 50$. Here, $\varepsilon_c$ is the cutoff energy of the order of $\gamma_0 \sim 3$ eV, where $-\gamma_0$ is the hopping integral in the simplest tight-binding model, and $n_c = \varepsilon_c^2 / (4\pi \gamma^2)$ is the concentration roughly corresponding to an impurity per several unit cells. With the increase of $\kappa_{\text{out}}$, the density of states in the vicinity of the Dirac point exhibits clear decrease, indicating the reduction of disorder. The conductivity does not increase so much, presumably due to the fact that the decrease of potential by dielectric screening is partly canceled by the reduction in the screening by electrons in graphene.

Figure 2 (c) shows the minimum conductivity at the Dirac point as a function of $\kappa_{\text{out}}$. It increases gradually with $\kappa_{\text{out}}$. The reason is that the effective potential tends to become of long range due to less screening by electrons in graphene. In fact, previous calculations for scatterers with Gaussian potential show that the minimum conductivity increases with the range except in the clean limit where the scattering strength is sufficiently small [16]. In fact, states at the Dirac point have higher $k$ components because of strong forward scattering caused by long-range scatterers. These higher $k$ states are weakly scattered in backward direction and therefore tend to have large contribution to the conductivity. For short-range scatterers, higher $k$ components do not contribute much to the conductivity and the minimum conductivity remains small.

Figure 2 (c) also shows ratio of transport relaxation time $\tau_t$ determining the conductivity and self-energy relaxation time $\tau$ corresponding to the inverse of the total scattering probability,
calculated using the Boltzmann transport equation [18]. For short-range scatterers we have \( \tau_\text{tr}/\tau = 2 \) because of the absence of backscattering [9]. For \( \kappa_{\text{out}} = 1 \) without environmental dielectric material, we have \( 2 < \tau_\text{tr}/\tau < 3 \) not so much different from that for short-range scatterers. This shows that charged impurities should be regarded as short-range scatterers for \( \kappa_{\text{out}} = 1 \) in contrast to the claim otherwise [19]. For sufficiently large \( \kappa_{\text{ox}} \), for which \( \tau_\text{tr}/\tau \) is much larger than two, charged impurities tend to have the nature of long-range scatterers. Experiments under different dielectric environments were reported [20, 21, 22], but results vary among them and therefore seem to remain inconclusive yet.

3. Band-gap opening in bilayer graphene

We consider a bilayer graphene which is arranged in the AB (Bernal) stacking as shown in Fig. 3. The upper layer is denoted as 1 and the lower layer denoted as 2. In each layer, the unit cell contains two carbon atoms denoted by \( A_1 \) and \( B_1 \) in layer 1 and \( A_2 \) and \( B_2 \) in layer 2. For the
Figure 3. Lattice structure of (a) AB stacked and (b) AA stacked graphenes. The nearest-neighbor interlayer hopping integral denoted by $\gamma_1$ determines essential features of the band structure. The next-nearest-neighbor hopping integrals in AB graphene denoted by $\gamma_3$ and $\gamma_4$ are neglected because of simplicity.

Figure 4. 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.

inter-layer coupling, we include only the coupling between vertically neighboring atoms. Then, electronic states are described by the $k \cdot p$ Hamiltonian [23, 12]:

$$
\mathcal{H} = \begin{pmatrix}
A_1 & B_1 & A_2 & B_2 \\
+eFd/2 & \gamma \hat{k}_- & 0 & 0 \\
\gamma \hat{k}_+ & +eFd/2 & \Delta & 0 \\
0 & \Delta & -eFd/2 & \gamma \hat{k}_- \\
0 & 0 & \gamma \hat{k}_+ & -eFd/2
\end{pmatrix},
$$

(4)

where $\Delta (= \gamma_1 \approx 0.4 \text{ eV})$ represents the inter-layer coupling between sites $B_1$ and $A_2$ and $eFd$ represents the potential difference between layers 1 and 2 ($F$ is the effective electric field and
$d = 0.334 \text{ nm is the interlayer distance})$. This potential difference should be determined by a self-consistent calculation [24, 25, 26]. Very roughly, $F$ becomes reduced by about factor two from field externally applied [26].

Figure 4 shows some examples of calculated (a) density of states and (b) conductivity for a symmetric bilayer with $\Delta = 0$. 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 for short-range scatterers [12] 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. 4 (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.

Figure 5 shows some examples for an asymmetric bilayer with nonzero gap. The density of states does not easily vanish and has low energy tail. This is partly due to the self-consistency between the screening constant and the density of states. In fact, smaller density of states causes less screening and causes effectively large scattering strength giving rise to long tail in the density of states. In spite of the considerable density of states, the conductivity within the gap region is much smaller than that outside, in particular for large gap $eFd/\Delta = 1$.

4. AA stacked bilayer graphene

The structure of an AA stacked bilayer graphene is shown in Fig. 3 (b). When we consider the strongest nearest-neighbor interlayer interaction, the Hamiltonian becomes

$$
\hat{H}_0 = \begin{pmatrix}
A_1 & B_1 & A_2 & B_2 \\
+eFd/2 & \gamma \hat{k}^- & \Delta & 0 \\
\gamma \hat{k}^+ & +eFd/2 & 0 & \Delta \\
\Delta & 0 & -eFd/2 & \gamma \hat{k}^- \\
0 & \Delta & \gamma \hat{k}^+ & -eFd/2
\end{pmatrix}.
$$

(5)

Let us define

$$
\Delta = \tilde{\Delta} \sin \psi, \quad \frac{eFd}{2} = \tilde{\Delta} \cos \psi, \quad \tilde{\Delta} = \sqrt{\Delta^2 + \left(\frac{eFd}{2}\right)^2},
$$

(6)

and

$$
V = \begin{pmatrix}
\cos(\psi/2) & 0 & -\sin(\psi/2) & 0 \\
0 & \cos(\psi/2) & 0 & -\sin(\psi/2) \\
\sin(\psi/2) & 0 & +\cos(\psi/2) & 0 \\
0 & \sin(\psi/2) & 0 & +\cos(\psi/2)
\end{pmatrix}.
$$

(7)

Then, we have

$$
V^{-1} \hat{H}_0 V = \begin{pmatrix}
\tilde{\Delta} & \gamma \hat{k}^- & 0 & 0 \\
\gamma \hat{k}^+ & \tilde{\Delta} & 0 & 0 \\
0 & 0 & -\tilde{\Delta} & \gamma \hat{k}^- \\
0 & 0 & \gamma \hat{k}^+ & -\tilde{\Delta}
\end{pmatrix}.
$$

(8)

This immediately shows that the band structure consists of two monolayer-like bands relatively shifted in energy by amount $\pm \tilde{\Delta}$. Further, scatterers with potential same in the top and bottom layers cannot cause scattering between the two bands, i.e., the conductivity is the sum of those of two monolayer bands. When the scattering potential is different between the top and bottom layers, interband scattering appears and can modify the conductivity. Possible
Figure 5. Calculated density of states (a) and (c), and conductivity (b) and (d) of asymmetric bilayer graphene. (a) and (b) $eFd/\Delta = 0.2$. (c) and (d) $eFd/\Delta = 1$.

The asymmetry between the top and bottom layers due to perpendicular electric field does not affect this conclusion and contribute only to the change of $\Delta$ into $\Delta$.

Figure 6 shows some examples of calculated (a) density of states and (b) conductivity as a function of energy for symmetric bilayer $eFd = 0$. Results for asymmetric bilayer can be obtained by replacing $\Delta$ with $\Delta$ given in Eq. (6). The density of states in the clean limit is independent of energy in the region given by $-\Delta < \varepsilon < +\Delta$ and starts to increase linearly outside this region, as shown by a dotted line in Fig. 6 (a). In the presence of charged impurities,
the density of states is enhanced symmetrically around $\pm \Delta$ corresponding to the Dirac points of the two bands given by Eq. (8). As a result, the total density of states is most strongly enhanced near zero energy.

For small impurity concentration $n_i/n_c = 0.05$, the conductivity exhibits a singularly sharp drop at $\pm \Delta$. This is a manifestation of the zero-mode anomaly appearing in the conductivity for short-range scatterers with strength independent of energy or electron concentration predicted previously [9]. In fact, the screening effect is essentially independent of the energy in the vicinity of $\pm \Delta$ as shown in Fig. 6(a), making charged impurities effectively “short-range scatterers” with energy independent strength. Therefore, the zero-mode anomalies characteristic of massless Dirac electrons can be experimentally observed in an AA stacked bilayer graphene even if scattering is dominated by charged impurities.

5. Summary
We have studied the conductivity in the presence of dominant charged impurities in graphenes, using the self-consistent Born approximation. In monolayer graphene, effects of environmental dielectric screening have been considered, showing that charged impurities should be regarded as short-range scatterers except in the case of very large dielectric constant. In bilayer graphene, effects of band-gap opening due to asymmetry between two layers caused by perpendicular electric field are considered, showing that the conductivity remains small even in the presence of appreciable density of states within the gap. The Hamiltonian in AA-stacked bilayer graphene can be decomposed into those of two monolayer graphenes with relative displacement of the Dirac points by the amount determined by the nearest-neighbor inter-layer interaction and asymmetry between two layers. Because of the near independence of the screening effect, a singularity at the Dirac point predicted in monolayer graphene with short-range scatterers with energy-independent strength appears also for charged impurities.
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