Charge screening and carrier transport in AA-stacked bilayer graphene: tuning via a perpendicular electric field

Yawar Mohammadi

Young Researchers and Elite Club, Kermanshah Branch, Islamic Azad University, Kermanshah, Iran

PACS 77.22.-d – Dielectric properties of solids and liquids
PACS 72.10.-d – Theory of electronic transport; scattering mechanisms
PACS 72.80.Vp – Electronic transport in graphene

Abstract – The static dielectric function in AA-stacked bilayer graphene (BLG), subjected to an electric field applied perpendicular to layers, is calculated analytically within the random phase approximation (RPA). This result is used to calculate the screened Coulomb interaction and the electrical conductivity. The screened Coulomb interaction, which here can be tuned by the perpendicular electric field, shows a power-law decay as \(1/(\gamma^2 + V^2)\) at long-distance limit where \(V\) and \(\gamma\) are the electrical potential and the inter-layer hopping energy respectively, indicating that the Coulomb interaction is suppressed at high perpendicular electric fields. Furthermore, our results for the effect of the short-range and the long-range (Coulomb) scattering on the electrical conductivity show that the short-range scattering yields a constant electrical conductivity which is not affected by the perpendicular electric field. While the electrical conductivity limited by the Coulomb scattering is enhanced by the perpendicular electric field and increases linearly in \(V^2\) at small \(V\) with a finite value at \(V = 0\), indicating that we can tune the electrical conductivity in AA-stacked BLG by applying a perpendicular electric field.

Introduction. – Single layer graphene (SLG), an isolated layer of graphite, shows many interesting properties \([1,2]\) originated from its chiral linear low energy spectrum dominated by a massless Dirac-like equation. Stacking order of graphene layers can change dramatically (or greatly) these properties leading, for example, to the gapless parabolic spectrum for AB-stacked BLG showing properties \([3,4]\) which are different from those in graphene. Recently a new stable order of few-layer graphene, few-layer graphene with AA stacking order, has been observed in experimental researches \([5,6]\). In this stacking order of graphene layers, each sublattice in a top layer is located directly above the same one in the bottom layer. They have a special band structure composed of SLG-like band structures with different doping which depend on the number of layer and the inter-layer hopping energy \([6,8]\). Recently, AA-stacked BLG has been studied in theoretically, leading to discovery of some interesting properties \([9,14]\) which mainly originate from its special low energy band structure.

One of the most fundamental physical quantities is static polarization function. Knowing this quantity is essential to study many fundamental properties, e.g., the RKKY interaction between magnetic adatoms, Kohn anomaly in phonon dispersion and the carrier transport through screened coulomb interaction by charged impurities. The static polarization function of SLG \([15,21]\) and AB-stacked BLG \([22,24]\), in recent years, have been studied extensively. The main result of these works is the vanishing (enhanced) 2\(k_F\) backscattering in SLG (BLG) \((k_F\) is the Fermi wave vector.), which plays a key role in determining low density and low temperature carrier transport, resulting in different features for SLG and BLG. In a recent research \([25]\), the AA-stacked BLG static polarization has been calculated analytically. One of aims of this paper is to calculate analytically the AA-stacked BLG static polarization in the presence of an electric field applied perpendicular to layers, which can be use to tune the properties of AA-stacked BLG.

The other purpose of our work is to calculate the carrier transport in AA-stacked BLG and to investigate effects of the perpendicular electric field on it. The carrier transport in SLG \([11,15,20,30]\) and AB-stacked BLG \([23,31,34]\) is controlled mainly by two scattering mechanisms, (i) the long-range Coulomb scattering by random charged impurities located in the substrate near the graphene layers
and (ii) the the short-range disorder scattering coming, for example, from the zero range point defects, or resonant short-range scattering, or other mechanisms. The first is often dominant in controlling the carrier transport in SLG, leading to linear dependence of its conductivity on carrier density beside weak temperature dependence of its conductivity. While the later becomes important in high mobility samples of SLG. On the other hand, both scattering mechanisms contribute significantly to determine the carrier transport in AB-stacked BLG, leading to the strong insulating temperature dependence of AB-stacked BLG conductivity beside the linear dependence of AB-stacked BLG conductivity on carrier density at high carrier densities. Moreover, AA-stacked BLG lattice has some similarities with both SLG and AB-stacked BLG. The band structure of AA-stacked BLG is composed of two SLG-like spectrum. In addition, the Thomas-Fermi screening wave vector in AA-stacked BLG, similar to AB-stacked BLG and in contrast to SLG, is constant and independent of chemical potential. This can lead to different stacked BLG and in contrast to SLG, is a spectrum. In addition, the Thomas-Fermi screening wave vector in AA-stacked BLG, similar to AB-stacked BLG and in contrast to SLG, is constant and independent of chemical potential. This can lead to different stacked BLG.

This paper is organized as follows. In the section II, we introduce the tight-binding Hamiltonian describing the low energy quasiparticle excitation in AA-stacked BLG, subjected to an electric field applied perpendicular to layers, and obtain corresponding eigenvalues and eigenfunctions. Section III is devoted to obtain an analytical relation for the static polarization function of AA-stacked BLG and we use this result to consider the effect of the perpendicular electric filed on the Coulomb interaction in AA-stacked BLG. In section IV, we consider the electrical conductivity, limited by short- and long-range scattering, and show how one can tune the electrical conductivity in AA-stacked BLG by making use of a perpendicular electric field. Finally, we end our paper by summary and conclusions in section V.

Model Hamiltonian. – In an AA-stacked BLG lattice which is composed of two SLG, each sublattice in the top layer is located directly above the same one in the bottom layer. The unit cell of an AA-stacked BLG consists of 4 inequivalent Carbon atoms, two atoms for every layer (fig. 1). Moreover, the presence of the bias voltage creates a potential +V in the top layer and −V in the bottom layer. Thus its Hamiltonian, in the nearest-neighbor tight-binding approximation, is given by

\[
H = \sum_{\mathbf{q}} \hat{\Psi}^\dagger_{\mathbf{q}} \hat{H}_{\mathbf{q}} \hat{\Psi}_{\mathbf{q}},
\]

where

\[
\hat{H}_{\mathbf{q}} = \begin{pmatrix}
V & \phi'(\mathbf{q}) & \gamma & 0 \\
\phi(\mathbf{q}) & V & 0 & \gamma \\
\gamma & 0 & -V & \phi'(\mathbf{q}) \\
0 & \gamma & \phi(\mathbf{q}) & -V
\end{pmatrix},
\]

and \(\hat{\Psi}^\dagger_{\mathbf{q}} = (a_{1\mathbf{q}}^\dagger, b_{1\mathbf{q}}^\dagger, a_{2\mathbf{q}}^\dagger, b_{2\mathbf{q}}^\dagger)\), \(a_{\lambda\mathbf{q}}^\dagger (b_{\lambda\mathbf{q}}^\dagger)\) are creation operators of an electron with momentum \(\mathbf{q}\) at A(B) sub-lattice in nth-layer. \(\gamma\) is the inter-layer hopping energy and \(\phi(\mathbf{q}) = -\mathbf{\gamma} \sum_{i=1}^3 e^{i\mathbf{q} \cdot \mathbf{d}_i}\), where \(\mathbf{d}_1 = (a\sqrt{3}/2, a/2)\), \(\mathbf{d}_2 = (-a\sqrt{3}/2, a/2)\) and \(\mathbf{d}_3 = (0, -a)\) are the nearest neighbor vectors (fig. 1) with \(a\) being the shortest Carbon-Carbon distance. To obtain the Hamiltonian dominates the low-energy excitations, which occur near Dirac points (K and K’), we must expand \(\phi(\mathbf{q})(\phi^* (\mathbf{q}))\) for |\(\mathbf{q}\)| \(\ll |\mathbf{K}|\) around Dirac points where \(\mathbf{q} = \mathbf{K} + \mathbf{k}\). If we expand the Hamiltonian around \(\mathbf{K} = (2\pi/3\sqrt{3}a, 2\pi/3a)\) point, we have \(\phi(\mathbf{q}) = h_F k_\perp (\phi^* (\mathbf{q}) = h_F k_{\perp}\) where \(k_\perp = k_x \pm i k_y\) and \(v_F = 3ta/2\hbar \approx 9 \times 10^3 m/s\) is Fermi velocity. Our results for the corresponding low-energy eigenvalues and eigenstates are given by

\[
\tilde{\varepsilon}^\lambda_{\mathbf{k}} = s\gamma' + \lambda h_F |\mathbf{k}|,
\]

\[
\psi_{\mathbf{k}}^\pm = \frac{\gamma}{2\sqrt{\gamma' - V}} \left( \begin{array}{c}
1 \\
\lambda e^{-i\theta_k} \\
\frac{\gamma'}{\gamma} \frac{V - e^{-i\theta_k}}{V} \\
\frac{\gamma'}{\gamma} \frac{V - e^{-i\theta_k}}{V}
\end{array} \right),
\]

where \(s = \pm, \lambda = \pm\) and \(\gamma' = \sqrt{\gamma^2 + V^2}\). Here \(|\mathbf{k}| = \sqrt{k_x^2 + k_y^2}\) is the amount of the two-dimensional momentum measured from Dirac points and \(\theta_k = tan^{-1}(k_y/k_x)\). Notice, the low energy band structure of AA-stacked BLG is a composition of two electron-doped and hole-doped SLG-like band structures \(\uparrow \uparrow \uparrow\), which for some properties behave like decoupled bands leading to many attractive

![Fig. 1: A segment of AA-stacked BLG lattice structure. \(\mathbf{d}_1, \mathbf{d}_2\) and \(\mathbf{d}_3\) are three vectors that are drown from a sub-site to its nearest neighbors.](image-url)
properties not been observed in the other graphene-based materials so far. The low energy density of states of AA-stacked BLG is
\[ D(E) = \frac{g |E - \gamma'| + |E + \gamma'|}{2\pi h^2 v_F^2}, \]
where multiple \( g = 4 \) is due to the spin and valley degeneracies. The low energy band structure and the density of states of AA-stacked BLG, for different values of the bias voltage, have been shown in fig. 2.

**Static polarization function and charge-carrier screening.** The static dielectric function in the low energy excitation limit, where inter-layer and intra-layer Coulomb interactions are approximately equal, and within RPA is given by
\[ \epsilon(q) = 1 + \frac{2\pi e^2}{\kappa q} \Pi(q), \]
where \( \Pi(q) \) is the static polarization function and \( \kappa \) is the background dielectric constant. The static polarization function of AA-stacked BLG is given by
\[ \Pi(q) = -\frac{g}{2A} \sum_{k\lambda' ss'} \frac{n^e_{k\lambda} n^h_{k'\lambda'} - n^e_{k'\lambda'} n^h_{k\lambda}}{\epsilon_{k\lambda} - \epsilon_{k'\lambda'}} F^{ss'\lambda\lambda'}_{kk'}, \]
where \( k' = k + q \), \( \Delta \theta_{k'} = \theta_{k'} - \theta_k \) and \( F^{ss'\lambda\lambda'}_{kk'} \) is the overlap of electron and hole wave-function, \( F^{ss'\lambda\lambda'}_{kk'} = \langle \psi_{k'\lambda'}^s | \psi_{k\lambda}^h \rangle^2 \), which becomes \( (1 + \alpha^2 \cos \Delta \theta_{k'k})/2 \) if \( s = s' \) and is zero if \( s \neq s' \). This indicates that only transitions between electron and hole bands with same \( s \) (or \( s' \)) band-index contribute to the polarization function of AA-stacked BLG. Here, \( n^e_{k\lambda} = 1/(1 + \exp((\epsilon_{k\lambda} - \mu)/k_B T)) \) is the Fermi-Dirac distribution function with \( k_B \) being Boltzmann constant.

In this paper, we only calculate the polarization function of the AA-stacked BLG in undoped regime at zero temperature. In this case the static polarization function of AA-stacked BLG can be written as sum of two SLG static polarization function with \( \mu = \gamma' \) and \( \mu = -\gamma' \) which, as it has been shown before [8], are equal. Therefore, the static polarization function of undoped AA-stacked BLG is equal to that of a doped SLG with \( \mu = \gamma' \) which can be written as
\[ \Pi(q) = \frac{gq}{2\pi h^2 v_F} \text{ for } q \leq 2\gamma'/h_F, \]
and
\[ \Pi(q) = \frac{gq}{16h_F} + \frac{g\gamma'}{2\pi h^2 v_F} (1 - \frac{1}{2} \sqrt{1 - 4g^2 h_F q^2 - 2\gamma'/h_F q}) \]
for \( q > 2\gamma'/h_F \). Notice that the static polarization function of AA-stacked BLG, for \( q \leq 2\gamma'/h_F \), (similar to that in doped SLG and ordinary 2DEG) is a constant metallic-like polarization, even in the absence of doping. This constant polarization, in zero limit of the perpendicular electric field, is only depend on the inter-layer hopping energy and on the Fermi velocity \( v_F \). Moreover, it can be tuned by a perpendicular electric field. For \( q > 2\gamma'/h_F \), AA-stacked BLG, similar to SLG, has an insulating-like polarization which increases linearly in \( q \). Furthermore, the value of a momentum, at which a crossover from metallic to insulating screening takes place (\( q = 2\gamma'/h_F \)), can be tuned electrically and this allow us to suppress the insulating screening effects via a perpendicular electric filed.

The static screening, in the long wave-length limit, is given by \( \epsilon(q) \approx 1 + q_T F/q \) where \( q_T F \) is the Thomas-Fermi wave-vector. For the biased AA-stacked BLG, Thomas-Fermi wave-vector is \( q_T F = 2\pi e^2 D(0)/\kappa = q_T \sqrt{\gamma^2 + V^2/2\pi \kappa v_F^2} \), which, similar to that in ordinary 2DEG and in contrast to that in SLG, is independent of carrier concentration.

Moreover, the electrical field dependence of the static dielectric function allow us to tune charge screening in AA-stacked via an electric field applied perpendicular to layers and manipulate some attractive properties of AA-stacked BLG arising from Coulomb interaction of electrons. This feature can be seen, explicitly, in electrical potential dependence of the long-distance behavior of...
Coulomb interaction. The long-distance behavior of long-range Coulomb interaction consist of two parts, a non-oscillatory term coming from long wave-length behavior of the static polarization (Thomas-Fermi approximation) and a Friedel-oscillation part arising from a discontinuity occurring in the second derivative of the static polarization. The non-oscillatory part, which can obtained by making use of Thomas-Fermi dielectric function, is given by

$$\phi(r) = \frac{Ze^2}{\kappa r} - \frac{\pi Ze^2 q_{TF}}{2\kappa} [H_0(q_{TF} r) - Y_0(q_{TF} r)],$$

where $H_0$ and $Y_0$ being the Struve and the Bessel functions of the second kind. The asymptotic form of this term at large distance is given by $Ze^2 q_{TF} / [\kappa(q_{TF} r)^3]$ where $q_{TF} = \frac{g e^2}{\sqrt{\gamma^2 + V^2}}$. It is evident that by increasing $V$ this part decreases as $1/(\gamma^2 + V^2)$ leading to a suppressed interaction at high electric field.

The Friedel-oscillation part, which originates from a discontinuity occurring in the second derivative of the static polarization, can be calculated by making use of a theorem of Lighthill. To obtain these terms we must use the asymptotic form of the the Bessel function. Therefore, we have

$$\phi(r) \simeq \frac{Ze^2}{\sqrt{\pi r}} \int_0^\infty \frac{\cos(k_F E x) + \sin(k_F E x)}{x} \sqrt{x} dx,$$

where $k_F = \sqrt{\gamma^2 + V^2}/\hbar v_F$, $x = q/k_F$. This integral can be easily calculated which becomes

$$\phi(r) \simeq \frac{3Ze^2}{4\kappa} \frac{\alpha k_F'}{(1 + \pi \alpha) (k_F E)^2},$$

where $\alpha = e^2/\kappa \hbar v_F$. Friedel-oscillation part, similar to non-oscillatory part, depend on electric potential as $1/(\gamma^2 + V^2)$, but with an extra oscillatory coefficient, $\cos(2r\sqrt{\gamma^2 + V^2}/\hbar v_F)$ whose periodicity can be tuned by the electric field.

**Carrier transport.** – We use Boltzmann equation to calculate the carrier transport in AA-stacked BLG, motivated by this fact that the theoretical results obtained from this equation for the carrier transport in SLG [11,15,20,29,30] and AB-stacked BLG [32,33] are in good agreement with the reported experimental results. It is logical to suppose that the charge carrier in AA-stacked BLG, even in absence of doping, behave like a homogenous electron gas. This is due to the large density of state at Fermi level, the average carrier density is always larger than the fluctuations in carrier density and this prevents from formation of electron-hole puddle structures induced by the charged impurities which is observed in SLG and AB-stacked BLG close to the charge neural point. Moreover, since the low energy bands with different $s$ index band in AA-stacked BLG behave like decoupled bands, the electrical conductivity of AA-stacked BLG can be written as sum of two terms for SLG electrical conductivity with $E_F = -\gamma$ and $E_F = +\gamma$. The electrical conductivity in a homogenous electron gas of massless chiral Dirac carriers is given by

$$\sigma = g \frac{e^2}{4\pi h^2} \int d\epsilon_k \tau(\epsilon_k) \epsilon_k \left( \frac{\partial f(\epsilon_k)}{\partial \epsilon_k} \right),$$

where $\epsilon_k = \hbar v_F |k|$, $f(\epsilon_k) = [1 + \exp((\epsilon_k - \mu)/k_BT)]^{-1}$ is Fermi distribution function with $\mu$ being chemical potential and $\tau(\epsilon_k)$ is the scattering time given by

$$\frac{1}{\tau(\epsilon_k)} = \frac{\pi}{\hbar} \int \frac{d\mathbf{k}}{2\pi^2} \frac{n_s |v_s(q)|^2 + n_l |v_l(q)|^2}{(\epsilon(q))^2} \times (1 - \cos^2 \theta_{kk'}) \delta(\epsilon_k - \epsilon_{k'}),$$

where $v_s(q)/v_l(q)$ is the matrix elements of the long (short)-range scattering potential between an electron and an charged impurity (a point defect) and $n_s(n_l)$ is the corresponding impurity density. The long-range Coulomb interaction is given by $v_l(q) = 2\pi e^2 e^{-qd}/\kappa q$ with $d$ being the average distance of charged impurity from AA-stacked BLG. The short-range interaction is $v_s(q) = v_0 = \text{const.}$ In this paper we only consider zero temperature case. Therefore we have $\sigma = \frac{e^2}{2\pi \hbar v_F} \tau(E_F)$ where $\tau(E_F)$ is the scattering time at zero temperature.

It is interesting to compare the role of the short-range and Coulomb scattering in controlling the electrical conductivity in AA-stacked and also to see how the perpendicular electric filed affects on each contribution. We can write the electrical conductivity as $\frac{1}{\tau} = \frac{1}{\tau_s} + \frac{1}{\tau_l} = \frac{1}{\tau_s} (\Lambda_s + \Lambda_l)$, where $\sigma_s^{-1}$ and $\sigma_l^{-1}$ are the electrical resistivity arising from short-rang and Coulomb scattering respectively, and $\Lambda_s$ and $\Lambda_l$ are given by

$$\Lambda_s = \frac{2 n_s v_s^2 \hbar v_F}{\pi \gamma^2 + V^2} \int_0^1 d\lambda \frac{\lambda^4 \sqrt{1 - \lambda^2}}{(\lambda + 4r_s)^2}$$

and

$$\Lambda_l = \frac{2 n_l v_l^2 \hbar v_F}{\gamma^2 + V^2} \int_0^1 d\lambda \frac{\lambda^2 \sqrt{1 - \lambda^2}}{(\lambda + 4r_s)^2} e^{-\frac{\sqrt{\gamma^2 + V^2}}{\hbar v_F r_s}}$$

with $\lambda = \hbar v_F q/2\sqrt{\gamma^2 + V^2}$ and $r_s = e^2/\hbar v_F k_B$ being the dimensionless Wigner-Seitz radius in graphene which is a constant. It is evident that, due to the nonzero density of state at Fermi energy level, even in the absence of doping and at $V = 0$, AA-stacked BLG shows a finite electrical conductivity. Moreover, Eq. (14) shows that the short-range scattering yields a constant electrical conductivity which only changes by varying the substrate resulting in different substrate dielectric constant (and consequently different $r_s$). Another result, which is more interesting, is that we can enhance $\sigma_l$ by applying a perpendicular electric filed (black line in fig. 3). This term increases linearly in $V^2$ (black line in fig. 3) with a nonzero value at $V = 0$ which depends on the interlayer hopping energy.
cal conductivity in AA-stacked BLG, examining the effects of Coulomb and short-range scattering mechanisms. Our results showed that the short-range scattering, which can arise for example from point defect, yields a constant electrical conductivity which is independent of the applied perpendicular electric field and can only change by varying the substrate and of course by varying the short-range impur density. On the other hand, we found that the Coulomb-scattering-limited electrical conductivity can be tuned by applying a perpendicular electric field, showing a linear dependence on $V^2$ at small perpendicular electric fields. Moreover we found that when $n_s/n_t$ increases the electrical conductivity shows a sub-linear dependence on $V^2$ at large perpendicular electric fields.

**Summary and conclusions.** In summary, we first calculated analytically the static dielectric function in AA-stacked BLG in the presence of an electric field applied perpendicular to layers within the random phase approximation. Then we obtained analytical relations for the Friedel-oscillation and the non-oscillatory parts of the long-distance limit of the screened Coulomb interaction, which shows explicitly their dependence on the applied perpendicular electric field. This expression revealed that the Coulomb interaction in AA-stacked BLG is suppressed at the high perpendicular electric fields. Finally we used the Boltzmann transport theory to calculate the electrical conductivity in AA-stacked BLG, examining the effects of Coulomb and short-range scattering mechanisms.
[26] Peres N. M. R., *Phys. Mod. Phys.*, **82** (2010) 2673.
[27] Ziegler K., *Phys. Rev. Lett.*, **97** (2006) 266802.
[28] Nomura K., and MacDonald A. H., *Phys. Rev. Lett.*, **98** (2007) 076602.
[29] Hwang E. H., Adam S. and Das Sarma S., *Phys. Rev. Lett.*, **98** (2007) 186806.
[30] Stauber T., Peres N. M. R., and Guinea F., *Phys. Rev. B* **76**, **76** (2007) 205423.
[31] Koshino M. and Ando T., *Phys. Rev. B*, **73** (2006) 245403.
[32] Das Sarma M. S., Hwang E. H., and Rossi E., *Phys. Rev. B*, **81** (2010) 161407.
[33] Lv M., and Wan Sh., *Phys. Rev. B*, **81** (2010) 195409.
[34] Yuan Sh., De Raedt H., and Katsnelson M. I., *Phys. Rev. B*, **82** (2010) 235409.
[35] Lighthill M. J., *Introduction to Fourier Analysis and Generalised Functions* (Cambridge University Press, Cambridge) 1958, p. 52.