Coulomb screening and collective excitations in a graphene bilayer

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We have investigated the Coulomb screening properties and collective excitations in a graphene bilayer. The static screening effect is anisotropic and is much stronger in the undoped graphene bilayer than in a monolayer graphene \([1]\). The dynamic screening shows the properties of a Dirac gas in the low frequency and that of a Fermi gas in the high frequency. The transition from the Dirac to the Fermi gas is also observed in the plasmon spectrum. Finally, we find that an electron gas in a doped graphene bilayer has quite similar properties as those of a Fermi gas in materials containing two energy valleys.

PACS numbers: 71.10.-w, 75.10.Lp, 75.70.Ak, 71.70.Gm

The realization of the monolayer and the bilayer graphene – the two-dimensional crystal of one and two layers of carbon atoms, has opened a new door for exploration of the fundamental physics and also fabrication of nanoelectronic devices [2, 3]. Being different from the multilayer graphene or graphite, the monolayer and the bilayer graphene are intrinsically zero-gap semiconductors. The monolayer graphene has the properties of a chiral Dirac gas while the graphene bilayer has the energy band of a chiral Fermi gas at high energies with several quasi-Dirac points at the bottom of the band [4, 5, 6, 7]. Consequently, a comparison of the physical properties between them would offer new understanding and provide interesting predictions about the different behaviors between the charged chiral-Dirac and the Fermi gases.

In normal two-dimensional semiconductors, the many-body effects on the Coulomb interaction has been extensively studied using different methods. One of the most successful and widely accepted approaches is the random-phase approximation (RPA). In this approximation it is assumed that only the single-particle excitations of the same wavevector as the Coulomb interaction plays an effective role in the screening process while the effects of others having different wavevectors cancel out. In the past years, there have been a few studies reported in the literature on the Coulomb screening and the collective excitation spectrum in the monolayer graphene using the RPA [8, 9, 10, 11, 12]. In this paper, we present some of the interesting properties of the Coulomb screening and the collective excitations in a graphene bilayer.

The graphene bilayer is formed by stacking two graphene layers in the same way as the stacking occurs in graphite, i.e., the Bernal stacking [4, 5, 6, 7]. Each graphene layer has a hexagonal (honeycomb) carbon lattice [Fig. 1(a)] which is composed of two periodic sublattices, A and B [Fig. 1(b)]. In other words, there are two inequivalent lattice sites with atoms A and B in each unit cell of the periodic lattice. The two sublattices are displaced from each other along an edge of the hexagons by a distance of \(a_0 = 1.42 \text{ Å}\). In a graphene bilayer, there are four inequivalent sites in each unit cell, with atoms A and B at the top and A’ and B’ at the bottom. In the case of the Bernal stacking, the two graphene layers are arranged in such a way that the A sublattice is exactly on top of the sublattice B’ with a vertical separation of \(b_0 = 4 \text{ Å}\) [13] as shown in Fig. 1(a) and (b). The system can be described by the tight-binding model [3] characterized by three coupling parameters, \(\gamma_0 = 3.16 \text{ eV}\) between atoms A and B or A’ and B’ (intra-layer coupling), \(\gamma_1 = 0.39 \text{ eV}\) between A and B’ (the direct inter-layer coupling), and \(\gamma_3 = 0.315 \text{ eV}\) between A’ and B, A and A’, or B and B’ (the indirect inter-layer coupling).

In the \(k\) space, the graphene bilayer has the same hexagonal Brillouin zone as that of a monolayer graphene. Its physical properties are mainly determined by the energy spectrum and the wavefunction near the two inequivalent corners of the Brillouin zone \(K\) and \(K’\), where the \(\pi\) conduction band and \(\pi\) valence band meet at the Fermi surface \([14]\). Due to the strong interlayer coupling (the \(\pi\) orbit overlap) both the conduction band and the valence band in a bilayer are split by an energy of \(\sim 0.4 \text{ eV}\) near the \(K\) and \(K’\) valleys \([7, 13, 14]\). Since this energy splitting is larger than the energy range we are interested in from the bottom of the energy band, we take into account only the upper valence band and the lower conduction band. The bilayer graphene cannot be treated as two independent monolayer graphenes with the interlayer coupling as a perturbation because of the strong interlayer overlap of the \(\pi\) orbits. In contrast, the perturbation treatment of the interlayer coupling is valid for a normal double quantum well system \([16]\) or in an intercalated graphite \([17]\).

In the effective-mass approximation, the electrons in the \(K\) valley is described by a Hamiltonian with a mixture of the linear and the quadratic terms of \(k\) [4, 5, 6, 7]

\[
H_K = \frac{\hbar^2}{2m^*} \begin{pmatrix} 0 & k_+^2 & 0 \\ k_+^2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} - \frac{\hbar^2k_0}{2m^*} \begin{pmatrix} 0 & k_+ \\ k_+ & 0 \end{pmatrix}
\]  

(1)

with \(k_\pm = k_x \pm i k_y\) and \(k = (k_x, k_y)\) being measured from the \(K\) point. The effective mass of the quadratic term is \(m^* = 2\hbar^2/\gamma_1(3a_0\gamma_0)^2 \approx 0.033\) and the ‘light’ velocity of the linear term is \(v_0 = \hbar k_0/2m^* = 3a_0\gamma_3/2\hbar \approx 10^5 \text{ m/s}\) with \(k_0 \approx 10^8/\sqrt{3} \text{ m}^{-1}\).

The eigenfunction of the above Hamiltonian is

\[
\Psi_k(r) = \frac{e^{i(k_x \cdot r)}}{\sqrt{2}} \left( e^{i\phi_k} \right) \text{ with the energy } E_k = ...
\]
\[ \lambda h k \sqrt{k^2 - 2k_0 k \cos 3 \varphi + k_0^2/2m^*} \text{ and the pseudospin angle } \lambda \theta. \text{ Here } \varphi = \arg(k_+), \phi = \arg(ke^{-2i \varphi} - k_0 e^{i \varphi}) \text{ with } \arg(z) \text{ being the argument } \theta \text{ of a complex } z = |z| e^{i \theta}, \text{ and } \lambda = 1(1) \text{ for the conduction (valence) band.} \]

For \( k \gg k_0 \) the electron states are chiral with \( \phi = -2 \varphi \) and have an approximately isotropic parabolic energy dispersion \( E^\lambda_k = \lambda h^2 k^2/2m^* \). Near \( k = k_0 \), the energy dispersion becomes highly anisotropic as shown in Fig. 1(c) and (d). The corresponding characteristic energy is \( E_0 = k_0^2/2m^* = 3.9 \) meV. At \( E = 0 \), where the Fermi energy is located in undoped graphene bilayer, there are four contact points between the conduction and valence bands: One at \( k = 0 \), the center of the valley and three satellites at \( k = k_0 \) in the directions of \( \varphi = 0, \pi/3, \text{ and } 2\pi/3 \). They can be treated as four quasi-Dirac points because the electronic states near each point has a linear energy dispersion and has the same chirality as those near a Dirac point in the monolayer graphene. However, compared to the monolayer graphene, the energy dispersion here is anisotropic and the ‘light’ velocity is about ten times slower. As illustrated in Fig. 1(c) and (d), there is an energy pocket with a depth of about \( E_0/4 \) at each quasi-Dirac point. The above peculiar characteristics of the graphene bilayer makes it quite different from the monolayer graphene in their Coulomb screening properties as described in the following.

Just as for the case of the monolayer graphene \( \lambda \) and other SU(2) spin systems \( \lambda \), we find that the dielectric matrix of a graphene bilayer is again a unit matrix multiplied by a dielectric function

\[ \varepsilon(q, \omega) = 1 - v_q \hat{\Pi}_0(q, \omega) \]

with the bare Coulomb interaction \( v_q = e^2/(2\varepsilon_0 q) \) and the electron-hole propagator

\[ \hat{\Pi}(q, \omega) = 4 \sum_{\lambda, \lambda'} |g^\lambda_{k}(q)|^2 \frac{f(E_{k+q}^\lambda) - f(E_k^\lambda)}{\omega + E_{k+q}^\lambda - E_k^\lambda + i\delta}. \]

The factor four comes from the degenerate two spins and two valleys at \( K \) and \( K' \), \( f(x) \) is the Fermi function, and the vertex factor reads \( |g^\lambda_{k}(q)|^2 = [1 + \lambda \lambda' \cos(\theta_k - \theta_{k+q})]/2 \). Near the central quasi-Dirac point at \( k = 0 \), the intraband backward scattering and interband vertical Coulomb scattering are forbidden and \( \langle g^\lambda_{k}(-\theta)(0) \rangle^2 = |g^\lambda_{k}(-2k)|^2 = 0 \). The same rules also hold for the three satellite quasi-Dirac points. For a large \( k \gg k_0 \), \( |g^\lambda_{k}(-\theta)(0) \rangle^2 = 0 \) but \( |g^\lambda_{k}(-2k)|^2 = 1 \), i.e. the intraband backward transition is allowed but both the interband backward and vertical transitions are forbidden. The above selection rules together with the energy dispersion of the carriers in the graphene bilayer indicate that electrons (holes) close to the bottom (top) of the conduction (valence) band have very different behaviors from those away from the bottom (top).

Note that in a monolayer graphene the dielectric function \( \varepsilon \) is invariant if all the parameters with the energy unit, \( \omega, E_F \), and \( k_B T \), and with the wavevector unit, \( k \)

and \( q \), vary proportionally because of the linear energy dispersion of the Dirac gas \( \lambda \). As a result, the dielectric function and the plasmon dispersion is uniform for systems with proportional parameters. In a graphene bilayer, however, this is not true anymore because of the nonlinear energy dispersion.

**Coulomb screening:** The static dielectric function at zero temperature versus \( \varphi \) is plotted in Fig. 2(a). Its long wavelength limit is given by the properties of the four quasi-Dirac points. The central point has an isotropic ‘light’ velocity \( v_0 = \hbar k_0/(2m^*) = 10^5 \) m/s while the satellite ones have the elliptic form of equienergy lines with a minimum ‘light’ velocity equal to \( v_0 \) along their radical direction and a maximum of \( 3v_0 \) along the azimuthal direction. The static dielectric constant at \( q = 0 \) is estimated to be \( \varepsilon_s = 1 + 3e^2/(8\varepsilon_0 \hbar v_0) \approx 105 \). This value is much bigger than the one for the monolayer graphene \( \lambda \). This means that the long-range Coulomb interaction is much more strongly screened for the bilayer system, thanks to a much bigger density of states near the Fermi energy in a graphene bilayer.

Another characteristic of the bilayer graphene is its screening anisotropy, especially for scattering at a distance range of about 10 nm. This is shown by the difference between the solid and the dotted curves in Fig. 2.
corresponding to the directions of \( q \) pointing to any satellite quasi-Dirac points (\( \alpha = 0 \)) or to the middle of any two satellites (\( \alpha = \pi/6 \)) respectively. Here \( \alpha \) is the angle between \( q \) and the \( x \)-axis. At \( q = \sqrt{3}k_0 = 10^8 \text{ m}^{-1} \), the wavevector distance between any two satellite quasi-Dirac points, the anisotropy of \( \varepsilon_x \) reaches its maximum whit a mismatch of 20% along the different directions. The shoulder near \( q = k_0 = 0.58 \times 10^8 \text{ m}^{-1} \) in the solid curve reflects the strong scattering between the carriers in the central and the \( \alpha = 0 \) satellite quasi-Dirac points. At a finite temperature, the energy pockets near the quasi-Dirac points are partially occupied and the intraband scattering strength is greatly enhanced. As a result, the static dielectric function near \( q = 0 \) increases rapidly, as shown in Fig. 2(b) at \( T = 4.2 \text{ K} \).

In order to have a complete picture of the Coulomb screening and an insight for understanding the plasmon spectrum in bilayer graphene, we have calculated the real and imaginary parts of the dynamic dielectric function versus the energy for a small wavevector \( q = 0.005 \) along \( \alpha = 0 \) at \( T = 0 \) and at \( T = 4.2 \text{ K} \) in Fig. 2(c) and (d).

For \( \omega > E_0/2 \), the dielectric function of a bilayer graphene is similar to that of a normal Fermi gas and its temperature dependence is weak. The step of \( \varepsilon_r \) and the peak of \( \varepsilon_i \) near \( \omega = E_0/2 = 2 \text{ meV} \) correspond to the single-particle excitation coupling states with a vanishing group velocity and having wavevectors located near the middle between the central and the satellite quasi-Dirac points. For small \( \omega \), however, the dielectric function becomes more sensitive to the temperature and shows characteristics of the Dirac gas. One sign of the Dirac gas is the lack of Coulomb screening (\( \varepsilon_r \approx 1 \)) in the energy window between 1 and 2 meV. Another sign is that a low-energy plasmon mode appears only at a finite temperature. As shown in Fig. 2(c), the \( \varepsilon_r \) has no negative value for the energy \( \omega < E_0/2 \) at \( T = 0 \) but evolves into a deep negative dip at a finite temperature \( T = 4.2 \text{ K} \), when the energy pockets near the quasi-Dirac points is partially occupied. As a result, one observes a weakly Landau damped plasmon mode of dispersion \( \omega \sim \sqrt{r} \) at \( T = 0 \) and a couple at finite temperatures.

**Collective excitation:** In Fig. 3(a), we calculate the plasmon spectrum of an intrinsic bilayer graphene (\( E_F = 0 \)). The dispersion of the weakly Landau damped mode is indicated by the thick curve and has a \( \sqrt{r} \) dependence. Interestingly, the plasmon mode exists only at the energy higher than \( E_0/2 \), i.e., double the depth of the energy pockets in the quasi-Dirac points. At a finite temperature \( T = 4.2 \text{ K} \), another weakly damped plasmon mode shows up at the energy lower than \( E_0/2 \) and also has a dispersion of \( \sqrt{r} \) near \( q = 0 \), as illustrated in Fig. 3(b). The plasmon mode of higher energy existing at \( T = 0 \) is not sensitive to the temperature. This temperature depen-
The plasmon spectrum of a doped bilayer graphene (solid curve) with a typical carrier density of $10^{12}$ cm$^{-2}$. Correspondingly, $E_F = 36.3$ meV and $k_F = 1.77 \times 10^6$ m$^{-1}$. The plasmon spectrum in the same system but without chirality is plotted as a dotted curve for comparison. Intra- (dark shaded) and inter- (light shaded) band single-particle continua are also shown.

The carrier density of the system can be changed by doping [7]. For a typical doping density of $10^{12}$ cm$^{-2}$, the Fermi energy is high enough from the conduction bottom and the linear $k$ term in the Hamiltonian can be neglected. The electrons then have a quadratic dispersion but with chirality and $\phi = -2\varphi$. Near $q = 0$, the plasmon dispersion in a doped bilayer graphene has again a $\sqrt{q}$ dispersion as shown by the solid curve in Fig. 4 and shares the same dispersion $\omega_p^{2D} = |n_e e^2 q / 2 \varepsilon_0 m^*|^{1/2}$ with a normal two-dimensional Fermi gas. To see the effect of the chirality, we plot as a dotted curve the plasmon dispersion of a normal two-dimensional Fermi gas with two valleys, for comparison. The two curves overlap for the small $q$ but separate as $q$ increases. The maximum difference in dispersion appears near $q = \sqrt{2} k_F$ when $k$ and $k + q$ form a right angle in the Fermi plane and the corresponding transition is forbidden in the graphene bilayer due to its chirality.

In summary, we have explored the Coulomb screening properties and the collective excitation modes in a graphene bilayer. In an undoped system, the static dielectric constant is much bigger than that in a monolayer graphene, due to the existence of four quasi-Dirac points in each energy valley and the much lower 'light' velocity of the quasi-Dirac points than the one in a monolayer graphene. The Coulomb screening also shows a strong anisotropy, especially near the wavevector $q = \sqrt{3} k_0$.

The work has been supported by the Canada Research Chair Program and a Canadian Foundation for Innovation (CFI) Grant.

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