Coulomb screening and collective excitations in biased bilayer graphene

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We have investigated the Coulomb screening properties and plasmon spectrum in a bilayer graphene under a perpendicular electric bias. The bias voltage applied between the two graphene layers opens a gap in the single-particle energy spectrum and modifies the many-body correlations and collective excitations. The energy gap can soften the plasmon modes and lead to a crossover of the plasmons from a Landau damped mode to being undamped. Plasmon modes of long lifetime may be observable in experiments and may have potentials for device applications.

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Bilayer graphene (BLG) has attracted much attention due to its unique electronic characteristics, distinct from the Dirac gas in monolayer graphene and the Fermi gas in traditional semiconductor quantum wells. In addition, an energy gap between the conduction and valence bands of a BLG can be opened and tuned by introducing an electrostatic potential bias between the two graphene layers. This can be easily realized via one or more external gates to perpendicularly bias BLG and make it a potential component for integrated electronics. It is then very intriguing to understand some fundamental properties such as correlation and screening properties of electron gases in a biased BLG. As collective excitations, plasmon modes are a direct result of electronic correlation due to Coulomb interaction between electrons. Experimental detection of plasmon modes has recently become feasible and has been used to determine the dynamical behavior of electrons in graphene layers.

Previously, assuming zero or nonzero spin-orbit interaction induced energy gap, we have studied the Coulomb screening and collective excitation spectrum of intrinsic and doped monolayer graphenes at zero and finite temperatures in the random-phase approximation (RPA). Later, Qaiumzadeh and Asgari assumed an unspecified energy gap of arbitrary width for doped monolayer graphene and studied the corresponding ground-state properties at zero temperature in RPA. They concluded that the conductance and charge compressibility decrease with the band gap. Furthermore, a THz source has been proposed based on the stimulated plasmon emission in graphene and the absorption of THz electromagnetic radiation in gapped graphene has been estimated. On the other hand, the Coulomb screening and the collective excitations in zero gap BLG have been studied in our previous work at zero and finite temperatures and by Hwang and Das Sarma for the zero-temperature case. In this Rapid Communication we report on our studies of the correlations, screening, and the plasmon spectrum of electron gases in a biased BLG.

In the effective-mass approximation, the Hamiltonian describing electrons of moderate energies in the K valley of a biased BLG reads as

\[ H_K = \frac{\hbar^2}{2m} \begin{pmatrix} 0 & \kappa^2 \\ \kappa^2 & 0 \end{pmatrix} + \frac{U}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \]
The factor four comes from the degenerate two spins and two valleys at \(K\) and \(K'\), \(f(\lambda)\) is the Fermi function, and the vertex factor reads \(|g_{k}^{\lambda\lambda'}(q)|^2 = \frac{1}{2} \left[ 1 + \lambda \lambda' \cos \alpha_k \cos \alpha_{k+q} + \lambda \sin \alpha_k \sin \alpha_{k+q} \cos (2\delta_k - 2\delta_{k+q}) \right]\). At \(q = 0\) or \(q = -2k\), \(|g_{k}^{\lambda\lambda'}(q)|^2 = (1 + \lambda \lambda')/2\). Similar to unbiased BLG, the intraband vertical and back scatterings are both forbidden but the intraband back scattering is allowed in biased BLG.

It has been shown that the interlayer indirect C-C interaction introduces anisotropic fine structures near the Fermi energy in the range of 2 meV and leads to some interesting dielectric and collective phenomena.\(^2\) For systems with energy gap \(U > 5\) meV or with Fermi energy \(E_F\) satisfying \(|E_F-kT| > 3\) meV, this anisotropy becomes negligible. For large \(U\) comparable to \(v_t\), the effect of the “Mexican hat” at the bottom (top) of the conduction (valence) band\(^1\) should be taken into account. Nevertheless, for moderate \(U\) and \(E_F\), the model described here should be valid. Furthermore, we assume that the BLG is far enough from the substrate and the gate so a unit background dielectric constant is used in the calculation.

In intrinsic BLG where no net carrier exists, i.e., \(N=0\) and the Fermi energy \(E_F=0\), intraband scattering is only allowed at nonzero temperatures. In Fig. 1, we have shown that the real part \(\epsilon_r\) (solid curve) and imaginary part \(\epsilon_i\) (dotted) of the dielectric function exist in the energy gap \(>3\) meV. Thus the anisotropy becomes negligible. For large \(U\) comparable to \(v_t\), the effect of the “Mexican hat” at the bottom (top) of the conduction (valence) band\(^1\) should be taken into account. Nevertheless, for moderate \(U\) and \(E_F\), the model described here should be valid. Furthermore, we assume that the BLG is far enough from the substrate and the gate so a unit background dielectric constant is used in the calculation.

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plasmon dispersion in BLG without bias which is just slightly modified from that of Fermi 2D gas, this dispersion is greatly softened for finite $q$ as also shown in Fig. 4. Our numerical analysis shows that this is a result of the deformation near the bottom and top of the energy bands. Note that the lowered plasmon group velocity may be helpful for making a stimulated plasmon oscillator. A Landau damped mode is located just below the intraband SPEC edge as usually happens in traditional 2D Fermi gas but is pushed to lower energy at larger $q$. The undamped mode can enter into the interband SPEC and becomes a slightly damped mode in some cases as shown in Fig. 3(a) under $U=30$ meV or merges with the damped mode and disappears near the cross of intra- and interband SPEC edges as shown in Fig. 3(b) under $U=60$ meV.

With the plasmon spectrum in mind, we now explore how $U$ affects the energy and damping properties of the modes. In the left panels of Fig. 4, we show $\omega$ versus $U$ at several typical $q$ when keeping the Fermi energy constant. As in Fig. 3, the light shadow indicates the interband SPEC and the dark shadow for the intraband one. At small $q$ as illustrated in (a), there is one undamped plasmon mode with energy located inside the SPEC gap of which the width is about $2E_F$ and one damped mode of low frequency. When $U$ reaches and passes $2E_F$, the Fermi level drops below the conduction bottom and the two plasmon modes merge and disappear. At larger $q$, the intraband SPEC edge shifts up and the interband one shifts down for $U<2E_F$ and $\omega$ increases as shown in (b) and also in Fig. 3. Then the two SPECs will merge and the previous undamped plasmon mode enter the interband SPEC and become slightly damped. In this case, we may open the SPEC gap again by applying a stronger bias and transfer the slightly damped plasmon mode into a undamped as shown in (c). The $\omega$ versus $U$ curve forms a shoulder when it meets the interband SPEC reflecting the strong coupling between the single-particle and collective excitations as also shown in other cases.$^{2,15,20}$

If $N$ remains constant as shown in the right panels, the Fermi vector is also constant but the $E_F$ shifts up with $U$. This is clearly shown in (d) by the interband SPEC edge of small $q$ which is located near $\omega=2E_F$. The undamped plasmon mode continues to exist as $U$ increases and its energy varies slowly. This is because $E_F$ is always higher than the conduction bottom with a constant Fermi vector. $\omega$ decreases with $U$ as the effective mass near $E_F$ increases. For a large $q$ the plasmon mode located inside the interband SPEC and is slightly damped at small $U$, one can always make it undamped by increasing the bias and widening the gap between the intra- and interband SPECs as shown in (f).

When an external gate voltage is applied to a BLG, the carrier density varies with the gate voltage as well as the energy gap. Although $N$ and $U$ can be dependent on each other in a nontrivial way, our result suggests that $\omega$ is proportional to $\sqrt{N}$ in almost the same way in both doped and undoped BLG. This happens because $\omega$ is mainly determined by $N$ as illustrated in the right panels of Fig. 4. The variation in $U$ of small amount affects $\omega$ only in a very limited scale. Nevertheless, as shown in Fig. 4, the higher $U$ opens a wider energy gap in the SPEC and prolongs the lifetime of the plasmon modes. In other words, a gate voltage can vary the imaginary part of the dielectric constant at the plasmon energy and the effect may be observed in experiments.

In summary, a potential bias can be applied between the two graphene layers of a bilayer graphene with the help of a gate voltage. We have studied the effect of the potential bias on electronic correlations, Coulomb screening, and collective excitations at both zero and finite temperature. The potential bias opens a gap in the single-particle energy spectrum and makes the semimetal bilayer graphene a semiconductor. As a result, the dielectric function for the Coulomb interaction and the propagator function are modified significantly. The potential bias also opens a gap in the single-particle excitation spectrum and softens the collective excitation modes. This
may result in undamped collective excitation modes that are observable in experiments. In the single gate configuration, the doping and gate voltage can vary the potential bias and the carrier density of the bilayer graphene and manipulate the energy and lifetime of the collective excitation modes inside.

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