Screening, Kohn Anomaly, Friedel Oscillation, and RKKY Interaction in Bilayer Graphene

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(Received 18 April 2008; published 8 October 2008)

We calculate the screening function in bilayer graphene (BLG) in both the intrinsic (undoped) and the extrinsic (doped) regimes within the random phase approximation, comparing our results with the corresponding single layer graphene and the regular two-dimensional electron gas. We find that the Kohn anomaly is strongly enhanced in BLG. We also discuss the Friedel oscillation and the RKKY interaction, which are associated with the nonanalytic behavior of the screening function at $q = 2k_F$. We find that the Kohn anomaly, the Friedel oscillation, and the RKKY interaction are all qualitatively different in the BLG compared with the single layer graphene and the two-dimensional electron gas.

DOI: 10.1103/PhysRevLett.101.156802 PACS numbers: 73.21.−b, 71.10.−w, 73.43.Lp

Single layer graphene (SLG), a single layer of carbon atoms arranged in a honeycomb lattice, has attracted a great deal of attention, both experimentally and theoretically, for its unusual electronic transport and the characteristics of relativistic charge carriers behaving like massless chiral Dirac fermions [1]. Bilayer graphene (BLG) consisting of two SLG is also of great current interest, for both technological applications and fundamental interest [1–3]. While the band structure of SLG has a linear dispersion, BLG has a quadratic dispersion [2] in the low energy regime making it similar to two-dimensional (2D) semiconductor systems except for the absence of a gap. The purpose of this work is to calculate the polarizability (or screening) function of bilayer graphene within the random phase approximation (RPA). Even though many theoretical works on Coulomb screening in graphene have been reported [4–7], the analytic investigation of Coulomb screening in BLG has not yet been performed. Recently, the screening of BLG was considered numerically in Ref. [8], but such a numerical calculation is less useful in any general context. Knowing the BLG screening function is crucial since it determines many fundamental properties: e.g., transport through screened Coulomb scattering by charged impurities [9], Kohn anomaly in phonon dispersion [10], and RKKY interaction [11]. In order to understand the electronic properties of BLG, it is therefore necessary to obtain its screening function.

The BLG is in some sense intermediate between the SLG and the regular semiconductor-based two-dimensional electron gas (2DEG) since it is chiral with a zero band gap at the Dirac point (where the electron and the hole bands touch) similar to the SLG but has the quadratic energy dispersion similar to the 2DEG. For example, the $2k_F$ backscattering is suppressed [4–7] in SLG due to its chiral nature, whereas in the 2DEG, the $2k_F$ backscattering plays a key role [12] in determining low density and low temperature carrier transport. We find that the $2k_F$ backscattering is restored (and even enhanced) in the BLG because of the quadratic dispersion and, more importantly, due to the symmetry imposed by the two-layer structure. This qualitative difference in the screening properties between BLG and SLG leads us to predict that transport and other electronic properties in BLG will be qualitatively more similar to 2DEG than to SLG in spite of the zero-gap chiral nature of BLG.

The effective BLG Hamiltonian is now well established in the theoretical literature. In the low energy regime, the Hamiltonian is reduced to the (2×2) matrix form and is given by (we use $\hbar = 1$ throughout this Letter) [2]

$$H_0 = -\frac{1}{2m}\begin{pmatrix} 0 & (k_x - ik_y)^2 \\ (k_x + ik_y)^2 & 0 \end{pmatrix}, \qquad (1)$$

where $m = \gamma_1/(2v_F^2)$, γ_1 is the interlayer tunneling amplitude, and v_F is the SLG Fermi velocity. The wave function of Eq. (1) can be written as $\psi_{s\mathbf{k}} = e^{i\mathbf{k}\mathbf{r}}(e^{-2i\theta_{\mathbf{k}}}, s)/\sqrt{2}$, and the corresponding energy is given by $\epsilon_{s\mathbf{k}} = sk^2/2m$, where $\theta_{\mathbf{k}} = \tan^{-1}(k_y/k_x)$ and $s = \pm 1$ denote the band index. Using the Hamiltonian of Eq. (1), we theoretically obtain the screening function of BLG by calculating the polarizability and the dielectric function within the RPA.

The static dielectric function can be written as

$$\epsilon(q) = 1 - \frac{2\pi e^2}{\kappa q}\Pi(q), \qquad (2)$$

where κ is the background dielectric constant and $\Pi(q)$ the polarizability. The static BLG polarizability is given by the bare bubble diagram

$$\Pi(q) = \frac{g}{L^2}\sum_{\mathbf{k}ss'}\frac{f_{s\mathbf{k}} - f_{s'\mathbf{k}'}}{\varepsilon_{s\mathbf{k}} - \varepsilon_{s'\mathbf{k}'}}F_{ss'}(\mathbf{k}, \mathbf{k}'), \qquad (3)$$

where g is the degeneracy factor (here $g = 4$ due to valley and spin degeneracies), $\mathbf{k}' = \mathbf{k} + \mathbf{q}$, $s, s' = \pm 1$ denote the band indices, $\varepsilon_{sk} = sk^2/2m$, and $F_{ss'}(\mathbf{k}, \mathbf{k}') = (1 + ss'\cos 2\theta)/2$, where θ is the angle between $\mathbf{k}$ and $\mathbf{k}'$, and f_{sk} is the Fermi distribution function $f_{s\mathbf{k}} = [\exp\{\beta(\varepsilon_{s\mathbf{k}} - \mu)\} + 1]^{-1}$, with $\beta = 1/k_BT$ and μ the chemical potential.

First, we consider intrinsic (i.e., undoped or ungated, with n and E_F both being zero) BLG where the conduction band is empty and the valence band fully occupied at $T = 0$. Then we have $f_{+\mathbf{k}} = 0$ and $f_{-\mathbf{k}} = 1$. Since the conduction band is empty, the polarization is induced by the virtual interband transition of electrons from the valence to the conduction band. The polarizability due to the interband transition becomes $\Pi(q) \equiv \Pi^0(q)$, where

$$\Pi^0(q) = \frac{g}{2}\int \frac{d^2k}{(2\pi)^2}\left[\frac{1-\cos 2\theta}{\varepsilon_{+\mathbf{k}} - \varepsilon_{-\mathbf{k}'}} - \frac{1-\cos 2\theta}{\varepsilon_{-\mathbf{k}} - \varepsilon_{+\mathbf{k}'}}\right], \quad (4)$$

where $\cos\theta = (|\mathbf{k}| + |\mathbf{q}|\cos\phi)/|\mathbf{k}+\mathbf{q}|$. Equation (4) can be calculated easily as

$$\Pi^0(q) = N_0 \log 4, \quad (5)$$

where $N_0 = gm/2\pi$ is the BLG density of states. Thus the intrinsic BLG polarizability is constant for all wave vectors. (Note that the polarizability of ordinary 2DEG is constant [11] only for $q \leq 2k_F$.) The dielectric function becomes $\epsilon(q) = 1 + q_s/q$, where the screening wave vector is given by

$$q_s = q_{\mathrm{TF}} \log 4, \quad (6)$$

where q_{TF} is the 2D Thomas-Fermi screening wave vector [11]: $q_{\mathrm{TF}} = gme^2/\kappa$. BLG static screening is thus enhanced by a factor of log4 compared with ordinary 2D screening [11]. For intrinsic BLG we can write the screened Coulomb potential as

$$\phi(r) = \frac{e}{\kappa r} - \frac{e}{\kappa}\frac{\pi q_s}{2}[H_0(q_s r) - N_0(q_s r)], \quad (7)$$

where $H_0(x)$ and $N_0(x)$ are the Struve function and the Bessel function of the second kind, respectively. The asymptotic form at large r is $\phi(r) \sim eq_s/\kappa(q_s r)^3$. Since the screening function is a constant for all q without any singular behavior, there is no oscillatory term in the potential. This is very different from the screening behavior of intrinsic SLG [4–6] or 2DEG [11].

For intrinsic SLG we have

$$\Pi^0(q) = N_0^{\mathrm{SLG}}\frac{\pi}{8}, \quad (8)$$

where $N_0^{\mathrm{SLG}} = gq/(2\pi v_F)$. The intrinsic SLG polarizability increases linearly with q, and $\epsilon(q) = 1 + (e^2 g/\kappa v_F) \times (\pi/8)$, which gives rise to only an enhancement of the effective background dielectric constant $\kappa^* = \kappa + (e^2 g/v_F)(\pi/8)$, i.e., the screened Coulomb interaction $V(q) = 2\pi e^2/\kappa^* q$. The Coulomb interaction in real space can be expressed by $V(r) = e^2/\kappa^* r$ for all r. Thus at large r the Coulomb potential decreases as $1/r^3$ in intrinsic BLG but only as $1/r$ in intrinsic SLG.

In the following we provide the zero temperature static polarizability of extrinsic (i.e., gated or doped) BLG where $n, E_F \neq 0$. At $T = 0$, $f_{-\mathbf{k}} = 1$ and $f_{+\mathbf{k}} = \theta(k_F - |\mathbf{k}|)$. Then we can rewrite Eq. (1) as $\Pi(q) = \Pi_{\mathrm{intra}}(q) + \Pi_{\mathrm{inter}}(q)$, where

$$\Pi_{\mathrm{intra}}(q) = -\frac{g}{L^2}\sum_{\mathbf{k}s}\left[\frac{f_{s\mathbf{k}} - f_{s\mathbf{k}'}}{\varepsilon_{s\mathbf{k}} - \varepsilon_{s\mathbf{k}'}}\right]\frac{1+\cos 2\theta}{2} \quad (9)$$

and

$$\Pi_{\mathrm{inter}}(q) = -\frac{g}{L^2}\sum_{\mathbf{k}s}\left[\frac{f_{s\mathbf{k}} - f_{-s\mathbf{k}'}}{\varepsilon_{s\mathbf{k}} - \varepsilon_{-s\mathbf{k}'}}\right]\frac{1-\cos 2\theta}{2}. \quad (10)$$

Π_{intra} (Π_{inter}) indicates the polarization due to intraband (interband) transition. After angular integration over the direction of $\mathbf{q}$, we have

$$\Pi_{\mathrm{intra}}(q) = \frac{gm}{2\pi}\int_0^{k_F}\frac{dk}{k^3}\left[k^2 - |k^2 - q^2| + \frac{(2k^2-q^2)^2}{q\sqrt{q^2-4k^2}}\theta(q-2k)\right], \quad (11)$$

$$\Pi_{\mathrm{inter}}(q) = \frac{gm}{2\pi}\int_{k_F}^{\infty}\frac{dk}{k^3}[-k^2 - |k^2 - q^2| + \sqrt{4k^4 + q^4}]. \quad (12)$$

Then

$$\frac{\Pi_{\mathrm{intra}}(q)}{N_0} = \begin{cases} 1 - \frac{q^2}{2k_F^2} & \text{if } q \leq k_F, \\ \frac{q^2}{2k_F^2} - 2\log\frac{q}{k_F} & \text{if } k_F < q < 2k_F, \\ \frac{q^2}{2k_F^2} - 2\log\frac{q}{k_F} - f(q) & \text{if } q > 2k_F, \end{cases} \quad (13)$$

$$\frac{\Pi_{\mathrm{inter}}(q)}{N_0} = \begin{cases} -1 + \frac{q^2}{2k_F^2} + g(q) & \text{if } q \leq k_F, \\ -\frac{q^2}{2k_F^2} + 2\log q + g(q) & \text{if } q > k_F, \end{cases} \quad (14)$$

with

$$f(q) = \frac{2k_F^2 + q^2}{2k_F^2 q}\sqrt{q^2 - 4k_F^2} + \log\frac{q - \sqrt{q^2-4k_F^2}}{q + \sqrt{q^2 - 4k_F^2}},$$
$$g(q) = \frac{1}{2k_F^2}\sqrt{4k_F^4 + q^4} - \log\left[\frac{k_F^2 + \sqrt{k_F^4 + q^4/4}}{2k_F^2}\right]. \quad (15)$$

Finally, we have the extrinsic BLG static polarizability as

$$\Pi(q) = N_0[g(q) - f(q)\theta(q - 2k_F)]. \quad (16)$$

Equation (16) with Eq. (15) is the basic result obtained in this Letter, giving the doped BLG polarizability analytically.

In Fig. 1, we show the calculated static polarizability as a function of the wave vector. Figures 1(a) and 1(b) show the calculated intraband and interband polarizabilities, respectively, with those of single layer graphene for comparison. Figure 1(c) shows total polarizability of bilayer graphene. At $q = 0$, we have $\Pi_{\mathrm{intra}}(0) = N_0$ and $\Pi_{\mathrm{inter}}(0) = 0$, which follow also from the compressibility sum rule $\Pi(q=0) = \int d\varepsilon[-df(\epsilon)/d\varepsilon]N(\varepsilon_q)$. For small

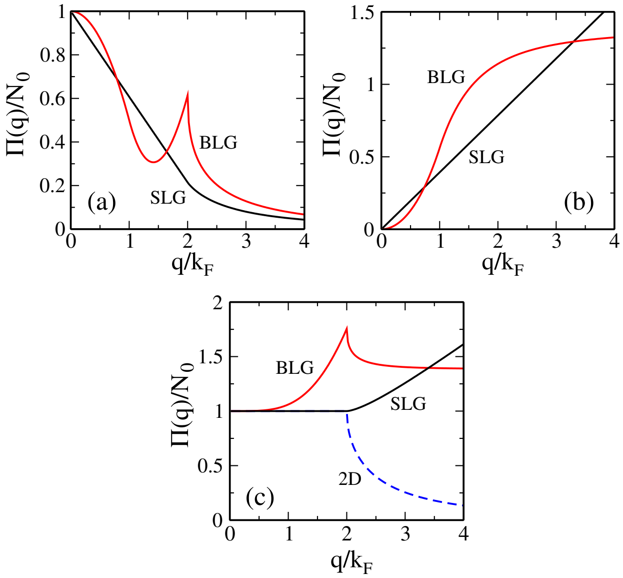

FIG. 1 (color online). Calculated (a) intraband, (b) interband, and (c) total static polarizability of bilayer graphene. For comparison, the single layer polarizabilities are shown. In (c), we also show the regular 2D static polarizability (dashed line).

q, $\Pi_{\rm intra}(q)$ decreases as $1 - q^2/2k_F^2$, and $\Pi_{\rm inter}(q)$ increases as $q^2/2k_F^2$. This behavior comes from the overlap factor $F_{ss'}$ in Eq. (3). For SLG, intraband (interband) polarizability decreases (increases) linearly as q increases, and these two effects exactly cancel out up to $q = 2k_F$, which gives rise to the total static polarizability being constant for $q < 2k_F$ as in the 2DEG. However, for BLG, the cancellation of two polarizability functions is not exact especially for $q > k_F$ because of the enhanced backscattering, so the total polarizability increases as q approaches $2k_F$, which means screening increases as q increases. Thus BLG, in spite of being a 2D system, does not have a constant Thomas-Fermi screening up to $q = 2k_F$ as exists in SLG and 2DEG.

A qualitative difference between SLG and BLG polarizability functions is at $q = 2k_F$. Because of the suppression of $2k_F$ backward scattering in SLG, the total polarizability as well as its first derivative are continuous. In BLG, however, the large angle scattering is enhanced due to chirality [i.e., the overlap factor $F_{ss'}$ in Eq. (3)], which gives rise to the singular behavior of polarizability at $q = 2k_F$. Even though the BLG polarizability is continuous at $q = 2k_F$, it has a sharp cusp and its derivative is discontinuous at $2k_F$, diverging as q approaches $2k_F$; i.e., as $q \to 2k_F$, $d\Pi(q)/dq \propto 1/\sqrt{q^2 - 4k_F^2}$. This behavior is exactly the same as that of the regular 2DEG, which also has a cusp at $q = 2k_F$ in addition to being constant in the $0 \le q \le 2k_F$ region. Note that in SLG this nonanalytic behavior of polarizability occurs in the second derivative: $d^2\Pi(q)/dq^2 \propto 1/\sqrt{q^2 - 4k_F^2}$.

In the large momentum transfer regime $q > 2k_F$, the BLG polarizability approaches a constant value (intrinsic polarizability Π^0), i.e., $\Pi(q) \to N_0 \log 4$, because the interband transition dominates over the intraband contribution in the large wave vector limit. This is very different from that of a 2DEG, where the static polarizability falls off rapidly ($\sim 1/q^2$) for $q > 2k_F$ [11], and SLG, where the polarizability increases linearly as q. Thus, the large q behavior of dielectric screening becomes $\epsilon(q \to \infty) \to 1 + g\pi e^2/(8\kappa v_F)$ for SLG and $\epsilon(q \to \infty) \to 1$ for both BLG and 2DEG.

The strong cusp in BLG $\Pi(q)$ at $q = 2k_F$ leads to Friedel oscillations in contrast to the SLG behavior. The leading oscillation term in the screened potential at large distances from a point charge Ze can be calculated as

$$\phi(r) \sim -\frac{e}{\kappa} \frac{4q_{\rm TF}k_F^2}{(2k_F + Cq_{\rm TF})^2} \frac{\sin(2k_F r)}{(2k_F r)^2}, \tag{17}$$

where $C = \sqrt{5} - \log[(1 + \sqrt{5})/2]$, which is similar to the 2DEG except for the additional constant C ($C = 1$ for 2DEG) but different from SLG where Friedel oscillations scale as $\phi(r) \sim \cos(2k_F r)/r^3$ [13]. The enhanced singular behavior of the BLG screening function at $q = 2k_F$ has other interesting consequences related to Kohn anomaly [10] and RKKY interaction, which we discuss below.

The strong cusp in the BLG polarizability at $q = 2k_F$, as can be clearly seen in Fig. 1(c), indicates that the screened BLG acoustic phonon frequency would manifest a strong Kohn anomaly, i.e., an observable dip structure in the phonon frequency at $q = 2k_F$. It is obvious from Fig. 1(c), and from the discussion above based on our analytical results for $\epsilon(q)$, that the screened phonon dispersion will exhibit a much stronger Kohn anomaly in the BLG than in the SLG with the 2DEG being intermediate. This arises from the stronger singularity at $q = 2k_F$ manifesting in the *first* derivative $d\Pi(q)/dq$ in the BLG rather than in the *second* derivative $d^2\Pi/dq^2$ in the SLG. Tuning the value of k_F by changing the carrier density through the applied gate voltage, it should be possible to verify that the Kohn anomaly is indeed associated with the $2k_F$ screening behavior in the BLG. In fact, the BLG Kohn anomaly would be, due to the very strong $q = 2k_F$ cusp in the polarizability, rather similar to the 1D Peierls instability [14] since the $q = 2k_F$ screening behavior in BLG is qualitatively similar to the 1D electron system [15].

The polarizability function in Eq. (16) also determines the RKKY interaction between two magnetic impurities due to the induced spin density (here we consider magnetic impurities located at the interface between BLG and substrate, so they do not break any symmetry). The RKKY interaction (or induced spin density) is proportional to the Fourier transform of $\Pi(q)$. The conventional form of the exchange interaction between the localized moment S and electron-spin density $s(r)$ is given by $V(r) = JS(\mathbf{R})s(\mathbf{r})\delta(\mathbf{R} - \mathbf{r})$, where J is the exchange coupling constant. The RKKY interaction between two localized moments via the conduction electrons may then be written in the following form: $H_{\rm RKKY}(r) = J^2 S_1 S_2 \Pi(\mathbf{r})$, where $\Pi(r)$ is the Fourier transform of the static polarizability $\Pi(q)$.

First, consider intrinsic BLG. The Fourier transform of Eq. (5) simply becomes a δ function because $\Pi^0(q)$ is a constant, i.e., $\Pi(r) = N_0 \log(4)\delta(r)$. This indicates that the localized magnetic moments are not correlated by the long range interaction and there is no net magnetic moment. In SLG, the Fourier transform of polarizability [Eq. (8)] diverges [even though $\Pi(r)$ formally scales as $1/r^3$, its magnitude does not converge], which means that intrinsic SLG is susceptible to ferromagnetic ordering in the presence of magnetic impurities [16,17] due to the divergent RKKY coupling.

In doped (or gated) BLG, the oscillatory term in RKKY interaction is restored due to the singularity of polarizability at $q = 2k_F$, and the oscillating behavior dominates at large $k_F r$. At large distances $2k_F r \gg 1$, the dominant oscillating term in $\Pi(r)$ is given by

$$\Pi(r) \sim N_0 \frac{k_F^2}{2\pi} \frac{\sin(2k_F r)}{(k_F r)^2}. \tag{18}$$

This is the same RKKY interaction as in a regular 2DEG, and it decreases as $1/r^2$, in contrast with $1/r^3$ behavior in SLG [6].

In conclusion, we calculate analytically the static wave vector dependent polarizability of both undoped and doped bilayer graphene within the RPA. For undoped BLG, we find that screening is enhanced by a factor of log4 compared with ordinary 2D screening. The RKKY interaction in undoped BLG is zero-ranged (δ function). The doped BLG screening function shows strongly enhanced Kohn anomaly at $2k_F$ compared with the corresponding SLG and 2DEG situations, which give rise to the usual RKKY interaction and Friedel oscillation. We show that BLG screening properties are qualitatively different from SLG screening behavior in all wave vector regimes ($q < 2k_F$, $q > 2k_F$, and $q = 2k_F$) with the BLG screening having a strong cusp at $q = 2k_F$. Our theory applies only in the density regime ($10^{10} < n < 5 \times 10^{12}$ cm^{-2}), where the band dispersion is quadratic and only the lowest subband is occupied [2], but the RPA should be well valid due to the interaction parameter r_s being generally small in graphene [3]. There are obvious implications of our results for BLG carrier transport limited by screened Coulomb scattering—in particular, the strong $2k_F$ anomaly in screening will lead to strong temperature dependence in dc transport at low ($T \ll T_F$) temperatures. This is in sharp contrast to SLG where $2k_F$ backscattering is suppressed.

This work is supported by U.S. ONR, NSF-NRI, and SWAN.

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