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Plasmon modes in Dirac/Schrödinger hybrid electron systems including layer-thickness and exchange-correlation effects

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Abstract

We calculate the plasmon dispersion relation and damping rate of collective excitations in a double-layer system consisting of monolayer graphene and GaAs quantum well at zero temperature including layer-thickness and exchange-correlation effects. We use the generalized random-phase-approximation dielectric function and take into account the nonhomogeneity of the dielectric background of the system. We show that the effects of layer thickness, electron densities and exchange-correlations are more pronounced for acoustic modes, while the optical branch depends remarkably on dielectric constants of the contacting media.

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Keywords: Graphene; Plasmon; Collective excitations.

1. Introduction

Graphene, a special two-dimensional electron gas (2DEG) system, has attracted a great deal of attention in recent years because of its unique electronic properties [1-3]. Charge carriers in graphene are Dirac-like massless, chiral fermions near the Dirac points, K and K' where the band structure of graphene is linear. The chiral electron wave function and linear dispersion lead to many properties significantly different from those of ordinary 2DEG systems [4].

Plasmon excitations in many-electron systems have been studied long time ago and have been used to create plasmonic devices [5]. It was revealed that plasmon modes of graphene possess special properties [6-7] and the plasmon dispersion relation in double-layer systems differs significantly from the single layer one [4, 8-13]. It has long been known that a two-component electron plasma has two branches of collective excitations. The higher-frequency (lower-frequency) branch corresponds to in-phase (out of phase) oscillations of densities in the two layers and has been called “optical plasmon” (“acoustic plasmon”). Acoustic plasmon in graphene systems has been studied intensively in recent years both theoretically [11-17] and experimentally [18-20]. Plasmons in double-layer structures formed by 2DEG and monolayer graphene (MLG) sheets, separated by a spacer, may have more interesting properties because the carrier densities of these massless-massive systems might be significantly different in both layers [14-17]. The authors of Refs. [14-16] have considered a MLG-2DEG double layers surrounding by a nonhomogeneous two dielectric medium. Their focus of interest was the derivation of analytical expressions for acoustic-plasmon group velocity at zero temperature. The thickness of 2DEG sheet was neglected and numerical results are very limited. Gonzalez de la Cruz has included the 2DEG thickness in the recent paper [17] but has still used the

model with two dielectric medium instead of realistic one with four dielectric constants. It was shown recently for systems consisting of two zero-thickness layers [21-22] that the differences between dielectric constants of contacting media can have significant effects on plasmon dispersions and must be taken into account to improve the results of models with one or two dielectric constants. The realistic model with finite thickness 2DEG and four dielectric medium has been used by the authors of Ref. [23] to calculate Coulomb drag resistivity. To our knowledge, up to now no calculations on plasmon dispersions have been done for such a realistic model.

Therefore, in this paper, we calculate frequency and damping rate of plasmon modes in a double-layer system consisting of doped MLG and GaAs quantum well of finite thickness w , separated by a spacer of width d assuming that 2DEGs in MLG and GaAs are electrically isolated [23-24]. We use the generalized random-phase-approximation (RPA) dielectric function, and take into account the nonhomogeneity of dielectric background [23] and the exchange-correlation effect which is very important for ordinary 2DEG with low electron density [10].

2. Theory

We consider a double-layer system consisting of a MLG flake placed onto modulation-doped GaAs/AlGaAs heterostructure hosting a 2DEG, with the effective mass m^* , in the GaAs quantum well as shown in Fig. 1.

Fig. 1. A MLG-2DEG double-layer system immersed in a three layered dielectric medium with the background dielectric constants κ_1 , κ_2 and κ_3 .

The plasmon dispersion relation of an electronic system can be obtained from the zeroes of dynamical dielectric function [10-11]

$$\varepsilon(q, \omega_p - i\gamma) = 0 \quad (1)$$

where ω_p is the plasmon frequency at a given wave-vector q and γ is the damping rate of plasma oscillations. In case of weak damping ($\gamma \ll \omega_p$), the plasmon dispersion and decay rate are determined from the following equations [10-11]

$$\operatorname{Re} \varepsilon(q, \omega_p) = 0 \quad (2)$$

and

$$\gamma = \operatorname{Im} \varepsilon(q, \omega_p) \left(\frac{\partial \operatorname{Re} \varepsilon(q, \omega)}{\partial \omega} \bigg|_{\omega=\omega_p} \right)^{-1} \quad (3)$$

In the RPA, the dynamical dielectric function of MLG-2DEG double-layer system has the form [21-22]

$$\begin{aligned} \varepsilon_{\text{MLG-2DEG}}(q, \omega) = & \left[1 + U_{2\text{DEG}}(q) [1 - G(q)] \Pi_{2\text{DEG}}(q, \omega) \right] \times \\ & \times \left[1 + U_{\text{MLG}}(q) \Pi_{\text{MLG}}(q, \omega) \right] - [U_{\text{MLG-2DEG}}(q)]^2 \Pi_{2\text{DEG}}(q, \omega) \Pi_{\text{MLG}}(q, \omega) \end{aligned} \quad (4)$$

where $\Pi_{2\text{DEG}}(q, \omega)$ ($\Pi_{\text{MLG}}(q, \omega)$) is the zero-temperature non-interacting density-density response function of the 2DEG (MLG) given in [10, 25] ([4]). $G(q)$ is a local-field correction (LFC) describing the exchange-correlation effects [26-27], $U_{2\text{DEG/MLG}}(q)$ and $U_{\text{MLG-2DEG}}(q)$ are the intra- and inter-layer bare Coulomb interactions in momentum space [23],

$$U_{2\text{DEG/MLG}}(q) = \frac{4\pi e^2}{q} f_{2\text{DEG/MLG}}(qd, qw), \quad (5)$$

$$U_{\text{MLG-2DEG}}(q) = \frac{8\pi e^2}{q} f_{\text{MLG-2DEG}}(qd, qw) \quad (6)$$

with

$$f_{\text{MLG-2DEG}}(x, y) = \frac{2\pi^2 \kappa_2 \{ \kappa_1 [\cosh(y) - 1] + \kappa_{2D} \sinh(y) \}}{y(y^2 + 4\pi^2) N(x, y)}, \quad (7)$$

$$f_{\text{MLG}}(x, y) = \frac{\kappa_2 \cosh(x) [\kappa_1 \sinh(y) + \kappa_{2D} \cosh(y)] + \kappa_{2D} \sinh(x) [\kappa_1 \cosh(y) + \kappa_{2D} \sinh(y)]}{N(x, y)}, \quad (8)$$

$$\begin{aligned} f_{2\text{DEG}}(x, y) = & \frac{\kappa_1 \kappa_2 [\kappa_2 \sinh(x) + \kappa_3 \cosh(x)] \{ 64\pi^4 [1 - \cosh(y)] + y(y^2 + 4\pi^2)(3y^2 + 8\pi^2) \sinh(y) \}}{2\kappa_{2D} y^2 (y^2 + 4\pi^2)^2 N(x, y)} \\ & + \frac{[\kappa_2 (\kappa_1 + \kappa_3) \cosh x + (\kappa_2^2 + \kappa_1 \kappa_3) \sinh x] [y(32\pi^4 + 20\pi^2 y^2 + 3y^4) \cosh y - 32\pi^4 \sinh y]}{2y^2 (y^2 + 4\pi^2)^2 N(x, y)} \\ & + \frac{\kappa_{2D} [\kappa_2 \cosh x + \kappa_3 \sinh x] y(y^2 + 4\pi^2)(3y^2 + 8\pi^2) \sinh y}{2y^2 (y^2 + 4\pi^2)^2 N(x, y)} \end{aligned} \quad (9)$$

where

$$N(x, y) = \kappa_2 \cosh x \left[\kappa_{2D} (\kappa_1 + \kappa_3) \cosh y + (\kappa_1 \kappa_3 + \kappa_{2D}^2) \sinh y \right] + \sinh x \left[\kappa_{2D} (\kappa_2^2 + \kappa_1 \kappa_3) \cosh y + (\kappa_1 \kappa_2^2 + \kappa_3 \kappa_{2D}^2) \sinh y \right] \quad (10)$$

3. Numerical results

In this section, we calculate the frequency and damping rate of plasmon oscillations in MLG-2DEG double-layer system with $\kappa_1 = \kappa_{\text{Al}_2\text{O}_3} = 9.1$, $\kappa_{2D} = \kappa_{\text{GaAs}} = 12.9$, $\kappa_3 = \kappa_{\text{air}} = 1$, $m^* = 0.067m_0$ where m_0 is the vacuum mass of the electron for several values of interlayer separation d , quantum-well width w , dielectric constant κ_2 , graphene density n_g and conventional 2DEG density $n_{2\text{DEG}}$ at zero temperatures. We show that Eq. (2) admits two solutions as in the case of semiconductor double quantum well systems. The higher (lower) frequency solution corresponds to in-phase (out-of-phase) oscillations of densities in the two layers. These two branches of collective excitations of double-layer systems are known as optical and acoustic plasmon modes. In the following we denote the Fermi energy and Fermi wave number of MLG by E_F and k_F , respectively.

In Fig. 2 we show the plasmon dispersion of MLG-2DEG double layer for $n_g = 10n_{2\text{DEG}} = 10^{11}\text{cm}^{-2}$, $d = 10\text{nm}$ and $\kappa_2 = \kappa_{\text{SiO}_2} = 3.9$ for a) $w = 20\text{nm}$ and b) $w = 0$. The solid (dashed) line is the optical (acoustic) plasmon dispersion and the dashed-dotted lines show the single particle excitations (SPE) boundaries of MLG and 2DEG. It is seen from Fig. 2 that the acoustic plasmon dispersion of MLG-2DEG system touches the edge of the continuum of 2DEG at a critical wave-vector as in semiconductor double quantum well systems [8-10]. We find that the acoustic plasmon merges into the SPE region at smaller wave-vector for larger quantum-well width.

Fig. 2. Plasmon dispersion of MLG-2DEG double layer for $n_g = 10n_{2\text{DEG}} = 10^{11}\text{cm}^{-2}$, $d = 10\text{nm}$ and $\kappa_2 = \kappa_{\text{SiO}_2} = 3.9$ for $w = 20\text{nm}$ (left) and $w = 0$ (right). The solid (dashed) line is the optical (acoustic) plasmon dispersion and the dashed-dotted lines show the single particle excitations (SPE) boundaries of MLG and 2DEG (color online).

To see the effect of the spacer width, we show in Fig. 3 the plasmon dispersion of a) acoustic and b) optical mode in MLG-2DEG systems with $\kappa_2 = \kappa_{\text{SiO}_2} = 3.9$, $n_g = 10n_{2\text{DEG}} = 10^{11}\text{cm}^{-2}$, $d = 10\text{nm}$ for $w = 0, 20$ and 100nm . We observe that both optical and acoustic plasmon frequencies decrease as the quantum-well

width increases. The dependence of acoustic mode on the quantum-well width is stronger than that of optical one.

Fig. 3. Plasmon dispersion of a) acoustic and b) optical mode in MLG-2DEG systems with $\kappa_2 = \kappa_{\text{SiO}_2} = 3.9$, $n_g = 10n_{2\text{DEG}} = 10^{11}\text{cm}^{-2}$, $d = 10\text{nm}$ for $w = 0, 20$ and 100nm (color online).

Fig. 4. Plasmon dispersion of a) acoustic and b) optical mode in MLG-2DEG systems with $\kappa_2 = \kappa_{\text{SiO}_2} = 3.9$, $n_g = 10n_{2\text{DEG}} = 10^{11}\text{cm}^{-2}$, $d = 100\text{nm}$ for $w = 0, 50$ and 500nm (color online).

In order to understand the combined effect of the spacer and quantum-well width we show in Fig. 4 the plasmon dispersion of a) acoustic and b) optical mode in MLG-2DEG systems with $\kappa_2 = \kappa_{\text{SiO}_2} = 3.9$, $n_g = 10n_{2\text{DEG}} = 10^{11}\text{cm}^{-2}$, $d = 100\text{nm}$ for $w = 0, 50$ and 500nm . It is seen from the inset of Fig. 4a that the system, with spacer width $d = 100\text{nm}$, admits a branch of acoustic plasmon as undamped modes for $w \geq 50\text{nm}$. The acoustic-plasmon dispersion, however, stays out the Dirac-fermion intra-band SPE for a very small range of wave numbers q . Similar behavior has been found by Principi and coworkers for $w = 0$ [15]. We note that in conventional double-layer 2DEG systems the acoustic mode is totally undamped at long wavelength when the distance between the layers exceeds a critical value d_c [8-9]. For given d , the acoustic plasmon emerges out of the SPE region and becomes undamped for $w > w_c$ because effective interlayer distance exceeds the critical value. We also see from Figs. 3a and 3b that the optical modes decrease as the spacer width d increases.

In order to understand the combined effect of the interlayer distance, quantum-well width and different electron densities, we show in Fig. 5 plasmon dispersions of acoustic (optical) modes in MLG-2DEG system with $\kappa_2 = \kappa_{\text{SiO}_2} = 3.9$, $n_{2\text{DEG}} = 10^{10} \text{ cm}^{-2}$, $n_g = n_{2\text{DEG}}$, $10 n_{2\text{DEG}}$ and $0.1 n_{2\text{DEG}}$ for a) $d = 10 \text{ nm}$, $w = 100 \text{ nm}$ and c) $d = 100 \text{ nm}$, $w = 500 \text{ nm}$ (b) $d = 10 \text{ nm}$, $w = 100 \text{ nm}$ and d) $d = 100 \text{ nm}$, $w = 500 \text{ nm}$). We observe that the acoustic plasmon merges into the SPE region at smaller q/k_F for larger graphene density n_g . The dependence of the optical plasmon dispersion on system parameters is weaker than that of acoustic one.

Fig. 5. Plasmon dispersions of acoustic (left) and optical (right) modes in MLG-2DEG systems with $\kappa_2 = \kappa_{\text{SiO}_2} = 3.9$, $n_{2\text{DEG}} = 10^{10} \text{ cm}^{-2}$, $n_g = n_{2\text{DEG}}$, $10 n_{2\text{DEG}}$ and $0.1 n_{2\text{DEG}}$ for $d = 10 \text{ nm}$, $w = 100 \text{ nm}$ (upper figures) and $d = 100 \text{ nm}$, $w = 500 \text{ nm}$ (lower figures) (color online).

In order to see the importance of nonhomogenous dielectric background, we show in Fig. 6 the plasmon dispersions, of MLG-2DEG systems with $d = 100 \text{ nm}$ and $n_g = 10 n_{2\text{DEG}} = 10^{11} \text{ cm}^{-2}$, calculated in two cases a) $w = 50 \text{ nm}$ and b) $w = 500 \text{ nm}$ for nonhomogenous dielectric background with $\kappa_2 = \kappa_{\text{SiO}_2} = 3.9$ (solid curves) and for homogenous dielectric background with an average permittivity $\bar{\kappa} = (\kappa_1 + \kappa_3) / 2 = 5.05$ (dashed curves). We find that the nonhomogeneity of the background dielectric environment increases remarkably the optical plasmon frequency while decreases slightly the acoustic one. This behavior is almost independent of the quantum-well width.

Fig. 6. Plasmon dispersions, of MLG-2DEG systems with $d = 100\text{nm}$ and $n_g = 10n_{2\text{DEG}} = 10^{11}\text{cm}^{-2}$, calculated in two cases a) $w = 50\text{nm}$ and b) $w = 500\text{nm}$ for nonhomogenous dielectric background with $\kappa_2 = \kappa_{\text{SiO}_2} = 3.9$ (solid curves) and for homogenous dielectric background with an average permittivity $\bar{\kappa} = (\kappa_1 + \kappa_3) / 2 = 5.05$ (dashed curves) (color online).

The effects of the spacer on acoustic (left) and optical (right) plasmon dispersions of MLG-2DEG systems with $d = 100\text{nm}$, $w = 50\text{nm}$ and $n_g = 10n_{2\text{DEG}} = 10^{11}\text{cm}^{-2}$ for $\kappa_2 = \kappa_{\text{SiO}_2} = 3.9$ (solid curves), $\kappa_2 = \kappa_{\text{Al}_2\text{O}_3} = 9.1$ (dashed curves) and $\kappa_2 = \kappa_{\text{AlGaAs}} = 12.9$ (dotted curves) are shown in Fig. 7. We observe that the energy of both optical and acoustical branches decreases when the dielectric constant of spacer increases.

Fig. 7. Acoustic (left) and optical (right) plasmon dispersions of MLG-2DEG systems with $d = 100\text{nm}$, $w = 50\text{nm}$ and $n_g = 10n_{2\text{DEG}} = 10^{11}\text{cm}^{-2}$ for $\kappa_2 = \kappa_{\text{SiO}_2} = 3.9$ (solid curves), $\kappa_2 = \kappa_{\text{Al}_2\text{O}_3} = 9.1$ (dashed curves) and $\kappa_2 = \kappa_{\text{AlGaAs}} = 12.9$ (dotted curves) (color online).

It is well-known that the many-body effect on properties of ordinary 2DEG systems is very important at low densities. We use the analytical LFC parameterized by three coefficients $C_{2i}(r_s)$, ($i = 1, 2, 3$) calculated numerically in Ref. [27] to take into account both exchange and correlation effects,

$G_{\text{GA}}(q) = r_s^{4/3} 1.402q / \sqrt{2.644C_{21}^2 q_s^2 + C_{22}^2 r_s^{4/3} q^2 - C_{23} r_s^{2/3} q_s q}$ where $r_s = 1 / \sqrt{\pi a^{*2} n}$ and $q_s = 2 / a^*$ with $a^* = \hbar^2 \kappa_{\text{GaAs}} / (m^* e^2)$ as the effective Bohr radius. We show in Fig. 8a the plasmon dispersions for MLG-2DEG systems with $\kappa_2 = \kappa_{\text{SiO}_2} = 3.9$, $d = 100\text{nm}$, $w = 50\text{nm}$ and $n_g = 10n_{2\text{DEG}} = 10^{11}\text{cm}^{-2}$ in two cases $G(q) = 0$ and $G(q) = G_{\text{GA}}$. It is seen from the figure that the exchange-correlation effect is remarkable only for acoustic branch. To make it more clear we plot in Fig. 8b acoustic plasmon dispersion curves for $\kappa_2 =$

$\kappa_{\text{SiO}_2} = 3.9$, $d = 100\text{nm}$, $w = 50\text{nm}$, $n_g = 10^{10}\text{cm}^{-2}$ and several values of density ratio $n_{2\text{DEG}}/n_g$. We observe that the exchange-correlation effect decreases the acoustic plasmon frequency at $q/k_F = 1.5$ about 10% for $n_{2\text{DEG}}/n_g = 0.1$ and about 3% for $n_{2\text{DEG}}/n_g = 10$. Our results indicate that it is necessary to take into account interaction effects in calculating acoustic plasmon dispersion of MLG-2DEG systems at low 2DEG densities.

Fig. 8. Plasmon dispersions for MLG-2DEG systems with $\kappa_2 = \kappa_{\text{SiO}_2} = 3.9$, $d = 100\text{nm}$ and $w = 50\text{nm}$ in two cases $G(q) = 0$ and $G(q) = G_{\text{GA}}$ (color online).

Finally, we show in Fig. 9 the damping rate of acoustic (left) and optical (right) modes of MLG-2DEG double layer with $\kappa_2 = \kappa_{\text{SiO}_2} = 3.9$, $d = 10\text{nm}$, $n_g = 10n_{2\text{DEG}} = 10^{11}\text{cm}^{-2}$ for $w = 0, 20$ and 100nm . It is found from Figs. 2 and 8 that, the acoustic branch always lies inside the MLG intraband SPE region and its damping first increases with increasing q , but then decreases to zero and acoustic plasmon mode gets overdamped when the plasmon dispersion touches the edge of the 2DEG continuum. We note that the acoustic branch of MLG-MLG systems is outside the graphene SPE region and undamped for small q . For larger q , its damping first increases with increasing q , then decreases to zero and acoustic mode becomes totally undamped again once the plasmon dispersion merges with the graphene intraband continuum. We find that by increasing w the acoustic modes of MLG-2DEG systems get overdamped at smaller wave-vectors. In the region of small q optical branch is outside the graphene SPE region and well-defined. At a critical wave-vector the optical plasmon dispersion enters the graphene interband SPE and its damping rate increases strongly from zero. The damping of optical plasmon starts at smaller q for smaller w and becomes less affected by quantum-well width for large w .

Fig. 9. The damping rate of acoustic (left) and optical (right) modes of MLG-2DEG double layer with κ_2

$= \kappa_{\text{SiO}_2} = 3.9$, $d = 10\text{nm}$, $n_g = 10n_{2\text{DEG}} = 10^{11}\text{cm}^{-2}$ for $w = 0, 20$ and 100nm (color online).

4. Conclusion

In summary, we calculate the frequency and damping rate of plasmon oscillations in MLG-2DEG double layer at zero temperature using the RPA dielectric function. We show that the properties of the optical and acoustical modes depend considerably on the spacer width, interlayer distance, electron densities and dielectric constants of the contacting media. It is found that the plasmon behavior of MLG-2DEG system is different from that of graphene double layer. Our results indicate that it is necessary to take into account exchange-correlation effects in calculating acoustic plasmon dispersion of MLG-2DEG systems at low densities.

We hope that our work might help in finding new applications of plasmonic modes of Dirac materials in such devices as terahertz detectors [28-29].

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