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Effects of temperature, doping and anisotropy of energy surfaces on behaviors of plasmons in graphene

S. Ta Ho [a], H. Anh Le [b], T. Le [c], D. Chien Nguyen [c], V. Nam Do [b,*]

[a] National University of Civil Engineering (NUCE), No. 55, Giai Phong Road, Hanoi, Viet Nam
[b] Advanced Institute for Science and Technology, Hanoi University of Science and Technology (HUST), Hanoi 10000, Viet Nam
[c] School of Engineering Physics, HUST, Viet Nam

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ABSTRACT

A numerical scheme based on the tight-binding description for p_z-electrons in graphene was developed to study the formation and behaviors of plasmons in this two-dimensional electron system. The random phase approximation has been used to calculate the dielectric function for arbitrary temperature and doping level. We show that at zero-doping, only one kind of plasmons of long wavelength is observed at sufficiently high temperature. At finite doping, such plasmons exist even at zero temperature, but strongly damped, due to the interplay between the intra- and inter-band transition processes. Particularly, we show a significant dependence of the plasmon spectrum on the wave-vector direction in the regime of high doping, which is the reflection of the anisotropy of the energy surfaces far from the Dirac point.

1. Introduction

Due to the special arrangement of carbon atoms in a hexagonal grid, the electronic structure of graphene exhibits many typical features [1–4]. Fundamentally, it was pointed out that only p_z electrons govern the electrical and optical properties of this material because the others, i.e., the s, p_x and p_y electrons, are totally confined in the σ-bonds between the carbon atoms [2]. The response of such a p_z electron system to static electric fields, generated by a dc bias voltage, for instance, has been intensively studied, showing many properties, such as high electron mobility and high saturation drift velocity at high fields, which are very attractive to applications in electronics [5].

Recently, studies of the dynamical response of graphene to external electromagnetic fields has also been focused [6]. Obtained results provide deep understandings of fundamental aspects of electronic properties in this material, for instance, the screening of Coulomb interaction induced by many-body effects, elementary excitation spectra and collective oscillation modes [7–12]. It was pointed out that graphene supports the propagation of not only transverse magnetic modes, but also transverse electric ones [13]. For the former one, it is accompanied by the formation of collective oscillations, or plasmons, of p_z electron density in graphene. In the limit of long wavelength, the square root law of the plasmon dispersion, $\omega_P(\mathbf{q}) \propto \sqrt{q}$, very similar to that in thin films of normal metals [14] was pointed out. This theoretical prediction was experimentally confirmed through the high resolution energy loss spectroscopy measurement [15]. So far, the theoretical studies were basically realized using the consideration of electrons in graphene as massless Dirac fermions and the random phase approximation (RPA) to derive analytical expressions for the dielectric function in the limit of zero temperature.

Since the plasmon spectrum is a result of the interplay between the contributions of the intra- and inter-band transition processes to the dielectric function, our aim in this work is to investigate explicitly such an interplay to understand the formation of plasmon modes in graphene. Our work is based on a full-band calculation using the framework of the tight-binding description for p_z electrons combined with the random phase approximation to calculate the dielectric function for different values of temperature and doping, i.e., going beyond the Dirac cone approximation and the zero temperature limit. Our numerical results qualitatively confirm available analytical ones and show differences such as the dependence of the plasmon frequency on the direction of the wave vector, which are essentially involved in the topological features of energy surfaces.

The paper is divided into four sections. In the next section, we will review basic concepts in the random phase approximation, which is used in this work. In Section 3 we review our analytical calculations for the dielectric functions. Practically, we use those results to check the correctness of our numerical scheme. In Section 4 we display results for the dispersion of plasmon in

* Corresponding author. Tel.: +84 904158559.
E-mail address: vannam.do@gmail.com (V. N. Do).

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graphene at finite temperature and different values of the chemical potential. Finally, Section 5 is for conclusions.

2. Dielectric function and random phase approximation

Though the contents presented in this section can be found in standard books [16–18], it would be still useful to summarize the key points of the dynamical response theory in order to understand how collective oscillation modes of an electron system can be formed and theoretically described. Basically, the dielectric function $\varepsilon(\mathbf{r},t;\mathbf{r}',t')$ is a physical quantity needed to be investigated. As the definition, it expresses the linear relationship between the external scalar potential $\phi_{ext}(\mathbf{r},t)$ and the total one $\phi_{tot}(\mathbf{r},t)$ inside the system. More precisely the definition is [17]

$$\phi_{tot}(\mathbf{r},t)=\int d\mathbf{r}'\int dt'\varepsilon^{-1}(\mathbf{r},t;\mathbf{r}',t')\phi_{ext}(\mathbf{r}',t') \tag{1}$$

$$\phi_{ext}(\mathbf{r},t)=\int d\mathbf{r}'\int dt'\varepsilon(\mathbf{r},t;\mathbf{r}',t')\phi_{tot}(\mathbf{r}',t') \tag{2}$$

According to the linear response theory, the dielectric function can be expressed through a retarded correlation function $\chi^R(\mathbf{r},t;\mathbf{r}',t')$ of the particle density operator $\hat{\rho}(\mathbf{r},t)$,

$$\varepsilon^{-1}(\mathbf{r},t;\mathbf{r}',t')=\delta(\mathbf{r}-\mathbf{r}')\delta(t-t')+\int d\mathbf{r}''V_c(\mathbf{r}-\mathbf{r}')\chi^R(\mathbf{r}'',t;\mathbf{r}',t') \tag{3}$$

where

$$V_c(\mathbf{r}-\mathbf{r}')=\frac{e_0^2}{4\pi\varepsilon_0\kappa|\mathbf{r}-\mathbf{r}'|} \tag{4}$$

is the Coulomb potential governing the mutual interaction of charged carriers ($e_0>0$ is the value of elementary charge, ε_0 the vacuum dielectric permittivity, and $\kappa$the relative static dielectric constant of system), and the retarded correlation function

$$\chi^R(\mathbf{r},t;\mathbf{r}',t')=-\frac{i}{\hbar}\theta(t-t')\langle[\hat{\rho}(\mathbf{r},t),\hat{\rho}(\mathbf{r}',t')]\rangle_0 \tag{5}$$

is also called the electron–hole propagator wherein i is the imaginary number, θ the conventional step function, the square bracket $[\ldots]$ the commutator, and the angle bracket $\langle\ldots\rangle_0$ implies that the expectation value of inside operator is calculated in the thermodynamic equilibrium.

Assuming the homogeneity of the system, it is more convenient to rewrite all the above equations in the frequency and momentum representation. The function $\chi^R(\mathbf{q},\omega)$ is usually solved using the method of equation of motion or the method of Feynman diagrams [17]. In the random phase approximation the electron–hole propagator and the corresponding dielectric function are given by

$$\chi^R_{RPA}(\mathbf{q},\omega)=\frac{\chi_0(\mathbf{q},\omega)}{1-V_c(\mathbf{q})\chi_0(\mathbf{q},\omega)} \tag{6}$$

$$\varepsilon_{RPA}(\mathbf{q},\omega)=1-V_c(\mathbf{q})\chi_0(\mathbf{q},\omega), \tag{7}$$

where $\chi_0(\mathbf{q},\omega)$ is determined from the simple pair-bubble diagram and formally takes the form [11]:

$$\chi_0(\mathbf{q},\omega)=\frac{1}{\Omega}\sum_{\mathbf{k},m,n}|\langle m,\mathbf{k}+q|e^{i\mathbf{q}\cdot\mathbf{r}}|n,\mathbf{k}\rangle|^2\frac{f(E_{m,\mathbf{k}+q})-f(E_{n,\mathbf{k}})}{E_{m,\mathbf{k}+q}-E_{n,\mathbf{k}}+\hbar\omega+i\hbar\delta} \tag{8}$$

wherein $\{|m,\mathbf{k}\rangle\}$ are the single particle Bloch states corresponding to the energies $\{E_{m,\mathbf{k}}\}$ which are labelled by the energy band index m and the $\mathbf{k}$-vector in the first Brillouin zone; $f(\varepsilon)=1/(1+e^{\beta\varepsilon})$, with $\beta=1/k_BT$ being the Fermi function; δ an positive infinitesimal number; and $V_c(\mathbf{q})$ the Fourier transform of the long-range Coulomb potential. In the two-dimensional (2D) space, $V_c(\mathbf{q})=e_0^2/2\varepsilon_0\kappa q$, and the volume Ω should be replaced by the area S of the 2D system.

In general, the vanishing of the dielectric function is the condition for the propagation of longitudinal electromagnetic fields in a medium [16] which are accompanied by the collective oscillation modes of electron system. However, due to the interplay between the inter- and intra-band transition processes, the dispersion of such oscillation modes $\omega_P(\mathbf{q})$ is determined as the zeros of the real part of $\varepsilon(\mathbf{q},\omega)$, i.e.,

$$\mathrm{Re}[\varepsilon(\mathbf{q},\omega_P)]=0 \tag{9}$$

The damping of such modes, however, is determined from the imaginary part $\mathrm{Im}[\varepsilon(\mathbf{q},\omega_P)]$. In the following sections we will use Eqs. (7) and (8) to calculate the RPA dielectric function and then solve Eq. (9) to find the plasmon dispersions of graphene.

3. Graphene electronic structure and long wavelength plasmon dispersion

Denote $\{a_i^\dagger,a_i\}$ and $\{b_j^\dagger,b_j\}$ the operators creating and annihilating a p_z electron at the nodes i and j of the A and B sub-lattices, which constitute the graphene hexagonal one, respectively. The Hamiltonian describing the dynamics of the p_z electron system is thus written in the tight-binding representation as follows:

$$H=-t_{cc}\sum_{i\in A}\sum_{j\in B}(a_i^\dagger b_j+b_j^\dagger a_i)+\mu\sum_{i\in A}a_i^\dagger a_i+\mu\sum_{j\in B}b_j^\dagger b_j \tag{10}$$

where $t_{cc}\simeq 2.67$ eV is the hopping energy between two nearest carbon atoms whose spacing is $a_{cc}\simeq 0.142$ nm, and μ the chemical potential away from half-filling induced by a gate or by doping. In the momentum space Eq. (10) is rewritten as [2]

$$H=\sum_{\mathbf{k}}X_{\mathbf{k}}^\dagger\begin{pmatrix}\mu & h_{\mathbf{k}}^*\\ h_{\mathbf{k}} & \mu\end{pmatrix}X_{\mathbf{k}}, \tag{11}$$

where $X_{\mathbf{k}}^\dagger=(a_{\mathbf{k}}^\dagger,\ b_{\mathbf{k}}^\dagger)$ is a two-component spinor and $h_{\mathbf{k}}=-t_{cc}[\exp(ik_xa_{cc})+2\exp(ik_xa_{cc}/2)\cos(\sqrt{3}k_ya_{cc}/2)]$ is a tight-binding function summed over the nearest neighbor sites. By diagonalizing the matrix in Eq. (11) we obtain the expressions for the eigen-energies $E_{n,\mathbf{k}}$ and for the corresponding eigen-wave-functions $X_{n,\mathbf{k}}$ ($n=1,2$):

$$E_{n,\mathbf{k}}=\mu+(-1)^n\sqrt{h_{\mathbf{k}}^*h_{\mathbf{k}}} \tag{12}$$

$$X_{n,\mathbf{k}}=\frac{1}{\sqrt{1+h_{\mathbf{k}}^*h_{\mathbf{k}}}}\begin{pmatrix}1\\ (-1)^nh_{\mathbf{k}}\end{pmatrix} \tag{13}$$

In Fig. 1(a) we display the well-known band structure of graphene resulted from Eq. (12). The touching of the two energy surfaces is clearly seen at six corner points of the hexagonal Brillouin zone whose coordinates are $K=(\pm 2\pi/3a_{cc},\ \pm 2\pi/3\sqrt{3}a_{cc})$ and $K'=(0,\ \pm 4\pi/3\sqrt{3}a_{cc})$. The energy surfaces around these K-points are zoomed out to clearly show the cone shape as seen in the figure. However, they are not the ideal isotropic Dirac cone, but just an approximation [see Eq. (14)]. In Fig. 1(b) we present the Fermi energy surface $E(\mathbf{k})=E_F$ to illustrate this fact. For $E_F=0.2$ eV and 0.3 eV we see the circular shape of the Fermi surface, but for $E_F=0.6$ eV, for instance, the anisotropy becomes significant. In the next section we will demonstrate that the anisotropy of the energy surfaces results in the dependence of the plasmon frequency ω_P on the direction of the wave vector $\mathbf{q}$.

Using the $\mathbf{k}\cdot\mathbf{p}$-method, around the K points Eqs. (12) and (13) are well approximated by [2,3]

$$E_{n\mathbf{k}}=\mu+(-1)^n\hbar v_F|\mathbf{k}| \tag{14}$$