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Mono-Mono-Mono and Bi-Bi-Bi three-layer graphene systems' optical conductivity

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ABSTRACT: Investigating the longitudinal optical conductivity of graphene systems, which is the most important property for opto-electronic devices, for three-layer graphene systems theoretically and numerically is the main purpose of this study. Each layer can be mono- or bi-layer graphene. Separation between layers has been denoted by d, selected to be about ten nanometers. The carrier densities in each layer can be tuned by changing gate voltage. In these two dimensional layered structures; the main contributions to the optical conductivity are from the intra- and inter-band transition channels in a same layer. In this paper the graphene structure is described primarily, and the three-layer graphene systems with composes of mono-mono-mono and bi-bi-bi has been defined. Using dielectric and electron density-density correlation tensors, the imaginary part of dielectric function for the three-layer graphene systems are calculated and optical conductivities are plotted as a function of photon energies in different broadening widths, for final stages.

Keywords: *Broadening width, Landau level, Optical conductivity, Three- layer Graphene.*

INTRODUCTION

Three-layer systems are formed by three isolated layers with an ultrathin insulating dielectric (such as $FeCl_3$, Al_2O_3 and so on) intercalation to separate the adjacent layers. Each layer can be cosisted by heterostructure, mono-layer graphene, and so on. Using the Raman spectrum analysis, experimental researchers indicate the dicoupling of the few layer graphene into separate mono-layer graphene. In these three-layer structures, the long-range inter-layer Coulomb interaction plays important roles in the many-body properties such as plasmon modes, polarizability, and drag conductivity. Min et al. Calculated the static polarizability and screening of multilayer graphene which is dependent on the layer number and includes the intra- and inter-band polarizability.The theoretical Thomas-Fermi screening wave vector results show different behaviours for several stacking sequences which implies the importance of the layer structure.The drag conductivity is induced by the Coulomb drag between passive and active layers.The electric field is applied in the passive layer and the current density is obtained in the other active layer, which is through the electron-electron scattering process. This drag conductivity, in the lowest leading order

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in the inter-layer potential, is related to the nonlinear susceptibility for each layer and screened inter-layer potential in the random phase approximation. Therefore, the optical coductivity and the drag conductivity are both related to the dielectric function for each layer and the inter-layer screened Coulomb interaction [1]. Graphene a 2D system with one atomic thick sheet of carbon, was fabricated experimentally in 2004 by Novoselov et al.. This ultra-thin material exhibits very novel physical properties because the energy dispersion can be expressed as linear relationship round the two nodal points k and k′ in the Brillouine zone. The electron dynamics obeys the 2D massless Dirac equation $H=\gamma\sigma$, $\gamma=h\nu_F$, $\nu_F=1/300$ c for graphene. k, which differs strongly from the case in a conventional two dimensional electron gas (2DEG) with the kinetic energy being proportional to k^2. $E_f=E_f^i$ the reference Fermi energy. σ, k are the Pauli matrix operator and wavevector, respectively. This exotic electronic structure has aroused the wide investigation on the fundamental physical properties in graphene which become a fast-growing research area in condensed matter physics.

In this paper, the structure with several isolated parallel two-dimension mono-layer graphene, and bi-layer graphene, separated by a distance d with an ultra-thin dielectric is studied. When an inter-layer distance d is about a few angstroms (d~3.5 Å), the out-of-plane π orbitals from two adjacent graphene sheets start to overlap. The inter-layer tunneling is obvious when (d~1-5 Å). Increasing the distance between the adjacent layers, the inter-layer tunneling decreases, and inter-layer electron-electron Coulomb scattering should be included. Here, we refer to the electron systems (i.e. extrinsic graphene systems) where the Fermi energy $E_f>0$ and $T\rightarrow 0$. The carrier density for each layer can be tuned both by the chemical doping and applied field (or gate voltage). The carrier densities in each layer can be independently controlled by using top and bottom gates. The carrier density in each layer can be obtained by the capacitance between graphene and the gates [2]. The properties of the optical conductivity in graphene have been widely investigated experimentally and theoretically. The experimental value of the optical conductivity per graphene layer (or optical sheet conductivity) is almost a constant and close to $\sigma_0=e^2/4h$, which is independent from the frequency and the inter-layer hopping. The second observation is that the optical sheet conductivity showed a threshold structure at two times the Fermi energy under an applied gate voltage and the turning points can be tuned by the gate voltage. In this paper, the optical conductivity for three-layer systems with composes mono-mono-mono and bi-bi-bi, is investigated analytically and numerically. The intra- and inter-layer contributions, the intra- and inter-band transition channels, the electron density, the broadening width for the optical conductivity are discussed.

THEORETICAL APPROACHES

For a n-layer graphene system, using the mean-field random phase approximation, The dielectric tensor elements, $\varepsilon_{l,m}(q,\omega)$, where l , m= 1,2,…, n denoting the different layer, can be written as:

$$\varepsilon_n = -\alpha B_n \Pi_n$$

Here, $\alpha=V_q=2\pi e^2/\kappa q$ is the intra-layer Coulomb interaction, κ is the static dielectric constant for graphene, Π_n is the density-density correlation tensor. For a several-layer graphene system, each layer separated by a dielectric $\pi_{lm}=0$, if $l\neq m$, and $\pi_{lm}=\pi_l$, if l=m. We can obtain:

$$\Pi_n = \begin{bmatrix} \pi_1 & 0 & 0 & \cdots & 0 \\ 0 & \pi_2 & 0 & \cdots & 0 \\ 0 & 0 & \pi_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & 0 & \cdots & \pi_n \end{bmatrix}$$

The matrix elements $\pi_l=\pi_l(q,\omega)$ are the density-density correlation functions, which for mono- and bi-layer graphene can be obtained as:
$\pi_l(q,\omega)=g_s g_v \sum_{s,s',k_m}(1+ss'A_{k_mq})/2\, f_{s,k_m}-f_{s',k_m+q})/\hbar\omega+E_{s,k_m}-E_{s',|k_m+q|)}+i\Gamma_m$. $g_s=2$ is spin degeneracy. There are two points k and k' at the corner of the graphene Brillouin zone, called the Dirac points. $g_v=2$ refers to this degeneracy, f_{s,k_m} is the Fermi-Dirac distribution function in the m-th layer. s,s'= ±1 refer to the conduction band (+1) and the valence band (-1). $(1+ss'A_{k_mq})/2$ Come from the overlap of carrier states. $A_{k_mq}=\cos\varphi_m$ and $A_{k_mq}=\cos 2\varphi_m$ in monolayer and bilayer graphene respectively, $\cos\varphi_m=(k_m+q\cos\Theta_m)/(|k_m+q|)$, Θ_m being

the angle between k_m and q. In monolayer graphene, $E_{s,k}=sh\nu_F|k|$ (ν_F being the Fermi velocity of graphene). In bilayer graphene $E_{s,k}=(sh^2k^2)/2m$, $m\approx0.033\ m_e$ is the effective mass of bilayer graphene with m_e being the free-electron mass. Γ_m is the broadening width induced by the carrier scattering process.

The B_n itself, can be written as:

$$B_n=-\frac{1}{\alpha}\Pi_n+\beta_n,$$

where,

$$\beta_n=\begin{bmatrix}1 & \beta & \beta^2 & \cdots & \beta^{n-1}\\ \beta & 1 & \beta & \cdots & \beta^{n-2}\\ \beta^2 & \beta & 1 & \cdots & \beta^{n-3}\\ \vdots & \vdots & \vdots & \cdots & \vdots\\ \beta^{n-1} & \beta^{n-2} & \beta^{n-3} & \cdots & 1\end{bmatrix}$$

Here,

$$\beta=e^{-qd}$$

In which, d is the distance between the adjacent layers. And:

$$\Pi_n=\begin{bmatrix}P_1 & 0 & 0 & \cdots & 0\\ 0 & P_2 & 0 & \cdots & 0\\ 0 & 0 & P_3 & \cdots & 0\\ \vdots & \vdots & \vdots & \cdots & \vdots\\ 0 & 0 & 0 & \cdots & P_n\end{bmatrix}$$

Here, $P_l=1/\pi_l$.

For a three-layer graphene system we obtain that:

$$\Pi_3=\begin{bmatrix}P_1 & 0 & 0\\ 0 & P_2 & 0\\ 0 & 0 & P_3\end{bmatrix}$$

And we can find:

$$\beta_3=\begin{bmatrix}1 & \beta & \beta^2\\ \beta & 1 & \beta\\ \beta^2 & \beta & 1\end{bmatrix}$$

As well as:

$$B_3=-\frac{1}{\alpha}\begin{bmatrix}\frac{1}{\pi_1} & 0 & 0\\ 0 & \frac{1}{\pi_2} & 0\\ 0 & 0 & \frac{1}{\pi_3}\end{bmatrix}+\begin{bmatrix}1 & \beta & \beta^2\\ \beta & 1 & \beta\\ \beta^2 & \beta & 1\end{bmatrix}=\begin{bmatrix}P_1 & \beta & \beta^2\\ \beta & P_2 & \beta\\ \beta^2 & \beta & P_3\end{bmatrix}$$

where,

$$P_l=1-\frac{1}{\alpha\pi_l}$$

Hence,

$$B_3=\begin{bmatrix}1-\frac{1}{V_q\pi_1} & e^{-qd} & e^{-2qd}\\ e^{-qd} & 1-\frac{1}{V_q\pi_2} & e^{-qd}\\ e^{-2qd} & e^{-qd} & 1-\frac{1}{V_q\pi_3}\end{bmatrix}$$

As we said:

$$\varepsilon_3=-\alpha B_3\Pi_3$$

$$\Pi_3=\begin{bmatrix}\pi_1 & 0 & 0\\ 0 & \pi_2 & 0\\ 0 & 0 & \pi_3\end{bmatrix}$$

So we can write:

$$\varepsilon_3=-V_q\begin{bmatrix}1-\frac{1}{V_q\pi_1} & e^{-qd} & e^{-2qd}\\ e^{-qd} & 1-\frac{1}{V_q\pi_2} & e^{-qd}\\ e^{-2qd} & e^{-qd} & 1-\frac{1}{V_q\pi_3}\end{bmatrix}\begin{bmatrix}\pi_1 & 0 & 0\\ 0 & \pi_2 & 0\\ 0 & 0 & \pi3\end{bmatrix}$$

Then ε_3 becomes as;

$$\varepsilon_3=\begin{bmatrix}1-V_q\pi_1 & -V_qe^{-qd}\pi_2 & -V_qe^{-2qd}\pi_3\\ -V_qe^{-qd}\pi_1 & 1-V_q\pi_2 & -V_qe^{-qd}\pi_3\\ -V_qe^{-2qd}\pi_1 & -V_qe^{-qd}\pi_2 & 1-V_q\pi_3\end{bmatrix}$$

Determination of the dielectric matrix function for three-layer graphene system yields;

$$\varepsilon_3(q,\omega)=1-V_q\left[\pi_1+\pi_2+\pi_3\right]$$
$$+V_q^2(1-e^{-2qd})\left[\pi_1\pi_2+\pi_2\pi_3\right]+V_q^2(1-e^{-4qd})\left[\pi_1\pi_3\right]$$
$$V_q^3\left(1-2e^{-2qd}+e^{-4qd}\right)\left[\pi_1\pi_2\pi_3\right]$$

Knowing that; $\pi_l=\pi_l(q,\omega)$. And we find imaginary part of dielectric function as;

$$\mathrm{Im}\varepsilon_3(q,\omega)=-V_q\left[\mathrm{Im}\pi_1+\mathrm{Im}\pi_2+\mathrm{Im}\pi_3\right]$$
$$+V_q^2\left(1-e^{-2qd}\right)\left[\mathrm{Im}\pi_1\pi_2+\mathrm{Im}\pi_2\pi_3\right]$$
$$+V_q^2\left(1-e^{-4qd}\right)\left[\mathrm{Im}\pi_1\pi_3\right]$$
$$+V_q^3\left(1-2e^{-2qd}+e^{-4qd}\right)\left[\mathrm{Im}\pi_1\pi_2\pi_3\right]$$

The longitudinal optical conductivity can be obtained by the dielectric function [3];

$$\sigma_{xx}(\omega)=-e^2\omega\lim_{q\to0}\frac{1}{q^2}\sum_m\mathrm{Im}\frac{\pi_m(q,\omega)}{\varepsilon(q,\omega)}$$

$\varepsilon(q,\omega)$ is the determination of the dielectric matrix

function. ω is the frequency of the incident light. q→0 reflects a fact that the electron-photon scattering does not change the wave vector of an electron, which can be understood from Maxwell equations with a complex dielectric function ε'=ε+i σ/ω being introduced to investigate the optical absorption problems. The longitudinal optical conductivity $\sigma_{xx}(\omega)$ is proportional to (ImπRe ε-ImεRe π). The intra- and inter-band d-d correlation functions contribute to the real and imaginary parts.

$$\pi_{L,i}(q,\omega) = R_e\,\pi_{L,i}(q,\omega) + l_m\pi_{L,i}(q,\omega)$$

Each part can be written as:

$$R_e\,\pi_{L,i}(q,\omega) = R_e\,\pi_{L,i}^{++}(q,\omega) + R_e\,\pi_{L,i}^{-+}(q,\omega)$$
$$l_m\pi_{L,i}(q,\omega) = l_m\pi_{L,i}^{++}(q,\omega) + l_m\pi_{L,i}^{-+}(q,\omega)$$

The real parts in the i-th layer are

$$R_e\,\pi_{L,i}^{++}(q,\omega) = L\frac{g_s g_v E_f^i q^2}{4\pi(\hbar\omega)^2}\frac{1-x_i^2}{(1+x_i^2)^2}$$

and:

$$R_e\,\pi_{L,i}^{-+}(q,\omega) = L\frac{g_s g_v q^2}{16\pi}\left[\frac{\hbar\omega}{2A_i}\ln\frac{k^{2L}}{R_i} + \left(\frac{(\hbar\omega)^2}{A_i} - 1\right)\frac{1}{\Gamma_i}\tan^{-1}\frac{\Delta}{\Gamma_i}\right]_{k_f^i}^{k_c}$$

The imaginary parts are:

$$l_m\pi_{L,i}^{++}(q,\omega) = -L\frac{g_s g_v E_f^i q^2\Gamma_i}{2\pi(\hbar\omega)^3}$$

and,

$$l_m\pi_{L,i}^{-+}(q,\omega) = -L\frac{g_s g_v q^2\Gamma_i}{16\pi A_i}\left[\frac{1}{1}\ln\frac{k^{2L}}{R_i} + \frac{\hbar\omega}{\Gamma_i}\tan^{-1}\frac{\Delta}{\Gamma_i}\right]_{k_f^i}^{k_c}$$

(++) and (−+) denoting intra- and inter channel transitions, respectively. Here L=1, 2 is for monolayer and bilayer graphene respectively. This coefficient is similar to the obtained plasmon results in MLG and BLG. These two plasmon analytical results are identical except for an extra factor of √2 in the BLG case. $x_i=\Gamma_i/\hbar\omega$, $A_i=(\hbar\omega)^2+\Gamma_i^2$, $\Delta=2\gamma k-\hbar\omega$, $R_i=(2\gamma k-\hbar\omega)^2+\Gamma_i^2$, $\gamma=\hbar V_f$ and k_c is the cutoff wave vector above which the linear energy dispersion approximation breaks down for graphene.

$$k_c \sim \frac{1}{a}$$

(a being the distance between C-C bond). The real and imaginary parts of intra- or inter-band d-d correlation function have much common factors, and have similar relationship to the broadening width, Fermi energy, q-wave vector, and the optical frequency. The contributions to the optical conductivity are from electron-hole excitations from the intra-layer and inter-layers. In each layer, there are two transition channels (intra- and inter-band transitions) contributing to the optical absorption. When the applied optical field is present, the carriers are excited from the occupied states to the unoccupied states. The intra-band contribution corresponds to electron excitation in the vicinity of the Fermi level within the conduction band. While the inter-band contribution corresponds to carrier excitation from the valance band to the conduction band and has a turning point at 2E_F. These two processes are intra-layer case given by the V_q term. The inter-layer contributions given by V_q^2 , V_q^3 terms. Finally the optical conductivity becomes:

$$\sigma_{xx}(\omega) = \omega l_m\varepsilon_3(q,\omega)$$

APPROACHES AND FINDINGS

Using dielectric tensor which has been obtained from electron density-density correlation function. The total optical conductivity has been calculated from imaginary part of three-layer graphene dielectric function, and plotted numerically as a function of photon energy for mentioned three-layer graphene systems, in different broadening widths, and constant electron densities in each layer. By using a MATLAB program the results have been collected and shown as below;

RESULTS AND DISCUSSIONS

By comparing Figures 1, 2 and 3 can be observed:
1- The longitudinal optical conductivity in bi-bi-bi, three-layer graphene system, is greater than the mono-mono-mono one, at all energy regions.
2- The second threshold structure in bi-bi-bi, three-layer graphene system, has an obvious difference with mono-mono-mono one, so as in bi-bi-bi system, the optical conductivity of second threshold structure, decreasing when photon energy increases, while, the mono-mono-mono system's optical conductivity is al-

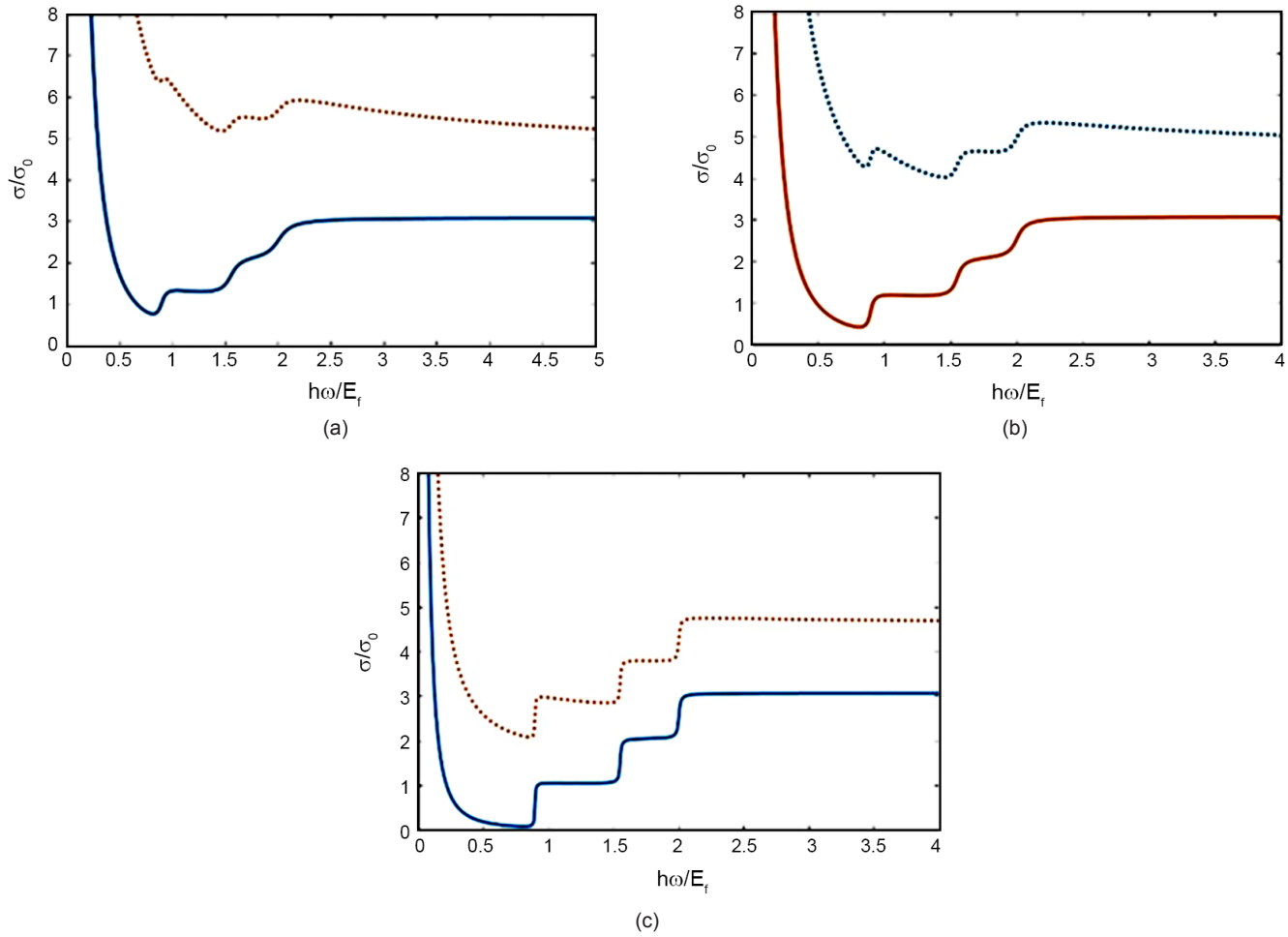

Fig. 1. The optical conductivity as a function of photon energy, for Three-layer graphene systems mono-mono-mono (solid line), and bi-bi-bi (dot line) in different broadening widths width values; a) $\Gamma=0.09E_f$; b), $\Gamma=0.05E_f$; c) $\Gamma=0.01E_f$; $ne_1=5\times10^{12}$ cm^{-2}; $ne_2=3\times10^{12}$ cm^{-2}; $ne_3=1\times10^{12}$ cm^{-2}; are electron densities in first-, second-, and third-layers respectively.

most constant.

3- At high energy regions, the optical conductivity of mono-mono-mono system tendency is three times of a sheet graphene's optical conductivity but in bi-bi-bi system this value is six times of it.

4- By decreasing the value of broadening width, turning regions between different threshold structures, sharply increase.

5- By decreasing the value of broadening width, the value of the optical conductivity decreases too.

REFERENCES

[1] Yang, C.H. Chen, Y.Y. Jiang, J.J. Ao, Z.M. (2016). The optical conductivity in double and three layer graphene systems. Solid State Comunications, 227, 23-27.

[2] Yang, C.H. Wan, P. Li, Q.F. Ao, Z.M. (2016). Coulomb screening effects on the optoelectronic far-infrared properties of spatially separated few-layer graphene. Physica E, 84, 324-329.

[3] Hwang, E.H. Das Sarma, S. (2009). Plasmon modes of spatially separated double-layer graphene. PHYSICAL REVIEW B, 80,205406,1-5.

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