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The longitudinal optical conductivity in bilayer graphene and other two-dimensional systems

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ABSTRACT

The longitudinal optical conductivity in bilayer graphene is calculated using the dielectric function by defining the density operator theoretically, while the effect of the broadening width determined by the scattering sources on the optical conductivity is also investigated. Some features, such as chirality, energy dispersion and density of state (DOS) in bilayer graphene, are similar to those in monolayer graphene and a traditional two-dimensional electron gas (2DEG). Therefore, in this paper, the bilayer graphene optical conductivity is compared with the results in these two systems. The analytical and numerical results show that the optical conductivity per graphene layer is almost a constant and close to $e^2/(4\hbar)$, which agrees with the experimental results.

1. Introduction

Graphene a two-dimensional material with honeycomb structure was fabricated experimentally by Geim et al. [1]. This ultra-thin material exhibits very unique and excellent physical properties, such as high mobility [2], unique quantum Hall effect [1], and Klein tunning [3]. Hence, graphene has been proposed as an advanced electronic and optoelectronic material and arouses wide investigation both experimentally and theoretically [4–10]. These excellent electronic and optical properties are related to the chirality of graphene and the linear and conical spectrum of band structure at the Dirac K/K' points. In monolayer graphene, the energy dispersion $E(k)=s\hbar v_F k$ is linear with the wavevector and has two branches $s=\pm 1$, which originates from the two sublattices. v_F is the Fermi velocity which is related to the hopping energy between the nearest-neighbor carbon atoms. In bilayer graphene, the 2×2 effective Hamiltonian [11–13] results in two parabolic bands. The energy dispersion with parabola and two branches have features similar to both monolayer graphene and traditional two-dimensional electron gas (2DEG) [11,13].

The properties of the optical conductivity have been widely investigated in graphene experimentally [14–16] and theoretically [9,17–22]. The experimental value of the optical conductivity per graphene layer (or an optical sheet conductivity) is almost a constant and close to $e^2/(4\hbar)$, which is independent of the frequency and the interplane hopping. The second observation is that the optical sheet conductivity at different carrier densities showed a threshold structure at two times the Fermi energy under an applied gate voltage. The Kubo formula and/or the Boltzmann transport theory were employed to investigate the optical conductivity theoretically. The Kubo formula starts from the current–current correlation function which is expressed as a product of two Green's functions. Using the linear response theory, the ac conductivity can be obtained. About the Boltzmann equation method, every collision term can be expressed directly. The mass- and energy-balance equations are employed to evaluate the optical conductivity and other electrical and optical properties self-consistently [23,24]. From Maxwell equation, the imaginary part of the dielectric function is related to the conductivity. Therefore, the longitudinal optical conductivity can be investigated from the polarization function (density–density correlation function).

In this paper, using the dielectric function, we examine the longitudinal optical conductivity with different broadening width in a bilayer graphene system. The results in monolayer graphene, bilayer graphene, and the conventional 2DEG are compared. The theoretical

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approach for calculating the optical conductivity induced by the dielectric function is developed in Section 2. The analytical and numerical results and discussion are presented in Section 3.

2. Theoretical approaches

From Maxwell equation $\nabla\times\mathbf{H}=\partial\mathbf{D}/\partial t+\mathbf{J}=-i\omega\varepsilon\mathbf{E}+\sigma\mathbf{E}$, a complex dielectric function $\varepsilon'=\varepsilon+i\sigma/\omega$ is introduced to study the electromagnetic transmission problems. It can be seen that the imaginary part of the dielectric function is related to the conductivity. The relationship between the optical conductivity and the dielectric function can be strictly solved in microscopic system. In the presence of an optical field, the transverse dielectric function $\varepsilon_T(\omega,q)$ of the solid can be obtained from the retarded form of the current–current correlation function. The longitudinal dielectric function $\varepsilon_L(\omega,q)$ can be derived from the density–density (d–d) correlation function. During the process of the electrons absorbing the optical energy to high energy states, the change of the wave vector q is very tiny. In the long wavelength limit $q\to 0$, the transverse dielectric function is exactly equal to the longitudinal one :$\varepsilon_T(\omega,q)=\varepsilon_L(\omega,q)=\varepsilon(\omega,q)$.

Applying the electron wavefunction and energy spectrum to a standard technique to derive the electron d–d correlation function for graphene, the dielectric function can be obtained as [13]

$$\varepsilon(\omega,q)=1-V_q\Pi(\omega,q) \tag{1}$$

$\Pi(\omega,q)=g_sg_v\sum_{s,s',\mathbf{k}}((1+ss'\cos(2\varphi))/2)\quad(f_{s,\mathbf{k}}-f_{s',\mathbf{k}+\mathbf{q}})/(\hbar\omega+E_{s,\mathbf{k}}-E_{s',|\mathbf{k}+\mathbf{q}|}+i\Gamma)$, $g_s=2$ 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. $f_{s,\mathbf{k}}$ is the Fermi–Dirac distribution function. $s,s'=\pm1$ refers to the conduction band $(+1)$ and the valence band (-1). $(1+ss'\cos(2\varphi))/2$ comes from the overlap of carrier states, with $\cos\varphi=(k+q\cos\theta)/|\mathbf{k}+\mathbf{q}|$, θ being the angle between $\mathbf{k}$ and $\mathbf{q}$, $\mathbf{k}'=\mathbf{k}+\mathbf{q}$. $E_{s,\mathbf{k}}=s\hbar^2k^2/(2m)$, $m\approx0.033m_e$ is the effective mass of bilayer graphene with m_e being the free-electron mass [25]. $V_q=2\pi e^2/(\kappa q)$ with κ being the static dielectric constant for graphene. Γ is the broadening width induced by the carrier scattering process. With the electron d–d correlation function, we can calculate the optical conductivity induced by electron–electron (e–e) interaction, $\mathrm{Im}\,\varepsilon(q,\omega)\sim V_q\,\mathrm{Im}\,\Pi(q,\omega)$. If a weak external light field polarized along the 2D plane (taken along the x direction) is present in graphene, the optical conductivity can be derived from Kubo formula [26,27], which is called as the longitudinal optical conductivity:

$$\sigma_{xx}(\omega)=-e^2\omega\lim_{q\to0}(1/q^2)\sum_{n',n}\mathrm{Im}\,\Pi_{n'n}(\omega,q), \tag{2}$$

where $q\to0$ reflects a fact that the electron–photon scattering does not change the wavevector of an electron. In the present study, gate voltage was used to tune the carrier density and the conduction band is occupied with electrons. The results of the optical conductivity contributed by two transition channels (intra- and inter-band transitions) can be obtained by the analytical and numerical calculation, $\sigma_{xx}(\omega)=\sigma_{xx}^{\mathrm{intra}}(\omega)+\sigma_{xx}^{\mathrm{inter}}(\omega)$.

The intra-band channel (i.e., $s'=s$) comes from the electronic transition in a same band. At a long-wavelength limit (i.e., $q\to0$), $\cos\varphi\approx1-(q^2/2k^2)\sin^2\theta$. $f_{+,\mathbf{k}}-f_{+,\mathbf{k}+\mathbf{q}}\approx-\mathbf{q}\cdot\hat{\mathbf{k}}\delta(k-k_F)$. A finite value Γ was taken for the broadening width. The intra-band transitions in a conduction band give rise to the optical conductivity:

$$\sigma_{xx}^{\mathrm{A-intra}}(\omega)=\sigma_{bi}^0\frac{8\Gamma E_F}{\pi(\hbar\omega)^2} \tag{3}$$

Here, the superscript "A" indicates the analytical results. $\sigma_{bi}^0=e^2/(2\hbar)$ which is two times larger than the value $\sigma_{mono}^0=e^2/(4\hbar)$ in monolayer graphene. It originates from the difference of the parabolic and/or linear energy dispersion. The dependence of the intra-band transition contribution to the optical conductivity on the broadening width and the Fermi energy and the optical energy is similar to the case in a conventional 2DEG, $\sigma_{xx-2DEG}(\omega)=(e^2/\hbar)\Gamma E_F/[\pi(\hbar\omega)^2]$ and the case in monolayer graphene [28].

The inter-band transition (i.e., $s'=-s$) refers to the electron transition from the valence band to the conduction band:

$$\sigma_{xx}^{\mathrm{A-inter}}(\omega)=\sigma_{bi}^0\frac{\hbar\omega\Gamma}{\pi\left[(\hbar\omega)^2+\Gamma^2\right]}\times\left[\frac{1}{2}\ln\frac{k^4}{R}+\frac{\hbar\omega}{\Gamma}\arctan\frac{\left(\hbar^2k^2/m-\hbar\omega\right)}{\Gamma}\right]_{k_F}^{k_c} \tag{4}$$

Here, $R=\left(\hbar^2k^2/m-\hbar\omega\right)^2+\Gamma^2$, and k_c is the cutoff wavevector for graphene, $k_c\sim1/a$ with $a\approx1.42$Å the carbon–carbon distance. $\hbar^2k^2/m$ is the energy difference $(E_{+,\mathbf{k}}-E_{-,\mathbf{k}})$, which is the main difference from that in monolayer graphene. In monolayer graphene, this term is $2\gamma k$ in Eq. (5) of Ref. [28]. When $\Gamma\ll\hbar\omega$, $\sigma_{xx}^{\mathrm{A-inter}}(\omega)\approx\sigma_{bi}^0\left[(1/\pi)\arctan\left(\hbar^2k^2/m-\hbar\omega\right)/\Gamma\right]_{k_F}^{k_c}$.

From the above analysis, the main contribution to the optical conductivity comes from the channel of the inter-band transition. The intra-band transition is linear with $\Gamma E_F/(\hbar\omega)^2$. Therefore, the contribution from intra-band transition is weak in a low density system or in the presence of a strong optical field. When the optical energy is larger than two times the Fermi energy $(\hbar\omega\geq2E_F)$ and the broadening width is taken to be a small value, using the relationship $\lim_{\Gamma\to0}1/(x+i\Gamma)\approx\mathrm{P}(1/x)-i\pi\delta(x)$, the optical conductivity can be obtained as $\sigma_{xx}\approx\sigma_{xx}^{\mathrm{A-inter}}\approx\sigma_{bi}^0$. It can be seen that the optical conductivity is close to a constant.

For an air–graphene–dielectric-wafer (e.g., SiO_2) system, the transmission coefficient can be obtained by [17]

$$T(\omega)=\sqrt{\frac{\epsilon_2}{\epsilon_1}}\frac{4(\epsilon_1\epsilon_0)^2}{\left|(\sqrt{\epsilon_1\epsilon_2}+\epsilon_1)\epsilon_0+\sqrt{\frac{\epsilon_1}{\sigma}(\omega)}c\right|^2} \tag{5}$$

Here, ϵ_2 is the effective high-frequency dielectric constant for substrate ($\epsilon_2=2.25$ for SiO_2 substrate). $\epsilon_1=1$, ϵ_0 are for the case of air and vacuum. c is the speed of light in vacuum.

3. Results and discussions

In this paper, we present the analytical and numerical results for the optical conductivity in bilayer graphene at a low-temperature limit $T\to0$ K. We take the typical sample parameters in the calculation. In our calculations, we consider a typical bilayer graphene devices in which the carriers are electrons, while electrons can be tuned by the gate voltage. The Fermi wavevector $k_F=\sqrt{4\pi n_e/g_sg_v}=\sqrt{2mE_F}/\hbar$ for the parabolic bilayer graphene energy curve. When $n_e=10^{12}$ cm^{-2} was taken, the Fermi energy $E_F^0=36.271$ meV, and the Fermi wave vector $k_F^0=1.7725\times10^6$ cm^{-1} were determined by the condition of electron number conservation. In the numerical calculation, the small wavevector during the electron–photon scattering process $q=0.01k_F^0$ was taken.

Fig. 1 shows the optical spectrum as a function of the radiation energy at a fixed electron density for different broadening width Γ. Here, using Eqs. (3) and (4), the optical conductivity was calculated analytically in a long wavelength limit (i.e., $q\to0$). There are two transition channels (i.e., intra- and inter-band) which contribute to the optical conductivity. Intra-/inter-band transition indicates that a carrier in a conduction/valence band is excited to the conduction band when the carrier absorbs the energy of the incident light field. From Fig. 1, it can be seen clearly that (1) the inter-band transition