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The anisotropic energy spectrum dependence of the optical conductivity in bilayer graphene

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ABSTRACT

In this paper, the longitudinal optical conductivity in bilayer graphene was calculated analytically and numerically. In addition to the quadratic terms in the effective-mass approximation Hamiltonian, the linear term, which relates to the indirect interlayer coupling, was included. The nonparabolic energy dispersion was obtained. Two intra- and inter-band transition channels for optical transition via carriers absorbing the optical energy are observed. The inter-band transition offers the main contribution and is almost a constant when the optical energy is larger than two times the Fermi energy. In the presence of the complex energy and pseudospin angle relationship, doing the numerical integration to the wavevector **k**, the contribution of the intra-band optical transition to the optical conductivity ($\sigma_{xx}^{\mathrm{intra}}(\omega)$) is strengthened in the low optical energy region, while the analytical results with parabolic energy curves contribute less to $\sigma_{xx}^{\mathrm{intra}}(\omega)$. In addition, the optical conductivity also depends on the electron density (or gate voltage) and the broadening width.

1. Introduction

A single layer of graphite, called graphene, was fabricated in 2004 by Geim group [1]. Since then, due to its excellent properties, such as abnormal quantum Hall effect [1], high mobilities [2], Klein tuning [3], there are a lot of investigations on the optical and electronic properties in the fields of condense matter physics and material science [4–7]. The most distinctive feature of monolayer graphene is the linear energy dispersion near the Dirac points, which can be analogized as the relativistic massless particles. The "isospin" originates from the two sublattice composition of electronic Bloch states. This linear energy spectrum at K/K' crossover points leads to a series of unique properties, which are different from those in traditional parabolic energy systems. The parabolic energy spectrum is obtained by the 2×2 effective Hamiltonian in bilayer graphene [8–10]. Through the angle-resolved photoelectron spectroscopy (SRPES), the energy anisotropy was observed, which can provide the information about the magnitude and sign of interlayer coupling parameters in bilayer graphene [11]. Wang et al. [12] considered an effective Hamiltonian with a mixture of linear and quadratic terms of wavevector. The anisotropic energy spectrum was obtained, which is different from the parabolic energy curves. Therefore, in bilayer graphene, the optical and electronic properties having both the similarities and differences with those in monolayer graphene and the tradition 2DEG systems can be anticipated.

The properties of the optical conductivity in graphene have been widely investigated experimentally [13–16] and theoretically [17–24]. The experimental value of the optical conductivity per intrinsic graphene layer is almost a constant and close to $e^2/(4\hbar)$, independent from the frequency and the interplane hopping when the optical energy is larger than two times the Fermi energy $2E_F$. Another phenomenon is that the optical sheet conductivity showed a threshold structure at $2E_F$ for different gate voltages (carrier densities). In the theoretical calculation, the linear/parabolic energy dispersion is employed to investigate the optical conductivity in monolayer/bilayer graphene respectively. In this paper, we focus on the effect of the anisotropic energy spectrum on the optical conductivity in bilayer graphene. Using the dielectric function, the optical conductivity can be calculated and the results are compared with those obtained by only parabolic energy spectrum. Due to the optical measurement methods can offer the potential for rapid and non-destructive characterization of large-area samples. Therefore, the theoretical optical sheet conductivity for graphene is a constant which indicates that the optical measurements can be employed to determine the optical constants and thicknesses of thin films.

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2. Theoretical approaches

In the presence of a weak external light field polarized along the 2D plane (taken as the x direction) in graphene, the optical conductivity can be derived from the Kubo formula [25–27], which reads for the longitudinal optical conductivity:

$$\sigma_{xx}(\omega) = -e^2\omega \lim_{q\to 0}(1/q^2)\sum_{n',n} \mathrm{Im}\,\Pi_{n'n}(q,\omega), \tag{1}$$

where e and ω are the electron charge and the incident optical frequency respectively. $q \to 0$ reflects a fact that the electron–photon scattering does not change the wavevector of an electron. $n(n')$ are the energy band indexes. $\Pi(q,\omega)$ is the electron density–density correlation function. Using Green's function method, $\Pi(q,\omega)$ is obtained by the definition of the density operator [10,12]:

$$\Pi(q,\omega) = g_s g_v \sum_{s,s',\mathbf{k}} F_{\mathbf{k}}^{s,s'}(q)\frac{f_{s,\mathbf{k}} - f_{s',\mathbf{k}+\mathbf{q}}}{\hbar\Omega + E_{s,\mathbf{k}} - E_{s',\mathbf{k}+\mathbf{q}} + i\Gamma} \tag{2}$$

where $g_s=2$ and $g_v=2$ are spin and valley degeneracy respectively. $f_{s,\mathbf{k}}$ is the Fermi–Dirac distribution function. $s, s' = \pm 1$ applies to the conduction band (+ 1) and the valence band (− 1) respectively. $E_{s,\mathbf{k}} = s\hbar^2 k\sqrt{k^2 - 2k_0 k\cos 3\theta + k_0^2}/(2m)$, $m \approx 0.033 m_e$ is the effective mass of bilayer graphene which relates to the intralayer coupling and direct interlayer coupling, with m_e being the free-electron mass [12]. $k_0 \approx 10^8/\sqrt{3}\ m^{-1}$ which relates to the indirect interlayer coupling. θ the angle between $\mathbf{k}$ and $\mathbf{q}$, $\mathbf{k}' = \mathbf{k} + \mathbf{q}$. $F_{\mathbf{k}}^{s,s'}(q) = [1 + ss'\cos(\phi_{\mathbf{k}} - \phi_{\mathbf{k}+\mathbf{q}})]$ comes from the overlap of carrier states. $\phi_{\mathbf{k}}$ is the argument of a complex $(ke^{-2i\theta} - k_0 e^{i\theta})$. Γ is the broadening width induced by the carrier scattering processes.

In the present study, gate voltage was used to tune the carrier density and the electrons are occupied. The results of the optical conductivity due to two transition channels (intra- and inter-band transitions) can be obtained by the analytical and numerical calculation, $\sigma_{xx}(\omega) = \sigma_{xx}^{\mathrm{intra}}(\omega) + \sigma_{xx}^{\mathrm{inter}}(\omega)$.

If the indirect interlayer coupling is neglected (i.e., $k_0 = 0$), the energy dispersion becomes parabolic curves $E_{s,\mathbf{k}} = s\hbar^2 k^2/2m$. The coefficient $F_{\mathbf{k}}^{s,s'}(q) = (1 + ss'\cos(2\varphi))/2$ with $\cos\varphi = (k + q\cos\theta)/|\mathbf{k}+\mathbf{q}|$. At a long-wavelength limit (i.e., $q \to 0$), $\cos\varphi \approx 1 - (q^2/2k^2)\sin^2\theta$. $f_{+,\mathbf{k}} - f_{+,\mathbf{k}+\mathbf{q}} \approx -\mathbf{q}\cdot\hat{\mathbf{k}}\delta(k - k_F)$. A finite value Γ was taken for the broadening width. The intra-band transitions in a conduction band give rise to the analytical 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 result with parabolic energy dispersion. $\sigma_{bi}^0 = e^2/(2\hbar)$ which is two times larger than the value of $e^2/(4\hbar)$ in mono-layer graphene. The contribution to the optical conductivity from intra-band transition depends on the broadening width, Fermi energy, and the incident optical energy.

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

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

Here, $R = (\hbar^2k^2/m - \hbar\omega)^2 + \Gamma^2$, and k_c is the cutoff wave vector for graphene, $k_c \sim 1/a$ with $a \approx 1.42$ Å being the carbon–carbon distance. When

$$\Gamma \ll \hbar\omega, \quad \sigma_{xx}^{\mathrm{A-inter}}(\omega) \approx \sigma_{bi}^0\left[\frac{1}{\pi}\arctan\frac{(\hbar^2k^2/m - \hbar\omega)}{\Gamma}\right]_{k_F}^{k_c}.$$

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 $T \to 0$ K. In our calculations, we consider that the carriers are electrons which can be tuned by the gate voltage. The typical sample electron density $n_e \approx 10^{12}$ cm^{-2} was taken. In the numerical calculation, the small wavevector during the electron–photon scattering process, $q = 0.01k_F$.

Fig. 1 shows the parabolic energy dispersion and the anisotropic energy spectrum as a function of the wavevector. An obvious feature is the Fermi wavevector. The Fermi wavevector $k_F = \sqrt{4\pi n_e/g_s g_v} = \sqrt{2mE_F}/\hbar$ for the parabolic energy curve, which satisfies the rotational symmetry of angle θ. While the wavevector takes a different value corresponding to a different angle θ with a linear term included in an effective Hamiltonian. In this case, at a given Fermi energy, the minimum and maximum values of the wavevector are respectively $k_F^{min} = \sqrt{2mE_F/\hbar^2 + (k_0/2)^2} - k_0/2$ and $k_F^{max} = \sqrt{2mE_F/\hbar^2 + (k_0/2)^2} + k_0/2$ above the characteristic energy $E = \hbar^2k_0^2/(2m) = 3.9$ meV. For example, when the Fermi energy E_F=36.271 meV, the Fermi wave vector $k_F = 1.7725 \times 10^6$ cm^{-1} and the electron density $n_e = 10^{12}$ cm^{-2} for the parabolic case. $k_F^{min} = 1.5071 \times 10^6$ cm^{-1}, and $k_F^{max} = 2.0845 \times 10^6$ cm^{-1} for the nonparabolic case. When E_F=7.2542 meV, $k_F = 0.79267 \times 10^6$ cm^{-1}, $n_e = 0.2 \times 10^{12}$ cm^{-2} for the parabolic case, $k_F^{min} = 0.55492 \times 10^6$ cm^{-1} and $k_F^{max} = 1.1323 \times 10^6$ cm^{-1} for the nonparabolic case. It should be noted that when the Fermi energy is given, the occupied carrier density is different for both parabolic and nonparabolic cases. In this paper, the Fermi energy is chosen to be a fixed value.

Figs. 2 and 3 show the analytical and numerical results for the optical conductivity respectively. From the figures, it is clearly shown that, (1) in the low energy region (or in the long-wavelength region), the optical conductivity is mainly contributed by the intra-band optical transition process. While in the high energy region (especially the optical energy is larger than $2E_F$), the

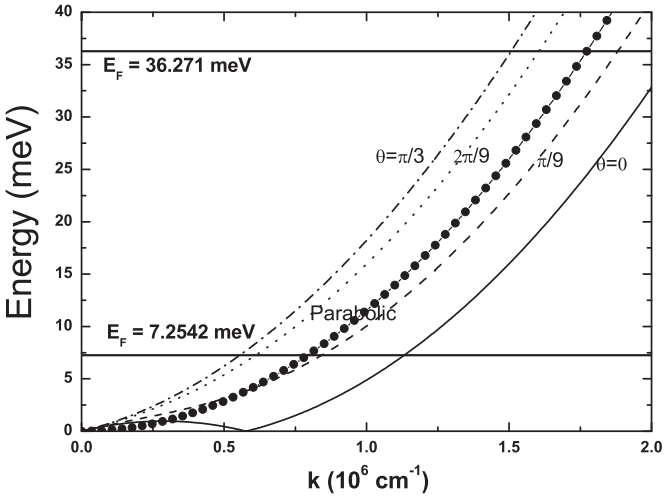

Fig. 1. The energy spectrum for equally separated θ from 0 to $\pi/3$. The curves for $\theta = 0$, $\pi/9$, $2\pi/9$, $\pi/3$ are denoted by solid, dashed, dotted, dash-dotted lines. The parabolic energy dispersion is drawn by line-symbol −•−. The horizontal lines indicate the Fermi energy at E_F=36.271 and 7.2542 meV.