Optical conductivity of ABA-stacked trilayer graphene*

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The optical conductivity of a trilayer graphene is studied using the Kubo–Greenwood formula. We calculate the real part of the diagonal optical conductivity of an ABA-stacked trilayer graphene with different Fermi energies. The optical conductivity arises from interband matrix elements of the electric current operator involving the transitions from the occupied states to the unoccupied ones. We study the dependence of the real part of the diagonal optical conductivity on the photon energy, and the role of the transitions.

Keywords: graphene, optical conductivity, photon energy

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1. Introduction

Since being discovered experimentally in 2004, graphene has attracted enormous interest in the field of condensed matter.[1–10] This is mainly a consequence of the chiral and massless character of the quasiparticles in graphene. The single layer graphene is a two-dimensional allotrope of carbon with a honeycomb structure. The multilayer systems containing a few layers of graphene have attracted much interest. The layers can be stacked differently with different horizontal shifts between graphene planes, leading to various band structures. Recent experimental realizations of trilayer graphenes[11–15] have opened the possibility of exploring their intriguing electronic properties and the field of device engineering. The trilayer graphene has two natural stable allotropes. One is of the ABA (Bernal) stacking, where the atoms of the topmost layer lie exactly on the top of those of the bottom layer; the other is of the ABC (rhombohedral) stacking, where one sublattice of the top layer lies above the centers of the hexagons in the bottom layer. For the ABA-stacked trilayer graphene, the low-energy band structure can be described by a combination of one massless and two massive sub-bands similar to the spectra of one single layer graphene and one bilayer graphene, respectively, while the band structure of the ABC-stacked trilayer graphene can be described approximately by cubic bands.

One of the most useful ways to study the properties of materials is to investigate their optical conductivity. It is known that the optical absorption is measured by the real part of the optical conductivity.[16–23] Among the interesting properties of graphene are its optical properties.[24–29] Ingenhoven *et al.*[25] calculated the optical conductivity of a disorder-free single graphene sheet in the presence of spin–orbit coupling. Interaction effects on the optical conductivity of a bilayer doped graphene was studied by Tse *et al.*[27] Yan *et al.*[29] investigated the effects of the surface states on the optical conductivity of an ABC stacked trilayer graphene. In this paper, we focus on the real part of the optical conductivity of an ABA-stacked trilayer graphene. We study the optical conductivity of the ABA-stacked trilayer graphene based on the linear response theory.

The paper is organized as follows. In Section 2, we present a brief account of the ABA-stacked trilayer graphene and a general formula for the optical conductivity. In Section 3, the optical conductivities with different Fermi energies are described. Conclusions are given in Section 4.

2. Model and general formula for optical conductivity

In a basis with components ψ_{A_1}, ψ_{B_1}, ψ_{A_2}, ψ_{B_2}, ψ_{A_3}, and ψ_{B_3}, the low energy effective Hamiltonian[30–34] of the ABA-stacked trilayer graphene around the K point is

$$\hat{H} = \begin{pmatrix} 0 & \upsilon p e^{i\phi} & 0 & -t & 0 & 0 \\ \upsilon p e^{-i\phi} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \upsilon p e^{i\phi} & 0 & 0 \\ -t & 0 & \upsilon p e^{-i\phi} & 0 & -t & 0 \\ 0 & 0 & 0 & -t & 0 & \upsilon p e^{i\phi} \\ 0 & 0 & 0 & 0 & \upsilon p e^{-i\phi} & 0 \end{pmatrix}, \tag{1}$$

where t is the interlayer hopping energy, υ denotes the Fermi velocity, p is the norm of the momentum vector $\boldsymbol{p} = (p_x, p_y)$, and $\tan\phi = p_y/p_x$. By performing a unitary transformation, the Hamiltonian can be rewritten as a combination of a monolayer Hamiltonian and a bilayer Hamiltonian with a modified interlayer hopping energy.[35,36] The basis function

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of the Hamiltonian is chosen as the linear combinations of the atomic orbits, namely, $[\psi_{A_1}-\psi_{A_3}]/\sqrt{2}$, $[\psi_{B_1}-\psi_{B_3}]/\sqrt{2}$, $[\psi_{A_1}+\psi_{A_3}]/\sqrt{2}$, $[\psi_{B_1}+\psi_{B_3}]/\sqrt{2}$, ψ_{B_2}, and ψ_{A_2}. The Hamiltonian can be expressed as

$$\tilde{\boldsymbol{H}} = \begin{pmatrix} \hat{\boldsymbol{H}}_1 & 0 \\ 0 & \hat{\boldsymbol{H}}_2 \end{pmatrix}, \tag{2}$$

where

$$\hat{\boldsymbol{H}}_1 = \begin{pmatrix} 0 & \upsilon p e^{i\phi} \\ \upsilon p e^{-i\phi} & 0 \end{pmatrix}, \tag{3}$$

$$\hat{\boldsymbol{H}}_2 = \begin{pmatrix} 0 & \upsilon p e^{i\phi} & -\sqrt{2}t & 0 \\ \upsilon p e^{-i\phi} & 0 & 0 & 0 \\ -\sqrt{2}t & 0 & 0 & \upsilon p e^{-i\phi} \\ 0 & 0 & \upsilon p e^{i\phi} & 0 \end{pmatrix}. \tag{4}$$

Now, the Hamiltonian has a block form, and it can be diagonalized.[33,37,38] The eigenvalues in the two blocks are $\mp\upsilon p$ and $[\mp t \mp \sqrt{t^2+2\upsilon^2 p^2}]/\sqrt{2}$, respectively.

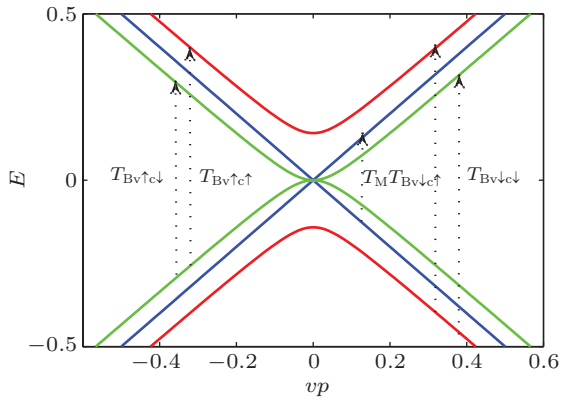


Fig. 1. (color online) Energy spectrum of ABA-stacked trilayer graphene.

Based on Green's function theory, the optical conductivity tensor $\sigma_{ij}(\omega)$ can be written as[39,40]

$$\sigma_{ij}(\omega) = \frac{\mathrm{i}}{\omega}\Pi_{ij}(\mathrm{i}\omega_n \to \omega + \mathrm{i}0^+), \tag{5}$$

$$\Pi_{ij}(\mathrm{i}\omega_n) = \frac{2T}{N}\sum_{m\boldsymbol{p}} \mathrm{Tr}\{e\hat{v}_i(\boldsymbol{p})\hat{G}(\boldsymbol{p},\mathrm{i}\omega_n+\mathrm{i}\nu_n) \times e\hat{v}_j(\boldsymbol{p})\hat{G}(\boldsymbol{p},\mathrm{i}\nu_n)\}. \tag{6}$$

By using the residue theorem, the ac optical conductivity tensor at zero temperature becomes

$$\sigma_{ij}(\omega) = -\mathrm{i}e^2 \sum_{\varepsilon_n<\varepsilon_F,\varepsilon_m\geq\varepsilon_F} \frac{1}{\varepsilon_m-\varepsilon_n}\left[\frac{\langle n|\hat{v}_i|m\rangle\langle m|\hat{v}_j|n\rangle}{\varepsilon_m-\varepsilon_n-\hbar\omega} - \frac{\langle n|\hat{v}_j|m\rangle\langle m|\hat{v}_i|n\rangle}{\varepsilon_m-\varepsilon_n+\hbar\omega}\right], \tag{7}$$

where ε_n is the eigenvalue corresponding to the eigenstate $|n\rangle$ of the low energy Hamiltonian $\tilde{\boldsymbol{H}}$, and $\hat{v}_i = \frac{\partial\tilde{H}}{\partial p_i}$ is the velocity operator. Now we study the real part of optical conductivity for photon energy ω and mark it as $\sigma_{xx}(\omega)$. From Eq. (7), we find that the optical conductivity is determined by the off diagonal matrix element of the velocity operator, which corresponds to the transition from the valence band to the conduction band in the same block. There are five types of such transitions: T_M, $T_{Bv\uparrow c\uparrow}$, $T_{Bv\uparrow c\downarrow}$, $T_{Bv\downarrow c\uparrow}$, and $T_{Bv\downarrow c\downarrow}$ (see Fig. 1). Here T_M denotes the transition from the valence band to the conduction band in the monolayer graphene, while the other four denote transitions in the bilayer graphene with a modified interlayer hopping energy, v and c stand for the valence and the conduction bands, respectively, and $\uparrow$ and $\downarrow$ are the band indexes of the splitting of energy band induced by the interlayer hopping.

3. Result and discussion

In this section, we give the dependences of optical conductivity on photon energy for fixed Fermi energies. We divide the location of the Fermi energy (E_F) into four ranges: (i) $E_F > \sqrt{2}t$, (ii) $0 < E_F < \sqrt{2}t$, (iii) $-\sqrt{2}t < E_F < 0$, (iv) $E_F < -\sqrt{2}t$. The off diagonal matrix element of the velocity operator is determined by the occupied and the unoccupied states, therefore we have

$$\sigma_{xx}(\omega) = 0, \tag{8}$$

in region (i). In region (ii),

$$\sigma_{xx}(\omega) = \frac{e^2}{16}\frac{\hbar\omega-2\sqrt{2}t}{\hbar\omega-\sqrt{2}t}\theta\left(-\sqrt{2}t+\frac{\hbar\omega}{2}\right) + \frac{e^2}{8}\frac{t^2}{\hbar^2\omega^2}\theta\left(-\frac{t}{\sqrt{2}}+\frac{\hbar\omega}{2}\right), \tag{9}$$

where $\theta(x)$ is the step function, and the two contributions arise from the transitions $T_{Bv\downarrow c\uparrow}$ and $T_{Bv\uparrow c\uparrow}$, respectively. In this region, the contribution from the monolayer is zero, because the two energy bands are fully occupied. From Eq. (9), we find that the dependence of optical conductivity on photon energy is independent of the Fermi energy. Figure 2 shows the real part of the diagonal optical conductivity σ_{xx} as a function of photon energy $\hbar\omega$. When $\hbar\omega < \sqrt{2}t$, σ_{xx} is zero. When the photon energy sweeps across $\hbar\omega = \sqrt{2}t$, σ_{xx} decreases with the increase of the photon energy, and $\sigma_{xx} = \frac{t^2}{\hbar^2\omega^2}\sigma_0$, which corresponds to the transition $T_{Bv\uparrow c\uparrow}$. When $\hbar\omega \geq 2\sqrt{2}t$, σ_{xx} reaches its minimum, and increases with the increase of the photon energy. In this region, $\sigma_{xx} \sim \frac{\hbar\omega-2\sqrt{2}t}{\hbar\omega-\sqrt{2}t}\sigma_0$, and σ_{xx} tends to σ_0 in the limit of $\hbar\omega \to \infty$. This is due to the fact that the contribution from the transition $T_{Bv\downarrow c\uparrow}$ plays a crucial role.

In region (iii),

$$\sigma_{xx}(\omega) = \frac{e^2}{16}\theta\left(-\frac{t}{\sqrt{2}}+\frac{\hbar\omega}{2}\right) + \frac{e^2}{16}\left[\frac{\hbar\omega+2\sqrt{2}t}{\hbar\omega+\sqrt{2}t}\theta\left(E_F+\frac{\hbar\omega}{2}\right) + \frac{2t^2}{\hbar^2\omega^2}\theta\left(E_F-\frac{t}{\sqrt{2}}+\frac{\hbar\omega}{2}\right)\right]$$

$$+\frac{e^2}{16}\left[\frac{\hbar\omega-2\sqrt{2}t}{\hbar\omega-\sqrt{2}t}\theta\left(-\sqrt{2}t+\frac{\hbar\omega}{2}\right)\right.$$
$$\left.+\frac{2t^2}{\hbar^2\omega^2}\theta\left(-\frac{t}{\sqrt{2}}+\frac{\hbar\omega}{2}\right)\right]. \quad (10)$$

In region (iv),

$$\sigma_{xx}(\omega)$$
$$=\frac{e^2}{16}\theta\left(-\frac{t}{\sqrt{2}}+\frac{\hbar\omega}{2}\right)+\frac{e^2}{16}\left[\frac{\hbar\omega+2\sqrt{2}t}{\hbar\omega+\sqrt{2}t}\theta\left(E_{\rm F}+\frac{\hbar\omega}{2}\right)\right.$$
$$\left.+\frac{2t^2}{\hbar^2\omega^2}\theta\left(E_{\rm F}-\frac{t}{\sqrt{2}}+\frac{\hbar\omega}{2}\right)\right]$$
$$+\frac{e^2}{16}\left[\frac{\hbar\omega-2\sqrt{2}t}{\hbar\omega-\sqrt{2}t}\theta\left(E_{\rm F}+\frac{\hbar\omega}{2}\right)\right.$$
$$\left.+\frac{2t^2}{\hbar^2\omega^2}\theta\left(E_{\rm F}+\frac{t}{\sqrt{2}}+\frac{\hbar\omega}{2}\right)\right]. \quad (11)$$

All the five transitions contribute to the optical conductivity in regions (iii) and (iv). On the right sides of Eqs. (10) and (11), the five terms correspond to the transitions $T_{\rm M}$, $T_{\rm Bv\uparrow c\downarrow}$, $T_{\rm Bv\uparrow c\uparrow}$, $T_{\rm Bv\downarrow c\uparrow}$, and $T_{\rm Bv\downarrow c\downarrow}$, respectively.

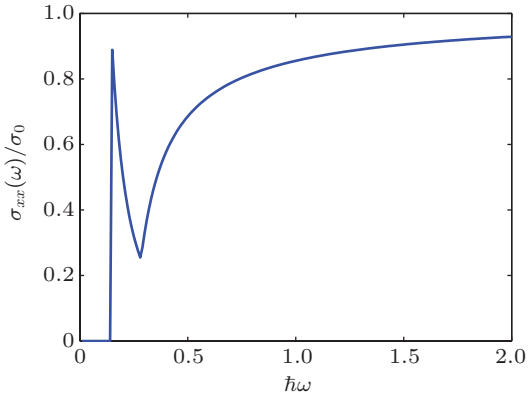


Fig. 2. (color online) Real part of diagonal optical conductivity σ_{xx} in units of $\sigma_0 = e^2/16$ as a function of photon energy $\hbar\omega$ in region (ii).

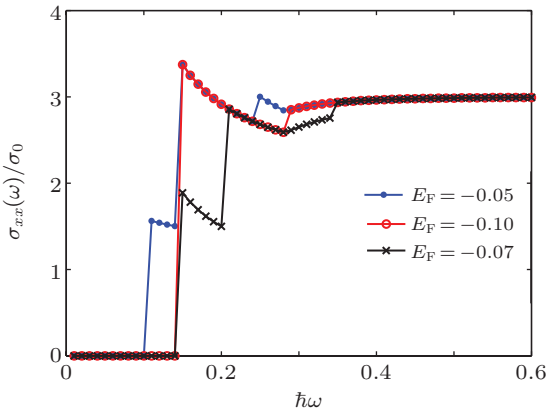


Fig. 3. (color online) Real part of diagonal optical conductivity σ_{xx} in units of $\sigma_0 = e^2/16$ as a function of photon energy $\hbar\omega$ with different Fermi energy $E_{\rm F}$ in region (iii).

In Fig. 3, we show the real part of the diagonal optical conductivity σ_{xx} as a function of the photon energy $\hbar\omega$ with different Fermi energy $E_{\rm F}$ in region (iii). We find that σ_{xx} equals 0 for $\hbar\omega < \sqrt{2}t$ when $E_{\rm F} \leq -t/\sqrt{2}$, and σ_{xx} equals 0 for $\hbar\omega < 2E_{\rm F}$ when $E_{\rm F} > -t/\sqrt{2}$. For $E_{\rm F} > -t/\sqrt{2}$, σ_{xx} equals $[(\hbar\omega+2\sqrt{2}t)/(\hbar\omega+\sqrt{2}t)]\sigma_0$ (corresponding to the transition $T_{\rm Bv\uparrow c\downarrow}$) when the photon energy sweeps across the region $[-2E_{\rm F}, \sqrt{2}t]$. With the increase of the photon energy, the transitions $T_{\rm M}$, $T_{\rm Bv\downarrow c\downarrow}$, and $T_{\rm Bv\uparrow c\uparrow}$ come to play their roles, but the change of σ_{xx} is determined by $(2t^2/\hbar^2\omega^2)\sigma_0$. For $E_{\rm F} \leq -t/\sqrt{2}$, the effects of the transitions $T_{\rm M}$, $T_{\rm Bv\downarrow c\downarrow}$, and $T_{\rm Bv\uparrow c\downarrow}$ ($E_{\rm F} = -t/\sqrt{2}$) become evident when the photon energy sweeps across $\hbar\omega = \sqrt{2}t$. The σ_{xx} includes the contribution from the transition $T_{\rm Bv\uparrow c\uparrow}$ with the increase of the photon energy. When $\hbar\omega > 2\sqrt{2}t$, σ_{xx} (corresponding to the transition $T_{\rm Bv\downarrow c\uparrow}$) increases with the increase of the photon energy, and σ_{xx} tends to $3\sigma_0$ in the limit of $\hbar\omega \to \infty$.

In Fig. 4, we show the real part of the diagonal optical conductivity σ_{xx} as a function of the photon energy $\hbar\omega$ with different Fermi energy $E_{\rm F}$ in region (iv). When $\hbar\omega < \sqrt{2}t$, σ_{xx} is zero. When the photon energy is smaller, the contribution from the transition $T_{\rm M}$ dominates in the contributions to σ_{xx}. When $\hbar\omega > -E_{\rm F}$, the transitions $T_{\rm Bv\uparrow c\downarrow}$ and $T_{\rm Bv\downarrow c\uparrow}$ both contribute to σ_{xx}. With the increasing photon energy, the contributions from $T_{\rm Bv\uparrow c\uparrow}$ and $T_{\rm Bv\downarrow c\downarrow}$ are trivial because of the term $1/\omega^2$. In the limit of $\hbar\omega \to \infty$, σ_{xx} tends to $3\sigma_0$.

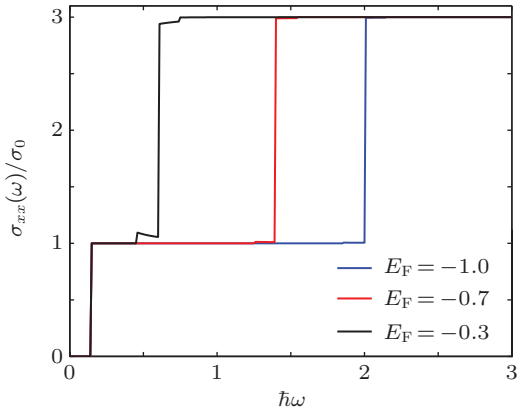


Fig. 4. (color online) Real part of diagonal optical conductivity σ_{xx} in units of $\sigma_0 = e^2/16$ as a function of photon energy $\hbar\omega$ with different Fermi energy $E_{\rm F}$ in region (iv).

4. Summary

In summary, the real part of the diagonal optical conductivity of an ABA-stacked trilayer graphene has been studied. The dependence of the real part of the optical conductivity on the photon energy with different Fermi energy is analyzed. The analytical expressions involving five transitions are obtained. Among the five transitions, three of them ($T_{\rm Bv\uparrow c\downarrow}$, $T_{\rm Bv\uparrow c\uparrow}$, and $T_{\rm Bv\downarrow c\downarrow}$) decrease with the increasing photon energy, one of them ($T_{\rm Bv\downarrow c\uparrow}$) increases with the increasing photon energy, and the last one ($T_{\rm M}$) is a constant. In the limit of

$\hbar\omega \to \infty$, the optical conductivity is a constant, σ_{xx} tends to $3\sigma_0$ for $E_F < 0$ and to σ_0 for $0 < E_F < \sqrt{2}t$. In the low photon energy region $\hbar\omega < \sqrt{2}t$ or $\hbar\omega < 2E_F$ (determined by the position of Fermi energy), $\sigma_{xx} = 0$.

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