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Absorption spectra of graphene nanoribbons in a composite magnetic field

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ABSTRACT

The low-frequency optical absorption properties of graphene nanoribbons in a composite magnetic field are investigated by using the gradient approximation. The spectral function exhibits symmetric delta-function like prominent peaks structure in a uniform magnetic field, and changes to asymmetric square-root divergent peaks structure when subjecting to a composite field. These asymmetric divergent peaks can be further classified into principal and secondary peaks. The spectral intensity and frequency of the absorption peaks depend sensitively on the strength and modulation period of the composite field. The transition channels of the absorption peaks are also analyzed. There exists an optical selection rule which is caused by the orthogonal properties of the sublattice wave functions. The evolution of the spectral frequency of the absorption peaks with the field strength is explored.

1. Introduction

Graphene is an one-atom thick layer of carbon atoms packed in a two-dimensional (2D) honeycomb lattice, and it can be regarded as a single atomic plane extracted from bulk graphite. The honeycomb lattice is a bipartite lattice consisting of two interpenetrating triangular sublattices, designated A and B. Each carbon atom is tied to its three nearest neighbors via σ bonds. Graphene has unusual electronic properties due to its unique energy dispersion, that is, its energy subbands are linear near the chemical potential (μ) and intersect at the Dirac point. From the viewpoint of its electronic properties, graphene is a zero-gap semiconductor with vanishing density of states at the chemical potential. With zero bandgap, graphene is not suitable for digital logic applications [1]. However, it is possible to open a bandgap by cutting 2D graphene into quasi one-dimensional (Q1D) graphene nanoribbons (GNRs) or by biasing bilayer graphene [2]. Graphene nanoribbons can be fabricated by plasma etching of masked graphene sheets [3], longitudinal unzipping of carbon nanotubes [4], or chemical vapor deposition [5]. Zigzag and armchair nanoribbons (ZGNRs and AGNRs) are the two basic types of GNRs, classified by the structure of their confining edges. Many studies of the electronic and transport properties of GNRs have been performed [6–10].

When a uniform magnetic field is applied to a 2D graphene, it will confine the electron motion and condenses the electron states into dispersionless Landau levels (LLs) [11], which follow a simple relation $|E_{n^{c,v}}| = (\hbar v_F/l_B)\sqrt{2n^{c,v}}$, where v_F is the Fermi velocity, and $n^{c,v}$ is the subband index. The magnetic length l_B is given by $\sqrt{\hbar/eB}$, and a typical value is $l_B \approx 46.9 Å$ for $B = 30$ T. Given a graphene nanoribbon is subjected to a uniform magnetic field, the carrier motion is restricted by both the magnetic potential and the nanoribbon boundary. The magnetic confinement will compete with the quantum confinement. When the magnetic field is strong, the carriers are confined solely by the magnetic potential, and quasi-Landau levels (QLLs) are formed. Recently, a number of investigations have been devoted to the optical properties of GNRs [12–16]. Liu and coworkers reported that the optical response of GNRs can be significantly enhanced and tuned by an applied magnetic field [12]. Raman spectroscopy measurements of etched GNRs were performed by Bischoff et al. [13]. Hsu and Reichl proposed a theory of optical transitions in GNRs [14]. The spin-dependent exciton effects in ZGNRs were investigated by Lu et al. [15]. Cordeiro and coworkers studied the optical dichroism in graphene nanoribbons by using gauge model [16]. In realistic circumstances, GNRs may have edge reconstructions. Among them the most important one is $zz(57)$, a reconstruction of a zigzag edge where hexagon carbon rings transforming into alternating pentagon-heptagon carbon rings [17–20].

In this work, we study the electronic and optical properties of GNR in a composite magnetic field, which consists of a uniform magnetic field and a spatially-modulated magnetic field. A spatially modulated magnetic field can be produced by putting an array of nanostructured ferromagnetic strips [21] on top of the samples. The band structures are calculated by employing the tight-binding method, and the spectral function $A(\omega)$ is obtained by using the gradient approximation [22,23]. The rest of the paper is organized as follows. The

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computational models are introduced in Section 2, and the energy dispersions and optical absorption spectra are discussed in Section 3. In Section 4, the conclusion is given.

2. The Peierls tight-binding method and the gradient approximation

The electronic properties of GNRs are briefly reviewed here. The nanoribbon width is specified by N_y, the number of dimer lines along the transverse ($\hat{y}$) direction, and the actual width W is given by $(3N_y-2)d_{CC}/2$, where $d_{CC}=1.42$ Å is the C–C bond length. Based on tight-binding calculations, zigzag GNRs are always gapless due to the partial flat bands at the chemical potential [24], while armchair GNRs can be either gapless or semiconducting, depending on N_y.

A schematic diagram of a zigzag GNR is given in Fig. 1. There are $2N_y$ carbon atoms in the unit cell, which is the dashed-line rectangle indicated in Fig. 1. The single-orbital nearest-neighbor tight-binding method is used to compute the electronic structure formed by the $2p_z$ orbitals. A composite magnetic field is a combination of a uniform magnetic field $\vec{B}_0=B_0\hat{z}$ and a spatially-modulated one $\vec{B}_m=B_m \sin(2\pi y/\lambda)\hat{z}$, where λ is the modulation period. In such field, the Hamiltonian matrix element is

$$\langle k|H|j\rangle=\gamma_0 \exp\left[i\vec{k}\cdot(\vec{R}_j-\vec{R}_k)+i\frac{e}{\hbar}\Delta G\right], \tag{1}$$

where $j(k)$ stands for A or B site, and $\vec{R}_j$ is the position vector of the j site. The π-bond hopping parameter between A and B atoms γ_0 has the value 2.598 eV. The vector potential $\vec{A}=B_0x\hat{y}-\lambda B_m\cos(2\pi y/\lambda)/2\pi\hat{x}$ causes a Peierls phase $\Delta G=\int_{\vec{R}_j'}^{\vec{R}_k'}\vec{A}\cdot dl$. The modulation period λ is in the unit of the nanoribbon width W.

The π-electronic wave function is the linear superposition of the $2N_y$ tight-binding functions. It is $\psi^{c,v}=\sum_{m=1}^{2N_y}a_m^{c,v}|\varphi_m>$, where c and v represent the conduction band and the valence band, respectively. $|\varphi_m>$ is the tight-binding function of the periodical $2p_z$ orbitals in the mth sublattice. In the subspace spanned by these tight-binding functions, the Hamiltonian is a $2N_y \times 2N_y$ Hermitian matrix. The dangling bonds on the edge sites are assumed to be terminated by hydrogen atoms, and they will not contribute to the electronic states near the chemical potential. The energy dispersion $E^{c,v}(k,n^{c,v})$ and the wave function $\psi^{c,v}(k,n^{c,v})$ are obtained by diagonalizing the Hamiltonian matrix, where k is the wave vector in the unit $\pi/\sqrt{3}d_{cc}$.

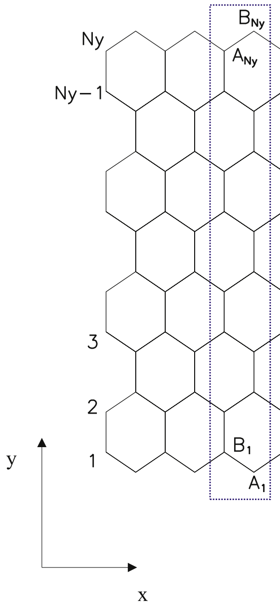

Fig. 1. (Color online) Schematic diagram of a zigzag graphene nanoribbon. The blue dotted-line rectangle is the primitive unit cell.

When a GNR is subjected to an electromagnetic field, the electrons are vertically excited from the occupied states to the unoccupied states in the momentum space; that is, the initial and final states have the same k. Based on Fermi's golden rule, the optical absorption function is given by

$$A(\omega)\propto\sum_{c,v,n^c,n^v}\int_{1stBZ}\frac{dk}{2\pi}\times \mathrm{Im}\left[\frac{f[E^c(k,n^c)]-f[E^v(k,n^v)]}{E^c(k,n^c)-E^v(k,n^v)-\omega-i\Gamma}\right] \times\left|\left\langle\psi^c(k,n^c)\left|\frac{\hat{\mathbf{E}}\cdot\vec{P}}{m_e}\right|\psi^v(k,n^v)\right\rangle\right|^2, \tag{2}$$

where f is the Fermi–Dirac distribution function. $\vec{P}$ stands for the momentum operator, and m_e is the bare electron mass. The electric polarization $\hat{\mathbf{E}}$ is along x-axis. $\Gamma=0.001\ \gamma_0$ is the phenomenological broadening parameter. The velocity matrix element $M^{vc}(k)\equiv\langle\psi^c(k,n^c)|\hat{E}\cdot\vec{P}/m_e|\psi^v(k,n^v)\rangle$ determines the possible transition channels. The gradient approximation [18,19] is used to evaluate $M^{vc}(k)$, and it is expressed as the first-order derivative of the Hamiltonian matrix element $\sum_{m,m'=1}^{2N_y}(a_{m'}^c)^*a_m^v\frac{\partial H_{m,m'}}{\partial k}$.

3. Low-energy electronic properties and optical absorption spectra

When a GNR is subjected to a uniform perpendicular magnetic field $\vec{B}=B_0\hat{z}$, $B_0=30$ T, the energy dispersion is a hybrid of parabolic and flat bands (Fig. 2a). The latter are the QLLs. Each subband is two-fold degenerate, and the conduction and valence subbands are symmetric with reference to the chemical potential $\mu=0$. The partial flat bands at $\mu=0$ are due to the mixing of localized edge states and Landau states. If a spatially-modulated magnetic field is superimposed on the uniform field, the energy dispersion is altered significantly (Fig. 2b). The band structure is now composed of partial flat bands at $\mu=0$ and oscillatory parabolic subbands. The curvature of the parabolic subbands increases with rising subband energy. The subbands nearest to $\mu=0$ have the lowest curvature. Each parabolic subband has one low-curvature concave downward central band-edge state at k_C, two high-curvature concave upward secondary band-edge states at the left (k_L) and right (k_R) of k_C. The subbands are left-right asymmetric with reference to k_C. The band-edge states at k_C and k_L are the states when the carriers are located at the maximum ($B=B_0+B_m$) and minimum ($B=B_0-B_m$) values of the composite magnetic field, respectively. As B_m increases to 12 T, the band-edge state energy shifts upward at k_C and downward at k_L, while their band curvatures rise (Fig. 2c). A larger modulation amplitude B_m has opposite effect on the band-edge state energy at k_C and k_L, but the band curvature is determined by the field gradient ∇B. A larger B_m leads to a larger ∇B at both k_C and k_L band-edge states. Furthermore, the rising band curvature indicates that a composite magnetic field with larger modulation amplitude has weaker capability to condense the electronic states.

At a longer modulation period ($\lambda=1.5$), the field varies more slowly in space, and the band curvature is reduced due to the smaller field gradient (Fig. 2d). On the other hand, the band-edge state energies at k_C and k_L, which are determined by B_0 and B_m, are almost unchanged. At $\lambda=0.5$, the field changes more rapidly in space, and the larger field gradient enhances the band curvature. In addition, extra band-edge states are created by such field (Fig. 2e). As λ decreases to