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Controlling absorption spectra of strained graphene nanoribbon by magnetic modulation

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ABSTRACT

This study shows that the optical absorption spectra of strained graphene nanoribbons can be effectively tuned by a spatially modulated magnetic field. The absorption spectra exhibit many asymmetric square-root divergent peaks structure due to the oscillatory parabolic subbands. These absorption peaks can be classified into primary and secondary ones. The number, spectral intensity, and frequency of the absorption peaks depend sensitively on the strength and period of the modulated field. The transition channels of the absorption peaks are identified and the optical selection rule is analyzed. There exists an optical selection rule for the primary absorption peaks. Such rule is originated from the orthogonal properties of the quasi-Landau level wave functions. A uniaxial stress changes the band-edge state energy and subband curvature, in turn modifying the optical absorption spectra. The evolution of the frequencies of the absorption peaks with the field strength is explored. They first show linear, then square-root dependence on the field strength. These theoretical predictions can be validated by absorption spectroscopy experiments.

1. Introduction

Graphene, a one-atom-thick honeycomb lattice made up of carbon atoms, has aroused many experimental and theoretical studies since the pioneering work performed by the Manchester group [1]. The honeycomb lattice consists of two interpenetrating triangular sublattices, designated A and B (a bipartite lattice). The sites of one sublattice are at the centers of the triangles defined by the other. Graphene exhibits many unusual electronic properties, such as the half-integer quantum Hall effect [2–4], the absence of backward scattering [5,6], and the weak localization phenomena [7–9]. They are caused by graphene's unique band structure, that is, the subbands are linear near the chemical potential (μ) and intersect at the Dirac point. Therefore, graphene is a zero-gap semiconductor with vanishing density of states at the chemical potential. Its electronic properties can be tuned by cutting it into one-dimensional (1D) graphene nanoribbons (GNRs).

Graphene nanoribbons can be obtained by lithographic patterning of graphene [8], unzipping carbon nanotubes [10], or chemical vapor deposition [11]. There are two basic categories of GNRs, namely, zigzag and armchair nanoribbons (ZGNRs and AGNRs), classified by the shape of their boundary edges. Because of topological reasons, ZGNRs have strongly localized electronic states at the boundary edges. These localized edge states give rise to the partial flat bands at the chemical potential, which occupy about one-third of the Brillouin zone [12]. On the other hand, AGNRs do not have localized edge states or partial flat bands. Many studies of the electronic properties [12–17], magnetic properties [18], transport properties [19,20], and synthesis [21] of graphene nanoribbons have been performed. When a graphene nanoribbon is immersed in a perpendicular magnetic field, the electron motion is restricted by both the magnetic potential and the ribbon boundary. There exists competition between the magnetic confinement and the quantum confinement. Furthermore, in the limit of a strong magnetic field, quasi-Landau levels (QLLs) are formed. The electrons are confined solely by the magnetic potential. The electronic properties are independent of the ribbon boundary, and the electronic states reproduce the LLs of a 2D graphene [19].

Optical absorption measurements are important diagnosis tools, and provide us with useful information about the materials. Those of graphene and graphene nanoribbons have been the focus of recent investigations [22–26]. The optical responses of multilayer graphene in the terahertz regime were measured by Lin and coworkers [22]. Computations of multilayer graphene magneto-optical absorption spectra were presented by Koshino [23]. The optical selection rule of bilayer graphene under mechanical deformations were reported by Li and collaborators [24]. Wright and coworkers studied the exceptionally strong optical response of bilayer GNRs in the terahertz domain [25]. The magneto-absorption spectra of bilayer GNRs were investigated by Huang and coworkers [26].

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Applying a periodic electric [27–29] or magnetic [30–32] field to graphene strongly affects its electronic properties and might lead to new phenomena. In this work, we study the electronic and optical properties of strained graphene nanoribbon in a spatially modulated magnetic field, which can be realized by placing an array of nanostructured superconductors [33] or ferromagnetic strips [34] on top of the sample. The electronic structures are calculated by using the Peierls tight-binding model, and the optical spectral function $A(\omega)$ is evaluated by employing the gradient approximation [35,36]. The rest of the paper is organized as follows. The theoretical models are introduced in Section 2, and the low-energy electronic properties and optical absorption spectra are discussed in Section 3. In Section 4, concluding remarks are given.

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

The electronic properties of GNR are briefly reviewed first. The ribbon width is determined by N_y, the number of dimer lines along the transverse $(\hat{y})$ direction, and the actual width W is $(3N_y-2)d_{CC}/2$. $d_{CC}=1.42$ Å is the C–C bond length. Within the tight-binding framework, all ZGNRs are gapless due to the partial flat bands at the chemical potential [14]. On the other hand, all AGNRs with $N_y=3I+2$ are predicted to be gapless, where I is an integer. Yet those with $N_y\neq 3I+2$ possess bandgap and are semiconductors. A layout of a ZGNR is presented in Fig. 1. There are $2N_y$ carbon atoms in the primitive unit cell, which is the dashed-line rectangle shown in Fig. 1. We use the single-orbital tight-binding method to compute the energy dispersions formed by the $2p_z$ orbitals. With the presence of a uniaxial stress along the longitudinal direction $(\hat{x})$, the C–C bond length is changed proportionally. Based on the elasticity theory, the position vector of the carbon atoms before $(\vec{R}_i)$ and after $(\vec{R}'_i)$ applying stress is described by

$$\vec{R}'_i=\begin{pmatrix}1+\varepsilon & 0\\ 0 & 1-\varepsilon/6\end{pmatrix}\vec{R}_i. \tag{1}$$

The strain ε is defined as the ratio of the deformed bond length to the original length. The positive and negative values of ε indicate tension and compression, respectively. The variations of the bond length alter the transfer integrals according to Harrison's formula [37], $\gamma'=\gamma_0 l^2/l'^2$, where l' and l are the bond lengths with and without deformation, respectively. The tight-binding formulation of strained graphene nanoribbons was given in the published work [38].

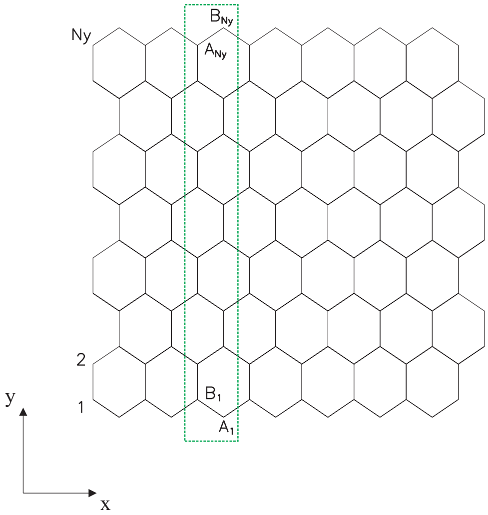

Fig. 1. Geometric structure of a zigzag graphene nanoribbon. The green dashed-line rectangle represents the primitive unit cell. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)

In a spatially modulated magnetic field $\vec{B}=B_m\sin(2\pi y/\lambda)\hat{z}$, where λ being the periodic length, the hopping integral becomes

$$\langle k|H|j\rangle=\gamma'(\vec{R}'_j,\vec{R}'_k)\exp\left[i\vec{k}\cdot(\vec{R}'_j-\vec{R}'_k)+i\frac{e}{\hbar}\Delta G\right], \tag{2}$$

where $j(k)$ stands for A or B site. The vector potential $\vec{A}=-\lambda B_m\cos(2\pi y/\lambda)/2\pi\hat{x}$ induces a Peierls phase $\Delta G=\int_{\vec{R}'_j}^{\vec{R}'_k}\vec{A}\cdot dl$. λ is in the unit of the ribbon width. The Bloch wave function is the linear superposition of the $2N_y$ tight-binding functions. It is $\psi^{c,v}=\sum_{m=1}^{2N_y}a_m^{c,v}|\varphi_m\rangle$, where c and v represent the unoccupied conduction band and the occupied valence band, respectively. $|\varphi_m\rangle$ is the tight-binding function of the periodical $2p_z$ orbitals in the mth sublattice. The Hamiltonian, which is built from the subspace spanned by these tight-binding functions, is a $2N_y\times 2N_y$ Hermitian matrix. All graphene nanoribbons are assumed to be edge hydrogenated to eliminate dangling bond effects. 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 the subband index $n^{c,v}$ specifies the subbands counting from μ. k is the wave vector in the unit $\pi/\sqrt{3}d_{cc}$.

In the presence of an electromagnetic field, the electrons are vertically excited from the occupied states to the unoccupied states; that is, the initial and final states have the same k. Based on Fermi's golden rule, the optical absorption function can be written as

$$A(\omega)\propto\sum_{c,v,n^c,n^v}\int_{1stBZ}\frac{dk}{2\pi}\times\mathrm{Im}\left[\frac{f[E^c(k,n^c)]-f[E^v(k,n^v)]}{E^c(k,n^c)-E^v(k,n^v)-\omega-i\Gamma}\right]\times\left|\left\langle\psi^c(k,n^c)\left|\frac{\hat{\mathbf{E}}\cdot\vec{P}}{m_e}\right|\psi^v(k,n^v)\right\rangle\right|^2, \tag{3}$$

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 the x-axis. $\Gamma=0.001\ \gamma_0$ is the phenomenological broadening parameter accounting for various deexcitation mechanisms. 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. Within the gradient approximation [35,36], it can be expressed as

$$\sum_{m,m'=1}^{2N_y}(a'^c_m)^*a^v_m\frac{\partial H_{m,m'}}{\partial k}.$$

3. Low-energy electronic properties and optical absorption spectra

When a strained GNR is immersed in a uniform perpendicular magnetic field $\vec{B}=B_0\hat{z}$, $B_0=40$ T, the energy dispersion is a hybrid of parabolic and flat bands, which are quasi-Landau levels (QLLs) (Fig. 2a). 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 the uniform magnetic field is changed to a spatially modulated one, the energy dispersion is modified severely (Fig. 2a). The band structure is now consisted of partial flat bands at $\mu=0$ and many oscillatory parabolic subbands. The curvature of the parabolic subbands increases with rising subband energy. The subbands nearest to $\mu=0$ have the