Trigonal warping and photo-induced effects on zone boundary phonon in monolayer graphene

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ABSTRACT

We have reported the electronic band structure of monolayer graphene when the combined effects arising from the trigonal warp and highest zone-boundary phonons having A_{1g} symmetry with Haldane interaction which induced photo-irradiation effect. On the basis of our model, we have introduced a diagonalization to solve the associated Fröhlich Hamiltonian. We have examined that, a trigonal warping effect is introduced on the K and K′ points, leading to a dynamical band gap in the graphene electronic band spectrum due to the electron-A_{1g} phonon interaction and Haldane mass interaction. Additionally, the bands exhibited an anisotropy at this point. It is also found that, photo-irradiation effect is quite smaller than the trigonal warp effects in the graphene electronic band spectrum. In spite of this, controllability of the photo induced effects by the Haldane mass will have extensive implications in the graphene.

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1. Introduction

Over the past decade, there has been a growing interest in studying the physical properties of graphene and graphene-based microstructures due to its experimental realization [1,2]. For this purpose, many efforts have been devoted to investigate various properties of graphene, such as the electronic and optical properties [3—6]. In particular, some studies have focused on the electron-phonon interaction dispersion relations which provide a basic information about the physical properties of graphene [7—11] when combined with information about the electronic structure. Recently, it has been shown that the interaction of doubly degenerate E_{2g}-phonons with Dirac carriers yield to Fermi velocity renormalization of these carriers [11] without opening a gap. However, the interaction of the Dirac electrons with A_{1g}-phonons induces a small band gap which has great importance for the electronic applications, especially in transistors [12—14]. Trigonal warping is a deformation of the Fermi lines with circular forms around the K-points tends to be trigonal forms due to the symmetry of the lattice. This phenomenon has a substantial effect on the low energy properties of graphene. In the pure graphene, the energy band in the edge of the hexagonal Brillouin zone meets each other. Interaction of charge carriers with doubly degenerate E_{2g}-phonons in the presence of trigonal warp, exhibit an anisotropy in the energy bands [15]. Moreover, this effects shows the asymmetry between the conduction and the valance bands of graphene [15]. The effects of trigonal distorsion also modify the transport characteristics and the value of minimal conductivity near the Dirac points, have been investigated for both theoretically [16—18] and experimentally [19,20]. Additionally, trigonal warping in the graphene have been analyzed not only

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for Dirac cone approximation but also the entire first Brillouin zone [21] because it has an important role on the physical properties of graphene for the entanglement spectrum of graphene. In 2005 [22], Kane and Mele proposed a generalization of the Haldane model includes the spin via the spin-orbit interaction which gives rise to a quantum spin Hall effect characterized by helical edge states. But Haldane [23] type intrinsic spin-orbit interaction model was motivated by Quantum Hall effect without strong magnetic field to break the time reversal symmetry by unit cell. This model describes a whole class of bands insulating phases with a nontrivial topological insulators namely a Chern insulator. By this model, both inversion symmetry and time reversal symmetry are simultaneously broken in a sheet of graphene. Inversion symmetry is broken by assigning different on site energies to the two inequivalent sublattices of the honeycomb lattice, while time reversal invariance is lifted by local magnetic fluxes organized so that the net flux per unit cell vanishes. To the best of our knowledge there has been no report on the band gap characteristics of graphene in the presence of simultaneous effects of trigonal warping and Haldane interaction induced by photo-irradiation which correspond to quantum Hall insulator [18] together with highest zone boundary phonon mode of A_{1g}. With this motivation; firstly, we found the energy eigenvalues and eigenfunctions of the system. Then, we considered electron-phonon interaction Hamiltonian giving rise to inter-valley scattering between K and K′ points as well as trigonal warping and photo-induced effects. Afterwards, to diagonalize the associated Hamiltonian, we performed a unitary transformation scheme based on Lee-Low-Pines (LLP) theory [24]. Finally, within the framework of this theory, we analyzed the energy spectrum of electrons interacting with phonons having A_{1g}-symmetry in trigonal distorted and photo-induced graphene.

2. Theory

In the long-wavelength regime, low-energy Dirac electrons interacting with A_{1g}-phonon mode can be written as,

$$\mathscr{H} = \mathscr{H}_0 + \sum_\tau \sum_q \hbar\omega_\tau(q) b^\dagger_{q,\tau} b_{q,\tau} + \mathscr{H}_{e-ph} \tag{1}$$

$$\mathscr{H}_0 = \begin{pmatrix} \mathscr{H}_0^K & 0 \\ 0 & \mathscr{H}_0^{K'} \end{pmatrix} \tag{2}$$

where $\mathscr{H}_0^K$ and $\mathscr{H}_0^{K'}$ are the unperturbed parts which represent the combine effects of trigonal warping and Haldane interaction in the vicinity of the K-point and K′-point of the graphene, respectively. The $\mathscr{H}_0^K$ effective Hamiltonian is described by,

$$\mathscr{H}_0^K = \begin{pmatrix} \Delta & \gamma k_- + \gamma\tilde{\beta}k_+^2 \\ \gamma k_+ + \gamma\tilde{\beta}^\dagger k_-^2 & -\Delta \end{pmatrix} \tag{3}$$

here $\tilde{\beta}$ is an adjustable parameter which represents the trigonal warping term described by $\tilde{\beta} = \frac{\beta a}{4\sqrt{3}}e^{3i\eta}$, $a = \sqrt{3}a_{cc}$ and a_{cc} is the lattice constant. The η in the definitions of trigonal warping term defined as a chiral angle. Regardless of the value of η chiral angle, $\tilde{\beta}$ parameter must take the value of 1 for the graphene material because the adjustable parameter depends on the distance between the a_{cc} neighbors of the graphene. In Eq. (2), $\gamma = \hbar v_F$ and v_F is the Fermi velocity of graphene charge carriers. k is the two component wave vector with $k_\pm = k_1 \pm k_2$. The eigenvector of the unperturbed part are given at K-point

$$\left| K\nu\mathbf{k} \right\rangle = \frac{1}{\sqrt{2E^K(2E^K + \Delta)}} \begin{pmatrix} \Delta + E_\nu^K \\ \gamma k_+ + \gamma\tilde{\beta}k_-^2 \end{pmatrix} \tag{4}$$

and the eigenvalues of the unperturbed part are given as,

$$E_\nu^\tau = \nu\sqrt{\Delta^2 + \gamma^2 k^2 + \gamma^2\tilde{\beta}^2 k^4 + \tau 2\gamma^2\tilde{\beta}k^3 Cos3\theta}. \tag{5}$$

$$E_\nu^\tau = \nu E^\tau \tag{6}$$

where the ν is the band index, τ is the valley index. Similarly, the eigenvector and eigenvalue of the unperturbed part at K′-point can be written

$$\mathscr{H}_0^{K'} = \begin{pmatrix} -\Delta & -\gamma k_+ + \gamma\tilde{\beta}k_-^2 \\ -\gamma k_- + \gamma\tilde{\beta}^\dagger k_+^2 & \Delta \end{pmatrix} \tag{7}$$

corresponding eigenvector can be written as,